

Numerical Study Model for Solidification and Melting of Nano-enhanced Phase Change Material by Enthalpy Porosity Method



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| ARTICLE INFO | ABSTRACT | | | | |
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| Article history: Received 2 May 2019 Received in revised form 5 August 2019 Accepted 12 September 2019 Available online 7 November 2019 | This paper presents numerical work on solidification and melting of nano-enhanced phase change material. In this work, we propose an improvised numerical solution for solidification and melting of nano-enhanced phase change material (NEPCM) by allowing different thermophysical properties in solid and liquid phase in enthalpy-porosity method. The solidification and melting of NEPCM will be conducted in a two-dimensional computational domain with adiabatic horizontal walls and isothermal vertical walls. In this approach, a single-domain formulation is coupled with porosity source term to the momentum equations to differentiate liquid and solid regions during the phase change process. A source term is also added to the energy equation via enthalpy terms to account for latent heat evolution during the same process. This research is expected to produce results closer to the experimental results relative to previous numerical works. This will indicate that the proposed model has contributed to the improvement on existing NEPCM solidification and melting numerical model. | | | | |
| Keywords: | | | | | |
| Nano-enhanced phase change material; | | | | | |
| PCM; enthalpy-porosity method | Copyright © 2019 PENERBIT AKADEMIA BARU - All rights reserved | | | | |

1. Introduction

Over the recent years, researchers have dedicated their works to enhance the effectiveness of Phase Change Materials (PCM) as thermal energy storage system for various purposes. PCM relies on its ability to absorb and remove latent heat during its phase changing process in order to store and release heat energy as required. Such latent heat storage system is attractive as it offers high energy storage capacity during the process within acceptable range of temperature change [1, 2]. Although phase change process may occur in other different phase combinations, the most practical phase changes for PCM applications are liquid-solid (Solidification) and solid-liquid (Melting) [3]. In other words, PCM solidification allows for latent heat 'discharging' while PCM melting enables latent heat 'charging'. Figure 1 shows the principle of PCM application to achieve its function.

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Fig. 1. Principle of Phase Change Materials (PCM) [4]

Nanotechnology is manipulation of nano-sized particles to achieve new technological innovations. Choi *et al.*, [5] proved that thermal conductivity of fluids may be enhanced by dispersing nanosized particles. In the following years, many studies have been performed on nanofluids which confirms its ability to enhance liquid thermophysical properties [6, 7]. Parallel with this advancement, nanoparticles have also been applied to improve the performance of PCM thus the term Nano-Enhanced Phase Change Materials (NEPCM) is introduced. Figure 2 shows the typical composition of NEPCM which is a nanofluid substance which consist of base-fluid (PCM) and nanoparticles.



Fig. 2. NEPCM Composition

In 2007, Khodadadi and Hosseinizadeh [8] added nanoparticles in PCM to investigate these fine particles influence on its performance during phase change process and the result was encouraging. The introduction of NEPCM calls for the need to further analyse the balance in between the benefits offered and the cost of developing the material. For such detail analysis and study, numerical simulation is a convenient and economical approach that have been widely used over the years. It allows various different conditions to be simulated by substituting the variables in the models used.

Currently, NEPCM phase change numerical simulations can be performed by macroscale or mesoscale approach where the latter approach is relatively more complex [9]. In macroscale, NEPCM phase change can be modelled in one domain or two domains. Single-domain modelling is simpler compared to multi-domain modelling because only one domain needs to be solved at each iteration. Therefore, this approach is widely used and preferred by most researchers. The enthalpy-porosity method is commonly used for this approach. However, in most applications involving this method for phase change, the thermophysical properties for each solid and liquid phase is simplified to be similar or averaged to a single value [10].

In the 19th century, some studies on modelling solidification and melting have been recorded. The process was understood as a transient problem where a boundary in between solid and liquid develops and moves in the domain throughout the process. The position of this boundary is unknown in advance thus need to be determined as function of time and space as part of the solution. Although



Lame and Clapeyron [11] initiated this study, it was made well known by Stefan later through his works thus the name; Stefan Problem [12]. Many of the early works in this area solved pure heat conduction equation which neglects the existence of convective effect. In reality however, convective effects were proven to significantly influence the phenomena or in some cases dominate the overall heat transfer process [13, 14]. In addition to this fact, early models were also unable to solve multidimensional problems.

A more practical approach was developed later to avoid tracing the moving boundary explicitly. The moving boundary is indirectly embedded in a different form of equation. The methods under this category is known as methods of latent-heat evolution. They are widely known as weak solutions for the problem as the special attention required on the moving boundary is no longer required. One of the prominent methods under this category is enthalpy method [15]. Compared to the other methods, the main characteristic of enthalpy method is the evolution of latent heat is accounted by enthalpy as well as the correlation in between enthalpy and temperature; in terms of the latent heat characteristics of the material under phase change.

With the advancement of numerical methods and computational capability in the mid-20th century, solution to Navier-Stokes equations which were earlier limited and deemed to be tedious received more attention. Newtonian thermal-fluid flow problems were able to be predicted quantitatively by solving the set of mass, momentum and energy conservation equations. This scenario enabled for solidification / melting simulations to be conducted by considering both conductive and convective heat transfer mechanisms. As a result, enthalpy-porosity method (EPM) was developed [16, 17]. This approach is a single-domain formulation which adds porosity source term to the momentum equations to differentiate liquid and solid regions during the phase change process. A source term is also added to the energy equation via enthalpy terms to account for latent heat evolution during the same process.

In the 21st century, progress have been made to develop other approach which are able to solve solidification and melting phenomena. Mesoscale methods such as Lattice Boltzmann Method (LBM) have been proven to be able to yield acceptable results by modelling fluid flow at mesoscopic level in terms of local interactions between particles. LBM was first implemented for phase change material simulations in 2001 by Miller *et al.*, [18].

Numerical simulations on NEPCM solidification & melting are mainly performed by researchers to study the parameters which influence the process such as nanoparticle fraction in the mixture, nanoparticle size, boundary conditions applied, and geometry. These factors have been investigated by many researchers by applying several different numerical models. Details on the numerical models used and findings of each research are summarized in Table 1 and Table 2. All works were validated by either previous experimental (E) or numerical (N) works and showed acceptable agreement.

Table 1 shows summary of numerical simulations for NEPCM solidification. The simulations were performed at various different nanoparticle characteristics (particle size and particle volume concentration) and different geometries. All of the works applied enthalpy-porosity method coupled with finite volume method (EPM-FVM) [8], [19-25] which is a single domain approach. All of the works also applied linear function mixture model [26] to obtain values for density, heat capacity and thermal expansion coefficient. Most of the works if not all, obtained values of dynamic viscosity and thermal conductivity using Brinkman [27] and Maxwell [28] correlation respectively.

Table 2 shows summary of numerical simulations for NEPCM melting. Similar to the previous phase change process, the simulations were also performed at various different nanoparticle characteristics and different geometries. Most of the works also applied enthalpy-porosity method coupled with finite volume method (EPM-FVM) [29-38] except for others which did not specify specifically the method applied [39] or applied mesoscale simulation by applying Lattice Boltzmann



Method (LBM) [40-43]. Other correlation [44-47] besides the mostly applied Brinkman and Maxwell were also used to represent the values of dynamic viscosity and thermal conductivity of the substance while all models still resorted to linear function mixture model to obtain values for density, heat capacity and thermal expansion coefficient.

| Ref | NEPCM | Particle size (nm) | Particle Volume (%) | Geometry | μ and k correlation | Properties value for solid / liquid | |
|------|-----------------------|-----------------------|---------------------------|-----------|-------------------------------|---|--|
| [8] | H ₂ O + Cu | 10 | 0, 10, 20 | Square | Brinkman[27] Maxwell [28] | Similar | ↑ Particle fraction results in ↑ heat release rate & k ↓ latent heat of fusion |
| [19] | H ₂ O + Cu | Not reported | 0, 2.5, 5 | Annulus | Brinkman[27] Maxwell [28] | Similar | ↑ Particle fraction results in ↑ heat transfer rate & k ↑ ΔT: ↓ solidification time |
| [20] | n-Octadecane + Cu | 45 | 0, 2, 8 | Rectangle | Brinkman[27] Maxwell [28] | Similar | ↑ Particle fraction results in ↑ solidification & heat discharge rate |
| [21] | $Paraffin + Al_2O_3$ | Not reported | 0, 2, 5, 10 | Annulus | Vajjha [44] | Different k f(T) = ρ & μ | ↑ Particle fraction results in ↑ charge-discharge rate ↑ heat transfer rate & k ↓ energy storage capacity |
| [22] | n-Hexadecane + Cu | 10 | 0, 3, 8 | Square | Corcione [45] Maxwell [28] | Similar except k | ↑ Particle fraction results in ↑ heat transfer rate & k + \downarrow wall T = ↑ solid fraction |
| [23] | H ₂ O + Cu | 10 | 0, 10, 20 | Trapezium | Brinkman[27] Maxwell [28] | Similar | ↑ Particle fraction &ΔT results in: ↑ solidification & heat transfer rate ↑ Incline angle results in: ↑ solidification rate |
| [24] | H ₂ O + Cu | 2, 5 | 10 (wt%) | Square | Brinkman[27] Maxwell [28] | Similar | ↓ Size particles results in: ↑ thermal conductivity ↓ frozen region thickness ≠ phase interface shape |
| [25] | H ₂ O + Cu | 1 | 0, 5, 10 | Wavy | Brinkman[27] Maxwell [28] | Similar except k | ↑ Particle fraction & waviness: ↑ solidification rate |

It should be noted that most models used similar thermophysical properties values for both in solid and liquid region during the phase change process. Others have different values, but they are dependent on temperature [21], [33-36] and not the phase condition. The models which have different value of property for both phases [22,25,37,40] are only for thermal conductivity which also includes the previously mentioned works.



Table 2

Summary of numerical simulations for NEPCM melting

| | NEPCM | Particle size (nm) | Particle Volume (%) | Geometry | Numerical Technique | μ and k correlation | Properties value for solid / liquid | Findings |
|------|---|-----------------------|---------------------------|----------------|------------------------|-------------------------------------|---|---|
| [29] | Eicosane + CNT | Not reported | | Rectangle | EPM -FVM | Brinkman[27] Gharagozloo [46] | Similar | ↑ Particle fraction results in: ↑ melting rate & k ↑ viscosity ↓ latent heat of fusion |
| [30] | n-octadecane + CuO | Not reported | 0, 2.5, 5 | Square | EPM - FVM | Brinkman[27] Maxwell [28] | Similar | ↑ Particle fraction results in: ↑ melting rate & k ↑ viscosity |
| [31] | RT 50 + Cu | 1 | 0, 3, 5 | Annulus | EPM - FVM | Brinkman[27] Maxwell [28] | Similar | ↑ Particle fraction results in: ↑ melting rate ↑ melt front penetration ↑ liquid fraction |
| [32] | Paraffin + Cu | Not reported | 0, 2.5, 5 | Square | EPM - FVM | Brinkman[27] Maxwell [28] | Similar | ↑ Particle fraction results in: ↑ melting rate & k ↑ Δ T results in: ↓melting time |
| [39] | NaNO3+ Al ₂ O ₃ | Not reported | 0, 3, 6 | Circle | FVM | Brinkman[27] Maxwell [28] | Different k $f(T)=\rho, \mu, Cp$ | ↑ Particle fraction results in: ↑ melting rate & k |
| [33] | Paraffin + CuO | 10 | 0-7 | Shell-tube | EPM - FVM | Vajjha [44] | Different k $f(T) = \rho \& \mu$ | ↑ Particle fraction results in: ↑ melting rate ↑ viscosity |
| [40] | $H_2O + Cu$ | 1 | 0, 5, 10 | Square | EB - LBM - DDF | Brinkman[27] Maxwell [28] | Similar except k | ↑ Particle fraction results in: ↑ melting rate & k |
| [41] | $H_2O + Cu$ | 100 | 0, 1, 2, 3 | Square | EB - LBM - DDF | Brinkman[27] Patel et.al[47] | similar | ↑ Particle fraction results in: ↑ melting rate & k ↓ latent heat of fusion |
| | | | | | | | | |
| [42] | $H_2O + Cu$ | 100 | 0, 2, 4 | Cylinder | EB - LBM - DDF | Brinkman[27] Patel et.al [47] | Similar | ↑ Particle fraction results in: ↑ melting rate & k ↓ latent heat of fusion |
| [43] | H ₂ O + Cu | 100 | 0, 2, 4 | Semi circle | EB - LBM - DDF | Brinkman[27] Patel et.al [47] | Similar | ↑ Particle fraction results in: ↑ melting rate & k ↓ latent heat of fusion ↑ viscosity |
| [34] | Paraffin + Al ₂ O ₃ | Not reported | 0, 2, 5 | Square | EPM - FVM | Vajjha [44] | Different k $f(T) = \rho \& \mu$ | Source-sink at dedicated walls and hot wall on top results in: = Highest melting rate |
| [35] | Paraffin + Al ₂ O ₃ | Not reported | 0, 2, 5 | Square | EPM - FVM | Vajjha [44] | Different k $f(T) = \rho \& \mu$ | Source-sink with alternate location & order on vertical wall results in: = Highest melting rate |
| [36] | Paraffin + CuO | 29 | 0, 1, 3 | Square | EPM - FVM | Vajjha [44] | $f(T) = \rho, k \& \mu$ | Bottom heating results in: ↑ melting rate ↑ stored energy |
| [37] | $P116 + Al_2O_3$ | 45 | 0, 2, 6, 8 | Rectangle | EPM - FVM | Brinkman[27] | | ↑ Aspect ratio results in: ↑ area for heat transfer |



| | | | | | | Maxwell [28] | Similar except k | ↑ melting / charging rate |
|------|-------------|---|--------------|---------|-----------|---------------|---------------------|---|
| [38] | RT 50 + CuO | 1 | 0, 2, 4 (wt) | Annulus | EPM - FVM | Not indicated | Similar | ↑ Particle fraction results in: ↑ melting rate & k ↑ Inclination angle: ↑ melting rate |

As can be seen in the literature, most numerical models for simulation of solidification and melting process of NEPCM have been established mainly by applying enthalpy-porosity formulation coupled with finite volume method. Most models solved a single macroscale domain at each iteration which resulted in no attempt to solve it in two domains which requires more complex approach. Such dilemma is avoided when mesoscale methods (Lattice Boltzmann Method-LBM) are applied but this method is less favourable as it is also relatively more complex. Regardless of the chosen scale, most models were simplified by assuming that the thermophysical properties values are similar throughout the phase change process regardless for liquid or solid. Such oversimplified model may result in critical deviation of the result relative to physical or experimental solution [10].

2. Methodology

In this research, the solidification and melting of NEPCM will be conducted in a two-dimensional computational domain with adiabatic horizontal walls and isothermal vertical walls. Figure 3 shows an example of the numerical domain for NEPCM melting process.



Fig. 3. NEPCM Melting Process Numerical Domain [65]

The system of equations for natural convection coupled with phase change will be applied to simulate NEPCM solidification and melting. These equations will be correlated with the phenomena by using FORTRAN code. The program will use the enthalpy-porosity method [16, 17] coupled with finite volume method (EPM-FVM) as this approach has been widely used by other researchers to represent the phenomena. This approach is a single-domain formulation which adds porosity source term to the momentum equations to differentiate liquid and solid regions during the phase change process. A source term is also added to the energy equation via enthalpy terms to account for latent heat evolution during the same process.

Assuming the mixture is incompressible, behaves as a Newtonian fluid; the continuity, momentum and energy conservation equations for 2-dimension are written as follows:

Continuity equation:

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

x-momentum equation:

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} = \frac{1}{\rho_{nf}} \left[-\frac{\partial P}{\partial x} + \mu_{nf} \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right) - C \frac{(1-\varepsilon)^2}{\varepsilon^3 + b} u \right]$$
(2)

y-momentum equation:

$$\frac{\partial v}{\partial t} + u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} = \frac{1}{\rho_{nf}} \left[-\frac{\partial P}{\partial y} + \mu_{nf} \left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} \right) - C \frac{(1-\varepsilon)^2}{\varepsilon^3 + b} v + (\rho\beta)_{nf} g \left(h - h_{ref} \right) \right]$$
(3)

Energy equation:

$$\frac{\partial h}{\partial t} + u \frac{\partial h}{\partial x} + v \frac{\partial h}{\partial y} = \frac{k_{nf}}{\left(\rho C_p\right)_{nf}} \left(\frac{\partial^2 h}{\partial x^2} + \frac{\partial^2 h}{\partial y^2}\right) \pm \left[\frac{\partial \left[\rho \Delta H\right]}{\partial t} + \frac{\partial \left[\rho \Delta H\right]}{\partial x} + \frac{\partial \left[\rho \Delta H\right]}{\partial y}\right]$$
(4)

Subscript *nf* denotes nanofluid (NEPCM). Three distinct regions will be present during the phase change process: a solid region, a liquid region, and a mushy region consisting of liquid and solid.

In a system going through a phase change via heat transfer, the total enthalpy is indicated as:

$$H = h + \Delta H \tag{5}$$

where it is the sum of sensible enthalpy, h and latent heat, ΔH . The latent heat component is temperature dependent and the phase change process should occur within a temperature range since NEPCM is a non-pure substance:

$$\Delta H = \varepsilon(T) = \begin{cases} L \text{ for } T > T_L \\ L(1 - \varepsilon) \text{ for } T_L > T > T_S \\ 0 \text{ for } T < T_S \end{cases}$$
(6)

where a parameter known as liquid fraction, ϵ is introduced to indicate the fraction of liquid in all cells and T_L and T_S is the melting and freezing temperature respectively while L is the latent heat of fusion. The liquid fraction is defined as follows:

$$\varepsilon = \frac{\Delta H}{L} \tag{7}$$

For linear phase change which should occur for NEPCM (non-pure substance):

$$\varepsilon = 0 \text{ if } T < T_S \text{ and } \varepsilon = 1 \text{ if } T > T_L$$
 (8)

For $T_S < T < T_L$, liquid fraction, ε is

$$\varepsilon = \frac{T - T_S}{T_L - T_S} \tag{9}$$

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This parameter is calculated for each cell in the domain at each iteration, based on an enthalpy balance. The mushy zone is a region in which the liquid fraction lies between 0 and 1. The mushy zone is modelled as a pseudo porous medium in which the porosity increases from 0 to 1 or decreases from 1 to 0 as the NEPCM liquefies or solidifies respectively. Porosity decreases to zero in the solid region and therefore the velocity in the region will also drop to zero as indicated in the source term.

The single value thermophysical properties will be estimated by linear function mixture model [26] for density, heat capacity and thermal expansion coefficient. Dynamic viscosity and thermal conductivity will be estimated using Brinkman [27] and Maxwell [28] correlations respectively.

Density of NEPCM will be defined by

$$\rho_{nf} = (1 - \emptyset)\rho_f + \emptyset\rho_s \tag{10}$$

Heat capacity of NEPCM will be defined by:

$$\left(\rho C_p\right)_{nf} = (1 - \emptyset) \left(\rho C_p\right)_f + \emptyset \left(\rho C_p\right)_s \tag{11}$$

Thermal expansion coefficient of NEPCM will be defined by:

$$(\rho\beta)_{nf} = (1 - \emptyset)(\rho\beta)_f + \emptyset(\rho\beta)_s \tag{12}$$

Dynamic viscosity of NEPCM will be defined by:

$$\mu_{nf} = \frac{1}{(1-\phi)^{2.5}} \mu_f \tag{13}$$

Thermal conductivity of NEPCM will be defined by:

$$k_{nf} = \frac{k_s + 2k_f + 2(k_s - k_f)\phi}{k_s + 2k_f - 2(k_s - k_f)\phi} k_f \tag{14}$$

Subscript *nf* denotes nanofluid (NEPCM), while *f* and *s* are the values for the base-fluid (PCM) and nanoparticle respectively. \emptyset is the volume fraction of nanoparticle dispersed in the PCM.

For single domain solution which will allow two values of thermophysical properties for solid and liquid region to be considered, the continuity, momentum and energy conservation will be amended and improvised as one of the objectives in this research.

The widely known algorithm Semi-Implicit Method for Pressure Linked Equations (SIMPLE) [66] will be used to solve the equations that govern the fluid flow and heat transfer phenomena. Figure 4 shows the overall flow chart for the methodology approach to be applied in this research. Finally, in order to visualize all the numerical values obtained from the simulation, Tecplot 360 EX shall be used.

2.1 Model Validation

Several diagrams will be constructed from the calculated domain for validation purposes. Melting or solidification front progress with time will be compared with predictions from experimental work of Gau and Viskanta [49] and numerical work of Brent *et al.*,[17]. The shape of the phase change front must be in acceptable agreement with these previous works.





Fig. 4. Research Methodology Flow Chart





Fig. 5. Prediction of melting front with time [17], [49]



Fig. 6. Predicted horizontal velocity component on the vertical mid-plane of the square cavity [48]

Next, the horizontal velocity component on the vertical mid-plane of the square cavity will be compared with the works of Khanafer *et al.*, [48]. This parameter must also be in acceptable agreement. The similarities mentioned above must be present to ensure the model satisfies the physics of the problem.

3. Conclusion

This research is expected to produce results which are even closer to the experimental results relative to previous numerical works. This will indicate that the proposed model has contributed to improvement on existing NEPCM solidification and melting numerical model. The limitations and



applicability of this proposed model will also be identified to avoid production of unacceptable or less accurate result during future model application. It is expected by completing this research, critical deviation of NEPCM phase change numerical simulation result relative to physical or experimental solution can be further reduced.

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