

Transient Numerical Models for Predicting the Performance of Encapsulated PCM Under Varying Ambient Temperatures for Cooling Application

Abasiafak N. Udosen

Abstract - This paper is aimed at presenting a single phase transient heat conduction model that mimics the effects of phase change present in paraffin wax under varying ambient temperatures for cooling application. The low energy encapsulated PCM-paraffin wax with initial temperature at 20°C, is modelled and numerically studied using the explicit finite difference method (FDM) and the effective heat capacity method (EHC). Numerical results obtained from Matlab showed that the melting temperature of the modelled paraffin varies but falls within the range of 23 – 26°C. The combination of the FDM and EHC numerical methods prove suitable for simplification and solving moving boundary phase change problems. Numerical results showed that encapsulating paraffin wax with high density polyethylene shells and exposing these capsules to ambient temperature conditions is capable of causing significant drop in ambient temperatures from 22 – 31.5°C to 14.2 – 20.3°C representing temperature depressions of 7.84 – 11.24°C.

Keywords - Phase Change, Mathematical Model, Stefan Problem, Nodal Temperature, Energy Balance, Finite difference, Paraffin wax.

1. INTRODUCTION

Phase change materials absorb heat from a high surrounding temperature fluid and releases that heat to a lower temperature fluid hence, causing a drop in temperature of the high temperature fluid. The application of a particular PCM is largely determined by its phase change temperature which can comfortably drop ambient temperature to levels used for space air conditioning. Phase change problems also referred to as Stefan or moving boundary problems are considered as nonlinear phenomenon because the phase change interface moves continuously during the melting or solidification processes and is usually difficult to track [8]. The aim of this paper is to use the energy balance method (EBM) to develop a single phase generalized heat conduction model that mimics melting and solidification effects of phase change present in PCMs and solve the model using FDM and EHC methods. The modelled PCM capsules are exposed to varying ambient temperatures for possible energy storage and cooling. The PCM used in this study is commercially available low energy paraffin wax encapsulated with high density polyethylene (HDPE) spherically shaped capsules and maintained at 20°C initial temperature.

The complexity of phase change problem is mainly a result of this unknown location of the phase change interface trajectory [3]. Phase change materials encapsulated in spherical geometries have attracted much attention for more than a century. This great interest is due to its direct relevance to thermal energy storage and other thermal management applications. Authors [1], presented a numerical and experimental study of solidification in a spherical shell. In their numerical simulations the PCM-air system was described using volume of fluid (VOF) model and for the phase change region inside the PCM, the enthalpy-porosity approach was used, where by the porosity in each cell is set equal to the liquid fraction in that cell and the porosity was assumed zero inside fully solid regions. The numerical results were obtained using FLUENT 6.2 software and convergence of solution was checked at each time step with convergence criterion of 10^{-5} . Similarly, a simple, rapid and generalized model, based on the energy balance technique, for solving heat transfer problems in phase change materials of liquid/solid type was formulated in [7]. The author considered the effect of natural convection in a rectangular cavity during sensible cooling and fusion processes. The results showed that the model based on the finite element method during the solidification process presented a very prolonged computer time (70h) as opposed to (>1h) by the energy balance technique. Authors [6], pointed that most precise analytical solution for a one-dimensional

• Abasiafak N. Udosen is currently a lecturer in the department of mechanical engineering, University of Nigeria, Nsukka, Nigeria, PH-+2348138188878. E-mail: Abasiafak.udosen@unn.edu.ng

phase change problem was originated by Neumann with different boundary conditions. Other analytical methods include methods like the quasi-stationary approximation, perturbation methods, the Megerlin method and the Heat-balance-integral method. The authors stated that the aforementioned methods are only suitable for calculating semi-finite or in-finite storages, however they added that real storages are finite and should be handled three or at least two-dimensionally so as to achieve a sufficiently accurate solution. The interfacial tracking method used by Zang and Yang [10] was developed for conduction-controlled melting and solidification problems which utilizes the advantages of both deforming and fixed grid methods. Numerical methods for solving PCM problems range from finite element method (FEM), finite difference method(FDM), finite volume method(FVM), variable grid method(VGM), Enthalpy method, fixed grid method etc. Caldwell and kwan [11] compared several effective methods for the numerical solution of one-dimensional Stefan problems. They examined the enthalpy method, boundary immobilization method, perturbation method, nodal integral method and the heat balance integral method. The difference among these methods is seen in the discretization approach but common to all the methods is that the phase change phenomenon has to be modeled separately due to the nonlinear nature of the problem. In the fixed grid method (FGM) as reported in [5], the phase change interface fitting was totally eliminated by formulating the energy equation in terms of the effective heat capacity where the fixed grid size and fixed time step can be employed to generate a single heat model equation used to predict the thermal profile of the PCM. Costa et al [2] used the enthalpy formulation with fully implicit finite difference method to analyse numerically the thermal performance of latent heat storage, modelled in both (2-D) conduction and (1-D) convection heat transfer modes. The authors concluded that the method is useful for designing thermal stores.

2. PROBLEM FORMULATION

The following assumptions are used to simplify the analysis:

1. Ambient air, Paraffin wax and HDPE shell temperature varies along the radial direction of each PCM capsule; $T_f = T_f(r)$, $T_w = T_w(r)$ and $T_p = T_p(r)$

2. One dimensional transient state is considered for the paraffin wax and HDPE shell hence; $\frac{\partial T}{\partial \theta} = 0$, $\frac{\partial T}{\partial \phi} = 0$, $\frac{\partial T}{\partial r} \neq 0$
3. No internal heat generation in the PCM capsules; $\dot{Q} = 0$
4. The PCM regime is assumed to be solid dominated, therefore the convective heat transfer during phase change in the solid-liquid or liquid-solid interface is neglected; $h_w = 0$
5. The PCM capsules are exposed to air (incompressible Newtonian fluid)flowing through an axial flow fan at varying ambient temperatures T_i ; $\rho_f = 0$
6. The momentum heat, fluid and mass transfer analysis is not considered.
7. The densities of the HDPE shells and paraffin wax are constant.
8. Radiant heat transfer coefficient between the capsules is negligible.
9. Thermophysical properties of HDPE shells and paraffin wax do not vary with time.

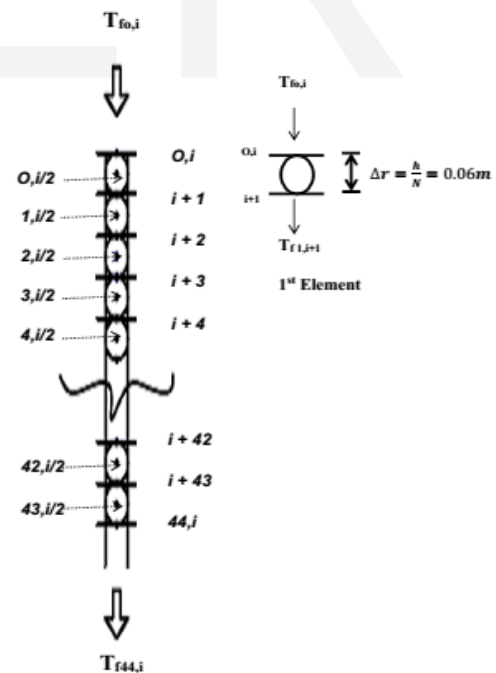


Fig.1: Nodal Network of 44 paraffin wax capsules in the axial flow direction.

3. GOVERNING EQUATIONS

To solve the PCM problem, it requires consideration of already stated assumptions hence a one-dimensional single phase transient heat conduction equation is developed for PCM capsule nodes 0 – 43, which interacts with the HDPE spherical shell boundaries. Mathematical the energy balance can be derived using the formula; Energy transferred from HDPE capsule walls to internal PCM nodes of control volume $A_s \Delta r$ equals energy increase in the paraffin wax within the control volume $A_s \Delta r$ due to energy storage.

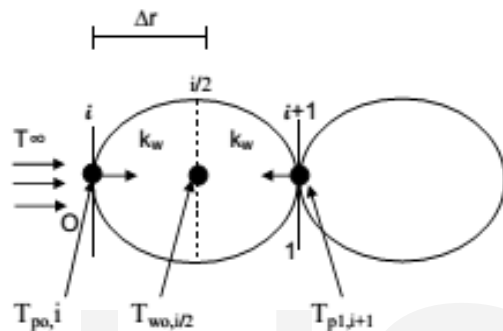


Fig. 2: Energy balance analysis of paraffin wax about internal center nodes 0 - 43

The applicable energy equation can be expressed as:

$$\ell_w C_{pw} A_s \frac{\partial T_w}{\partial t} = \phi + \frac{k_w}{r^2} A_s \frac{\partial}{\partial r} \left[r^2 \frac{\partial (T_{p0} - T_{w0,i/2})}{\partial r} \right] + \frac{k_w}{r^2} A_s \frac{\partial}{\partial r} \left[r^2 \frac{\partial (T_{p1} - T_{w0,i/2})}{\partial r} \right] + A_s \partial r \quad (1)$$

Applying assumption 3, and simplifying equation (1) yields;

$$\ell_w C_{pw} A_s \frac{\partial T_w}{\partial t} = \frac{k_w}{r} A_s \frac{\partial^2 (r(T_{p0} - T_{w0,i/2}))}{\partial r^2} + \frac{k_w}{r} A_s \frac{\partial^2 (r(T_{p1} - T_{w0,i/2}))}{\partial r^2} + A_s \partial r \quad (2)$$

Initial Conditions:

$$T_w(r_h, 0) = T_{w\text{initial}} = T_{p\text{initial}} \quad (3)$$

$$T_w(r_0, 0) = T_{w\text{initial}} = T_{p\text{initial}} \quad (4)$$

$$T_w\left(\frac{r_h}{2}, 0\right) = T_{w\text{initial}} = T_{p\text{initial}} \quad (5)$$

Boundary Conditions:

$$T_w(r_0, t) = -\frac{h_w}{k_w} \left[T_{p(0,t)} - T_w\left(\frac{r_0}{2}, t\right) \right] \quad (6)$$

$$T_w(r_h, t) = -\frac{h_w}{k_w} \left[T_{p(43,t)} - T_w\left(\frac{r_h}{2}, t\right) \right] \quad (7)$$

The initial and boundary conditions in equation (6) - (7) can be used to solve equation (2) analytically. To simplify the governing equation (2) for numerical approach, we define the following applicable dimensionless parameters.

$$r^* = \frac{r}{r_h}, \tau^* = \frac{t}{t_0}, \theta = \frac{T - T_w}{T_p - T_w}$$

Where τ_0 is some arbitrary time interval, r is radius at any internal node points on the PCM capsule and r_h is the HDPE exit capsule external node, τ is the dimensionless time.

In figure 1, the nodal position $\frac{r_0}{2} = \frac{i}{2}$ represents the mid-point of each capsule where ; $r = \text{node } 0, r_0 = \text{node } 1, r_1 = \text{node } 2, \dots, r_h = \text{node } 44$

Let $T_w = T_{p0} - T_{w0,i/2}$ and $T_p = T_{p1} - T_{w0,i/2}$ in equation (2) for simplicity thus substituting the dimensionless parameters into equation (2) gives

$$\ell_w C_{pw} A_s t_0 r^* r_h \frac{\partial T_w}{\partial \tau} = k_w A_s t_0 \frac{\partial (T - T_w) + T_p}{\partial r^* \partial \theta} + k_w A_s t_0 r^* r_h \frac{\partial (T - T_w) + T_w}{\partial r^* \partial \theta} + A_s t_0 r^* r_h \partial r \quad (8)$$

Dividing through by $A_s t_0 r^* r_h$ gives

$$\ell_w C_{pw} \frac{\partial T_w}{\partial \tau} = \frac{k_w}{r^* r_h} \frac{\partial (T - T_w) + T_p}{\partial r^* \partial \theta} + \frac{k_w}{r^* r_h} \frac{\partial (T - T_w) + T_w}{\partial \theta} + \frac{\partial r}{r^* r_h} \quad (9)$$

Dividing equation (9) through by k_w and multiplying

by $\alpha_w = \frac{k_w}{\ell_w C_{pw}}$ gives

$$\frac{\partial T_w}{\partial \tau} = \frac{\alpha_w}{r^* r_h} \frac{\partial (T - T_w) + T_p}{\partial r^* \partial \theta} + \frac{\alpha_w}{r^* r_h} \frac{\partial (T - T_w) + T_w}{\partial \theta} + \alpha_w \frac{\partial r}{r^* r_h} \quad (10)$$

By order of magnitude analysis of equation (10) we

compare necessary terms, hence there's no justification to neglect a term in preference to the other. Also, Substituting $T_w = T_{p0} - T_{w0,i/2}$,

$T_p = T_{p1} - T_{w0,i/2}$ and $\theta = \frac{T - T_w}{T_p - T_w}$ back to equation (10) yields

$$\frac{\partial T_w}{\partial \tau} = \frac{\alpha_w}{r^* r_h} \frac{\partial (T_{p0} - T_{w0,i/2})}{\partial r^*} + \frac{\alpha_w}{r^* r_h} \frac{\partial (T_{p1} - T_{w0,i/2})}{\partial r^*} + \alpha_w \frac{\partial r}{r^* r_h} \quad (11)$$

Multiplying through by $\frac{r^* r_h}{\alpha_w}$ gives

$$\frac{r^* r_h \partial T_w}{\alpha_w \partial \tau} = \frac{\partial (T_{p0} - T_{w0,i/2})}{\partial r^*} + \frac{\partial (T_{p1} - T_{w0,i/2})}{\partial r^*} + \partial r \quad (12)$$

Equation (12) is multiplied by $\alpha_w = \frac{k_w}{\ell_w C_{pw}}$ to yield

$$\frac{\partial T_w}{r \partial \tau} = \frac{k_w}{\ell_w C_{pw}} \frac{\partial (T_{p0} - T_{w0,i/2})}{\partial r^*} + \frac{k_w}{\ell_w C_{pw}} \frac{\partial (T_{p1} - T_{w0,i/2})}{\partial r^*} + \frac{k_w}{\ell_w C_{pw}} \partial r \quad (13)$$

Rearranging equation (13) gives

$$\frac{k_w}{\ell_w C_{pw}} \frac{\partial(T_{p0} - T_{wo,i/2})}{\partial r^*} + \frac{k_w}{\ell_w C_{pw}} \frac{\partial(T_{p1} - T_{wo,i/2})}{\partial r^*} = \frac{\partial T_w}{r \partial \tau} - \frac{k_w}{\ell_w C_{pw}} \partial r \quad (14)$$

Multiplying equation (14) by r^* gives

$$\frac{k_w}{\ell_w C_{pw}} (T_{p0} - T_{wo,i/2}) + \frac{k_w}{\ell_w C_{pw}} (T_{p1} - T_{wo,i/2}) = \frac{\partial T_w r^*}{\partial \tau} - \frac{r^* k_w \partial r}{\ell_w C_{pw}} \quad (15)$$

Discretizing equation (15) using the simple explicit and first-order finite difference formulation gives:

$$\frac{k_w}{\ell_w C_{pw}} (T_{p0,i}^n - T_{wo,i/2}^n) + \frac{k_w}{\ell_w C_{pw}} (T_{p1,i+1}^n - T_{wo,i/2}^n) = \frac{T_{wo,i/2}^{n+1} - T_{wo,i/2}^n}{\Delta t} \Delta r^2 - \frac{k_w \Delta r^2}{\ell_w C_{pw}} \quad (16)$$

Collecting like terms and multiplying through by $\frac{\ell_w C_{pw}}{k_w}$ gives

$$T_{p0,i}^n - 2 T_{wo,i/2}^n + T_{p1,i+1}^n = \frac{\ell_w C_{pw} \Delta r^2}{k_w \Delta t} (T_{wo,i/2}^{n+1} - T_{wo,i/2}^n) - \Delta r^2 \quad (17)$$

Further rearranging gives

$$T_{p0,i}^n - 2 T_{wo,i/2}^n + T_{p1,i+1}^n + \Delta r^2 = \frac{\ell_w C_{pw} \Delta r^2}{k_w \Delta t} (T_{wo,i/2}^{n+1} - T_{wo,i/2}^n) \quad (18)$$

Hence, equation (18) becomes

$$T_{p0,i}^n - 2 T_{wo,i/2}^n + T_{p1,i+1}^n + \Delta r^2 = \frac{\Delta r^2}{\alpha_w \Delta t} (T_{wo,i/2}^{n+1} - T_{wo,i/2}^n) \quad (19)$$

Multiplying equation (19) by $\frac{\alpha_w \Delta t}{\Delta r^2}$ gives

$$\frac{\alpha_w \Delta t}{\Delta r^2} T_{p0,i}^n - \frac{2\alpha_w \Delta t}{\Delta r^2} T_{wo,i/2}^n + \frac{\alpha_w \Delta t}{\Delta r^2} T_{p1,i+1}^n + \alpha_w \Delta t = T_{wo,i/2}^{n+1} - T_{wo,i/2}^n \quad (20)$$

Rearranging equation (20) gives

$$T_{wo,i/2}^{n+1} - T_{wo,i/2}^n = \frac{\alpha_w \Delta t}{\Delta r^2} T_{p0,i}^n - \frac{2\alpha_w \Delta t}{\Delta r^2} T_{wo,i/2}^n + \frac{\alpha_w \Delta t}{\Delta r^2} T_{p1,i+1}^n + \alpha_w \Delta t \quad (21)$$

Where $F_o = \frac{\alpha_w \Delta t}{\Delta r^2}$ is the Fourier number so that equation (21) becomes

$$F_o (T_{p0,i}^n + T_{p1,i+1}^n + \alpha_w \Delta t) + (1 - 2F_o) T_{wo,i/2}^n = T_{wo,i/2}^{n+1} \quad (22)$$

Rearranging equation (22) gives

$$T_{wo,i/2}^{n+1} = F_o (T_{p0,i}^n + T_{p1,i+1}^n + \alpha_w \Delta t) + (1 - 2F_o) T_{wo,i/2}^n \quad (23)$$

Applying the stability criterion, requires that the coefficient $T_{wo,i/2}^n$ be greater than or equal to zero so that Δt - simulation time is selected to be well within

the stability limit which corresponds to the value of F_o hence from the stability criterion equation

$$(1 - 2F_o)F_o \geq 0; F_o \leq \frac{1}{2}; \Delta t = \frac{F_o \Delta r^2}{\alpha_w} \approx 1 \text{hr.}; F_o = \frac{\alpha_w \Delta t}{\Delta r^2} = 0.49$$

When substituting parameters for Δr^2 , F_o and α_w for convergence and stability of numerical results, the minimum permissible value for the computation time interval is $\Delta t \approx 1 \text{hr.}$

By substituting F_o into equation (23) gives

$$T_{wo,i/2}^{n+1} = 0.49 (T_{p0,i}^n + T_{p1,i+1}^n + \frac{k_w}{\ell_w C_{pw}} \Delta t) + 0.02 T_{wo,i/2}^n \quad (24)$$

Where C_{pw} is the specific heat capacity of paraffin wax with melting and solidification boundary conditions stated as follows:

$$C_{pw(\text{solid})} = \frac{1800 \text{kJ}}{\text{kg}} \text{K}, T_{wo,i/2}^n < 20.99^\circ \text{C}, \ell_w = 850 \text{kg/m}^3$$

$$C_{pw(\text{solid-liquid})} = \frac{18,067 \text{kJ}}{\text{kg}} \text{K}, 20.99^\circ \text{C} \leq T_{wo,i/2}^n \leq 27.99^\circ \text{C}, \ell_w = 850/780 \text{kg/m}^3$$

$$C_{pw(\text{liquid})} = 2400 \frac{\text{kJ}}{\text{kg}} \text{K}, T_{wo,i/2}^n > 27.99^\circ \text{C}, \ell_w = 780 \frac{\text{kg}}{\text{m}^3}$$

Source: [6]

Equation (24) is the generalized single phase heat conduction model used to predict phase change phenomenon at node 0 and can be written for nodes 0 - 43 at new time steps forming a set of N-algebraic linear equations solvable using MATLAB. The Authors [6], obtained this boundary conditions based on their correlation of effective heat capacity which states that the effective heat capacity of a material C_{eff} is directly proportional to the stored and released energy during phase change and also to the specific heat capacity but inversely proportional to the width of the solidification temperature range.

$$C_{\text{eff}} = \frac{L}{(T_{w2} - T_{w1})} + C_p \quad (25)$$

Where L is the latent heat of fusion, T_{w1} is the temperature where melting or solidification begins and T_{w2} is the temperature where the paraffin is totally melted or solidified [6]. This method can be applied to equation (25) and values of C_{pw} for liquid, solid and solid-liquid phases are obtained for fixed temperature conditions. Thermophysical properties of commercially available paraffin and HDPE materials where used to solve equation (6) as detailed in [9].

3.1 GOVERNING EQUATION FOR HDPE INTERNAL NODES 1-43 IN TRANSIENT MODE

The energy balance about HDPE internal capsule nodes 1-43 at transient state is expressed mathematically, as the *sum* of heat quantity transferred by conduction from node 1 to node 2 across capsule space Δr and heat transfer by conduction from node 3 to node 2 across capsule space Δr *equals* rise in temperature at node 2 within the control volume $A_s \Delta r$ due to energy accumulation at node 2. The governing applicable equation can be written as

$$\ell_p C_{pp} A_s \frac{\partial T_p}{\partial t} = \emptyset + \frac{k_p}{r^2} A_s \frac{\partial}{\partial r} \frac{r^2 \partial (T_{p1} - T_{p2})}{\partial r} + \frac{k_p}{r^2} A_s \frac{\partial}{\partial r} \frac{r^2 \partial (T_{p2} - T_{p3})}{\partial r} \quad (26)$$

By applying assumptions, setting the initial and boundary conditions equation (26) is either solved analytically or numerically. The numerical solution for equation (27) is expressed as

$$T_{p1,i+1}^{n+1} = 0.499 (T_{po,i}^n + T_{p2,i+2}^n) + 2 * 10^{-3} T_{p1,i+1}^n \quad (27)$$

Equation (27) is the numerical algorithm use to predict the temperature at node 1 and can be written for nodes 2 - 43 at new time steps forming a set of N algebraic linear equations.

3.2 GOVERNING EQUATION FOR HDPE EXTERNAL NODES IN TRANSIENT MODE

The energy balance about HDPE external nodes 0 and 44 within the control volume $A_s \Delta z$ is expressed mathematically, as the *sum* of the heat transfer by convection from ambient air flowing through an axial fan to node 0 *and* heat transfer by conduction from node 1 to node 0 within control volume $A_s \Delta z$ which *equals* the rate at which the shell temperature raises at node 0 within the control volume $\frac{A_s \Delta z}{2}$ due to the energy accumulation at that node. The governing equation is thus derived for nodes 0 and 44 and is given as

$$\ell_p C_{pp} A_s \frac{\partial r}{2} \frac{\partial T_p}{\partial t} = \frac{k_p}{r^2} A_s \frac{\partial}{\partial r} \frac{r^2 \partial (T_{p1} - T_{p0})}{\partial r} + h_f A_s (T_{f0} - T_{p0}) \quad (28)$$

By setting the initial and boundary conditions, equation (28) is either solved analytically or numerically. The numerical solution for equation (28) is expressed as

$$T_{po,i}^{n+1} = 0.98 (T_{p1,i+1}^n + 1.52 * 10^{-4} T_{fo,i}^n) + 3.3 * 10^{-4} T_{po,i}^n \quad (29)$$

Equation (29) can be used to predict the temperature fluctuations of nodes 0 and 44 only and can be written for new time steps forming a system of N-algebraic linear equations.

4. RESULTS AND DISCUSSION

The single heat conduction numerical transient model developed in equation (24) has the capability to predict the effects of phase change present in solid-liquid paraffin wax where the melt fraction regime is assumed as conduction dominated. A combination of the explicit-first order finite difference (FDM) and the effective heat capacity (EHC) methods was adopted as numerical methods used in discretizing and solving the PCM equation. It is the authors view that all numerical predictions derived in this study, give considerable estimation of melting and solidification processes. The graph in figures 3-8 were plotted in EXCEL using numerical results obtained from Matlab and shows the PCM-paraffin wax temperature behavior at nodes 0,20 and 43 undergoing phase change from solid sensible heating mode to the latent melting transition mode to solidification mode. The graphs also showed the HDPE temperature profile of the exist capsule node 44 and a significant drop in ambient temperatures from initial values of 22 – 31.5°C to final values of 14.2 – 20.3°C for 6 days, which represents temperature depressions of 7.84 – 11.24°C. The melting /phase change temperature of the modelled paraffin wax varies but falls within the range of 23 – 26°C and the solid sensible heating and the latent transition modes occurred between 12am – 2am while the solidification mode starts immediately till 12am, the next simulation day.

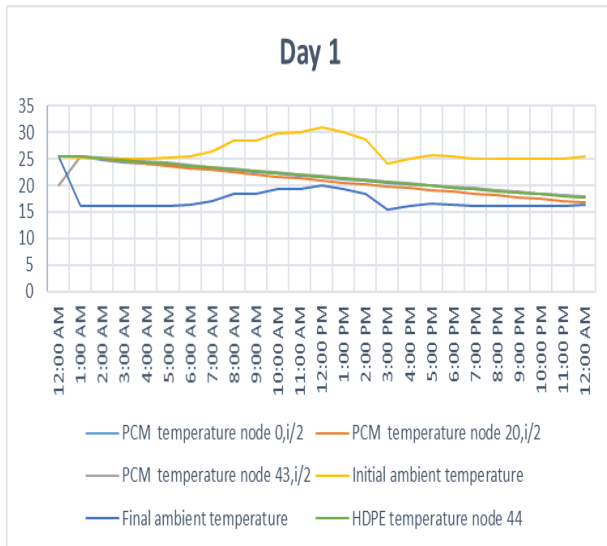


Fig.3: Graph of temprature against time for Day 1.

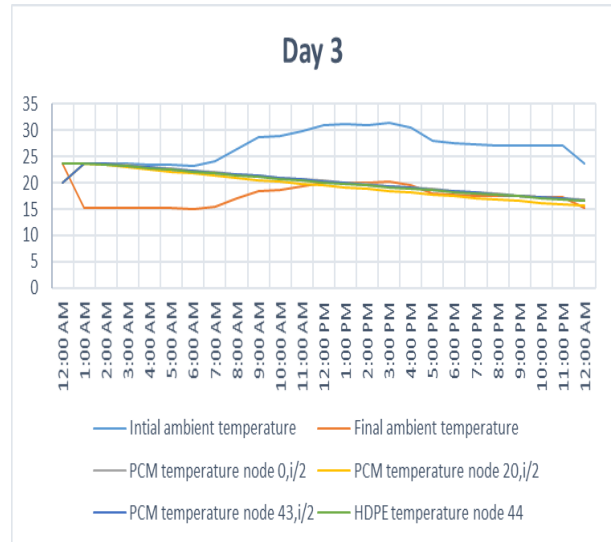


Fig. 5: Graph of temprature [°C] against time for Day 3.

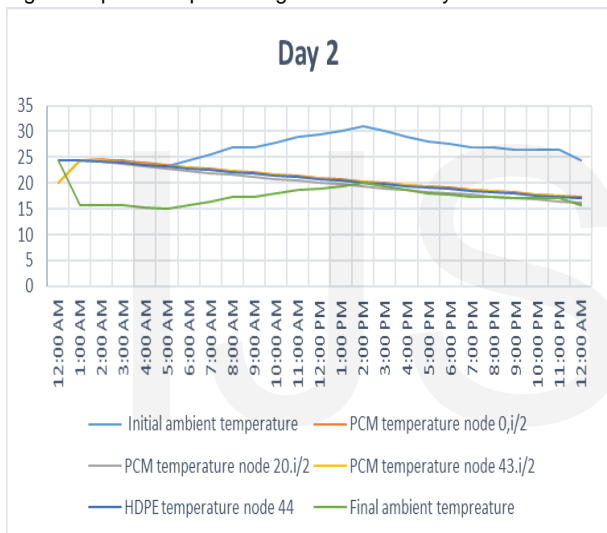


Fig.4: Graph of temprature[°C]against time for Day 2.

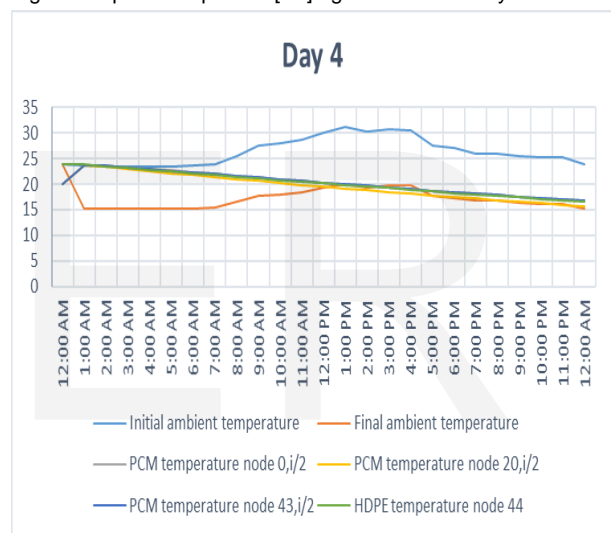


Fig. 6: Graph of temprature[°C] against time for Day 4.

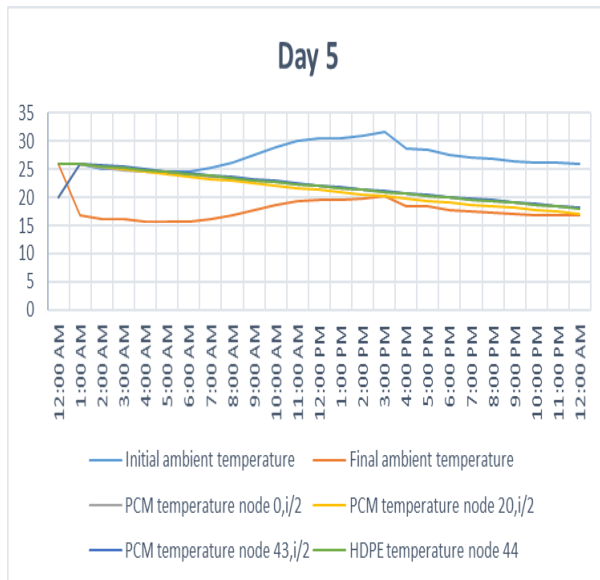


Fig. 7: Graph of temperature[°C] against time for Day 5.

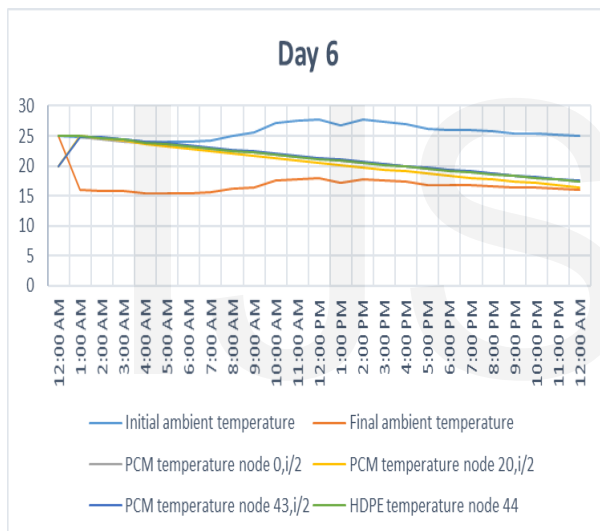


Fig. 8: Graph of temperature against time for Day 6.

5. CONCLUSION

The formulation of a single phase transient heat conduction model, to predict the performance of encapsulated phase change material under varying ambient temperatures has been successfully carried out and was necessary to solve the “moving boundary” phase change problem. The results obtained are simplified energy models analyzed to mimic the effects of phase change present in solid-liquid PCMs where the melt fraction regime is assumed as conduction dominated. In this paper, it can be established that the combination of the explicit-

first order finite difference method (FDM) and the effective heat capacity method (EHC) used in discretizing the PCM energy equation is suitable for simplification and solving of the moving boundary phase change problems. The numerical results also showed that encapsulating paraffin wax with high density polyethylene shells and exposing these capsules to varying ambient temperatures, is useful for significant cooling application.

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