Numerical Study of PCM-Based Energy Storage System Using Finite Difference Method

C. Abhijith and Ranjith Maniyeri

Abstract Energy storage systems incorporating phase change material (PCM) are becoming the answer to intermittent energy availability in the area of solar cooking vessels and solar room heating systems. These thermal energy storage systems are efficient, reliable and can reduce running costs and investments. The present work investigates the melting of n-octadecane using enthalpy formulation method by using finite difference method-based discretization. Accordingly, a numerical model is developed in MATLAB which is validated first by comparing with previous works. Further using the developed model studies on wall materials, thickness, different PCMs and temperatures are carried out. It is found that metal containers with higher thermal conductivities provided significant boost in energy storage. The increased thickness of walls adds significant change only if containers are of lower thermal conductivity such as steel. Different PCMs are analysed, and their operating temperature and energy storage capabilities are studied. In addition, enthalpy equation in cylindrical coordinates is solved since practical PCM storages are commonly cylindrical in shape. At the end, the numerical results are compared with an experimental case with paraffin wax as PCM.

Keywords Energy storage · Enthalpy formulation · Finite difference method · Melt fraction · Phase change materials

1 Introduction

Thermal energy storage systems are increasingly becoming attractive since many renewable energy supplies must deal with inconsistent demand and supply. Latent heat storage systems store energy while melting and solidification of phase change materials (PCM) as latent heat. PCM-based systems have the advantage of high

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storage capacity and relatively constant operating temperature. Such systems can be employed to bridge the mismatch between supply and demand of renewable systems such as solar cooking vessels and room heating systems. Two-dimensional (2D) numerical heat transfer studies of PCM materials have been done by Chen et al. [1] and Costa et al. [2] using enthalpy formulation method. Research works were reported on the studies of Melting characteristics with respect to temperature and storage vessel materials. It is understood that melting characteristics such as melting and solidification time, latent energy stored, wall temperature and container material should be studied in detail. Most of the studies considered rectangular coordinate system for the simulation but in reality PCM containers are of cylindrical shape and hence solving enthalpy equations in cylindrical coordinates is of practical significance. Inspired by this, we propose finite difference-based simulation model to study PCM-based energy storage system under different wall temperatures, metal containers and wall thicknesses. We also aim to see how our numerical model relate with that of experimental works on solar box cooker embedded with a PCM developed by Anilkumar et al. [3].

2 Literature Review and Objective

Several researchers have studied the melting and energy storage capabilities of PCM materials. The challenging part of a phase change problem exists due to the moving boundary between phases. Costa et al. [2] used enthalpy formulation method to simulate PCM melting in 1D and 2D domains. Enthalpy formulation solves one single enthalpy equation for both liquid and solid domains and hence the interface does not need any extra conditions. Costa et al. [2] used finite difference method and an additional melt fraction update equation to simulate the melting of n-octadecane PCM material.

Many researchers have studied to incorporate the PCM into useful applications. Buddhi and Sahoo [4] developed a latent heat storage-based box solar cooker to demonstrate feasibility of using a phase change material (stearic acid) in Indian climatic conditions. They demonstrated the variation of temperature with time. Sharma et al. [5] studied the operation of a cylindrical PCM storage system that uses erythritol as PCM. They studied temperature and melt fraction variation during operation. Halawa et al. [6] used enthalpy formulation to investigate the freezing characteristics of thin slabs of PCM with variation in wall temperatures. Chen et al. [1] studied melt fraction variation of PCM storage system with time and wall conduction using enthalpy formulation in 2D domain.

Zivkovic and Fujii [7] compared rectangular and cylindrical PCM storage melting and validated the enthalpy formulation method by experiment. Vyshak and Jilani [8] expanded upon this work to compare rectangular, cylindrical and cylindrical shell PCM storages and concluded that cylindrical shell configuration provided more favourable energy storage rates.

Recently, Anilkumar et al. [3] conducted experiments on a cooking pot of solar box cooker integrated with a cylindrical PCM storage system and analysed its ability to retain favourable temperatures. Paraffin wax was used for analysis and optimum amount of PCM was calculated and different PCMs were analysed and best PCM for the application was recommended to be erythritol.

Deriving inspiration from previous studies and to contribute further the present work aim to develop a computational model using finite difference method to predict PCM melt fraction in thermal energy storage systems and to study the effect of parameters such as PCM materials, container material, container thickness, boundary condition on melting and energy storage. In addition, melting and solidification in a cylindrical storage to compare with an experimental case is also studied.

3 Materials and Methods

3.1 Mathematical Model

Enthalpy formulation is employed as the mathematical model to solve the given problem where the variable is enthalpy. Assumptions involved in enthalpy formulation method are.

1. PCM thermal properties are not dependent on temperature. Thermal properties of liquid and solid phases can be different.
2. Initial condition of PCM is solid.
3. PCM is assumed to be isotropic and homogenous.
4. PCM is subjected to only conduction heat transfer.

For any phase change problem, the total volumetric enthalpy can be represented by

$$\frac{\partial H}{\partial t} = \Delta(k_k(\Delta T)) \tag{1}$$

k_k denotes the thermal conductivity of phase k. Total volumetric enthalpy represented in terms of sensible and latent heat is

$$H = h(T) + \rho\lambda f(T) \tag{2}$$

ρ denotes the density, f(T) is the melt fraction and λ is the latent energy of the PCM. Sensible heat h can be written as

$$h = \int_{T_m}^{T} \rho_k c_k dT \tag{3}$$

The melt fraction f at different temperature is

$$f = \begin{cases} 0 \;\; if \;\; T < T_m \;\; (solid) \\ 0 \;\; to \;\; 1 \;\; if \;\; T = T_m \;\; (mushy) \\ 1 \;\; if \;\; T > T_m \;\; (Liquid \end{cases}$$

Enthalpy at each phase can be written as

$$H = \begin{cases} \int_{T_m}^{T} \rho_s c_s dT \; T < T_m \;\; (solid) \\ \rho_l f \lambda T_m \;\; (mushy) \\ \int_{T_m}^{T} \rho_l c_l dT \; T > T_m \;\; (liquid) \end{cases}$$

Value of temperature can be obtained from enthalpy as

$$T = \begin{cases} T_m + \frac{H}{\rho_s c_s} H < 0 \;\; (solid) \\ T_m 0 < H < \rho_l \lambda \;\; (mushy) \\ T_m + \frac{H - \rho_l \lambda}{\rho_l c_l} H > \rho_l \lambda \;\; (liquid) \end{cases}$$

From (2) and (3), two-dimensional heat transfer equation while melting of a PCM is given as

$$\frac{\partial h}{\partial t} = \frac{\partial}{\partial x}\left(\alpha \frac{\partial h}{\partial x}\right) + \frac{\partial}{\partial y}\left(\alpha \frac{\partial h}{\partial y}\right) - \rho_l \lambda \frac{\partial f}{\partial t} \tag{4}$$

3.2 Numerical Solution

The fully implicit finite difference approach can be used to solve Eq. (4). For uniform grids the discretisation leads to

$$h_p = h_p^0 + \alpha R\left[h_E - 4h_p + h_S + h_N + h_S\right] + \rho_l \lambda [f_p^0 - f_p^k] \tag{5}$$

$$a_E h_E + a_W h_W + a_P h_P + a_N h_N + a_S h_S = Q \tag{6}$$

where

$$a_E = a_W = a_N = a_S = -\alpha R,$$

$$a_P = 1 - a_E - a_W - a_N - a_S$$

$$Q = h_p^0 + \rho_l \lambda [f_p^0 - f_p^k],\ R = \frac{dt}{dx^2}$$

Here superscript 0 denotes the preceding time step and k means the kth iteration for updating the melt fraction Voller [9] derived the formula as

$$f_p^k = f_p^0 + \frac{-a_E h_E - a_W h_W - a_N h_N - a_S h_S + h_p^0}{\rho_l \lambda} \tag{7}$$

The algorithm developed by Voller [9] is.

1. Compute the coefficients.
2. To constrain sensible enthalpy h_p while melting or solidification, a_p value is set to 10^{15} during phase change.
3. Solve for enthalpy and update liquid fraction at each iteration. Along with under and over correction for the melt fraction

$$f = \begin{cases} 0\ if\ \ f < 0 \\ 1\ if\ \ f > 1 \end{cases}$$

4. Repeat calculation until convergence. Large a_p value is retained until phase change is completed or convergence is reached.

Convergence is reached at a time step where total enthalpy is less than the given tolerance

$$\frac{ABS(H^k - H^{k+1})}{\rho_k c_k} < TOL$$

Tolerance for the present work is taken as 10^{-4}.

Interface Properties

Because properties of the two phases differ, the domain will have non-uniform thermal conductivity, Specific heat and density As a result, the equivalent properties of the mushy control volume must be calculated. As an example thermal conductivity of mushy control volume is

$$k_{mushy} = k_s(1 - f) + k_f f \tag{8}$$

Boundary and Initial Conditions

Initial temperature of PCM is fixed at 5^0C lower than the melting point of the PCM. Temperature at the left boundary is kept as 10^0C (or 15^0C) and other boundaries

are given adiabatic condition. All the equations listed above have been solved by developing a code in MATLAB.

4 Results and Discussion

4.1 Grid Independence Study and Validation

Grid independence study is carried out by choosing 32 × 32 grid and 64 × 64 grid and melt fraction vs time graph is plotted as shown in Fig. 1. There is very little difference between both grids hence 32 × 32 grid is computationally much efficient. But while plotting melt front progression 62 × 62 grid provides much clearer picture hence 62 × 62 grid is selected as optimum grid for further simulations.

Then, by comparing our results with that of Costa et al. [2] the developed code is validated as depicted in Fig. 2. The PCM used is n-octadecane in an aluminium container. From the figure, it can be inferred that there is good agreement with our results with that of Costa et al. [2] results which proves the reliability of our code. Further, the progression of melt front with time is also recorded at 2,10,30,60,150 and 240 min to illustrate the melting of PCM which also shows excellent agreement with that of Costa et al. [2] studies as represented in Figs. 3 and 4 (Table 1).

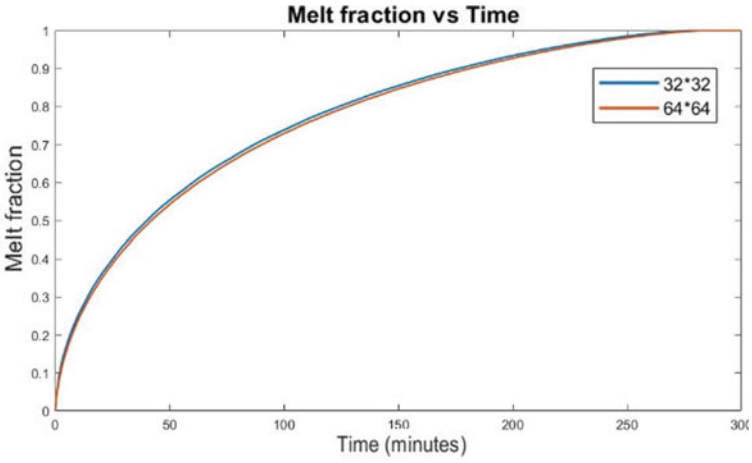

Fig. 1 Melt fraction versus time for two different grids

Table 1 Properties of n-octadecane

N-octadecane	
Melting temperature	300.7 K
Latent heat of fusion	243.5 kJ/kg
Density (liquid)	777.0 kg/m^3
Thermal conductivity	
Liquid	0.148 W/mK
Solid	0.358 W/mK
Thermal diffusivity	
Liquid	8.64*10^{-8} m^2/s
Solid	2.14*10^{-7} m^2/s

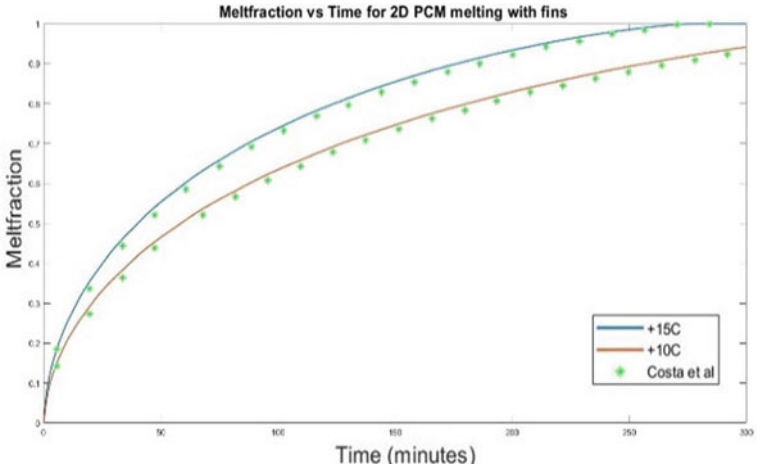

Fig. 2 Melt fraction vs time for current code versus Costa et al. [2] results

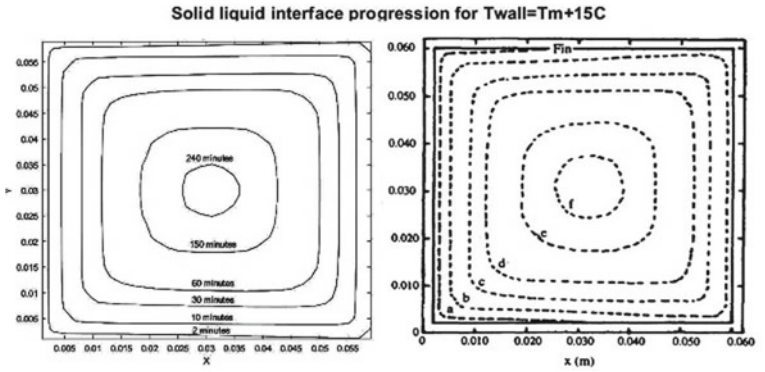

Fig. 3 Solid liquid interface progression with wall temperature 15 °C for **a** Current code (left) **b** Costa et al. [2] (right)

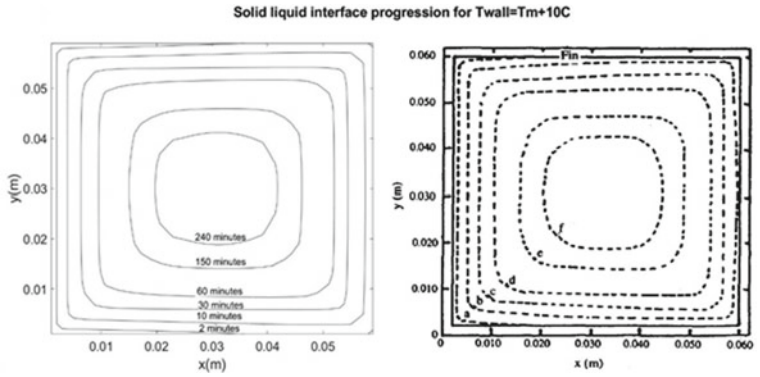

Fig. 4 Solid liquid interface progression with wall temperature 10 °C for **a** Current code (left) **b** Costa et al. [2] (right)

4.2 Factors Affecting Heat Transfer

4.2.1 Heat Transfer with Different Container Materials

Numerical simulations are performed for various container materials like copper, tin, stainless steel and glass to see the change in melting characteristics. The thermal conductivity values of these metals result in different melting characteristics.

While investigating the melt front propagation, we can see significant changes in low-conductivity materials such as steel and glass since they take significantly more time for melting. With metals such as copper and tin which have appreciable conductivity change in melting time is minimal. There is very little improvement in using copper in place of aluminium. Figure 5 depicts these observations (Fig. 6).

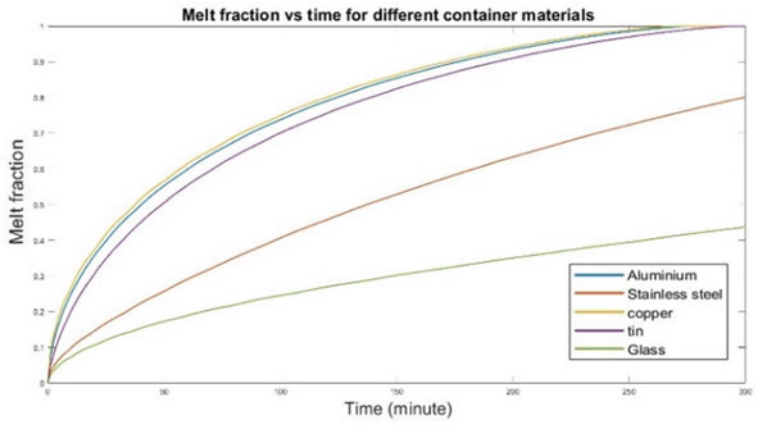

Fig. 5 Melt fraction versus time for different container materials

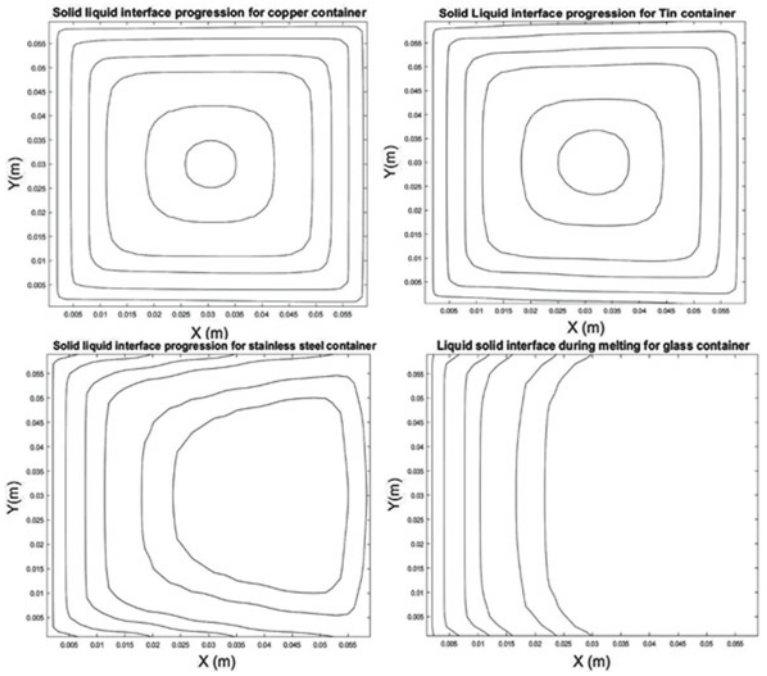

Fig. 6 Solid liquid interface progression for different fin materials **a** Copper **b** Tin **c** Stainless steel **d** Glass

The melting in copper and tin are very similar to aluminium container but for lower thermal conductivity metals such as steel more melting is done near the heated wall and the right end melts slower than the other side. In the glass container, there is very little heat conduction hence melt front is essentially flat progressing from left to right. It is apparent that glass does not provide any heat transfer benefit and only acts as a container for PCM.

4.2.2 Heat Transfer with Different Thickness of Metal Container

The previously mentioned simulations are done for 2 mm metal containers. To see the effect of change in thickness of the metal containers the simulations are repeated for 1mm, 2 mm, 3 mm and 4 mm thicknesses. Total melting time computed in each case shed light on the effectiveness of melting.

From the total melting time values shown in Table 2, with higher thickness heat transfer is improved and time for melting is decreased. The effect is more pronounced in metals with lower thermal conductivity such as steel where a decrease of 38.2% in time is observed when thickness is increased from 1 to 4 mm while in copper this change is merely 2.46%.

Table 2 Total melting time for different metal thickness

	Total melting time (minutes)			
Thickness (mm)	Aluminium	Copper	Tin	Steel
1mm	291.6	279.9	328.2	706.3
2mm	282	275.3	302.8	537.9
3mm	279	273.7	294.9	472.7
4mm	277.4	273.05	289.4	436.4

Table 3 Total melting time for different PCMs

PCM	Latent heat (kJ/Kg)	Time (minutes)
n-Octadecane	243.5	282.033
Stearic Acid	160	100.3667
Acetamide	263	210.4
Acetanilide	222	186.35
Erythritol	339.8	368.3

4.2.3 Melting Characteristics of Different PCMs

Different PCM materials operate at different melting temperatures as shown in Table 3. PCMs such as n-octadecane, stearic acid, acetamide, acetanilide and erythritol are subjected to melting at excess temperature of 15 °C from their respective melting temperature. Melt fraction as well as latent energy stored per unit length with respect to time is plotted for each PCM which is illustrated in Figs. 7 and 8.

Even though erythritol seems to store more energy during its melting, fixing PCM for a particular usage is heavily dependent upon the operating temperature available.

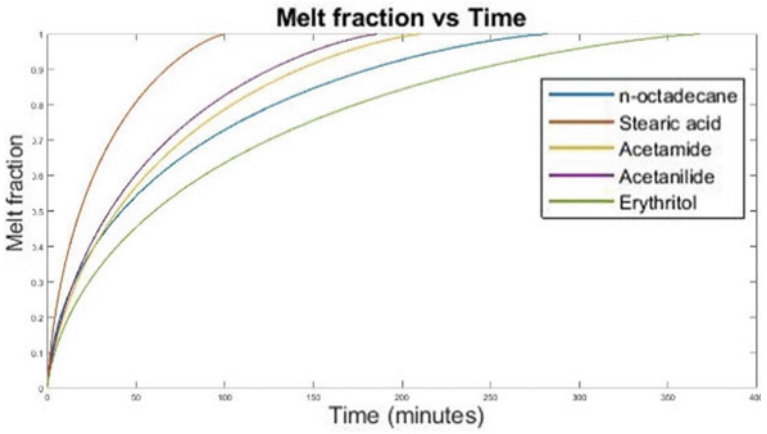

Fig. 7 Melt fraction versus time for different PCMs

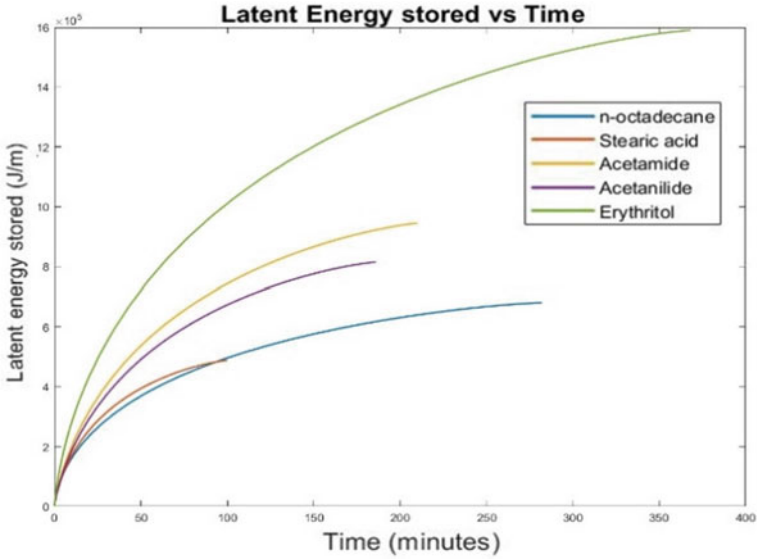

Fig. 8 Latent energy stored during melting for different PCMs

So PCMs with high energy storage may not be suitable since they also require high operating temperature. It is important to select PCM based on both energy storage and operating temperature requirements.

4.3 Cylindrical PCM Geometry

In the next stage, we extend the developed model for the case of cylindrical geometry. Accordingly, the governing equation describing the problem in cylindrical coordinates is given by

$$\frac{\partial h}{\partial t} = \frac{1}{r}\frac{\partial}{\partial r}\left(\alpha \frac{\partial h}{\partial r}\right) - \rho_l \lambda \frac{\partial f}{\partial t} \tag{9}$$

Again, the code in cylindrical coordinate system is first validated by comparing with that of Zivkovic and Fujii [7] where the melting of a cylinder calcium chloride hexahydrate ($CaCl_2.2H_2O$) with radius 20 mm kept in air temperature of 60 °C is studied. Outer surface of the cylinder is given a convective boundary condition. Temperature at the centre of the cylinder is plotted to monitor the process which is illustrated in Fig. 9. Both results are in good agreement.

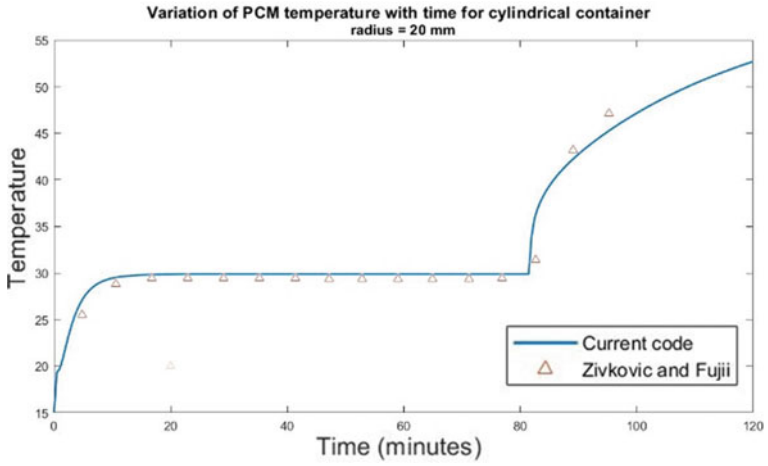

Fig. 9 Centreline temperature for current code versus Zivkovic and Fujii [7] results

Cylindrical Thermal Energy Storage Unit Experiment

In the final stage, we attempt to implement our developed computational model for the study reported by Anilkumar et al. [3] in which an experiment consisting of cylindrical PCM unit filled with paraffin wax is performed for a solar box cooker. Cylinder has diameter of 16 cm and height of 18 cm. To ascertain the PCM's ability to retain specific temperature a 6-h experiment is done by filling the cavity with hot water and measuring the lateral surface temperature of the unit. The unit is partially heated and PCM is partially melted at the start of the experiment and 78 °C water is filled and temperature is measured throughout the span of experiment. The present code is used to analyse this case by employing convective boundary condition at both water and air side of the cylinder.

Figure 10 shows the comparison of lateral surface temperature variation with time for present work and that of Anilkumar et al. [3]. From the plot, it can be seen that for both experimental and numerical works the temperature is very close to the melting temperature of the PCM and is successful in maintaining that temperature. More variation in experimental result is due to the isothermal assumption taken while in reality paraffin wax has melting range of 55 °C–60 °C. Hence more drop in temperature is expected. Both results show that PCM units are successful in maintaining desired temperature over the duration of operation. Maximum error between Experimental and Numerical study was found at the 1-h mark where the deviation is found to be 4 °C.

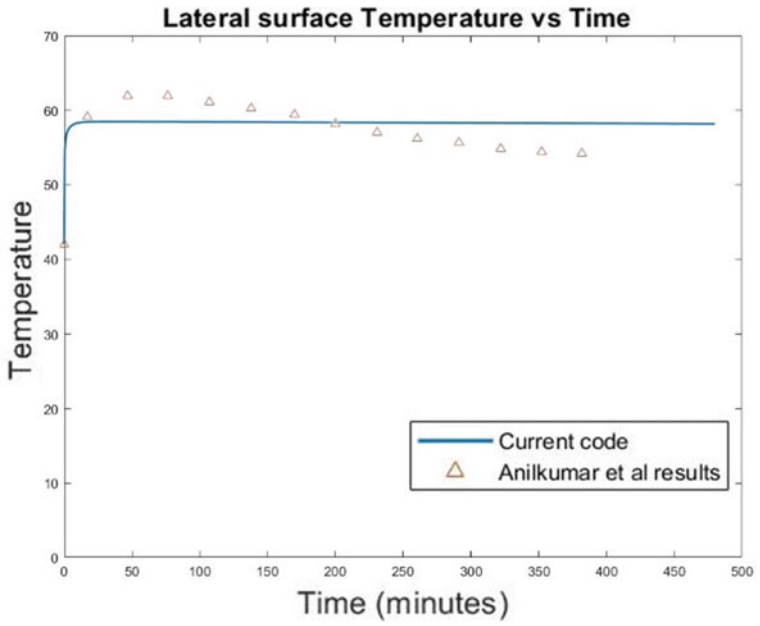

Fig. 10 Lateral surface temperature (°C) for current code versus Anilkumar et al. [3] experiment

5 Conclusion

In the present work, numerical simulation of melting of PCM is done through enthalpy formulation and fully implicit finite difference method. Initially, the developed code is validated. Then, the changes in melting characteristics for different container materials, wall thickness, wall temperature and using different PCMs are observed. The increasing of wall thickness imparted little improvement in melting except for material with low thermal conductivity. Similarly, changing container material does not have much influence on melting unless it is a material with low conductivity. PCMs operating at different melting temperatures gives different amount of latent energy stored and different total melting time. These characteristics of the system can be manipulated for optimal conditions according to a specific use. A model for enthalpy formulation in cylindrical coordinate is also developed and validated. The ability of paraffin wax PCM to maintain desired temperature is analysed using developed code and compared with available experimental results.

Nomenclature

h Sensible enthalpy (J/Kg)
T Temperature (°C/K)

λ Latent energy (J/Kg)
f Melt fraction (−)
ρ Density (Kg/m^2)
k Thermal conductivity (W/mK)
C Specific heat (J/KgK)
α Thermal diffusivity (m^2/s)

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