

Numerical Investigation of Melt Fraction of PCMs in a Latent Heat Storage System

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Abstract: Theoretical investigations of Phase Change Material (PCMs) for energy storage system have been conducted in this study. The selected PCMs were $\text{CaCl}_2 \cdot 6\text{H}_2\text{O}$, $\text{Na}_2\text{SO}_4 \cdot 10\text{H}_2\text{O}$, n-Octadecane, paraffin wax, lauric acid and stearic acid. For the two-dimensional simulation model based on the enthalpy approach, calculations have been made for the melt fraction with conduction only. Glass, stainless steel, tin, aluminium mixed, aluminium and copper were used as heat exchanger materials in the numerical calculations. Theoretical results show that the paraffin wax has good compatibility with latent heat storage system. The large value of thermal conductivity of heat exchanger container material did not make significant contribution on the melt fraction except for at very low thermal conductivities. Numerical results also showed that the effect of thickness of container material on melt fraction is not significant. It is also found that initial temperature of the PCM does not have very important effects on the melting time, while the boundary wall temperature plays an important role during melting and has a strong effect on melt fraction.

Key words: Phase change, enthalpy, heat transfer, (PCM), melt fraction

INTRODUCTION

Over a last couple of decades there has been a lot of interest in thermal energy storage applications. The need of thermal energy storage arises when the supply and demand of energy do not match. Basically, there are three methods of storing thermal energy: sensible, latent and thermo-chemical heat or cold storage. Thermal energy storage in solid-to-liquid phase change employing PCMs have attracted much interest in storage systems due to the following advantages, it involves PCMs that have high latent heat storage capacity, the PCMs melt and solidify at a nearly constant temperature, The phase change from solid to liquid or vice-versa is preferred because the operating pressure is lower than liquid to gas or solid to gas phase change, a small volume is required for a latent heat storage system, thereby the heat losses from the system maintains in a reasonable level during the charging and discharging of heat. The interest on thermal energy storage by using salt hydrates, paraffin's and fatty acid as PCMs has risen in recently times since they have desired thermodynamic and kinetic criteria for low temperature latent heat storage applications. A large number of solid-liquid PCMs have been investigated for applications in the area of spacecraft, refrigeration and air-conditioning systems, solar energy systems, heating and cooling of buildings, backup for active systems and energy conservation given by Lane^[1], Abhat^[2], Zelba *et al.*^[3]; Farid *et al.*^[4]; Tyagi and Buddhi^[5].

The main components of a latent heat storage system are, PCMs, Heat exchanger and Container material. In order to provide accurate design data and to optimize the thermal energy storage system, it is necessary to analyze the heat transfer of melting and solidifying processes of PCMs. Therefore, melting and solidification problems have been studied extensively in recent years. When the PCM changes state, both liquid and solid phase are present and they are separated by the moving interface between them. The difficulty in solving a phase change problem is the presence of a moving boundary or region on which heat and mass balance conditions have to be met.

Generally, two approaches of the finite difference and finite element techniques are used to solve the phase change problems numerically. One of the methods to solve the moving boundary problem is enthalpy formulation by Comini *et al.*^[6], Dalhuijsen and Segal^[7], Costa *et al.*^[8]. The enthalpy method is used in a particular way so that the only unknown variable is the temperature of the phase change material and the solidification occurs at a uniform temperature. Enthalpy method treats the enthalpy as a temperature dependent variable and constructs the latent heat flow through the volume integration with the use of the enthalpy of the system by Voller *et al.*^[9], Swaminathan and Voller^[10], Alexiades and Solomon^[11]. Heat transfer with moving boundary involving phase change is very important in latent heat storage application i.e. ice formation, freezing of food,

Table 1: Thermophysical properties of phase change materials

Properties	CaCl ₂ .6H ₂ O	Na ₂ SO ₄ .10H ₂ O	N-Octadecane	Lauric acid	Paraffin wax	Stearic acid
Melting temperature (°C)	29.85	39.15	27.7	42.2	53.3	66
Latent heat of fusion (kJ kg ⁻¹)	187.49	180	243.5	181	164	155
Density (kg/m ³)	1710	1460	777	862	822	847
Specific heat (kJ/kg°C)						
Solid	1.46	2.0	2.15	1.6	1.77	2.46
Liquid	2.13	2.0	2.20	1.6	1.77	2.46
Thermal conductivity (W/m°C)						
Solid	1.09	0.54	0.36	0.15	0.29	0.17
Liquid	0.54	1.08	0.15	0.15	0.21	0.17

Table 2: Thermophysical properties of various container materials

Name of material	Conductivity (W/m°C)	Density (kg/m ³)	Specific heat (kJ/kg°C)
Glass	0.78	2700	0.840
Stainless Steel	7.7	8010	0.500
Tin	64	7304	0.226
Aluminum Mixed	137	2659	0.867
Aluminum	204	2707	0.896
Copper	386	8954	0.383

castings, metallurgy, crystal growth and various other solidification techniques. The predication of temperature distribution and rate of melting or solidification is very important in order to design such storage device.

A number of theoretical efforts were made to study the thermal performance of latent heat storage systems by Voller^[12], Lacroix^[13], Laoudi and Lacroix^[14], Banaszek *et al.*^[15], Zivkovic and Fujii^[16], Lamberg *et al.*^[17] and Saman *et al.*^[18]. Costa *et al.*^[8] have used the enthalpy formulation with a fully implicit finite difference method to analyze numerically the thermal performance of the latent heat storage systems. The method takes into account both conduction and convection heat transfer in a one-dimensional model and conduction in a two-dimensional model. Liu and Ma^[19] and Sharma and Buddhi^[20] studied dimensionless numerical analysis of melting with constant heat flux heating in a thermal energy storage system at its surfaces to investigate the influences of various parameters on the melting process. None of the authors analyzed the effect of thermo-physical properties of different PCMs with different heat exchanger container material for numerical calculation in a latent heat storage system. While the container material properties is important as the properties of the PCMs i.e., salt hydrates, paraffin's and fatty acid in the latent heat storage system. The heat transfer studies of the PCMs with differential heat exchanger material would be very helpful to design the latent heat storage systems more accurately.

In this study, two-dimensional theoretical model based on enthalpy formulation of a latent heat storage system has been used. The thermophysical properties of PCMs used in the program are given in Table 1 and the properties of various heat exchanger materials presented in the Table 2. Calculations were made to study the effect of thermal conductivity, thermal capacity of CaCl₂.6H₂O, Na₂SO₄.10H₂O, n-Octadecane, paraffin wax, lauric acid and

stearic acid with different type of heat exchanger container material and their effect on melt fraction. The effect of thickness of the container material, initial PCM temperature (T_{mit}) and boundary wall temperature (T_{wal}) on the melt fraction has been also calculated through the programme.

NUMERICAL SIMULATION

Following assumptions were made to analyze the latent heat storage system:

- Thermophysical properties of the PCMs and fin material are independent of temperature. But they are different for solid and liquid phases of PCM.
- PCM is initially in solid phase.
- PCM is homogeneous and isotropic.
- The mode of heat transfer is conduction only.

Enthalpy formulation: By introducing an enthalpy method, the phase change problem becomes much simpler and has the following advantages, the governing equation is similar to the single phase equation, there is no condition to be satisfied at the solid-liquid interface as it automatically obeys the interface condition and the enthalpy formulation allows a mushy zone between the two phases. Phase change problems are usually solved with finite difference or finite element methods in accordance with the numerical approach. The enthalpy formulation is one of the most popular fixed-domain methods for solving the Stefan problem. The major advantage is that the method does not require explicit treatment of the moving boundary. To introduce the formulation we define an enthalpy function *h* as a function of temperature and equation are applied over the whole fixed domain as given by Voller and Costa *et al.*^[8].

For a phase change process involving either melting or freezing, energy conservation can be expressed in terms of total volumetric enthalpy and temperature for constant thermophysical properties, as follows:

$$\partial H/\partial t = \nabla(k_i(\nabla T)) \tag{1}$$

where H is, - the total volumetric enthalpy. It is the sum of sensible and latent heat of the PCM i.e.

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

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

In study of isothermal phase change, the liquid fraction of melt is given by

$$f = \begin{cases} 0 & \text{if } T < T_m & \text{(solid)} \\ 0 - 1 & \text{if } T = T_m & \text{(mushy)} \\ 1 & \text{if } T > T_m & \text{(liquid)} \end{cases} \tag{4}$$

Following Eq. 2 and 3 the enthalpy of PCM is

$$H = \int_{T_m}^T \rho_s c_s dT, \quad T < T_m \text{ (Solid)} \tag{5a}$$

$$H = \rho_l f \lambda, \quad T = T_m \text{ (melting)} \tag{5b}$$

$$H = \int_{T_m}^T \rho_l c_l dT + \rho_l \lambda, \quad T > T_m \text{ (Liquid)} \tag{5c}$$

Eq. 5a represents the sensible enthalpy from the initial temperature (T_{mit}) to the melting temperature (T_m). Solving the Eq. 5 for the PCM temperature, one gets

$$T = T_m + H/\rho_s c_s \quad H < 0 \quad \text{(Solid)} \tag{6a}$$

$$T = T_m \quad 0 \leq H \leq \rho_l \lambda \quad \text{(Interface)} \tag{6b}$$

$$T = T_m + (H - \rho_l \lambda) / \rho_l c_l \quad H > \rho_l \lambda \quad \text{(Liquid)} \tag{6c}$$

Using Eq. 2 and 3, an alternative form of equation (1) for two-dimensional heat transfer in the PCM can be obtained as

$$\frac{\partial h}{\partial t} = \frac{\partial}{\partial x} \left(\alpha \frac{\partial h}{\partial x} \right) + \frac{\partial}{\partial y} \left(\alpha \frac{\partial h}{\partial y} \right) - \rho_l \lambda \frac{\partial f}{\partial t} \tag{7a}$$

and for the heat exchanger container material is

$$\frac{\partial h_r}{\partial t} = \frac{\partial}{\partial x} \left(\alpha_r \frac{\partial h_r}{\partial x} \right) + \frac{\partial}{\partial y} \left(\alpha_r \frac{\partial h_r}{\partial y} \right) \tag{7b}$$

NUMERICAL SOLUTION

In order to obtain the algebraic equations using the control volume technique developed by Patankar^[21], it is necessary to divide the domain into elementary control volumes and then integrate the equation in these control volumes. Equation (7a) is solved using a fully implicit finite difference solution method. The finite difference equation for the PCM is obtained on integrating Eq. 7a over each control volume. The discretization of Eq. (7a) for $\Delta x = \Delta y$ leads to the following scheme (Fig. 1):

$$h_p = h_p^o + \alpha R [h_E - 4 h_p + h_W + h_N + h_S] + \rho_l \lambda [f_p^o - f_p^k] \tag{8}$$

$$a_E h_E + a_W h_W + a_P h_P + a_N h_N + a_S h_S = Q \tag{9}$$

Where

$$a_E = a_W = a_N = a_S = -\alpha R, \quad a_P = 1 - a_E - a_W - a_P - a_N - a_S$$

and

$$Q = h_p^o + \rho_l \lambda [f_p^o - f_p^k], \quad R = dt/(dx)^2$$

Equation 9 has been solved using a Tri-Diagonal Matrix Algorithm (TDMA). The central feature of the present fixed grid enthalpy method is the source term Q. Here, h_p^o and f_p^o refer to the enthalpy and the melt fraction, respectively, from the previous time step. The source term Q keeps track of the latent heat evolution, and its driving element is the melt fraction. Its value is determined

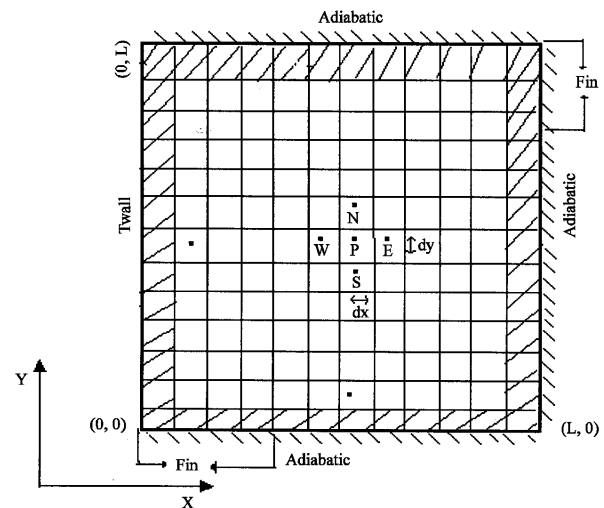


Fig. 1: Two-dimensional domain

Table 3: Melt fraction of PCMs with various container materials in 300 min

Name of material	CaCl ₂ .6H ₂ O		Na ₂ SO ₄ .10H ₂ O		N-Octadecane		Lauric acid		Paraffin wax		Stearic cid	
	t*	f	t*	f	t*	f	t*	f	t*	f	t*	f
Glass	300	0.45	300	0.39	300	0.46	300	0.54	300	0.66	300	0.51
Stainless steel	300	0.76	300	0.72	300	0.83	300	0.95	260	1.00	300	0.94
Tin	300	0.94	300	0.88	300	0.95	268	1.00	183	1.00	298	1.00
Aluminum mixed	264	1.00	300	0.98	265	1.00	190	1.00	129	1.00	214	1.00
Aluminum	242	1.00	300	1.00	248	1.00	176	1.00	119	1.00	200	1.00
Copper	172	1.00	223	1.00	181	1.00	129	1.00	87	1.00	148	1.00

iteratively from the solution of the enthalpy equation. Hence, after the (k + 1)th numerical solution of the enthalpy equation of the Pth node, Eq. 9 may be rearranged as

$$a_p h_p = -a_e h_e - a_w h_w - a_n h_n - a_s h_s + h_p^o + \rho_1 \lambda [f_p^o - f_p^k] \quad (10)$$

If phase change is occurring about the Pth node (i.e. 0 ≤ f ≤ 1), the (k + 1)th estimate of the melt fraction needs to be updated such that the left side of Eq. 10 is zero, i.e.,

$$0 = -a_e h_e - a_w h_w - a_n h_n - a_s h_s + h_p^o + \rho_1 \lambda [f_p^o - f_p^{k+1}] \quad (11)$$

Eq. 11 may be rearranged as

$$f_p^{k+1} = (-a_e h_e - a_w h_w - a_n h_n - a_s h_s + h_p^o) / \rho_1 \lambda + f_p^o \quad (12)$$

The melt fraction update Eq. 12 is applied at every node after the (k + 1)th solution of the Eq. 9 for sensible volumetric enthalpy (h), along with under/over correction, i.e.

$$f = 0 \quad \text{if } (f)^{k+1} \leq 0$$

$$1 \quad \text{if } (f)^{k+1} \geq 1$$

Further details concerning the numerical implementation of the present enthalpy method may be found in the work of Costa *et al.*^[8]. Convergence at a given time step is declared when the difference in the total enthalpy fields falls below a given tolerance, i.e.,

$$\text{ABS}[(H) - (H)] / \rho_k c_k < \text{TOL} \quad (13)$$

For the present case, the value of TOL is set to 10⁻⁴.

The Eq. 7 has been solved by the same method and used the same boundary condition in the program given by Sharma and Buddhi^[20].

RESULTS AND DISCUSSION

In order to analyze the performance of the PCM storage system, author considers the effect of thermophysical properties of the PCMs and container

materials. A grid level of 32x32 (2 mm x2 mm each) with time step 20 s has been used where the grid level for the PCM was 30x30 and surrounded by the grid of the heat exchanger container materials (Fig. 1). The thickness of the used container materials is 2 mm. The initial temperature of the PCMs were assumed 5°C less than the melting temperature and the heating wall temperature was maintained at 15°C higher than the melting temperature. Numerical calculations were made for various types of heat exchanger container materials having different thermal conductivity, density and specific heat with different PCMs and their effect on melt fraction with in 300 min. To see the effect of the thickness of the heat exchanger container material, initial temperature of PCM and wall temperature on the melt fraction, calculations have been made.

Effect of the thermophysical properties of the heat exchanger container material and PCMs on melt fraction:

To see the effect of the thermophysical properties of the heat exchanger container materials on the melt fraction, calculation have been made for six PCMs with glass, stainless steel, tin, aluminum mixed, aluminum and cooper. Table 3 shows the numerical results of PCMs for the melt fraction with various container materials with in 300 min. The values of thermal conductivity of the container materials increase, the value of melt fraction also increase. The continuous melt fraction with time has been plotted in Fig. 2 for six PCMs with copper only. For copper material, the time taken for complete melting was 87 min for paraffin wax, while it was 223 min for Na₂SO₄.10H₂O. It can be seen from the Table 3 and Fig. 2, paraffin wax showed good compatibility with the latent heat storage systems. The melt fraction of the paraffin wax was high as compare to the other PCMs at the same time. It can also be seen from this Fig. the effect of thermophysical properties of the PCMs make significant contribution on the melt fraction.

For paraffin wax, the time taken for complete melting was 87 min for copper, while it was 0.66 for the glass with in 300 min. Comparisons of melt fraction for various heat exchanger container materials with in 87 min are plotted in Fig. 3. It can be observe from the figure, the melt fraction with copper is very high as compare to the glass due to

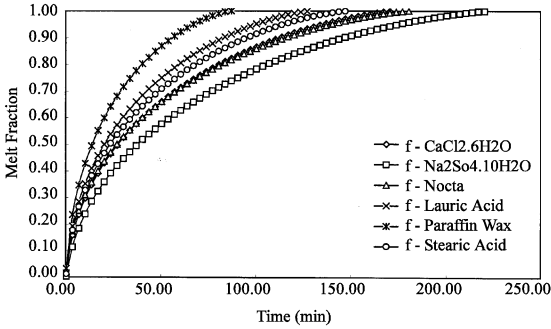


Fig. 2: Timewise prediction of melt fraction of PCMs with copper

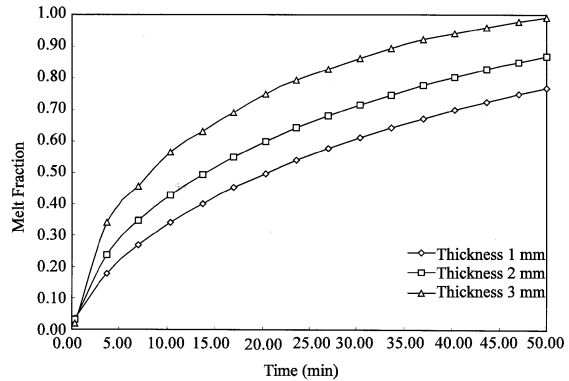


Fig. 4: Variation of melt fraction of paraffin wax with different thickness of the container materials with copper only

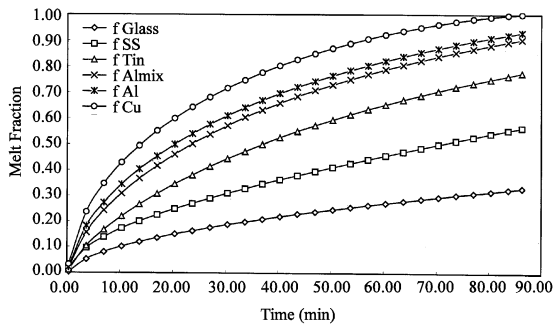


Fig. 3: Variation of melt fraction of Paraffin Wax for various container materials with in 87 min

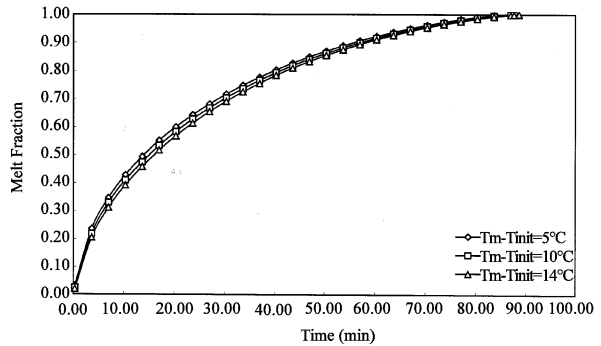


Fig. 5: Comparison of melt fraction of Paraffin Wax with different values of $(T_m - T_{ini})$ for copper with constant value of $T_{wall} - T_m = 15^\circ\text{C}$

the effect of the thermal conductivity, while aluminum and aluminum mixed also showed the good melt fraction during the prediction time. It can also be seen from the table and figure, the effect of thermal conductivity of heat exchanger container materials was dominating at its lower values on melt fraction. Any increase in thermal conductivity value of $100 \text{ W/m}^\circ\text{C}$ did not make significant contribution on the melt fraction.

Effect of thickness of the container material on melt fraction: To study the effect of thickness of the various heat exchanger container materials on the melt fraction, calculations have been made for paraffin wax with 1, 2 and 4 mm thickness, which have been presented in Table 4. It can be seen from the table as the value of thickness increases the melt fraction also increases. For copper the melt fraction was 0.77 with 1 mm thickness, while it was 0.87 and 0.99 for 2 mm and 4 mm thickness, respectively with in 50 min and plotted in Fig. 4. When more of the total volume consisting of PCM and heat exchanger container materials, is occupied by using thicker container walls for the same amount of melting, obviously the melt fraction must increase. But from the table and figure its clear that melt fraction increases with increasing the thickness of the container, while the difference of the melt

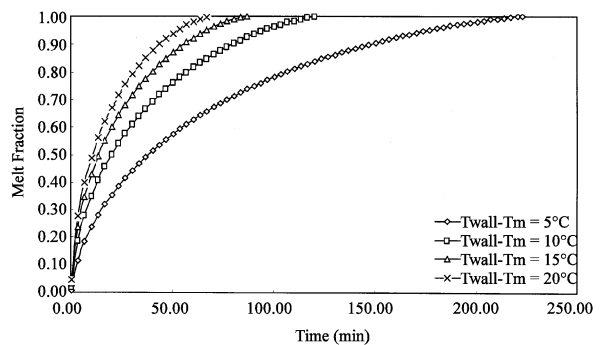


Fig. 6: Comparison of melt fraction of paraffin wax with different values of $(T_{wall} - T_m)$ for copper with constant value of $T_m - T_{ini} = 5^\circ\text{C}$

fraction was not too much high as compare with the increasing the thickness. It can be seen from the table and figure that the thickness of heat exchanger container material is having in-significant effect on the melt

Table 4: Variation in thickness of various container materials and melt fraction of paraffin wax in 50 min

Thickness (mm)	Glass		Stainless steel		Tin	Aluminum mixed		Aluminum		Copper	
	f	f	f	f	f	f	f	f	f	f	f
1	0.23		0.34		0.44	0.59		0.64		0.77	
2	0.25		0.41		0.59	0.73		0.76		0.87	
4	0.30		0.62		0.79	0.90		0.92		0.99	

Table 5: Variation of melt fraction of the paraffin wax for different values of $(T_m - T_{init})$ with various container materials

$T_m - T_{init}$	Glass		Stainless steel		Tin		Aluminum mixed		Aluminum		Copper	
	t*	f	t*	f	t*	f	t*	f	t*	f	t*	f
5	300	0.66	260	1.00	183	1.00	129	1.00	119	1.00	87	1.00
10	300	0.64	268	1.00	186	1.00	131	1.00	120	1.00	88	1.00
15	300	0.63	275	1.00	188	1.00	132	1.00	122	1.00	89	1.00

Table 6: Variation of melt fraction of the paraffin wax for different values of $(T_{wall} - T_m)$ with various container materials

$T_{wall} - T_m$	Glass		Stainless steel		Tin		Aluminum mixed		Aluminum		Copper	
	t*	f	t*	f	t*	f	t*	f	t*	f	t*	f
5	300	0.38	300	0.65	300	0.86	300	0.98	300	1.00	223	1.00
10	300	0.54	300	0.92	263	1.00	183	1.00	168	1.00	122	1.00
15	300	0.66	260	1.00	183	1.00	129	1.00	119	1.00	87	1.00
20	300	0.76	204	1.00	142	1.00	101	1.00	93	1.00	69	1.00

Effect of the initial PCM temperature (T_{init}) on melt fraction: Calculations were made to study the effect of initial temperature of PCM (T_{init}) on the melt fraction with paraffin wax only. Influence of T_{init} on the melting process, in reality, the T_{init} is not at its fusion point; hence the whole melting process is divided into two different stages, that is, the premelt stage and the melting stage. During the premelt stage, melting does not start actually until the solid is heated to its fusion point. This not only affects the total melting time but also the melting process. This is because when melting actually starts, the temperature of the solid is below its fusion point except that at the interface. To see the effect of initial temperature of the PCM on the melt fraction, calculation have been made for paraffin wax with 5, 10 and 15°C temperature differences between the melting temperature and initial temperature. Table 5 shows the results of the effect of T_{init} i.e. $(T_m - T_{init})$ with various container materials on the melt fraction. It can be seen from the table the value of T_{init} decreases the melt fraction of the PCM slightly decreases. It is also found that initial temperature of the PCM does not have very important effects on the melt fraction and melting time. However, increasing the thermal conductivity of the container materials, the melt fraction increases with same time. It can be seen from the table, melt fraction with copper was 1.0 with in 87 min for 5°C temperature difference, while melt fraction was 1.0 with in 88 and 89 min at 10 and 15°C temperature differences, respectively, which is not high as per the temperature difference increase. Figure 5 shows the comparison of melt fraction for paraffin wax with 5, 10 and 15°C temperature differences between the melting temperature

and initial temperature with copper only. From the figure it's clear that initial temperature of the PCM does not have a sharp effect on melting process.

Effect of the boundary wall temperature (T_{wall}) on melt fraction: To see the effect of wall temperature on the melting rate, calculation have been made for paraffin wax with 5, 10, 15 and 20°C temperature differences between the wall temperature and the melting temperature. Table 6 shows the effect of the volumetric enthalpy of the known boundary i.e. difference between boundary wall temperature and melting temperature ($T_{wall} - T_m$) with various container materials on melt fraction. From table it's clear that for the higher values of the enthalpy at the known boundary, higher melt fraction was obtained. Table also shows the comparison of the melt fraction with various container materials. From the Table, It can also be seen that the melt fraction with copper was 1.00 with in 223 min for 5°C temperature difference, while melt fraction was 1.0 with in 122, 87 and 69 min at 10, 15 and 20°C temperature differences respectively. Figure 6 shows the effect of the difference between boundary wall temperature and melting temperature ($T_{wall} - T_m$) on melt fraction with copper only. It can be observed from this figure that the melt fraction was always high, when the difference between wall temperature and melting temperature was 20°C as compare to other temperature differences. From the figure it can also be seen that boundary wall temperature of the container material play an important role during the melting process and it has strong effect on melt fraction.

CONCLUSION

A theoretical two-dimensional theoretical model based on the enthalpy formulation and fully implicit finite difference method was developed to predict the melt fraction of PCMs i.e. salt hydrates, paraffin's and fatty acid. From the obtained results it can be conclude that

- The selection of the thermal conductivity of the heat exchanger container material and effective thermal conductivity of the PCM also very important as these parameters has effect on the melt fraction.
- As the thermal conductivity of container material increases, time required for complete melting of the PCM decreases.
- Effect of thickness of heat exchanger container material on melt fraction is in-significant
- The initial PCM temperature does not have very important effect on the melt fraction, while the boundary wall temperature plays an important role during the melting process and has a strong effect on the melt fraction.

Finally, from the theoretical results it can be concluded for the latent heat storage system, the design parameter of the heat exchanger container materials should be selected carefully in order to optimize the performance of the storage system. The higher value of thermal conductivity of the container material did not make significant contribution on the melt fraction except for at very low thermal conductivities.

NOMENCLATURE

c	=	Specific heat (J/kg °C)
c _k	=	Specific heat of phase k in PCM (J/kg °C)
dx, Δx	=	Length of control volume (m)
dy, Δy	=	Height of control volume (m)
f	=	Melt fraction
h	=	Sensible volumetric enthalpy (J/m ³)
H	=	Total volumetric enthalpy (J/m ³)
k _k	=	Thermal conductivity of phase k in PCM (W/m°C)
L	=	Length (m)
t	=	Time (s)
t*	=	Time (min)
T	=	Temperature (°C)
X, x	=	Space coordinate (m)
Y, y	=	Space coordinate (m)
Greek Letters		
α	=	Thermal diffusivity of PCM (m ² /s)
α _t	=	Thermal diffusivity of container material (m ² /s)

ρ	=	Density (kg/m ³)
ρ _k	=	Density of phase K in PCM (kg/m ³)
λ	=	Latent heat of fusion (J/kg)
Subscript		
f	=	Heat exchanger container material
init	=	Initial
l	=	Liquid
m	=	Melting
s	=	Solid
wall	=	wall temperature
W, E, P, N, S	=	West, East, Centre, North and South node
Superscript		
k	=	Interaction level
o	=	Old value

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