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COMPUTER MODELLING OF PHASE CHANGE MATERIALS USING THE ORTHOGONAL COLLOCATION METHOD

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ABSTRACT

A computer program had been developed for aone-dimensional, orthogonal collocation model of a packed bed heat storage system. The system comprised of a cylindrical storage tank filled with phase change material (PCM) encapsulated in spherical containers. This paper also presented the thermal performance simulation of packed bed heat storage system using PCM during charging and discharging process. Paraffin wax was chosen as PCM, and air was chosen as heat transfer fluid (HTF).The enthalpy method was used in the model to accommodate the phase change behaviour of PCM over a range of temperature. It was shown that the governing equations were two energy conservation equations written for HTF and PCM. Both governing equations were numerically solved by applying orthogonal collocation approach implemented using MATLAB. The results obtained by solving the model using the orthogonal collocation method were initially validated with experimental results in the literature. The model covered through-flow conditions for charging and discharging the thermal heat storage within the air. In this paper, the complete computational model was simplified and efficient enough to interface with a larger program simulating a heat storage system. The simulations were conducted in order to derive the temperature profiles of HTF and PCM as well as to estimate the time required to complete charging and discharging of PCM.

Keywords: phase change material, orthogonal collocation, modelling, simulation.

1. INTRODUCTION

Nowadays, thermal heat storage plays an important role in rationale use of energy, as it allows the decoupling between production and demand of energy. The thermal storage technology based on the use of PCM has recently raised an important practical interest. PCMs are a well-established category of materials with many possible applications, ranging from the stabilization of temperature to heat storage.

Basically, there are three methods of storing thermal heat, which are thermochemical, sensible and latent heat storage. In a thermochemical heat storage process, thermal heat is absorbed or released by breaking and reforming molecular bonds in a completely reversible chemical reaction. In a sensible heat storage unit, thermal heat is stored by changing the temperature of the storage medium, which can be in liquid or solid phase. In a latent heat storage unit, thermal heat is accumulated by means of a reversible change phase occurring in the medium. In fact, the latent heat of most materials is much higher than their sensible heat, thus requiring a much smaller mass of storage medium for storing and then recovering a given amount of thermal heat. The heat storage in the form of latent heat can be effectively achieved by means of PCMs, which materials are characterized by high latent heat of fusion. PCMs can absorb or release high latent heat during melting or solidifying process, have been receiving attention for various applications such as waste heat recovery, solar heating system and building energy conversation in recent years.

There are three types of PCMs, which are organic, inorganic and eutectic. PCMs are usually composed of several substances, which are suitable for particular application. Organic materials are further described as paraffin and non-paraffin. Organic materials are congruent melting, self-nucleation, non-corrosiveness and high heat of fusion. However, there are several undesirable properties of organic materials such as low thermal conductivity, non-compatible with the plastic container and moderately flammable. Inorganic materials are classified as salt hydrate and metallic. Inorganic materials are high latent heat of fusion per unit of volume, relatively high thermal conductivity and small volume changes on melting. Most of salt hydrates are cheap (Lane, 1978). The disadvantages of most salt hydrates are incongruent melting and corrosiveness. The solution of salt hydrates is supersaturated at the melting temperature. This result in an irreversible melting-freezing of the salt hydrate goes on decreasing with each charge-discharge cycle. On the other hand, eutectic PCMs are subdivided in organic-organic, organic-inorganic and inorganic-inorganic. The main advantage of eutectic PCMs is that they consist of advantages of organic and inorganic in a material but the cost of eutectic materials are 3 to 5 times higher than organic and inorganic materials.

Modelling of heat transfer in charging and discharging processes has been discussed widely in the scientific literature for decades. A very good review on thermal heat storage, particularly on moving boundary problems, a numerical simulation in different heat exchanger constructions, is presented by (Zalba, *et al,* 2010). In this paper, the formulation of a mathematical model provides the definition of moving solid-liquid interfaces and hence varying boundary conditions. This is due to phase change is considered as non-linear because phase change interfaces moves continuously during

charging or discharging and its position is not known in the solution. Different studies and investigations have been presented for the solution of PCM problem including analytical, experimental and numerical methods where energy equation is formulated in various ways. The most common approach used throughout the literature is the enthalpy method due to its reliability and simplicity to implement the numerical algorithm without the need to satisfy conditions at phase change front (Agyenium *et al*, 2013). The enthalpy method procedure is based on the solution of multiple differential equations governing the PCM performance where temperature and enthalpy are two variables to be computed (Voller and Cross, 1981). There are several methods being adopted to model and solve for the temperature variation in the domain of interest. The numerical methods for such problems are reported in two broad categories, which are temperature based model and enthalpy model. In this paper, the temperature based model is used. The phase change interface is either captured on a grid at each fixed time step. Therefore, non-uniform grid spacing is constructed, or captured on a uniform grid. Then, a non-uniform time step is used. In 2013 Wang studied heat charging or discharging performance of a shell-and-tube PCTES unit (Wang *et al*, 2013). They concluded that discharging process needs shorter time than charging process does due to discharging process has larger heat transfer rate than charging process (Tan and Leong, 1999). Hence, it would reach steady-state quickly under same inlet temperature and mass flow rate of HTF in charging and discharging process.

In this paper, the charging and discharging processes are investigated in one-dimensional, orthogonal collocation model of packed bed heat storage. The objective is to develop an approximate numerical solution of the one-dimensional heat transfer problem for a packed bed heat storage which is being charged and discharged isothermally by HTF. A computer program can be developed which will predict the solid-liquid interface location and the temperature profile of PCM and HTF as a function of time during charging and discharging processes in packed bed heat storage.

2. PHYSICAL MODEL

Figure-1 shows the physical arrangement of the packed bed considered for the numerical modelling. PCM encapsulated in plastic spherical containers are packed randomly inside the storage tank. This provides a porous structure in the storage tank with a void fraction of 'ε'. The void fraction provides space and passage for the flow of HTF. At time, $t > 0$, HTF at constant temperature flows in through the bottom of the storage tank. During charging or discharging processes, PCM undergoes three different regimes, which are sensible heating below phase change temperature, phase change process, and sensible heating above phase change temperature. The maximum velocity used in this model is 'v_{max}' which is calculated from the flowrate of HTF across porous cross section of the packed bed. In fact, PCMs require accurate and reliable methods for determining their physical properties, since for numerical modelling the thermophysical properties of materials and their proper determination indicate a significant issue that considerately affects the accuracy and credibility of numerical simulations and their outcomes. The thermal properties of PCM are obtained by differential scanning calorimetry (DSC), based on temperature and heat measurement of investigated and reference materials.

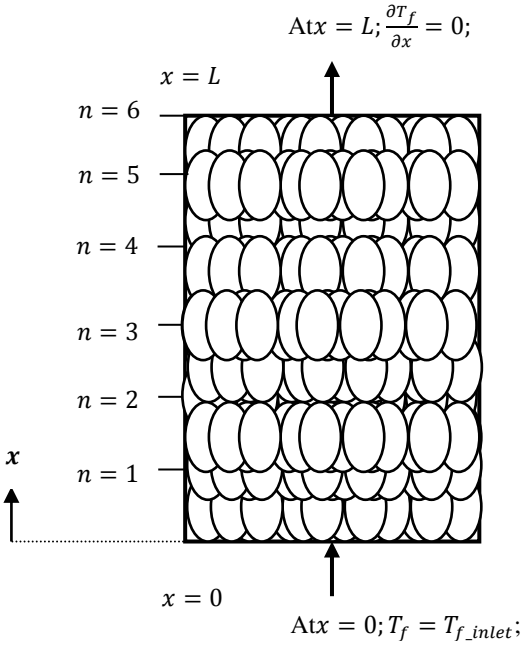


Figure-1. Physical arrangement of the packed bed model.

A simplified one-dimensional model is introduced to determine numerically the temperature distribution of the PCM and the HTF as well as the location of the solid-liquid interface during charging and discharging. The following assumptions have been made for the model:

a) HTF and PCM are two different domains and separate equations for each region.
b) The thermophysical properties of the PCM are different for the solid and liquid phases. The variation of properties with respect to temperature during the phase change is considered as linear.
c) The inlet temperature of the HTF is constant during the entire charging or discharging processes.
d) The initial temperatures of the HTF and the PCM are uniform.
e) The resistance offered by the thin wall of the spherical capsule is neglected.
f) Radiant heat transfer is ignored.
g) The tank is perfectly insulated.
h) Heat loss from the tank surface to the surrounding is neglected.

2.1 Governing equations

An energy balance between PCM and HTF is presented in one-dimensional phase change problem (Equation 1). In this model, the PCM capsules behave as a continuous medium and not as a medium comprised of individual particles. With the assumptions above, the governing equations for PCM and HTF are stated.

For PCM:

$$(1-\varepsilon)\rho_p A_c L c_p \left(\frac{\partial T_p}{\partial t}\right) = h_s a_p (T_f - T_p) \quad (1)$$

The equation (1) represents the rate change of latent energy of PCM is equal to the heat transfer by convection from HTF to PCM capsules.

For HTF:

$$\varepsilon\rho_f A_c L c_f \left(\frac{\partial T_f}{\partial t} + v_{max}\frac{\partial T_f}{\partial x}\right) = h_s a_p (T_p - T_f) + h_w a_w (T_w - T_f) \quad (2)$$

where $T_w = T_{sur}$

The first term of the left hand side of equation (2) represents the rate change of internal energy of HTF, while the second term accounts for energy change due to the HTF flow. The two terms on right hand side of equation (2) represent the heat transfer by convection between PCM and HTF and the heat leak through the wall of cylindrical container, respectively.

2.2 Initial and boundary conditions

The initial and boundary conditions for the above set equations are:

For PCM:

Initial condition: $T_p(x, t=0) = T_{p\_ini}$ (3)

For HTF:

Initial condition: $T_f(x, t=0) = T_{f\_ini}$ (4)

Boundary condition: $T_f(x=0, t) = T_{f\_inlet}$ (5)

$$\frac{\partial T_f(x=L,t)}{\partial x} = 0 \quad (6)$$

The equations (1−6) were solved numerically using orthogonal collocation method. The mathematical model was developed and the numerical solution procedure was implemented using the advanced high-level technical computing language and interactive environment of MATLAB R2008a. The program flowchart of the model is given in Figure-2.

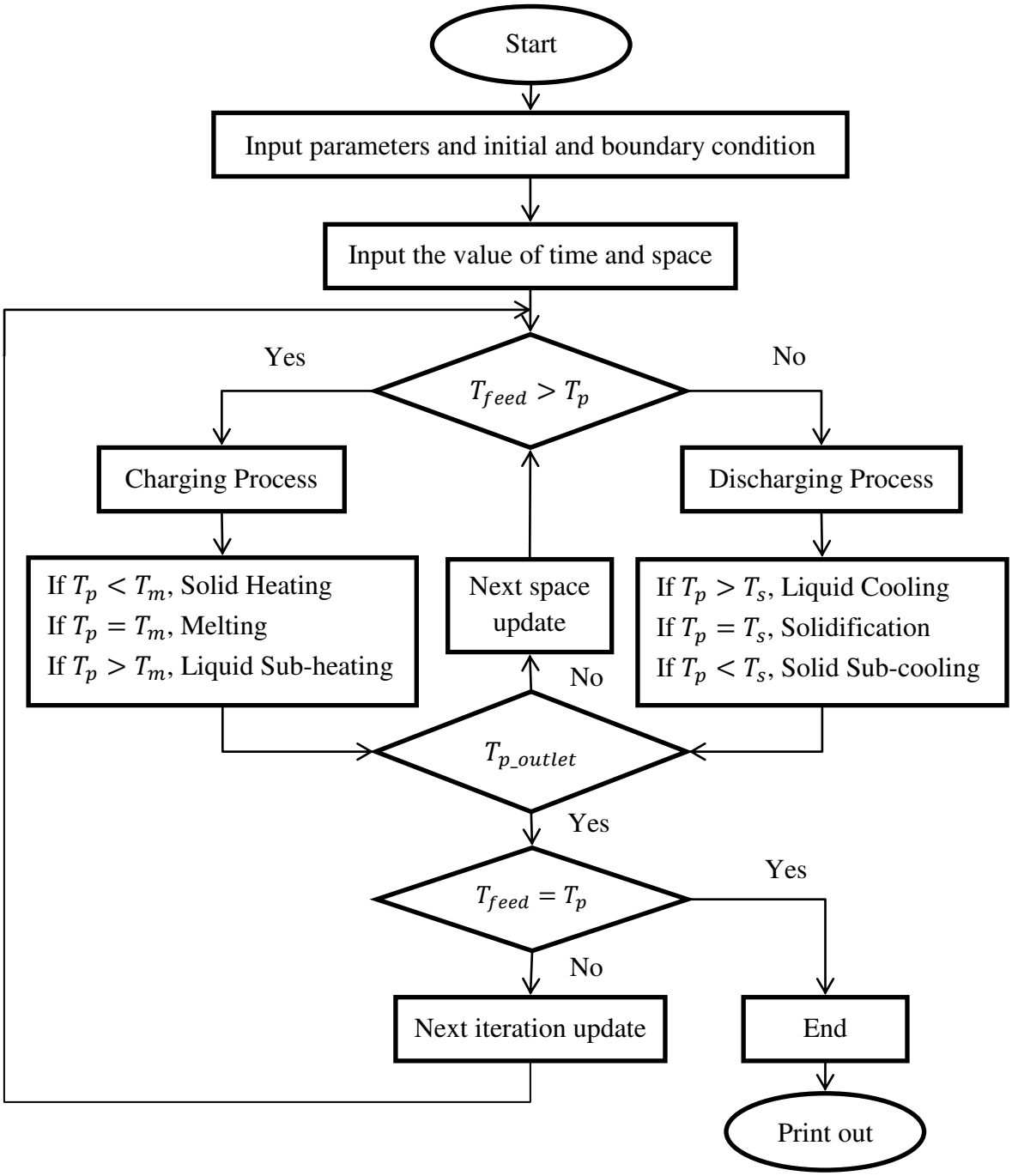


Figure-2. Program flowchart of the model.

2.3 Numerical procedure

The packed bed heat storage model is filled with spherical capsules encapsulated PCM to a length of 0.7 m and a diameter of 0.35 m, which was cylindrical shape. The bed void fraction is 0.52. The PCM encapsulated in plastic balls of an outer diameter with 0.07 m with a total number of 260 balls are packed inside the tank. The mass flow rate of HTF is 0.05 kg/s. The simulated heat storage model is in one-dimensional. Temperature data is simulated every 10s. Commercial grade paraffin wax is selected as PCM while air is selected as HTF in this model. Thermophysical properties of paraffin wax were: latent heat, 142.7 kJ kg^{-1}; specific heat, 1.8 kJ kg^{-1} K^{-1}; thermal conductivity, 0.2 W $m^{-1}K^{-1}$; phase change temperature, 60℃; and bulk density, 640 kg m^{-3}. When all temperatures of PCM are above the melting temperature and reach the same temperature as HTF, it shows the process is fully charged. On the other hands, for fully discharge process, all temperatures of PCM are below the solidification temperature and reach the same temperature of inlet HTF.

2.4 Method of solution

The equations for the HTF and PCM are discretised by the orthogonal collocation method. The discretised equation of HTF and PCM are solved

simultaneously for the new values of temperature of the HTF and PCM at increasing time step. The calculation steps are repeated by considering this new set of temperatures values as the present values for finding the temperature in the next time step. The simulation is continued until the temperature of HTF and PCM at all the nodes of the storage tank reaches the inlet temperature of HTF. The simulated temperature is computed using MATLAB program.

2.4.1 Model discretization of HTF and PCM

In this model, the orthogonal collocation method is used for one-dimensional boundary value problems. The term orthogonal collocation method is used to signify that the solution of a Partial Differential Equation (PDE) for a one-dimensional region is obtained by using the zeros of Jacobi orthogonal polynomials as the interior and boundary collocation points, which are also the Gauss-points in numerical integration. Since the results obtained by this method are the function values at the zeros of a Jacobi orthogonal polynomial, the numerical integration formula can be immediately applied to a problem that requires integration over the domain. This is one of the advantages of collocating at the roots of a Jacobi orthogonal polynomial (Villadsen, 1970).

Finlayson (1972) stated that in higher approximations the choice of collocation points is not crucial, but a choice in a certain way is possible and will make the calculations both convenient and accurate (Finlayson, 1972). Furthermore, Villadsenand Michelsen (1978) have pointed out, that a positioning of the collocation abscissas at the zeros of orthogonal polynomials leads to a rapidly convergent interpolation scheme, even for the functions that are poorly represented by polynomials (Villadsen and Michelsan, 1978). Therefore, it appears to be a natural choice to use the zeros of a Jacobi orthogonal polynomial as the collocation points (Chang and Finlayson, 1977).

In the orthogonal collocation method, by giving as the only input N, the degree of the Jacobi orthogonal polynomial in computer program, the zeros of the Jacobi orthogonal polynomial are calculated and chosen as the interior collocation points. The space domain is first transformed into the range [0, 1]. This inclusion is to ensure the continuity of both the function and the normal first derivative values across element boundaries, also to provide collocation points on the regional boundaries where the boundary conditions for the problem should be imposed. Therefore, the total number of collocation points on the interval will be $(J+2)$ points.

A one-dimensional approximate solution in the form of a Lagrange interpolation polynomial is taken, the matrices $A_{j,m}$ and $B_{j,m}$ representing the first and second derivatives, respectively, are established. These derivatives are expressed in term of the values of the function at the collocation points. The coefficients of matrix $A_{j,m}$ are obtained by differentiation of the Lagrange interpolation polynomial and then evaluated at the collocation points. The coefficients for the matrix $B_{j,m}$are computed by simply squaring $A_{j,m}$. Hence, the discretization matrices $A_{j,m}$ and $B_{j,m}$ are both $(J+2)\times(J+2)$. When i^{th} row of $A_{j,m}$ is multiplied by the values of the function at the collocation points on the interval under consideration, one obtains the first derivative at point which correspond to row number i.

In order to construct an approximate solution, the orthogonal collocation method makes use of the classical method of Lagrange in approximating a function with given values at a discrete number of points by a finite sum of polynomials. They provide a systematic procedure for evaluating their derivatives at collocation points. Importantly, the procedure can be easily implemented and automated for computers. For the same reason, the Lagrange formulation is widely used in the finite element method (Bathe and Wilson, 1976).

In the one-dimensional case, the normalised space domain is then divided into $(J+2)$ grid points consisting of Jinterior collocation points, and the two boundary points, $j=1$and $j=J+2$. The interior collocation points are not equally spaced, but chosen to be the roots of the Jacobi orthogonal polynomial, $P_J^{(\alpha+\beta)}$. These are polynomials of degree J which satisfy

$$\int_0^1 \xi^{\beta}(1-\xi)^{\alpha}\xi^{j}P_J^{(\alpha+\beta)}(\xi)d\xi = 0 \quad j=0,\dots,J-1 \qquad (7)$$

whereα and β are integers. Here, α and β are chosen as zero, which gives rise to a subset of Jacobi polynomials known as the Legendre polynomials. At a specific collocation point j and at dimensionless time, τ, any dependent variable, S, is expressed as

$$S(\xi_j,\tau) = \sum_{m=1}^{J+2} \ell_m(\xi_j) S_m(\tau) \qquad (8)$$

$$\ell_m(\xi_j) = \prod_{\substack{i=1 \\ i\neq m}}^{J+2} \frac{\xi_j-\xi_i}{\xi_m-\xi_{ij}} \qquad (9)$$

Since the Langrangian interpolation polynomial in equation (7) is a continuous function, it can be differentiated at the collocation point *j* to give

$$S'(\xi_j,\tau) = \sum_{m=1}^{J+2} \ell'_m(\xi_j) S_m(\tau)$$

$$= \sum_{m=1}^{J+2} A_{j,m} S_m(\tau) \qquad (10)$$

and

$$S''(\xi_j,\tau) = \sum_{m=1}^{J+2} \ell''_m(\xi_j) S_m(\tau)$$

$$= \sum_{m=1}^{J+2} B_{j,m} S_m(\tau) \qquad (11)$$

The application of the orthogonal collocation method is as follow. The required number of interior collocation points, J, is first decided and the collocation points are calculated to be the roots of the Jacobi orthogonal polynomial of degree J which satisfy equation

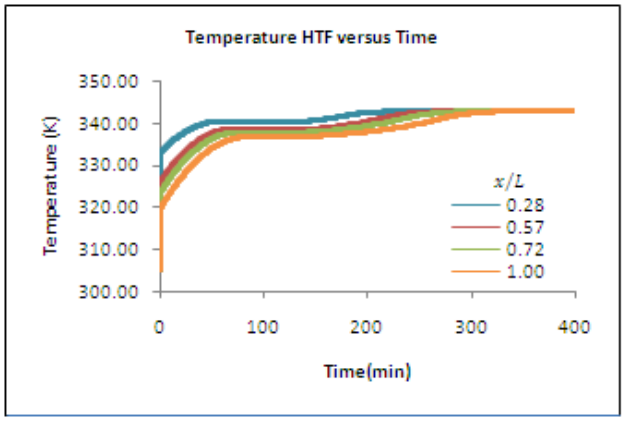
(7). The PDEs are then discretised into ordinary differential equations (ODEs) on the collocation points chosen, with spatial derivatives of the dependent variables replaced with the derivatives of the Langrangian interpolation polynomials.

3. SIMULATION RESULTS AND DISCUSSION

3.1 Modelling of PCM in charging mode

The HTF at inlet is maintained at a constant temperature of 70℃ (343 K) during the charging process. The initial temperature of HTF and PCM are 32℃ (305 K). The temperature variations of HTF and PCM at various heights of the storage tank are recorded and these measurements are used to evaluate the complete charging time for any given height.

Figures 3 (a) and (b) show the temperature profile of HTF during charging process. $x/L$is the dimensionless distance of the packed bed where x is the location of packed bed and L is the length of bed. During charging process, the heated air is forced from the bottom to top of the container. PCM absorbs the heat transferred from HTF. From Figure-3 (a), the result implies that the higher the location of packed bed, the lower temperature of HTF. In fact, when the heat is transferred from the HTF to the first cell of the PCM, a portion of it is accumulated while the remaining portion is transmitted to the adjacent cells far away. Therefore, only a small amount of the heat flux is received. From Figure-3 (a), the temperature of HTF increases rapidly at beginning. After that, it increases slowly in certain temperature because it is absorbed by PCM which needs heat for phase change from solid to liquid phase. Then, the temperature of HTF increases rapidly again after PCM absorbs enough heat for phase change. Finally, the temperature of HTF no longer increases over time. When the temperature of HTF at packed bed is equal to the inlet temperature of HTF, it is shown that it reaches in steady-state at particular location. Figure-3 (b) indicates the temperature of HTF increases drastically within few seconds. This is because the temperature difference between the initial and inlet of HTF is large. After a while, the temperature of HTF increases slowly because the heat is transferred to PCM capsules. Figure-3 (c) shows the temperature profile of PCM at particular locations. It is clearly seen that PCM undergoes 3 stages during charging process. There are solid sensible heat absorb, melting latent heat absorb and liquid sensible heat absorb. The temperature of PCM increases rapidly at solid sensible heat absorbs stage, then it increases slowly at temperature range of phase change until the melting process terminates. After the temperature range of phase change, the temperature increases rapidly to attain the temperature of HTF at particular location as shown in Figure-3 (d). Figure-3 (d) shows the temperature profile of HTF and PCM at$x/L = 0.57$ during charging process. The charging process is completed when the temperature of PCM is equal to the temperature of HTF. Result implies that the closer to the outlet location ($x/L = 1$), the longer the time required for fully charged.



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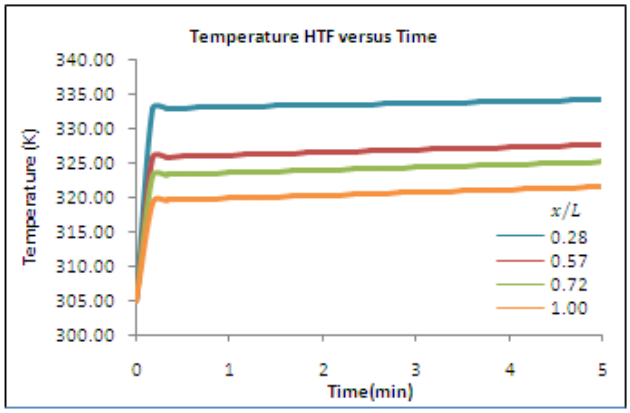

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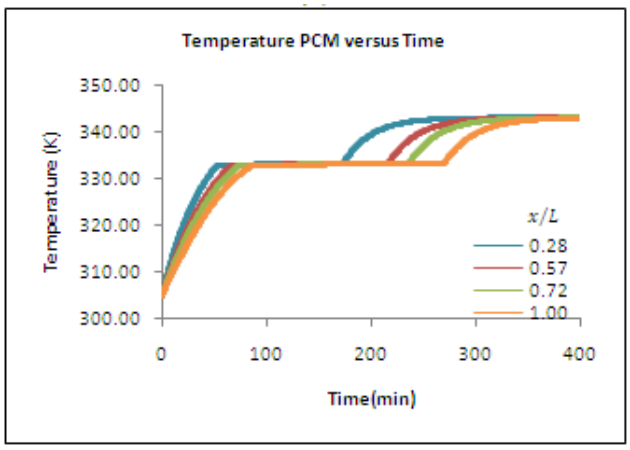

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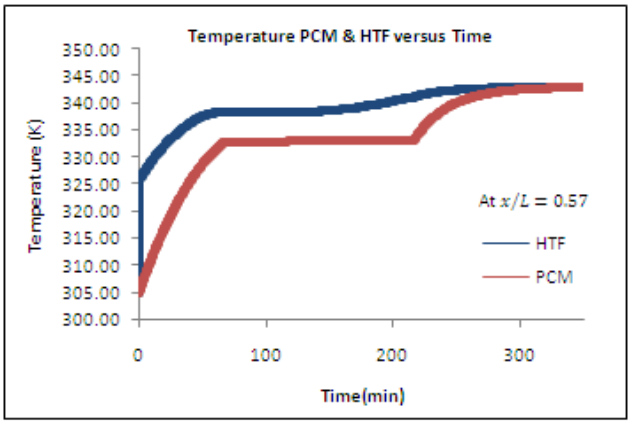


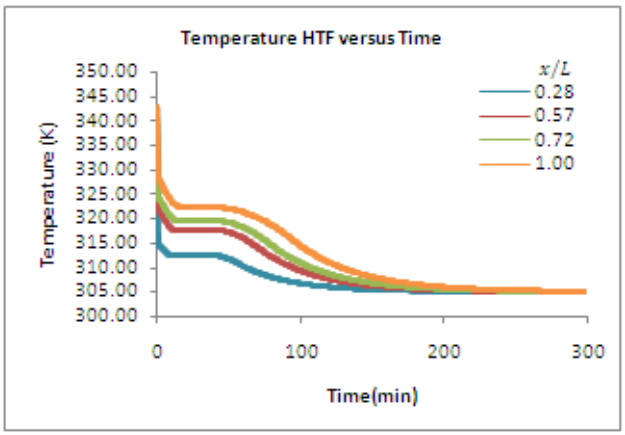
(d)

Figure-3. The variation temperature of PCM and HTF with time at different locations during charging process.

3.2 Modelling of PCM in discharging mode

The HTF at inlet is maintained at a constant temperature of32℃ (305 K) during the discharging process. The initial temperature of HTF and PCM are 70℃ (343 K). The temperature variations of HTF and PCM at various heights of the storage tank are recorded and these measurements are used to evaluate the complete discharging time for any given height.

Figure-4 (a) and (b) show the temperature profile of HTF during discharging process. During discharging process, the air is forced from the bottom to top of the container. PCM releases the heat to HTF. From Figure-4 (a), the result implies that the higher the location of packed bed, the higher temperature of HTF. From Figure-4 (a), it shows the temperature of HTF decreases rapidly at beginning. Then, it decreases slowly because the heat released by PCM is absorbed by HTF at certain temperature, which is the temperature range of phase change. After PCM successfully change phase from liquid to solid phase, the temperature of HTF decreases rapidly again. Finally, the temperature of HTF at packed bed no longer increases and equal to the inlet temperature of HTF. It is shown that HTF reaches in steady-state at particular location. Figure 4 (b) indicates the temperature of HTF decreases drastically within few seconds. This is because the temperature difference between the initial and inlet of HTF is large. Hence, the heat transfer rate is high. After a while, the temperature of HTF would decrease slowly because heat transfer rate decreases. Figure-4 (c) shows the temperature profile of PCM at particular locations. It is obviously seen that PCM undergoes 3 stages during discharging process. There are liquid sensible heat release, solidifying latent heat release and solid sensible heat release. The PCM temperature decreases rapidly at liquid sensible heat release stage, then it decreases slowly at temperature range of phase change until the solidifying process terminates. After the temperature range of phase change, the temperature decreases rapidly to reach the temperature of HTF at particular location as shown in Figure-4 (d). Figure-4 (d) shows the temperature profile of HTF and PCM atat$x/L = 0.57$ during discharging process. The discharging process is completed when the temperature of PCM is equal to the temperature of HTF. Result implies that the closer to the outlet location ($x/L = 1$), the longer the time required for fully discharged.



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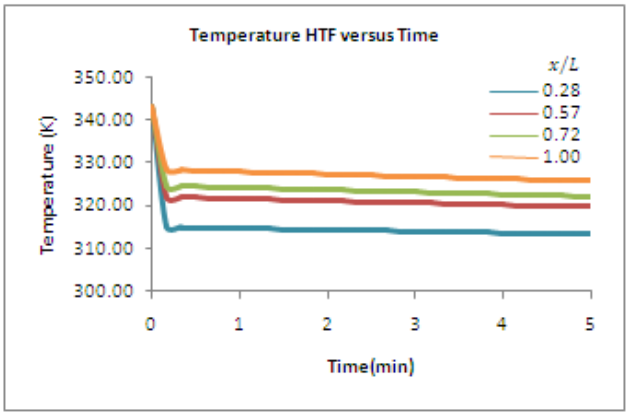

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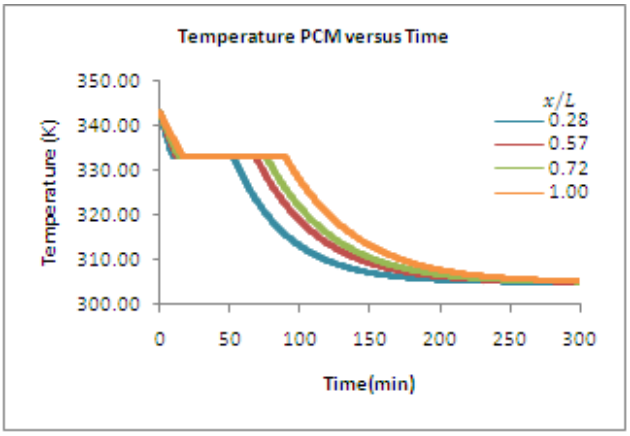

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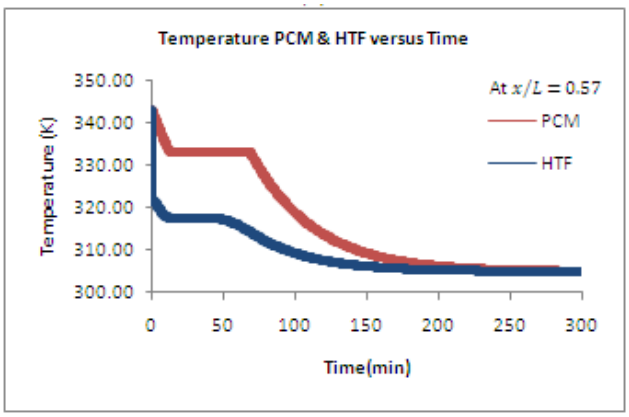

(d)

Figure-4. The variation temperature of PCM and HTF with time at different locations during discharging process.

3.3 Validation

In order to validate the model and assumptions, numerical simulation is conducted for the conditions of the experimental measurement in the literature (Nallusamy *et al*, 2007). The developed computer code has been validated by simulating charging and discharging of commercial grade of paraffin wax. The software has been set up to reproduce utilized experimental conditions. Experimental data have been then compared with the simulated computational data. In the literature, the experimental setup consists of an insulated cylindrical storage tank with diameter of 0.36 m and length of 0.46 m, which contains PCM, encapsulated spherical capsules (Nallusamy *et al,* 2007). The spherical capsule is made of high-density polyethylene (HDPE) with an outer diameter of 0.055 m and a wall thickness of 0.0008 m. The total number of capsules in the storage tank is 264 and the spherical capsules are uniformly packed in eight layers and each layer is supported by wire mesh. In numerical simulation for the experimental results (Nallusamy *et al,* 2007), the paraffin is used as PCM that a melting temperature of 60℃ and water is used as HTF. The inlet temperature of HTF is 32℃ and the mass flow rate of HTF 2 kg min^{-1}. The initial temperature of PCM is 70℃.

4. CONCLUSIONS

In this paper, a one-dimensional, orthogonal collocation model has been developed. The heat exchange between a HTF and a PCM is studied. The temperature distribution of PCM and HTF is simulated by numerically solving the two differential equations governing the physical problem. The differential equation of the HTF is involved the partial differential equation. Therefore, it has been discretised in time with orthogonal collocation method. It has an initial condition and two boundary conditions. On the other hand, the differential equation of the PCM is only involved the ordinary differential equation. Thus, only initial condition is set. The numerical model is valid and able to solve the problem very fast (about 1 hour of simulation with a standard PC for 5 physical hours of the transient problem). Simulation results also show the thermal performance of packed bed heat storage system using PCM. It implies that the model is validated. The main advantage of this computer program is the great computational simplicity with consequent high calculation speed, obtaining simulation results that accurately show the dynamic characteristic of heat storage system during charging and discharging process.

ACKNOWLEDGEMENTS

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Nomenclature

$A_{j,m}$	first derivatives of the Lagrange interpolation polynomial	*Greek Symbols*	
A_c	cross sectional area of bed (m^2)	ε	bed void fraction
a_p	surface area of the PCM sphere (m^2)	ρ_p	density of PCM (kg/m^3)
a_w	surface area of the wall of cylindrical container (m^2)	ρ_f τ	density of HTF (kg/m^3) dimensionless time
$B_{j,m}$	second derivatives of the Lagrange interpolation polynomial		
c_p	specific heat of PCM (J/kg K)		
c_f	specific heat of HTF (J/kg K)	*Superscripts*	
d_p D_c h_s	diameter of the PCM spherical ball (m) diameter of column (m) heat transfer coefficient between HTF and	i	the global number of collocation point on the boundary
h_w	PCM (W/m^2 K) heat transfer coefficient between HTF and	j	The interior collocation point
k_f	wall of cylindrical container (W/m^2 K) thermal conductivity of PCM (W/m K)	J	Jacobi orthogonal polynomial
L	length of bed (m)	k	iteration k

m_f	mass flow rate of HTF (kg/s)	m	the collocation point
N_{ball}	number of encapsulated ball		
N	number of interior collocation points	*Subscripts*	
T	temperature (K)	f	HTF
t	time (s)	p	PCM
S_m	value of the dependent variable at the collocation point m	w	wall of cylindrical container
S'	first spatial derivatives of the dependent variable	sur ini	surrounding initial
S''	second spatial derivatives of the dependent variable	$inlets$	Inlet solid phase of PCM
v_{max}	velocity of HTF along the bed void fraction (m/s)	l $latent$	liquid phase of PCM latent heat of PCM
x	coordinate along axial direction (m)		
x/L	dimensionless axial distance of bed	*Abbreviation*	
ξ	dimensionless axial co-ordinate	PCM	phase change material
ℓ_m	Lagrange interpolation polynomial	HTF	heat transfer fluid

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