Numerical Investigations on Latent Heat Storage Unit using Phase Change Material

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Abstract. Many renewable energy sources are not available at any time in nature so the development of energy storage technologies is very important to conserve the available energy and improve its utilization. Thermal energy storage by using Phase Change Materials (PCM) is considered one of the promising technology to store thermal energy. The numerical study of the shell and tube storage unit is carried out. Paraffin wax was filled in the shell side and the Heat Transfer Fluid (HTF) flowed inside the tube. The validation among numerical and experimental results was conducted. It is found that the effect of natural convection is important and should be taken to perform the model of the heat storage unit.

1. Introduction
Solar energy is one of the sources of sustainable energy. This energy is used in many fields such as generating electricity, heating water, domestic and commercial heating system, etc. Despite the importance of solar energy, it is not available throughout the day or throughout the year. Therefore, it is important to store solar energy and use it in times when it is not available. Solar energy systems require efficient thermal energy storage to store the heat during sunshine hours and to use the heat stored during the night. Thermal energy storage is very important in many engineering applications such as space heating and air conditioning, solar cooking, greenhouses, and solar water heating systems [1]-[4].

The charging process of paraffin wax with Al2O3 was numerically investigated [5]. The enthalpy-porosity procedure was utilized in FLUENT. It was noted that utilizing a small volumetric concentration of alumina particles in paraffin wax and the nanoPCM have great potential for thermal energy storage applications. The Boussinesq approximation and the enthalpy formulation were used by Eslami M. and Bahrami M.A. [6] for the melting and solidification model. It was found that conduction is the prevailing process at the starting of the charging process in a PCM. The effect of the convection mechanism is important and should be used to design an optimal latent thermal energy storage system. Ye W.B. et al [7] carried out a numerical study of the heat transfer inside paraffin in a plate-fin unit. It was noted that, as the temperature differences are less than 20°C, it plays an important role in the performances of energy storage. Darzi A. R. et al [8] performed numerical simulations on the melting process of two cylinders in state of concentric and eccentric. The result shows that the melting rate in the beginning time (15 min) for concentric is similar to the eccentric state. Then, the
melting rate is reduced in the concentric state as a result of the effect of pure conduction between the hot tube and the cold solid PCM.

In this study, the combined conduction convection heat transfer model was used during the melting process to investigate the heat transfer mechanism of the vertical shell and tube latent heat storage unit. The numerical results were validated against the experimental results of M. K. Rathod and J. Banerjee [9].

2. System model description
Rathod and Banerjee [9] experimentally studied the transient melting of the PCM (paraffin wax) in the shell-and-tube storage unit with the PCM on the shell side, and the HTF flowing inside the tube. Additionally, they conducted a series of experiments to study the effect of different flow rate and heat transfer fluid temperature on the heat transfer process.

Figure 1 shows the schematic diagram of the shell and tube of 1 m length. The inner diameter of the HTF tube is 0.033 m and the outer diameter is 0.035 m. The inner diameter of the shell is 0.128 m. Paraffin wax is filled in the shell side and the HTF flows inside the tube. Water is used as the heat transfer fluid. The properties of HTF and paraffin wax are shown in table 1. The outer surface of the cylinder is well-insulated. The hot water flows through the inner tube at the charging process.

![Figure 1. A schematic diagram of shell and tube.](image)

| Properties                        | Value            |
|-----------------------------------|------------------|
| Liquid density, $\rho_l$          | 778 kg/m³        |
| Solid density, $\rho_s$           | 861 kg/m³        |
| Thermal conductivity, $k$         | 0.15 W/m.k       |
| Liquid specific heat, $C_p$       | 2500 J/kg        |
| Latent heat, $L$                  | 213 kJ/kg        |
| Thermal expansion coefficient, $\beta_{t,ec}$ | 0.000091 1/K   |
| Melting temperature, $T_m$        | 331-333 K        |
| Initial temperature of solid PCM  | 303 K            |
| Charging temperature (HTF)        | 358 K            |
| Mass flow rate (HTF)              | 0.0833 kg/s      |
3. Numerical model

ANSYS Fluent was used to solve the 2D axisymmetric vertical slice of the cylinder model. ANSYS Fluent solved the melting process model using an enthalpy-porosity formulation for laminar flow with Navier-Stokes equations [10]. The viscous dissipation term was ignored. The change in volume of PCM due to phase change was ignored. The continuity, energy and momentum equations are written as:

**The Continuity equation:**

\[
\frac{\partial}{\partial t} (\rho) + \nabla \cdot (\rho \mathbf{v}) = 0
\]  

(1)

**The energy equation**

\[
\frac{\partial}{\partial t} (\rho H) + \nabla \cdot (\rho vH) = \nabla \cdot (k \nabla T) + S
\]  

Where \( H \) is the enthalpy, \( \rho \) is the density, \( v \) is fluid velocity, \( k \) is the thermal conductivity, \( S \) is the source term and \( t \) is the time. The enthalpy of the material is calculated as the sum of the sensible heat, \( h \), and latent heat, \( \Delta H \):

\[
H = h + \Delta H
\]  

(3)

The sensible heat is calculated as:

\[
h = h_{ref} + \int_{T_{ref}}^{T} C_p dT
\]  

(4)

Where \( h_{ref} \) is the reference enthalpy, \( T_{ref} \) is the reference temperature and \( C_p \) is the specific heat at constant temperature. The latent heat is also calculated as:

\[
\Delta H = \beta L
\]  

(5)

The liquid fraction, \( \beta \) can be calculated as

\[
\beta = \begin{cases} 
0 & T < T_S \\
\frac{T - T_S}{T_L - T_S} & T_S \leq T \leq T_L \\
1 & T > T_L 
\end{cases}
\]  

(6)

The source terms are used to modify the momentum equations in the mushy region.

\[
S = \nu A_{mush} \frac{(1-\beta)^2}{\beta^3 + \varepsilon}
\]  

(7)

Where viscosity \( \beta \) is the liquid fraction, \( \varepsilon \) is a small number (0.001) to prevent division by zero, and \( A_{mush} \) is the mushy zone constant and set to \( 10^5 \).

**The momentum equation**

\[
\frac{\partial}{\partial t} (\rho_0 \mathbf{v}) + \nabla \cdot (\rho_0 \mathbf{v} \mathbf{v}) = -\nabla P + \nabla \cdot (\mu \nabla \mathbf{v}) + (\rho - \rho_0) g + \nu \frac{A_{mush} (1-\beta)^2}{\beta^3 + \varepsilon}
\]  

(8)

The Boussinesq approximation was used where the fluid density has been assumed constant in all solver equations of the momentum equation except the body force term.

\[
(\rho - \rho_0) g = -\rho \beta_{tec}(T - T_0)
\]  

(9)
4. Initial and boundary conditions
1. The initial temperature of all zones is set to 303K.
2. The change in volume of PCM due to phase change is ignored.
3. The outer wall surface of the shell and the top and bottom caps are well insulated.
4. The temperature and the mass flow rate of HTF are at 358 K and 0.0833 kg/s.

5. Results and discussion
For ensuring grid and time independence solution, simulations were carried out with three different
 grids sizes (1000, 2000 and 4000 for the PCM zone) and three time-step sizes: 0.05 s, 0.1 s, and 0.2 s
 as shown in figure 3. It is found that the model with 2000 cells and time steps of the 0.05 s, 0.1s, and
 0.2 s produces a similar temperature variation. Increasing the number of elements to 4000 produces no
 significant change. Furthermore, the selected 2000 cells grid and 0.1 s time step are sufficient to
 achieve a convergence level of 1E-6 for the energy equation.

Figure 4 shows the contours of the liquid fraction and the temperature of PCM (paraffin wax) during the
 charging process. At the starting of heating PCM, the heat transfer takes place by conduction only where
 the energy is absorbed in the form of sensible heat. After 1 h of heating PCM by HTF, the average liquid
 fraction was about 28.4% and the average temperature of PCM was about 331 K. When the liquid
 film of molten PCM is formed during phase transition, the heat transfer takes place by buoyancy-induced
 natural convection in the melted PCM as a result of temperature differences. The average liquid
 fraction increases rapidly with time in the initial 4 h of the melting

Where $\rho_0$ is the reference density, $P$ is the pressure, $\mu$ is the dynamic viscosity $\beta$ is the liquid
fraction, $\beta_{tec}$ is the thermal expansion coefficient and $T_0$ is the operating temperature.

The 2D axisymmetric vertical slice of the cylinder model is created to reduce computational time.
The Coupled algorithm and the pressure staggering option (PRESTO) scheme are utilized in the
simulation. Simulations are performed with a second order upwind scheme for momentum and energy
equations. The numerical results are validated by comparison with experimental results of M. K.
Rathod and J. Banerjee [9] as shown in figure 2. This comparison shows that numerical results have a
good agreement with the experimental data.
process in which the average liquid fraction reaches about 80.3%. This is due to the fact that the PCM reaches high temperatures and the effect of natural convection is dominated. The average temperature of PCM reaches 349 K. Then, the rate of increasing the liquid fraction is reduced. This is due to the reduction in the temperature differences between the heat transfer fluid and PCM and hence the rate of heat transfer becomes slowly. The PCM (paraffin wax) takes about 8 hours to be completely melted. The average temperature of PCM reaches 357.3 K. The phase transition interface moves faster in the radial direction near the top of the cylinder as compared to the bottom. Therefore, a conical path of the phase transition can be observed in the PCM during the melting process.

Also, the mushy zone can be seen in the contours of the liquid fraction. The volume of mushy zone is about 11% of total volume of PCM after 1 h of the charging process and it increases and reaches 14.7% after 2 h. This is due to the fact that the effect of buoyancy natural convection in the melted PCM is dominated. Then, the volume of mushy zone is reduced and reaches about 1.9% and 0.6% after 7 h and 8 h, respectively. This is due to increasing in the melted PCM and decreasing in the solid PCM and then the volume of mushy zone is reduced.

Figure 3. (a) Grid size independency (b) Time independency.
Figure 4. The contours of (a) liquid fraction (b) the temperature of PCM during the charging process.
6. Conclusion
The numerical study was performed using ANSYS FLUENT. The shell and tube were utilized as Latent Heat Thermal Energy Storage Unit (LHTESU) where the paraffin wax was filled inside the shell and water flowed through the tube. The inlet temperature of the water was 85 °C during the charging process. The effects of natural convection and conduction heat transfer were studied in the model. It was noted that at the beginning of the charging process the heat transfer by conduction was dominated. Then, the temperature differences were increased inside the PCM and the heat transfer took place by the influence of buoyancy natural convection. The effect of natural convection heat transfer was important in the melting process.

Nomenclature

| Symbol | Definition                                                      |
|--------|-----------------------------------------------------------------|
| PCM    | Phase Change Material                                            |
| HTF    | Heat Transfer Fluid                                              |
| TES    | Thermal energy storage                                           |
| LHTESU | Latent Heat Thermal Energy Storage Unit                          |
| K      | Thermal conductivity (W/m.K)                                     |
| Cp     | Specific heat of PCM (J/kg)                                      |
| L      | Latent heat of fusion (J/kg)                                     |
| h      | Sensible enthalpy (J/kg)                                         |
| H      | Enthalpy (J/kg)                                                  |
| T      | Temperature (°C or K)                                            |
| v      | Velocity (m/s)                                                   |
| g      | Gravity acceleration (m/s²)                                      |
| Amush  | Mushy zone constant (kg/m³.s)                                    |

Greek letters

| Symbol | Definition                                                      |
|--------|-----------------------------------------------------------------|
| ρ      | Fluid density (kg/m³)                                           |
| βTEC   | Thermal expansion coefficient (1/K)                             |
| β      | Liquid fraction                                                 |
| μ      | Dynamic viscosity (kg/m.s)                                      |
| ε      | A small number (0.001)                                          |

Subscripts

| Symbol | Definition                                                      |
|--------|-----------------------------------------------------------------|
| l      | Phase change material at liquid state                            |
| s      | Phase change material at solid state                             |
| m      | Melting of phase change material                                 |
| mush   | Mushy zone                                                      |
| ref    | Reference                                                       |

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