Numerical and experimental investigation of melting process in spherical pcm capsule used for low-temperature thermal energy storage systems

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Abstract. The present work deals with the experimental and numerical investigation of melting process of phase change material used for low temperature thermal energy storage applications. Thermal energy storage is a good solution to bridge the gap between energy supply and energy demand. The unconstrained melting of paraffin wax having melting range of 57°C to 61°C was studied in simple spherical glass capsule. The objective of the subject work is to perform the experimental and numerical analysis of melting process in spherical capsule subjected to constant wall temperature. Ansys Fluent 18 is used for computation purpose. In experimental analysis, melting process was observed through visual capturing of interface between solid and liquid. Melting fraction and temperature at the centre of PCM capsule are monitored both experimentally and numerically. Good consistency in results were observed.

Keywords: Thermal energy storage, phase change material, unconstrained melting, melting fraction, constant wall temperature.

1. Introduction
Energy requirement in the industry, and utility sectors vary on every day or week and seasonal basis. These requirements can be fulfilled with the help of thermal energy storage (TES) systems that operate synergistically. The use of TES for thermal applications are on a fast track such as in solar applications like domestic water heating, air-conditioning etc. [1] - [4]. Such TES systems have a tremendous potential for large scale thermal applications in effective manner. Atul Sharma and V.V. Tyagi [5] in their paper have detailed the applications of thermal energy storage along with the investigation and analysis of PCM used in thermal energy storages. Sarada Kuravi and Jamie Trahan [6] in their paper have focused thermal energy storage design along with its integration in solar power plant. Also, paper explained some economic aspects based on the integration of system. Basically, TES stores the energy by heating, melting, or vaporizing of a material. The thermal energy becomes available by reversing the above processes. Storage by phase change (the transition from solid to liquid or from liquid to vapor with no change in temperature) is a mode of TES known as latent heat storage. Manish K. Rathod, Jyotirmay Banerjee [7] in their paper detailed a comprehensive study on phase change
materials considering the reliability and stability of PCM. This review will help in choosing a best PCM material for application. Kinga Pielichowska and Krzysztof Pielichowski[8]in their review have explained the recent advancements in PCM materials along with the improvement in thermophysical properties viz. thermal conductivity. Francis Agyenim, Neil Hewitt Ulster [9]and Zakir Khan, Zulfiqar Khan[10] have discussed in their review about phase change materials, it has been observed that paraffin, salt hydrates have better thermal performance with least cost. Thus, commercial paraffin wax as a phase change material is chosen for this work. Review also discusses the techniques for improving the thermal conductivity of PCM, different geometrical configurations. Syukrihimran, Aryadisuwono[11] in their paper discusses about use of paraffin waxes and alkanes as phase change material. It has been evaluated that a family of n-alkanes is a good choice for PCM as it involves large spectrum of latent heats, melting points, densities.

Different structural configurations of thermal energy storage systems have been proposed by researchers in past few decades. Bin Li, Xiaoqiang Zhai[12] have done the theoretical and experimental analysis of composite phase change material for mid temperature solar storage systems. Saeid Seddegh, Xiaolin Wang[13] have performed the heat transfer analysis of shell and tube (horizontal and vertical) storage systems for low temperature applications. Robynne Murray, Louis Desgrosseilliers[14] in the paper outlined the solar domestic hot water system with the help of lauric acid as a phase change material. Due to the low thermal conductivity of lauric acid, fins structure is implemented in the thermal energy storage system. Rathod Manish K, Banerjee Jyotirmay[15] have developed correlation of melting time of phase change material used for thermal energy storage system. Recently, some spherical geometrical configurations have been explored by different researchers as it gives more area to volume ratios when compared to other geometries [16] - [18]. The same spherical configuration is chosen for current study.

Based on the literature review, it has been observed that There has been less attempt of complete modelling and experimentation of thermal energy storage system with use of encapsulation and paraffin as a phase change material. There is a lack of understanding of unconstrained melting of phase change material and of interface between solid and liquid while melting in process.

2. Material and method:

2.1 Experimental Setup and phase change material selection:

The experimental tests were carried out in the laboratories of BITS PILANI, Pilani. An experimental setup is designed considering the uniform and symmetrical melting of phase change material in spherical capsule. Fig. 1 shows the experimental setup of thermal energy storage system model. It consists of a hot water bath setup kept at constant temperature (63°C) above melting point of phase change material. Heat is supplied to water in the container with the help of water heater and uniform temperature throughout the container is maintained with the help of stirrer. A thermocouple which is kept in water bath measures the temperature of water in the container and it is ensured that it remains constant throughout the experiment. Front side of hot water bath is kept transparent (a glass wall) to allow camera to capture the images of melting of phase change material kept in the round bottom flask. One thermocouple is kept at the centre of round bottom flask in order to monitor temperature at the centre. Inner diameter of spherical round bottom flask is 80mm. The amount of phase change material is same as taken for numerical analysis. The phase change material is poured in the flask gradually ensuring that it gets solidified uniformly at all locations of flask.
Commercial paraffin wax was used as PCM in the experimental and numerical investigation. In order to understand the specific heat capacity variation over temperature of the PCM during melting, samples of paraffin wax (~2mg) were sent to Bits Pilani chemical department for differential scanning calorimetry (DSC). The DSC scanning results in Figure 2 show that the peak melting temperature is 59 °C with latent heat of ~166 kJ/kg. The summarized thermo-physical properties are detailed in Table 1.

Before starting of experiment, water in the container is heated to a temperature of 63 °C and kept constant throughout the experiment. By keeping the flask filled with solid paraffin, is inserted in the hot water bath and experiment started. With the help of digital camera, images of melting patterns are taken at every 5 minutes of interval. Images captured are further processed for

Table 1: Material Properties of Paraffin wax and glass material

| Property                        | PCM Material                  | Glass Material |
|---------------------------------|-------------------------------|----------------|
| Melting Temperature, $T_m$ (K)  | 330-334                       | ______         |
| Heat of fusion $\lambda$ (kJ/Kg)| 166                           | ______         |
| Specific heat capacity $C_p$ (kJ/kg K) | 1.7 (Liquid) 2.3 (Solid)          | 0.754          |
| Thermal conductivity, $k$ (W/m K) | 0.25 (Liquid) 0.14 (Solid)       | 1.13           |
| Density, $\rho$ (kg/m$^3$)      | 780 (Liquid) 860 (Solid)        | 2230           |
| Liquid Viscosity (kg/ms)        | 3.42* 10$^{-3}$                | ______         |
calculation of the melting fraction i.e. fraction of phase change material melted. With the help of image processing toolbox in MATLAB, they are converted to binary images. Thus, area of whole flask and a melted phase change material are calculated which gives the melting fraction value. Also, the temperature at centre of round bottom flask is recorded at every 5 minutes of time interval with the help of respective thermocouple.

2.2 Physical model:
A numerical model for this PCM based system is developed to study the theoretical performance based on enhancement of thermal storage capacity. A two-dimensional axisymmetric model is developed for transient heat transfer analysis of the problem as shown in figure 3. A sphere of diameter 80 mm is chosen. Outer wall temperature is kept at 40°C above the mean melting temperature of phase change material. The selected paraffin wax has a melting range of 57°C to 61°C.

![Figure 3: 2d axisymmetry spherical sphere (diameter = 80 mm) encapsulated with PCM](image)

The model developed in this study distinguishes itself from those discussed in the literature review, in that it employs the following combination of features:

- All thermos-physical properties of paraffin (thermal conductivity, density, specific heat capacity, dynamic viscosity) are assumed to be constant for respective phases viz. solid and liquid.
- Only radial and axial variation in heat transfer through the system is considered.
- Because of small volume and low Rayleigh's number, no convective heat transfer mode is considered during simulation.
- Effect of volume expansion of solid and liquid phases for the PCM material is neglected.

2.3. Computational Methodology
Figure 4 indicates the meshing details of the physical model described above. A 2d axis symmetry model is meshed with 1678 quadrilateral elements with maximum element size of 0.548 mm. The computational analysis is done in Ansys fluent with solidification and melting solver.
Figure 5: Comparison of Melting fraction contours for experimental and numerical work at (A) 0 min, (B) 40 min, (C) 80 min, (D) 120 min

Semi implicit pressure linked equations as a discretization scheme is chosen. Computational domain consists of a phase change region for which enthalpy porosity approach is used. In this approach, each cell is given a value of liquid fraction as porosity. Numerical analysis is performed using Ansys 18. The grid size and time step has been chosen performing grid independence and time step independence tests. A time step of 0.01 has been set. It took 7 days of continuous run for simulation to complete. Simulation has been run on 4 cores and 1 graphics configuration PC.

3. Results and discussion

3.1 Comparison of melting fraction

Figure 5 shows a comparison of numerical and experimental contours of melting fraction at different time intervals of 0 min, 40 min, 80 min and 120 min. Numerical results are simulated by considering the gravity effect and show a fair consistency in results when compared to experimental one. The interface between solid and liquid phase and thus the melting fraction is in good agreement with both contour plots Figure 5 (B) has a solid portion suspended in upper half of sphere because of sticking of pcm to thermocouple inserted at the center of system.
Figure 6: Melt fraction (%) vs time (min) for numerical and experimental work

Figure 7: Temperature contours for numerical work at (A) 0 min, (B) 40 min, (C) 80 min, (D) 120 min
Figure 6 shows a plot of melting fraction vs time for experimental as well as numerical work. Initially for less than 10 minutes, melting fraction remains 0 because it takes time for melting to start as some amount of heat is absorbed as sensible heat. Further melting fraction shows a linear trend up to 100 min. It starts decelerating after 100 minutes. As remaining solid portion lies at the center of system, it requires more time for heat to reach at the center of system. Both experimental and numerical curves show a good agreement in results of melting fraction.

3.2 Comparison of temperature
Figure 7 shows contour plots of temperature behaviour during the melting of phase change material paraffin wax at different time intervals. Also figure 8 shows a temperature vs. time plot at the centre of sphere containing a phase change material. Temperature plot shows a linear behaviour till 100 minutes and it starts decelerating afterward. It indicates more time needed to rise a temperature after 100 minutes. A good agreement in experimental and numerical results of temperature plot is observed.

Figure 8: Temperature (K) at the center of PCM capsule vs time (min) for numerical and experimental work

4. Conclusions
The behavior of melting fraction and temperature at the center of sphere during the melting of phase change material was studied. Also, the interface between solid and liquid during melting was tracked successfully. Numerical modelling takes 131 minutes of time while Experimental analysis gives 136 minutes of time for complete melting of paraffin wax. From the plot of melting fraction Vs time (fig 6), it is observed that Numerical and experimental results of melting fraction are in good agreement with maximum deviation of 14.67 %. From the plot of temperature Vs time (fig 8), it is observed that Numerical and experimental results of temperature at a centre of spherical capsule is in good agreement with maximum deviation of 9.25 % It can be concluded that the numerical simulation could be further improved by considering few changes in modelling viz. three-dimensional model, temperature dependent thermo-physical properties.
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