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A Numerical Investigation Of The Thermal Behavior Of Different Phase Change Materials In Thermal Energy Storage Systems

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Abstract: Phase change materials (PCM) are widely used in thermal energy storage systems due to their high heat storage properties. However, due to the low thermal conductivity of PCMs, different surface areas are employed in order to increase the amount of energy. One of these methods is to use fins with high thermal conductivity. This study numerically investigated the thermal behavior of different PCMs (paraffin, paraffin wax, polyethylene glycol 6000) during the melting process in a thermal energy storage system with 15 fins. A FOX 50 heat flow meter was used for thermal conductivity measurements of these PCMs, and TA DSC Q200 (Differential Scanning Calorimetry) devices were used for specific heat measurements. The thermal property data of these measured PCMs were used in a time-dependent analysis. With the PCM data obtained, time-dependent thermal analyses were carried out using the Ansys-Fluent program based on the Computational Fluid Dynamics (CFD) method. The effect of these different PCMs on the melting processes was investigated by using water at 75°C in a 15-fin thermal storage system by observing their thermal behavior in the thermal energy storage system. In addition, cost analyses were conducted by determining the required amount of PCMs for the thermal storage system.

Keywords: Phase Change Materials, Thermal Energy Storage, CFD

1.INTRODUCTION

The sustainable development of the modern world is based on energy resources and their intended use. Most of today’s energy comes from fossil fuels. As a result of the depletion of fossil fuel reserves and their negative impact on the environment, the world has seen an increased demand for clean, efficient and reliable energy sources. Renewable energy sources, despite their lack of continuous availability, offer sustainable alternatives to fossil fuels as candidates with low environmental impact. A viable solution to such a situation is to store energy when available and use it as needed, especially as energy storage technology evolves.

Traditional energy storage systems have been used to recapture various forms of energy, such as flywheels to store mechanical energy, batteries to store electrochemical energy, and biofuels to store chemical energy. In recent years, renewable thermal energy storage has gained popularity in many parts of the world due to the abundance of renewable resources in the form of solar energy. Solar radiation can be used to store energy in the form of sensible energy, where energy is stored by increasing the temperature of a material, or in the form of latent energy, where energy is stored by changing the phase of a phase change material (PCM). In this context, passive cooling systems based on phase change materials have become very popular in recent years. The use of such materials in building structures can significantly reduce temperature fluctuations and energy consumption to maintain a comfortable thermal regime indoors [1–6]. The use of PCM is a broad research topic as it includes many factors affecting...
heat transfer that must be considered in structures of various geometries and under different thermal conditions. Such factors include climatic conditions, material selection, geometric properties, the relative positions of materials and, in some cases, heat transfer enhancers such as high thermal conductivity fins, metal foam and others [7]. Due to their high heat storage properties, phase change materials (PCM) are used in many areas like solar energy storage, passive cooling in bioclimatic buildings, protection of food and electronic devices, thermal comfort in vehicles, cooling of engines, and the thermal systems of space vehicles. It is understood that the thermal conductivity of phase change materials is relatively low. Therefore, in order to increase the heat transfer to the PCM, it is preferred to use materials with high thermal conductivity [8–10].

ul Hasnain et al. [11] numerically investigated the effect of different fins and nanoparticles to increase the melting of phase change material (PCM) placed in a horizontally structured latent heat thermal energy storage unit. The effects of different fin designs on PCM melting performance and heat transfer were investigated, and it was observed that the energy storage capacity increased at the same rate as the number of fins. Then, the effects of the most efficient blade design and the melting performance of Al₂O₃ nanoparticles were evaluated. However, they found that the corresponding energy storage decreased with an increase in nanoparticle concentration. Jmal and Baccar [12] numerically investigated the solidification of a PCM (ParaffinC18) and the effect of fins on heat transfer in internal and external horizontally finned thermal storage tubes for two air conditioning systems. They found that the amount of energy transfer increased due to the finned structure, and the outlet temperature of the fluid increased. Ogoh and Groulx [13] numerically investigated the effects of fin numbers and their distribution on the energy storage properties of a cylindrical thermal energy storage system. Analyses were conducted by making the inlet velocity of the hot water between 0.05 and 0.5 m/s and the number of fins from 0 to 27. They observed that the total heat transfer to the phase change material increased with an increasing number of fins. Augspurger and Udaykumar[14] investigated the effect of aluminum metal fins on the performance of a thermal storage device with phase change material (a mixture of NaNO₃ and KNO₃) for heat dissipation and recovery. They found that the best design in terms of their ability to absorb and give off heat is the one with the highest number of fins. Abdulateef et al. [15] investigated the heat transfer in PCM-latent heat thermal energy storage vessels using fins embedded in the PCM. In addition, they investigated the geometric dimensions, the dimensionless numbers and the blade position through numerical and experimental studies to evaluate the effects of this system on thermal performance. They observed that the best thermal performance was with longitudinal fins in a cylindrical thermal energy store. They said that as the number and size of the fins increased, the heat transfer surface area between the fin and PCM increased, so the thermal performance increased.

Osterman et al. [16] studied a system in which phase change materials (PCM) were used as thermal energy storage to reduce energy consumption in buildings. Analyses of a thermal energy storage system
consisting of plates filled with paraffin RT22HC were performed using the Fluent program and computational fluid dynamics (CFD). They observed that the two-dimensional analyses were experimentally consistent with each other. Matt et al. [17] numerically investigated the melting process in an RT82 triple tube heat exchanger with phase change material (PCM) using the Fluent program. They observed the effect of inner, outer and inner–outer fins to improve heat transfer between the PCM and the heat transfer fluid with three heating methods to melt the PCM from the inner tube, outer tube and both tubes. They calculated that the melting time could be reduced by 43% in a three-tube heat exchanger with internal and external fins. Hosseini et al. [18] experimentally and numerically investigated the effect of increasing the inlet temperature of the heat transfer fluid on the charging process of PCM during the melting of phase change materials (PCM) in a two-tube heat exchanger. They showed that when the inlet temperature of the heat transfer fluid was increased from 70°C to 80°C, the total melting time was reduced from 37% to 19%.

Li and Kong [19] numerically investigated the phase change and thermal performance of a two-pipe thermal storage unit using paraffin wax (as the PCM) and air and water as the heat transfer fluid. In the analyses, the melting temperature of the paraffin wax was 41°C and the latent heat was 140 kJ/kg. In the final stages of the melting process – when air was used during the phase change in the two-pipe thermal storage unit – they found that the heat transfer was very low, and the desired air temperature and speed were not sufficient. When water was used, they said that since the density and specific heat capacity of water are large, the melting process increased rapidly and occurred in a very short time compared to air. Koşan and Aktaş [20] investigated the thermal behavior of the phase change material (PCM) during the melting process in a nested tube heat exchanger used in thermal energy storage systems. They used the Ansys Fluent program for time-dependent models with and without fins, in two dimensions. In their model, the temperature of the heat transfer fluid was 50°C, 60°C and 70°C, and they observed the effect on the melting time of the PCM. Then, 6, 9, 12, and 15 fins were added to this model and the effect of the number of fins on the melting time of the PCM was investigated. It was emphasized that as the temperature of the heat transfer fluid and the number of fins increased, the melting time of the PCM decreased, so that the PCM stored heat more quickly. Agarwal and Sarviya [21] thermally investigated the casing tube-type latent heat storage system for a solar dryer. Using paraffin wax and heat transfer fluid with air as the heat storage material, the thermal and heat transfer properties of the latent heat storage system were observed during the charging and discharging process. They stated that the heat storage system achieved an air temperature increase in the range of 17°C to 5°C in 10 hours.

When the research literature was examined, the design of the thermal energy storage is seen to be very important for a PCM with low thermal conductivity and to store heat energy in a short time. It has been observed that the number of fins and the temperature of the heat transfer fluid affect the melting time in the thermal storage system.
In this study, a thermal energy storage system and heat transfer fluid temperature were determined by using the studies in published literature. For this purpose, the effect of five different PCMs on the melting processes was observed by using water at 75°C in a 15-fin thermal storage system. Measurements were made for thermal conductivity and specific heat values, which are usually taken as a constant value. A FOX 50 Heat Flow Meter was used for thermal conductivity measurements and TA DSC Q200 (Differential Scanning Calorimetry) devices were used for specific heat measurements. The thermal property data of these measured PCMs were used in time-dependent analyses. With the PCM data obtained, time-dependent thermal analyses were carried out using the Ansys Fluent program based on the Computational Fluid Dynamics (CFD) method. The thermal behavior of these PCMs was observed in the thermal energy storage system.

2. MATERIALS AND METHOD

2.1. Thermal Storage System Design, Boundary Conditions and Measurement of PCM Properties

The design parameters of the thermal storage system to be determined included the structure of the system and the number of fins. A thermal storage system with 15 fins was designed by making use of literature research to aid the system design and arrive at the ideal number of fins. In addition, the type of phase change material and heat transfer fluid, flow rate and fluid temperatures are other important parameters. The thermal storage system geometry is shown in Figure 1. In addition, the geometric dimensions of the thermal storage system are given in Table 1.

In the thermal storage system, the outer pipes were filled with phase change material and hot water was passed through the inner pipe with heat transfer taking place between these two pipes. The outer tube material was selected to be stainless steel with a diameter of 80 mm. The inner tube and fins were made of copper material with a high thermal conductivity and a diameter of 16 mm. The inlet temperature of the water, which was used as the heat transfer fluid in the analyses was 75°C and its speed through the pipes was 0.2 m/s. In order to examine the thermal behavior of the melting process in the thermal energy storage system, analyses were carried out for different PCMs (pure paraffin, paraffin wax and polyethylene glycol).

In the study, the thermophysical properties of the pipes were assumed to be constant, the fluid incompressible and Newtonian. A FOX 50 Heat Flow Meter was used for thermal conductivity measurements of the thermophysical properties of PCMs, and TA DSC Q200 (Differential Scanning Calorimetry) devices were obtained for specific heat measurements. Figure 2 shows the pictures of the FOX 50 Heat Flow Meter and TA DSC Q200 devices. In addition, in Figure 3, samples of PCMs that were prepared for analysis and measured in specially prepared containers are shown. The
thermophysical properties of pipes and PCMs are given in Table 2. The \( C_p \) and \( k \) values of pure paraffin, paraffin wax and polyethylene glycol 6000 that are given in Table 2 were calculated using the data obtained as a result of these measurements.

2.2. Numerical Analysis

In CFD analysis, the region to be calculated is divided into many small elements (cells) and governing equations are applied to each small element. The smaller these elements are, the better the resolution precision. However, if a suitable network structure is not selected according to the geometry and size of the model being analyzed, CFD analysis may either take longer than necessary or require the use of high-capacity computers. The computational cost increases as the time step gets smaller in time-dependent analyses.

In the CFD (Computational Fluid Dynamics) analysis, a numerical network structure was created. A tetrahedral digital mesh geometry was used for the flow volume of the thermal storage system. Figure 4 shows the network structure created for the thermal storage system analysis. In this model, there are an average of 390576 elements and 374604 nodes. In Table 3, the approaches used in numerical calculations and the determined parameters are given.

2.3. Fluent Basic Equation and Methods of Analysis Used in Analysis Software

Ansys Fluent or other modeling programs are used in this method, which is based on the finite volume method. The solution of the system is achieved by applying boundary conditions and parameters to the digital network structure files taken from the programs. Three-dimensional and time-dependent continuity, conservation of mass, momentum and energy equations are solved in the programs to be used in the numerical studies. The Ansys Fluent program uses the following equations in the background to solve the system [22].

The mass conservation equation is shown in Equation 1:

\[
\nabla \cdot \vec{v} = \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z}
\]

The momentum equation is given in Equations 2 to 4 for the X, Y and Z axes:

\[
\rho \left( \frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} + w \frac{\partial u}{\partial z} \right) = \mu \left( \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} \right) - \frac{\partial p}{\partial x}
\]

\[
\rho \left( \frac{\partial v}{\partial t} + u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} + w \frac{\partial v}{\partial z} \right) = \mu \left( \frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} + \frac{\partial^2 v}{\partial z^2} \right) - \frac{\partial p}{\partial y}
\]

\[
\rho \left( \frac{\partial w}{\partial t} + u \frac{\partial w}{\partial x} + v \frac{\partial w}{\partial y} + w \frac{\partial w}{\partial z} \right) = \mu \left( \frac{\partial^2 w}{\partial x^2} + \frac{\partial^2 w}{\partial y^2} + \frac{\partial^2 w}{\partial z^2} \right) - \frac{\partial p}{\partial z}
\]
\[ \rho \left( \frac{\partial w}{\partial t} + u \frac{\partial w}{\partial x} + v \frac{\partial w}{\partial y} + w \frac{\partial w}{\partial z} \right) = \mu \left( \frac{\partial^2 w}{\partial x^2} + \frac{\partial^2 w}{\partial y^2} + \frac{\partial^2 w}{\partial z^2} \right) - \frac{\partial P}{\partial x} \]  

(4)

In addition, the energy balance equation given in Equation 5 was taken into account to analyze the thermal behavior of the PCM:

\[ \frac{\partial}{\partial t} (\rho H) + \nabla \cdot (\rho \vec{v} h) = \nabla \cdot (k \nabla T) + S_E \]  

(5)

Here, \( h \) enthalpy (J); \( \rho \) is density (kg/m\(^3\)), \( \vec{v} \) flow velocity (m/s) and \( S_E \) is the source term (J/m\(^3\)s).

The total enthalpy \( h \) of the PCM in Equation 5 is calculated using Equation 6:

\[ h = h_{\text{sen}} + h_{\text{lat}} \]  

(6)

For the PCM used in this equation, \( h_{\text{sen}} \) sensible enthalpy and \( h_{\text{lat}} \) hidden latent enthalpy are calculated from the equations given in Equation 7-8, respectively.

\[ h_{\text{sen}} = h_{\text{hreb}} + \int_{T_{\text{ref}}}^{T} C_p \Delta T \]  

(7)

Here, \( h_{\text{hreb}} \) represents the latent enthalpy referenced in calculations. The latent enthalpy \( h_{\text{sen}} \) during phase change in Equation 8 is calculated based on the liquid volume ratio for the PCM.

\[ h_{\text{sen}} = \beta LH \]  

(8)

Here, LH (J/kg) represents the heat or latent heat fusion required to melt one kg of PCM, the liquid volume ratio indicated by \( \beta \) represents the ratio of the liquid volume in any cell to the entire metal volume in the same cell. \( \beta \) ranges from 0 to 1, 0 represents solid phase while 1 represents liquid phase. The 0<\( \beta \)<1 region is defined as the musy region. For \( \beta \), depending on the PCM temperature (T):

- \( T < T_{\text{solid}} \) \( \Rightarrow \) \( \beta = 0 \)
- \( T > T_{\text{solid}} \) \( \Rightarrow \) \( \beta = 1 \)
- \( T_{\text{solid}} < T < T_{\text{liquid}} \) \( \Rightarrow \) \( \beta = \frac{T - T_{\text{solid}}}{T_{\text{liquid}} - T_{\text{solid}}} \)

values are taken.
3. RESULTS

In this thermal storage system, the temperature of the water used as the heat transfer fluid and the thermal behavior of the PCM that melts (stores the energy) were modeled in three dimensions in the Ansys Fluent program over time. In the analyses, the data used were obtained by using the FOX 50 Heat Flow Meter for thermal conductivity measurements of thermophysical properties of PCMs and TA DSC Q200 (Differential Scanning Calorimetry) devices for specific heat measurements. In the analyses, temperature distributions and melting processes were investigated by considering three different PCM materials, namely pure paraffin, paraffin wax and polyethylene glycol. Figure 5 shows the temperature distribution contours that changed over time during the melting process of the PCM in the nested tube thermal storage system with a water temperature of 75°C.

In Figure 5, it is seen that with the initiation of the melting process, the temperature of the PCM increased with time. Following this the temperatures of the PCMs stabilized as thermal equilibrium was approached. According to these results, it was seen that the melting rate of paraffin was faster than paraffin wax and polyethylene glycol 6000.

As seen in Figure 6, time-varying liquid volume ratios (liquid fraction) are shown during the melting process of PCM in a nested tube thermal storage system with a water temperature of 75°C. The blue color (the region where the liquid ratio is 0) indicates the amount of PCM in the solid state, and the red color (the region where the liquid ratio is 1) indicates the amount of PCM in the liquid state. The solid–liquid interface that separates the two phases is called the mushy zone. The green–yellow color formed between the solid–liquid phase (the region where the liquid ratio is between 0 and 1) shows the mushy zone. With the initiation of the melting process, the heat transfer from the inner hot wall to the solid PCM caused the PCM to melt. Initially, there was heat transfer by conduction in all regions. Then, with the melting of PCM, it started to show the effects of natural convection.

Initially, the melting rate was very fast, but it started to slow down over time. The PCM takes the heat from the water and stored it as melting began. Paraffin completely melted in 190 minutes. Paraffin wax melted in 370 minutes and polyethylene glycol 6000 melted in 640 minutes.

In Figure 7, the graph of the total heat transfer rate required for the melting of PCMs is given. In addition, a cost analysis of PCMs is given in Figure 8.

As can be seen in Figure 7, less energy is required to melt the paraffin. Paraffin wax and polyethylene glycol 6000 needed more time and energy to melt. Paraffin wax required 141.17 W of energy, while
paraffin wax required 274.91 W and polyethylene glycol 6000 required 475.521 W of energy. In the graph given in Figure 8, a cost analysis was conducted according to the amount of PCMs required in the thermal storage system. According to the calculations, the amount of paraffin and paraffin wax required for the thermal storage system were similar, while the amount of polyethylene glycol is 1.6 times higher than paraffin. In addition, when calculations were made according to unit prices, both energy costs and quantities of other PCMs increased compared to paraffin. Paraffin is a suitable PCM for this thermal storage system with less energy and cost compared to other PCMs.

4. CONCLUSIONS

In this study, the melting process of paraffin, paraffin wax and polyethylene glycol 6000 used as PCM was modeled for a 15-fin heat storage system and a numerical analysis was carried out. In the numerical analysis, data obtained by using a FOX 50 Heat Flow Meter for thermal conductivity measurements of the thermophysical properties of PCMs, and TA DSC Q200 (Differential Scanning Calorimetry) devices were used for specific heat measurements. In this study, the design of a thermal storage system was carried out. In addition, the analyses were three-dimensional and time dependent, and were performed using the Ansys Fluent software simulation program. The data obtained in this study can be briefly summarized as follows:

• The thermal behavior of the thermal storage system filled with PCM and the time-dependent melting process of PCMs were investigated.
• Cost analyses of PCMs used in the system were carried out.
• The applicability of this numerical study can be analyzed in detail by conducting an experimental study.
• By using organic PCMs different from the PCMs used in this study, numerical analyses can be made and their thermal behavior in the thermal storage system can be examined.
• A FOX 50 Heat Flow Meter for thermal conductivity measurements of the thermophysical properties of different PCMs, and TA DSC Q200 (Differential Scanning Calorimetry) devices for specific heat measurements were used to make measurements, and the resulting thermal storage system could be developed.
• Different from the design parameters in this study, new fin designs compatible with PCM can be made and the melting and solidification processes of PCM can be examined.
DECLARATIONS

Availability of data and material: Availability of data and material is clearly stated in the text.

Conflicts of interest/Competing interests: There are no conflicts of interest/competing interests.

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Ethics approval: Suitable.

Consent to participate: Suitable.

Consent for publication: Suitable.

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Figures

Figure 1

The thermal storage system geometry is shown in Figure 1

Figure 2

Figure 2 shows the pictures of the FOX 50 Heat Flow Meter and TA DSC Q200 devices

![Paraffin, Paraffin wax, Polycethylene glycol 6000](image)

Figure 3

In Figure 3, samples of PCMs that were prepared for analysis and measured in specially prepared containers are shown
Figure 4

A tetrahedral digital mesh geometry was used for the flow volume of the thermal storage system. Figure 4 shows the network structure created for the thermal storage system analysis.

Figure 5

Figure 5 shows the temperature distribution contours that changed over time during the melting process of the PCM in the nested tube thermal storage system with a water temperature of 75°C.

Figure 6

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Figure 7

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Figure 8
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