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Performance evaluation of fatty acids as phase change material for thermal energy storage

Karunesh Kant*, A. Shukla, Atul Sharma

Non-Conventional Energy Laboratory, Rajiv Gandhi Institute of Petroleum Technology, Rae Bareli 229316, India

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ABSTRACT

Thermal energy storage (TES) systems using Phase Change Materials (PCM) are very attractive due to high storage density and economic viability. Use of fatty acids as phase change material for various TES applications: buildings, solar heating systems, air-conditioning systems have been widely accepted. It is highly desired to study the performance of PCMs for a particular application, in terms of heat transfer mechanism and geometry/structure of the container, as it helps in optimizing the cost and quality of TES systems. In the present work, authors studied the performance of five different fatty acids (Capric acid, Lauric acid, Myristic acid, Palmitic acid and Stearic acid) when used with aluminum containers. The numerical simulation of heating and cooling of PCMs has been conducted using finite element analysis (FEM). The results are reported in term of melt fraction, temperature variation, the transition of solid-liquid interface and the quantity of thermal energy stored in different fatty acids with time for melting and solidification. Based on the simulated results it can be concluded that the Capric takes minimum time for melting and solidification with the same boundary conditions, among the studied PCMs in this work. Such studies could be quite helpful in developing fatty acid based TES applications.

1. Introduction

Solar energy is environmentally clean, free and everlasting source of energy. The radiant energy reaching the Earth from the Sun is thousands of times higher than the present total consumption including all domestic as well as commercial requirements. This makes it one of the most promising renewable energy sources. However, due to its intermittent and unpredictable nature; tapping solar energy through various ways including efficient and economical solar thermal energy storage devices is the need of the hour. Among the different possibilities to store Solar Thermal energy, systems using PCMs are of much interest due to its consistency in latent heat storage. Latent heat thermal energy storage (LHTES) can accomplish a greater energy storage density, reduced size of the system and a narrower temperature range throughout the melting and solidification of PCMs [1–3]. PCMs have received considerable interest for their various applications in building energy efficiency, solar water heating systems, solar air heating system and air-conditioning systems [4–8].

Thermal energy storage system mainly consists of heat exchanger container materials and PCM. The efficiency of TES systems gets limited due to the lower thermal conductivity of PCMs. To overcome this drawback, the container material having highly thermal conducting materials is preferred and closely spaced with PCMs. During melting and solidification of PCMs, the melting interface moves away and present to the heated surface respectively. This imposes a challenge on solving and analyzing the heat transfer phenomena associated with the PCMs as the presence of a moving boundary or region on which heat balance conditions have to be met. Heat transfer with moving interface involving phase change is very important in TES systems for the prediction of temperature distribution, quantity of energy stored and rate of melting or solidification, consequently for performance evaluation of the different PCMs.

The interest on thermal energy storage by using fatty acid as PCM has risen in recent times since; they have desired thermodynamic and kinetic criteria for low-temperature latent heat storage [9] such as solar drying [10], solar desalination etc. [11]. Fatty acids have superior properties over many PCMs such as melting congruency, good chemical stability, and non-toxicity. More important of their characteristics is their smaller volume change during phase transition and high latent heat of fusion per unit mass and suitable melting temperature range for solar passive

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* Corresponding author.
E-mail addresses: k1091kant@gmail.com, kantrgipt@yahoo.in (K. Kant).

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Nomenclature

q	Heat flux by conduction
S	Strain-rate tensor
ξ	Viscous stress tensor
Q	Heat sources other than viscous dissipation
L	Latent heat of fusion
ΔT	Transition temperature
ρ	Density
ρ_{solid}	Density in solid state
ρ_{liquid}	Density in liquid state
H	Specific enthalpy
θ	Fraction of phase
C_p	Specific heat capacity at constant pressure
k	Thermal conductivity
u	Velocity field
αm	Mass fraction
C_{eq}	Equivalent heat capacity
C_L	Distribution of latent heat
T_{wall}	Heated wall temperature
T_m	Melting temperature

heating applications (i.e. Solar dryer, Solar Desalination etc.). An added advantage is that fatty acids are derived from the common vegetable and animal oils that provide an assurance of continuous supply despite the shortage of fuel sources [9–12]. Amongst the studied fatty acids, the Capric acid, Lauric acid, Myristic acid, Palmitic acid and Stearic acid are potential materials for heat storage in solar space and water heating systems from points of view of melting temperature and latent heat of fusion and thermal performance [13,14].

A number of experimental and theoretical studies have been done on the thermal performance of PCMs using fatty acid as the material for thermal energy storage for various applications [15–19]. Costa et al. [20] analyzed the heat transfer (one and two-dimensional both) in PCM using an enthalpy formation with a fully implicit finite difference method. Suppes et al. [21] carried out a study using the mixture of fatty acids and their work demonstrated that it is possible to develop high-performance PCMs from natural fatty acids. Lamberg et al. [22] carried out a numerical study with the FEMLAB simulation software and compared to experimental data. Both numerical methods gave good estimations for the temperature distribution of the storages in both the melting and freezing processes. However, the effective heat capacity method, which uses a narrower temperature range, $dT = 2\,^{\circ}\mathrm{C}$, was the most precise numerical method when the numerical results were compared with the experimental results. Lamberg et al. [23] developed an approximate analytical model for two-phase solidification problem in a finned PCM storage and the model gives a satisfactory estimation of the fin temperature and the solid–liquid interface when the length-to-height ratio of the storage cell is smaller than 6.0 and the fin length, is smaller than 0.06 m. The error made in the fraction of solidified PCM is ±10% when the analytical model is used rather than the two-dimensional numerical model.

In the present study, two-dimensional numerical studies of fatty acids as PCMs have been carried in COMSOL Multiphysics 5.0 version [24]. The two-dimensional studies are carried out with the effect of natural convection during melting by using an effective thermal conductivity of the liquid phase of the PCM. The calculations were made for the effect of mesh size, enthalpy stored; melt fraction and two-dimensional variation of melting interface and temperature of PCMs at three wall temperature.

2. Numerical formulation and physical model

The numerical simulation has been conducted for conjugate heat transfer in solid (container material for this study) and PCMs. The mathematical formulations used for the study are given in brief for solid as well as during the phase change process. The following assumptions have been made for the present study:

- Thermophysical properties of container material are independent of temperature.
- Properties of PCMs is different in solid and liquid phase.
- PCM is homogeneous and isotropic.
- The effect of natural convection during melting is taken into account by using an effective thermal conductivity of the liquid phase of the PCM [25].

The fundamental law governing heat transfer is the first law of thermodynamics, commonly referred to as the principle of conservation of energy. However, internal energy, U, is a rather inconvenient quantity to measure and use in simulations [26]. Therefore, the basic law is usually rewritten in terms of the temperature, T in Eq. (1). For a fluid, the resulting heat equation is:

$$\rho C_p\left(\frac{\partial T}{\partial t}+(u\bullet\nabla)T\right)=-(\nabla\bullet q)+\tau : S-\frac{T\partial\rho}{\rho\,\partial t}\Big|_p\left(\frac{\partial\rho}{\partial t}+(u\bullet\nabla)\rho\right)+Q \tag{1}$$

where

$$S=\frac{1}{2}\left(\nabla u+(\nabla u)^{\xi}\right)$$

In deriving Eq. (1) it is assumed that the mass is always conserved, which means that the density and the velocity must be related through

$$\partial\rho/\partial t+\nabla\bullet(\rho v)=0 \tag{2}$$

According to the Fourier law of heat conduction, the heat flux is proportional to the temperature gradient. Where k is the thermal conductivity of solid and it can be anisotropic (that is, it has different values in different directions). Then k becomes a tensor$k=\begin{bmatrix}k_{xx} & k_{xy} & k_{xz}\\ k_{yx} & k_{yy} & k_{yz}\\ k_{zx} & k_{zy} & k_{zz}\end{bmatrix}$ and the conductive heat flux is given by$q_i=-\sum_j k_{ij}\frac{\partial T}{\partial x_j}$. Inserting Eq. (2) in Eq. (1) and ignoring viscous dissipation and pressure work put the heat equation into a more familiar form

$$\rho C_p\frac{\partial T}{\partial t}+\rho C_p u\bullet\nabla T=\nabla\bullet(k\nabla T)+Q \tag{3}$$

The heat transfer in fluids interface solves this equation for the temperature, T. If the velocity is set to zero, the equation governing purely conductive heat transfer is obtained

$$\rho C_p\frac{\partial T}{\partial t}+\nabla\bullet(-k\nabla T)=Q \tag{4}$$

Instead of adding a latent heat L in the energy balance equation when the material reaches its phase change temperature T_m, it is assumed that the transformation occurs in a temperature interval between $T_m-\Delta T/2$ and $T_m+\Delta T/2$ [27]. In this interval, the phase of materials is modeled by a smoothed function θ, representing the fraction of phase before transition, which is equal to 1 before $T_m-\Delta T/2$ and to 0 after $T_m+\Delta T/2$. The density, ρ, and the specific enthalpy H, are expressed by Eq. (5) and Eq. (6) respectively:

$$\rho=\theta\rho_{solid}+(1-\theta)\rho_{liquid} \tag{5}$$