Thermal analysis of phase change materials inside a square enclosure

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Abstract. Rising challenges in electric mobility and computing domain to control and condition the temperatures inside circuit boards and motor control drivers call for efficient and effective heat sink designs. Phase change materials come handy and have applications in conditioning temperatures in electronic devices. They prevent failures and increase their efficiencies at different temperatures and conditions. In the present study, the complex flow physics of phase change materials during melting is studied, inside a square enclosure with a heat source mounted at the bottom wall. The walls are assumed to be adiabatic, the material properties of heat source are that of silicon at 330K. The turbulent natural convection flow is modeled by the computational fluid dynamics (CFD) approach using Reynolds averaged Navier-Stokes equation (RANS) with Lambrerhorst k-ε turbulence model. A finite difference method is employed to discretize the governing equations. An in-house CFD code was computed for simulating the convective heat transfer characteristics. The flow physics of three different phase change materials (n-Octadecane, PEG900, and Paraffin (RT60)) have been analysed for a fixed Grashof number value of $10^3$. The transient flow characteristics are examined by plotting the stream function, velocity, and temperature variation with time of the phase change materials.

1. Introduction

Heat transfer properties of phase change materials in an enclosure have been of great interest to researchers, which is mainly due to their applications in heat storage devices, thermal management, and thermal protection systems. PCMs have found major applications in space exploration shuttle designs and aerospace. They were used in recent space exploration programs and space-crafts such Mars rover change-1 satellite and NASA’s manned spacecraft new Orion as stated in [1], [2], [3]. PCMs are also used in controlling and conditioning temperatures of electronic devices. An experimental investigation has been conducted by Ganatraa et al. [4] where PCMs were used for thermal management of hand held devices. They evaluated the major aspects which influence the design of a thermal management system based on PCMs. A similar study by Ahmeda et al. [5], where the authors examined the continuous operation of the device and confirmed the use of PCM based Thermal Energy storage unit for thermal management of tablet PCs. Their results showed temperature drop of 8°C in the back cover during continuous operation. The authors also established that more convection at different inclination angles results in more heat transfer and lower the back cover temperature, conditioning the temperature below allowable chip temperature (85 °C). They also observed a significant delay in reaching heat saturation (27 min.). Another numerical simulation for cooling electronic devices was carried out by Yang and Wang [6] where they used n-eicosane as the operating phase change material for power levels of 2W to 4W. Using a laminar Navier Stokes model for momentum and energy equation, they found that n-eicosane can be used to maintain more stable operating temperatures for the electronic devices. They conducted their simulation with a maximum operating temperature of 320K for a melting time shorter than 6801.2 seconds. It has also been observed that the number of heat cycles influence the performance of the phase change material. This effect has been investigated by Vasa et al. [7] where the degradation of thermophysical properties due to variation in thermal cycle has been investigated for a sample mass of 200 cycles at 600 °C. They reported that the thermal conductivity increased with the number of cycles and the paraffin
(PCM) was stable up to 175 °C, regardless of the number of cycles it went through. The simulation for PCM storage based on direct and indirect solar organic Rankine cycle has also been conducted by Alvi et al. [8]. They found that the direct system outperformed the indirect system in terms of thermal efficiency and net power. While the energy storage in indirect system was 9.24MJ more than direct system. A numerical mathematical model was used to plot temperature profile of PCM that varies with time. Similar study for heat transfer analysis by encapsulated PCM was carried by Zhao et al. [9] for solar power applications. They established that the size of the capsules impacts the heat transfer. Since gravity sinks the solid phase of PCMs, it shortens the total energy storage time in encapsulated PCMs. The buoyancy driven convection can also shorten the storage time. The 7 arrays of PCMs were used with (capric acid, eicosane, decahydrated Sodium carbonate and octadecane), they established that thermal management with PCM is suitable for racing electric cars and small vehicles where space-constraints, weight and aerodynamics are a design challenge. Shamberger and Bruno [10] critically reviewed the thermo-physical properties and melting phenomenon of metallic phase change materials and developed a quantitative matrix to compare the performance of different compounds.

Composite PCMs have also been a significant topic of research due to its enhanced thermo-physical properties. One such composite PCM has been discussed by Wang and Liu [11], where composite of PEG and HAP has been used for investigations. There DSC results showed that the composite melted at 58.2 °C with an enthalpy of 128.9KJ/Kg and solidified at 46.9 °C with enthalpy of 109.2KJ/Kg. They concluded that the composite offered good thermal transition capacity with a thermal conductivity of 0.162W/mK and even with 200 thermal cycles there was no significant change recorded in the properties of the composite.

A review by Jaguemont et al. [12] established the facts more profoundly that how phase change materials can be used for thermal management in automobiles and how they are a better choice than conventional choice of cooling methods. Since forced air cooling and liquid air cooling is more complex and bulky, it is a viable option to use PCMs for thermal management in automobiles. Such research to employ a cooling array system for vehicles has been conducted by Ren at al. [13]. Madruga et al. [14] carried an experimental and numerical study, where the authors compared their experimental and numerical simulation results of melting phenomenon in a cubical enclosure, heated at 80°C from the bottom using tetracosane as the PCM. A similar study was carried out by David et al. [15], where they investigated the natural convection near a wall containing PCM. They examined the complexities of the flow interactions between the wall and the natural convection boundary layer. They also established that convective heat transfer doesn’t depend upon ambient temperature growth rate. The effectiveness of a CFD simulation for PCMs to predict their performance was studied by Gowreesunker [16] and found that their model predicted a reduction in peak temperature by 3K which was in accordance with the experimental results. Bondareva and Sheremet [17] have numerically simulated the natural convection of PCM in a square cavity with a heat source mounted at the bottom wall. The evolution of temperature fields and streamlines were examined by them.

The presented brief literature review of buoyancy driven melting of PCMs evidently show lack of a comparative study for different PCMs inside an enclosure, which would help in understanding the flow physics inside an enclosure. Such elemental study can be profound in designing efficient cooling systems for electronic devices. Hence, in the present study we investigate the flow physics of three different PCMs in a square enclosure whose Prandtl number range from 0.433 to 118 and Stefan number from 2.65 to 13.19. Based on the literature survey presented above and authors’ knowledge, the comparative study for three different phase change materials inside an enclosure with a heated source is introduced for the first time.
2. Methodology

![Cavity with boundary conditions](image)

Figure 1. Cavity with boundary conditions (Front view).

The square enclosure with adiabatic walls is assumed to be filled with PCM (n-Octadecane, PEG (900), Paraffin (RT60)). The boundary conditions have been represented in Figure 1. The material for the heat source is considered as silicon at 330K [13]. The melted material is supposed to be a viscous Newtonian fluid, satisfying the Reynolds averaged Navier-stokes equation (RANS) with Lambremhorst $k-\varepsilon$ turbulence model for a two dimensional analysis.

The system of energy transfer and momentum is described by the system of unsteady two-dimensional Boussinesq-Oberbeck equations as followed below [17, 18, 19].

\[
\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0
\]  \hspace{1cm} (1)

\[
\rho_m \left( \frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} \right) = -\frac{\partial p}{\partial x} + \mu_m \left( \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right)
\] \hspace{1cm} (2)

\[\rho_m \left( \frac{\partial v}{\partial t} + u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} \right) = -\frac{\partial p}{\partial y} + \mu_m \left( \frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} \right) + (\rho \beta)_{m} g (T - T_p)
\] \hspace{1cm} (3)

$\rho_m$ is the density of the phase change material and $u$ and $v$ are the velocities in x and y direction respectively. $\mu_m$ is the viscosity of the phase change material at the melting phase.

\[
\frac{\partial h}{\partial t} + u \frac{\partial h}{\partial x} + v \frac{\partial h}{\partial y} = k_m \left( \frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \right)
\] \hspace{1cm} (4)

\[
\frac{\partial h}{\partial t} = k_s \left( \frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \right)
\] \hspace{1cm} (5)

\[\rho c_h \frac{\partial T}{\partial t} = k_h \left( \frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \right) + Q
\] \hspace{1cm} (6)
and are the thermal conductivity of the melt (liquid PCMs), solid PCMs and heat source material.

The thermo-physical properties of the Phase Change Materials used has been specified in Table 1. Where \( \mu \) is the viscosity and \( T_m \) is the melting temperature.

| PCM         | Density(Kgm\(^{-3}\)) | \( \mu \)(Kgm\(^{-1}\)s\(^{-1}\)) | \( T_m \)(K) | Prandtl No. | Stefan No. | Thermal conductivity (W/mK) |
|-------------|------------------------|-----------------------------------|---------------|-------------|------------|----------------------------|
| n-Octadecane| 746                    | 1.81                              | 301.35        | 48.36       | 3.84       | 0.153                     |
| PEG(900)    | 1100                   | 9.9                               | 305           | 118         | 2.65       | 0.188                     |
| Paraffin(RT60)| 770                   | 3.75                              | 326.15        | 0.433       | 13.19      | 0.2                       |

### 3. Result and Discussion

In this paper we have discussed the effects of convective heat transfer for different phase change materials. Calculations are performed for three different phase change materials inside a square enclosure, heated by a source at the bottom wall. The temperature contours, streamlines, velocity at different sections and temperature change with time has been discussed in this study.
In Figure 2. and Figure 3, the temperature contours and the stream functions of the PCMs (n-Octadecane, PEG (900) and Paraffin (RT60)) has been shown at \(T=15\) seconds and 35 seconds. While in Fig.2 the conductive regime is evidently dominant for n-Octadecane, PEG (900) and Paraffin (RT60). In Fig.3 the convective plumes for n-Octadecane and PEG (900) are evidently visible. While the plumes are more developed in n-Octadecane than PEG (900) indicating that n-Octadecane reaches the melting phase before PEG (900). The plumes can be observed developing vertically upwards from the source. The stream functions are symmetric and more concentric at \(T=25\).
In Figure 4, a narrow region is formed in the domain just above the heat source in n-Octadecane and PEG (900). Due to the weak buoyancy forces the convective plume rises. It is also observed that the convective plume reaches the top wall faster than the side walls in all the three phase change materials. Plumes in n-Octadecane rise faster than PEG (900) indicating a higher melting rate. The plumes can also be observed to have merged and then rising upwards from the heat source. The streamlines are observed to be symmetric along a central axis, while the temperature distribution is asymmetric.
In Figure 5, the velocity profile for the phase change materials has been shown at $\mathcal{T} = 25$ and $\mathcal{T} = 35$. It is observed that the maximum velocity for the convective regime in PEG (900) increases by 23.92%. A gradual change is observed for n-Octadecane as the maximum velocity decreases by 19.08%. A decrease of 20.3% is observed in the case of Paraffin (RT60). At $\mathcal{T} = 25$, the velocities of n-Octadecane and Paraffin (RT60) were 71.5% and 112% higher than the maximum velocity of PEG (900). At $\mathcal{T} = 35$, the maximum velocity of n-Octadecane was 22.76% higher than that of PEG (900), while maximum velocity of Paraffin (RT60) was 36.17% higher. The high velocities illustrate that the convective plumes reaches faster for n-Octadecane than PEG (900).

In the Figure 6, the temperature profile for all the three phase change materials is shown. The stable phase change starts around 3 minutes for n-Octadecane and PEG (900), both the materials attain the phase change at almost same times but at different temperatures. As the Steffan’s number for n-Octadecane is higher than that of PEG (900), n-Octadecane starts melting slightly before PEG (900).
While the Stefan’s number for Paraffin (RT60) is the highest with the highest melting point, the phase change occurs later in time. This illustrates that for higher Stefan numbers, more time is consumed in melting.

4. Conclusion
The buoyancy driven convection heat transfer characteristics of three different phase change materials inside a square enclosure with internal heat source mounted at the bottom surface are numerically investigated. The turbulent flow is modeled by the computational fluid dynamics (CFD) approach using Lambrechtsen k-ε turbulence model and the governing equations are discretized using finite difference method. The temperature contours and streamline functions are analysed, while a comparative study is established for velocities at $\Upsilon = 15$, $\Upsilon = 25$, and $\Upsilon = 35$. The velocities at $\gamma=0.5$ cross-section is also analysed, where the maximum velocities of all the three phase change materials at $\Upsilon = 25$ and $\Upsilon = 35$ is compared. The highest velocities are observed for Paraffin (RT60) which has the highest Stefan’s number and the lowest Prandtl number. Finally the temperature profiles for all three phase change materials has been shown which indicates the time at which the melting starts and the durations of phase change for a material. This also illustrates that for a higher Stefan number more time is consumed in melting, as it was observed for Paraffin (RT60). A phase change material can be selected on the basis of its Stefan’s number for conditioning temperatures in electronic devices. The results from the present study will be suitable for selecting suitable Phase change materials for designing effective thermal management systems of electronic devices.

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