Numerical Simulation of Thermal Process in a Phase Change Material Exposed to Solar Heating in a Tropical Region

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Abstract. The capacity for phase change material (PCM) to absorb and release latent heat has led to its applications in heating/cooling strategies in solar heating systems, air-conditioning system, electronics cooling and food preservation. The use of PCM in building construction through micro/macro-encapsulation to passively cool/heat a living space has attracted a lot of experimental and simulation research work, especially after the turmoil caused due to worldwide energy crises. In this paper, the thermal behaviour of a PCM exposed to solar heating in a tropical climate is studied numerically over a 24-hour period using the ANSYS fluent Software. A grid dependency test is initially devised to establish the most appropriate grid sizes and time steps to be used for the subsequent simulations with acceptable accuracy. PCM is setup to be in contact with one side of a concrete block. The other side of the concrete is exposed directly to a typical daily solar radiation profile of a tropical region. Results, in terms of temperature distribution and liquid fraction, show that a two-layer of a commercially available PCM is sufficient to flatten the temperature fluctuations arising from solar heating in the tropical regions.

1. Introduction

Phase change materials (PCMs) are substances that can absorb thermal energy from the environment or release heat to the surroundings to reduce indoor temperature swings and consequently improve indoor thermal comfort at lower energy costs [1]. Numerical analysis is often employed to understand the physics of the phase change process under different working conditions since devising an experimental setup is costly and time consuming. Chauhan & Yadav [2] have numerically studied the effect of applying a constant heat flux of 2500 W/m² to a rectangular domain, filled with paraffin wax as PCM, in ANSYS Fluent. This paper extends the simulation work of [2], using the Discrete-Ordinates method, to incorporate a typical daily solar radiation profile in the tropical region that would heat up a concrete block. The effect of placing several layers of commercially available PCM plates in between the concrete block and the living space is then determined.

The main contributions are as follows: A simple procedure for the selection of the grid discretization sizes, taking into consideration the trade-off between computational speed and accuracy, is proposed. The model results are validated with experimental data carried out in [3]. The phase change process within a PCM subjected to tropical solar heating is visualised and the effect of increasing the number of PCM layers on the temperature is studied. This enables the determination of the optimal number of PCM plates required in a building construction to flatten the temperature fluctuations.
2. Materials and methods

2.1. The model studied
Figure 1(a) shows the schematic layout of a concrete block which is directly exposed to horizontal solar irradiance on the left surface and connected to the PCM on the right surface. The top and bottom surfaces are treated as adiabatic (no heat flux). Therefore, a two-dimensional model is employed as the effects of gravity along the vertical axis can be considered. A natural convection boundary condition is imposed on the right side of the PCM with a free stream initial temperature of 20 °C. The thermal parameters of the concrete block are: density is 2000 kg/m³, specific heat capacity of 920 J/(kg °C) and a heat transfer coefficient of 2.46 W/(m² °C). Table 1 lists the thermal properties of the PCM used, which is the SP25E2 from Rubitherm AG, Germany. This PCM is commercially [4] available in packed aluminium plates of dimensions 450 mm × 300 mm and thickness 15 mm as shown in figure 1(b).

![Figure 1.](image)

Figure 1. (a) Schematic layout example consisting of a concrete block and three PCM plates. (b) Phase change materials plate available commercially from Rubitherm AG, Germany [4].

| Parameters                        | Notation | SP25E2 [4] | Calcium Chloride Hexahydrate [3] |
|-----------------------------------|----------|------------|---------------------------------|
| Melting Temperature               | \( T_m [{}^\circ C] \) | 24 – 26    | 29.9                            |
| Liquid Specific Heat Capacity     | \( C_{p,l} [kJ/kg{}^\circ C] \) | 2          | 2.2                             |
| Solid Specific Heat Capacity      | \( C_{p,s} [kJ/kg{}^\circ C] \) | 2          | 1.4                             |
| Liquid Thermal Conductivity       | \( \kappa_L [kJ/ms{}^\circ C] \) | 0.5        | 0.53                            |
| Solid Thermal Conductivity        | \( \kappa_S [kJ/ms{}^\circ C] \) | 0.5        | 1.09                            |
| Liquid Density                    | \( \rho_L [kg/m^3] \)         | 1400       | 1530                            |
| Solid Density                     | \( \rho_S [kg/m^3] \)         | 1500       | 1710                            |
| Latent Heat                       | \( L [kJ/kg] \)               | 180        | 187                             |
| Dynamic Viscosity                 | \( \mu [kg/ms] \)             | \( 8\times10^{-2} \) | \( 1.21\times10^{-3} \)          |
Figure 2. Plot of average solar global horizontal irradiance on 14 September 2021 in Vacoas [5].

An average of the global horizontal solar irradiance shown in figure 2 has been utilized [5]. This data was measured over a whole day-period on the 14th September 2021 for Vacoas, a small tropical town located on the high lands of the island of Mauritius. Sunrise was at 05:45 and sunset at 18:00.

2.2. The governing equations
The mathematical equations which are solved numerically by ANSYS to simulate the heat and mass transfer in the model studies are the energy, momentum and mass (continuity) conservation given in [6].

The energy equation is given by
\[
\frac{\partial \rho H}{\partial t} + \nabla \cdot (\rho \vec{v} H) = \nabla \cdot [\kappa (\nabla T)] + S,
\]
where \( S \) is a heat source term, \( \vec{v} \) is a velocity vector, \( \rho \) is the density and \( T \) denotes the temperature. The enthalpy, \( H \), is calculated by:
\[
H = h_{\text{ref}} + C_p \frac{dT}{ds} + \beta L.
\]
Here, \( h_{\text{ref}} \) is the reference enthalpy, \( L \) is the latent heat, \( C_p \) is the heat capacity and \( \beta \), which represents the liquid fraction, can be obtained from:
\[
\beta = \frac{T - T_{\text{solidus}}}{T_{\text{liquidus}} - T_{\text{solidus}}}, \quad \beta \in [0,1].
\]

The continuity equation is:
\[
\frac{\partial \rho}{\partial t} + \frac{\partial \rho \vec{u}_i}{\partial t} = 0, \quad i, j = x, y, z,
\]
and using the velocity vector \( \vec{u}_i \) and source term \( S_i \) along coordinate \( i \), as well as the pressure \( P \), the momentum equation can be written as:
\[
\frac{\partial \rho \vec{u}_i}{\partial t} + \frac{\partial \rho \vec{u}_i u_j}{\partial i} = \mu \frac{\partial^2 \vec{u}_i}{\partial \vec{e}_j} - \frac{\partial P}{\partial i} + A_C \vec{u}_i + S_i,
\]
ANSYS solves the above governing equations using the finite volume method. The porosity term,\n\[
A_C = -\frac{A_{mush}(1 - \beta)^2}{\beta^3 + \epsilon},
\]
with \( \epsilon \) being a computational constant (1×10^{-3}), used to avoid division by zero, contains the mushy zone constant \( A_{mush} \). The default value for the latter is set as 10^{5} in ANSYS but can be modified as discussed in [6]. It is to be noted that \( A_C \) becomes zero in the fully liquid phase as \( \beta = 1 \).
2.3. A procedure for determination of Mesh Grid Sizes in ANSYS Fluent

The spatial and temporal grid sizes are determined using a 2-D Meshing of a 300 mm high and 15 mm thick rectangular PCM container for stability and accuracy. The solution at the coordinate locations of three equally spaced points are considered. The three points are placed at a horizontal distance of 7.5 mm away from the origin and are vertically located at 75 mm, 150 mm, and 225 mm respectively. The temperature variations in the PCM plate can be compared using the algorithm described below:

**Step 1** A minimum spatial grid size $\Delta x = \Delta y$, of 1 mm, is selected. This choice is motivated by the fact that a grid size which is too small will lead to a high computational burden whilst a grid size which is chosen too large will lead to inaccurate numerical results.

**Step 2** The time step is then varied, $\Delta t \in [0.05, 0.1, 0.25, 0.5, 1, 2]$ seconds, and the simulation is performed over 1 hour.

**Step 3** Taking the referenced temperature and referenced liquid fraction after 1 hour for the most refined grid choice, that is for $\Delta t = 0.05$ seconds, the relative difference of the remaining solutions for the other time steps is calculated with respect to the referenced values.

**Step 4** The maximum percentage relative difference of the temperature and liquid fraction at the three locations are plotted on the y-axis and the different time steps on the x-axis.

**Step 5** The optimal time step is selected as the maximum time step such that maximum percentage relative difference is within an acceptable tolerance.

The Percentage Relative Difference (PRD) is calculated as

$$\text{PRD} = \frac{\text{Compared Solution} - \text{Referenced Solution}}{\text{Referenced Solution}} \times 100\%.$$  

From figure 3(a), it can be observed that compared to the reference values for temperature and liquid fraction for $\Delta t = 0.1$ second, the PRD is quite small for time step sizes up to 1 second. The maximum PRD over the three measured points was less than 0.1%. However, for $\Delta t = 2$ seconds, the PRD is seen to increase significantly for both the temperature and liquid fraction such that $\Delta t = 1$ second is optimal.

Next, using $\Delta t = 1$ second, the spatial grid size $\Delta x = \Delta y \in [1.5\text{mm}, 3\text{mm}, 5\text{mm}]$ are considered to obtain an integer number of grid points, of equal lengths, over the whole computational domain. Here, the case $\Delta x = \Delta y = 1$ mm is the referenced solution. It can be seen from figure 3(b) that both the temperature and liquid fraction values deviate significantly from this referenced solution when the spatial sizes are greater than 1.5 mm. Although the temperature solution would remain accurate to the nearest degree Celsius for spatial steps of 1.5 mm, the liquid fraction was 3% less at the centre showing some discrepancy in the computational results. The solutions have also been compared to those of a more refined grid by taking $\Delta t = 0.1$ second and $\Delta x = \Delta y = 0.5$ mm. The differences in the solutions were not significant enough compared to the increase in the computational burden of such a refined grid. As such, it is concluded that choosing $\Delta t = 1$ second and $\Delta x = \Delta y = 1$ mm is appropriate.

![Figure 3](image-url)

**Figure 3.** Percentage relative difference for temperature and liquid fraction solutions for varying time step sizes for $\Delta x = \Delta y = 1$ mm.
2.4. Verification of numerical results with experimental data

The test case of Zivkovic & Fujii [3] which consists of a rectangular test container depicted in figure 4(a) with \( l = b = 100 \text{mm} \) and \( \delta = 20 \text{mm} \), filled with calcium chloride hexahydrate, is considered. The thermo physical properties of this PCM are listed in table 1. The lateral sides of the container are insulated with polystyrene. The temperature in the middle of the container is measured with time. The PCM, initially at 17.5 °C, is immersed in a constant temperature bath maintained at \( T = 60 \text{ °C} \). The convective heat transfer coefficient of the material used to make the container is 16 W/(m² °C). The 3-D mathematical model in section 2.2 with the grid sizes determined in section 2.3 are used to build the geometry of the domain as shown in figure 4(a). The computed temporal evolution of temperature at the centre of the PCM is shown in figure 4(b). This transient simulation is performed over 120 minutes and the numerical results obtained are seen to agree well with the observed experimental data in [3].

3. Results, analysis and discussion

The contour plots of temperature and liquid fraction for the simulation model in section 2.1, over twelve hours and twenty-four hours after sunrise, are shown in figure 5. It is seen that the PCM layers absorb a significant part of the solar heat preventing the right wall from radiating outside heat indoors. It is also seen from figure 5(c) that half of the PCM layers have melted after twelve hours and from figure 5(d), it is to be noted that almost all the PCMs have turned to the liquid state after twenty-four hours.

![Figure 4](image1.png)

(a) Numerical simulation of PCM in rectangular container (a), experimentally validated (b).

![Figure 5](image2.png)

(a) Temperature contours after (a) 12 Hours (b) 24 Hours and liquid fraction after (c) 12 Hours and (d) 24 Hours of simulation for a three PCM plates setup.
This is seen to occur in figure 6 after approximately 4 hours, 13 hours and 16 hours for a one-layer, two-layer and a three-layer PCM setups, respectively. This would correspond roughly to a clock time of 10:00, 19:00 and 22:00, respectively. The daily average temperature of the right wall for the one-, two-, and three-layer PCMs are 38.91 °C, 27.70 °C and 24.62 °C, respectively. This shows a 28.79% decrease for the two-layer PCM and a 36.71% decrease for the three-layer PCM in the relative temperature compared to the one-layer PCM. Considering the cost and space implications of a three-layer PCMs in a building construction, it can be deduced that a two-layer PCM would be optimal to flatten the temperature fluctuations due to tropical solar heating. Moreover, it is noted that the temperature of the right wall of the multi-layered PCM would start rising only after sunset such that free night air cooling to regenerate the PCM could be very promising, especially because the outside air temperature at night is lower than the air temperature during the day.

4. Conclusion
In this work, the numerical simulation of heat and mass transfer through a PCM exposed to solar heating in a tropical climate was performed using ANSYS fluent. A procedure for determining the most effective grid size and time step was proposed. The numerical model was then validated with an experimental work in literature and used to study the temperature distribution and the phase changes during the heating process. Finally, the optimal number of PCM plates required to flatten the temperature fluctuations due to the tropical solar heating was determined.

A 3-D model can be studied in a future work for a more accurate prediction of the temperature profile. A comparison about the thermal performance of several other commercially available PCMs can also be done to choose the best performing PCM in the tropical regions. Also, further investigation is required to determine the passive night cooling effect.

5. References
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