

Numerical study on melting process of Phase Change Material as thermal energy storage

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Abstract. The use of phase change material (PCM) as thermal energy storage is increasingly in demand. This is because PCM has high storage capacity. Thermal energy can be stored, not only as sensible heat, but also in the form of latent heat. A model for investigating the melting process of paraffin wax which is used as thermal energy storage, was developed in the ANSYS FLUENT simulation software environment, then the results were analyzed and compared with the results of previous experiments. The simulation results show that the melting process occurs relatively faster than the melting process in the actual experiment, due to the construction of the paraffin wax container. Also due to the construction of a cube-shaped paraffin wax container, paraffin wax remains in the lower right corner of the container. The effect of placing thermocouples in paraffin wax container, which when compared to the relatively small size of the container, can be significant. This certainly needs further investigation. The choice of heat source and how to keep its temperature constant in experiment need also to be investigated further. Based on the results obtained through this study, the use of PCM as cold storage in solar photovoltaic air conditioning system is worth considering, as thermal backup or even to substitute the battery storage system that has been used all this time.

1. Introduction

One of the biggest energy users in the building is the air conditioning system. The portion of energy use for the system can reach 60% of the total energy use in buildings[1]. The use of phase change material (PCM) in buildings has been in the spotlight, because PCM can be used as thermal energy storage, so that it can reduce conventional energy use and at the same time reduce greenhouse gases emission which is the cause of global warming.

PCM as thermal energy storage has advantages, because energy can be stored not only as sensible heat, but also as latent heat. This causes PCM to be known as material that has high storage capacity[2]. The use of PCM can be found in many applications, especially in buildings.

This study was conducted to assess numerically what had been done experimentally by Ambarita, H., et al. [3], who investigated the melting and solidification of phase change material as thermal energy storage to reduce electrical heater energy in solar water heater system.

In this study, a model was developed in ANSYS FLUENT simulation software based on what had been done in previous experiments by Ambarita, H., et al. [3], but restricted only to the melting process of paraffin wax. The results of the simulation were then compared with

the experimental results. Unlike the results of previous experiments, which was to support the study of the use of PCM on solar water heater, the information obtained through this study aims to explore the possibility of using PCM as cold storage in solar photovoltaic air conditioning system, as thermal backup or even to substitute the battery storage system completely.

2. Methods

This study was conducted to assess numerically what had been done experimentally by Ambarita, H., et al. [3] as shown in figure 1. Three glass chambers each with the size of 10 cm x 10 cm x 10 cm with glass thickness of 2 mm, were used sequentially from left to right as hot water container, PCM container and cold water container. The hot water container was used as heat source, which would cause heat flow to the cold container through the PCM container. The heat through PCM was used by PCM to transform into liquid. The hot water container was kept at a temperature of 90°C with an electric heating element that operates with a $\pm 2^\circ\text{C}$ hysteresis loop, while the temperature of the coldwater container was maintained at 27°C by using water from the hydrant. The three containers were then isolated with 2 mm thick aluminium plate, except for the front side of the PCM container, which was used to observe the melting process of PCM using a camera. The temperature of PCM was measured using nine thermocouples mounted inside the PCM container. PCMs studied in the experiment were paraffin wax and stearic acid, but for this study only the melting process of paraffin wax would be simulated.

2.1. Model Description

Figure 2 shows the simulated area which is the PCM container. This study concerned only the melting process of paraffin wax. The size of the area to be simulated is 10 cm x 10 cm, where the top and the bottom part of the chamber are isolated, the left side of the chamber is the high temperature part, and the right side is the low temperature part. Because of the symmetry from the area to be simulated and its relatively small size, which is considered that there is no significant change in the direction of the z axis, the simulation was carried out in 2D simulation. Paraffin wax properties were taken from the table listed in [3] and shown in table 1.

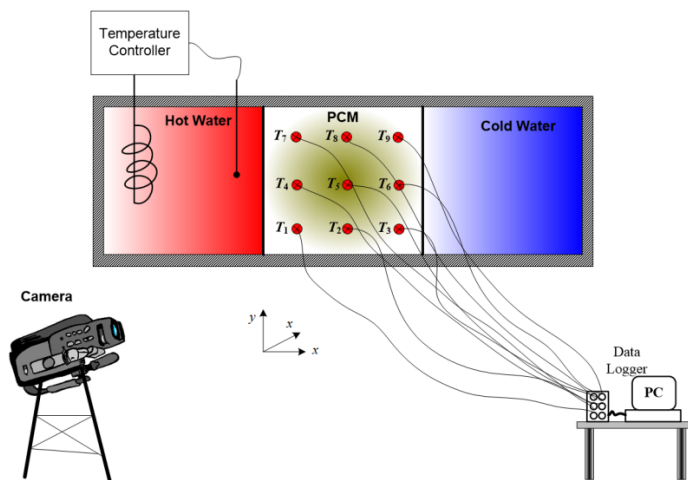


Figure 1. The experimental setup to study the melting and solidification of PCM as thermal energy storage[3].

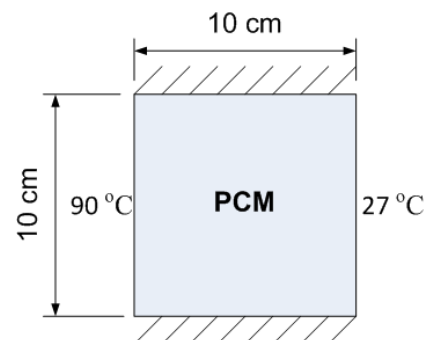


Figure 2. The model of the middle chamber containing PCM which would be simulated.

2.2. Model Usage and Limitation

The models that were activated in ANSYS FLUENT for this simulation are multiphase - volume of fluid, energy, viscous - laminar, and solidification and melting model. Solidification/melting model in ANSYS FLUENT has some limitation. It can be used only with the pressure-based solver. It cannot be used for compressible flows and only the VOF (volume of fluid) model can be used with it [5].

Solidification/melting model in ANSYS FLUENT does not track the liquid-solid front explicitly, as a substitute it uses an enthalpy-porosity formulation. The model treats the liquid-solid mushy zone as a porous zone with porosity equal to the liquid fraction.

Table 1. Thermo-physical properties of the paraffin wax.

Properties	Paraffin wax[4]
Melting temperature (°C)	59.8
Latent heat (kJ/kg)	190
Density (kg/m ³) when it is:	
Solid	910
Liquid	790
Specific heat (kJ/(kg °C)) when it is:	
Solid	2.0
Liquid	2.15
Thermal conductivity (W/m·K) when it is:	
Solid	0.24
Liquid	0.22

2.3. Data Input for the Model

The simulated model was drawn and then meshed and simulated in the ANSYS FLUENT program. Paraffin wax data that needed to be filled in ANSYS Fluent are density, specific heat, thermal conductivity, dynamic viscosity, molecular weight, standard state enthalpy, reference temperature, pure solvent melting heat, solidus temperature, and liquidus temperature.

Data regarding density, specific heat and thermal conductivity are assumed to be piecewise linear. Some of the required data above are not available in table 1 so that they were taken from other sources. Data on liquidus temperature was taken from melting temperature in table 1, while solidus temperature was taken from [6] which is 37°C (310.15 K). Data for dynamic viscosity as measured by Anton Paar viscometer for paraffin wax with a melting temperature of around 60°C is 6.89 mPa.s or 6.89×10^{-3} kg/m.s. Paraffin wax which is commonly found is paraffin wax with the molecular formula C₃₁H₆₄ with molecular weight 436 g/mol. The standard state enthalpy was calculated using equation (1) which was presented by Prosen, E.J., Rossini, F.D.[7], where the value is a function of the number of carbon atoms n contained in paraffin wax as follows:

$$\Delta H_f^\circ = -10.887 - 6.106n \pm \sqrt{0.1654 - 0.03898n + 0.002903n^2} \quad (1)$$

By ignoring the tolerance term and after being converted from kcal/mol to J/kmol, the value of the standard state enthalpy is -8.375×10^8 J/kmol at reference temperature of 25°C.

2.4. Equation to be Solved

The equation involved in this simulation is first and foremost the equation to calculate the enthalpy of paraffin wax. The enthalpy of paraffin wax (H) is the sum of its sensible heat (h) and its latent heat content (ΔH) according to equation(2) below:

$$H = h + \Delta H \quad (2)$$

where the value of h itself is obtained from the equation (3):

$$h = h_{ref} + \int_{T_{ref}}^T c_p dT \quad (3)$$

where h_{ref} is reference enthalpy, T_{ref} is reference temperature, and c_p is specific heat at constant pressure.

The liquid fraction (β) is defined as in equation (4)

$$\begin{aligned} \beta &= 0 & \text{if } T < T_{solidus} \\ \beta &= 1 & \text{if } T > T_{liquidus} \\ \beta &= \frac{T - T_{solidus}}{T_{liquidus} - T_{solidus}} & \text{if } T_{solidus} < T < T_{liquidus} \end{aligned} \quad (4)$$

The latent heat content is then written as the function of the liquid fraction as in equation (5), so that its value can be deviated between zero (if the paraffin wax is in solid form) and the latent heat of the paraffin wax L (if the paraffin wax is in liquid form).

$$\Delta H = \beta L \quad (5)$$

The following equation (6) is the energy equation applied for the melting simulation of paraffin wax.

$$\frac{\partial}{\partial t}(\rho H) + \nabla \cdot (\rho \vec{v} H) = \nabla \cdot (k \nabla T) + S \quad (6)$$

Where H is the enthalpy from equation (2), ρ is the density of the paraffin wax, \vec{v} is the fluid velocity, and S is the source term.

Enthalpy-porosity procedure treats mushy zone as a porous material with porosity from each cell is the same as the liquid fraction. For regions that are all solid, the porosity is zero and the velocity (\vec{v}) of paraffin wax is zero, which also means the momentum is zero. Equation (7) is used to calculate reduced momentum in the area of the mushy zone.

$$S = \frac{(1 - \beta)^2}{(\beta^3 + \varepsilon)} A_{mush} (\vec{v} - \vec{v}_p) \quad (7)$$

Where β is the liquid fraction, A_{mush} is the mushy zone constant, \vec{v} is the velocity of paraffin wax in the simulation zone, \vec{v}_p is the pull velocity (if there is paraffin wax being pulled out of the simulation zone, here is zero), and ε is a small number (0.001) to avert division by zero.

3. Results and Discussion

Simulation must be carried out with a small time step size (0.1 s) to obtain convergent results, whereas to observe the melting process of paraffin wax the overall simulation needs to be run with a large time value. Based on [3] it took up to 600 minutes (10 hours) until the whole paraffin wax melted. This causes the time needed to run the entire simulation was relatively

long. Figure 3 shows the simulation results in the form of liquid fraction from 0 minute to 600 minute. The standard color code in ANSYS FLUENT report is according to color sequences, where longest wavelength color (here orange color) is where the most liquid part and shortest wavelength color (here blue color) is the solid part of the paraffin wax. Figure 3 also shows the mushy zone of the paraffin wax, which is stretch from light green color to light blue color part. These results were then compared with the experimental results reported in [3].

In figure 3, the simulation results show a melting process that was slightly faster than the experimental results. This can occur considering that the front part of the paraffin wax container is intentionally not isolated because the observation of the experiment was carried out using a camera.

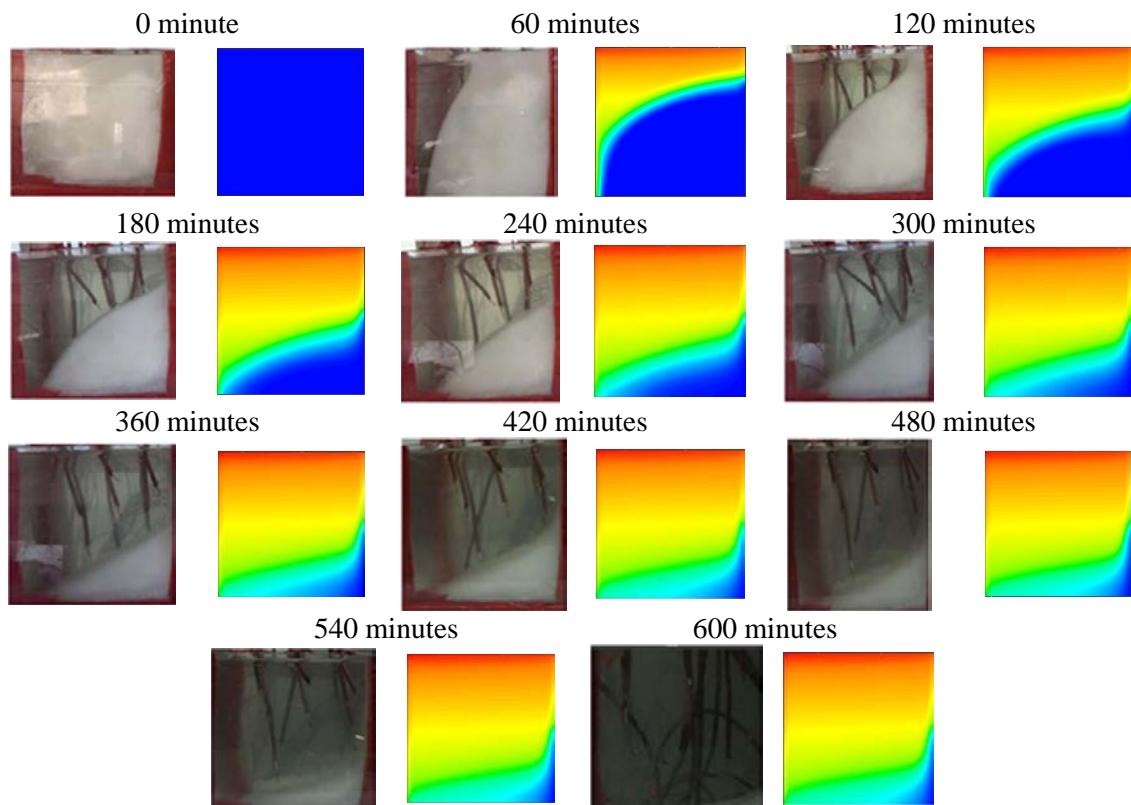


Figure 3. Comparison of the paraffin wax liquid fraction from the experimental results [3] with the simulation results.

This caused heat was transferred through the front side of the container to the environment where the experiment was carried out. This of course would slow down the melting process of paraffin wax, because the heat that was supposed to be used to melt paraffin wax, lost to the environment. This is particularly obvious in the early stages of the experiment, because at the beginning of the simulation, heat could only be transferred through conduction, because at that time paraffin wax was entirely solid. This results in the heat that should be transferred from the left side of the container, which is the heat source, to the right side of the container, which is the cold side, was transferred partially towards the front side of the paraffin wax container.

Figure 4 shows the velocity vectors for the 180 minutes, 360 minutes, and 600 minutes real time step of the simulation. As with the experimental results, the simulation results also show

that after 10 hours there is still a small amount of paraffin wax left in the lower right corner of the chamber. Paraffin wax, which has mostly melted at that time, would circulate in the container due to the natural convection as shown in figure 4. The scale used here is also according to color sequences, where longest wavelength color (here orange color) is where the most liquid part with the highest speed (7.73×10^{-4} m/s) and shortest wavelength color (here blue color) is the solid part of the paraffin wax with zero speed. Because the heat source came from the left side of the simulation zone, the temperature of paraffin wax in the left side increased and its density decreased. The relatively hotter and lighter paraffin wax rised to the upper left part of the zone and circulated clockwise. When it reached the upper right end of the zone, the temperature decreased and the density increased. The relatively colder and heavier paraffin wax than sinked towards the bottom of the zone, but when it encountered the mushy zone, its momentum dropped rapidly because the brake effect of the mushy zone. That is why the circulation slowed down before it reached the bottom and then moved to the left part of the simulation zone to continue the next cycle of the natural convective circulation. As we can see in figure 4, the mushy zone, which is stretch from light green color to light blue color part, grew bigger as time flew. This increased the momentum sink effect. That is why after 10 hours and more has passed, there is still paraffin wax left in the lower right corner of the simulation zone.

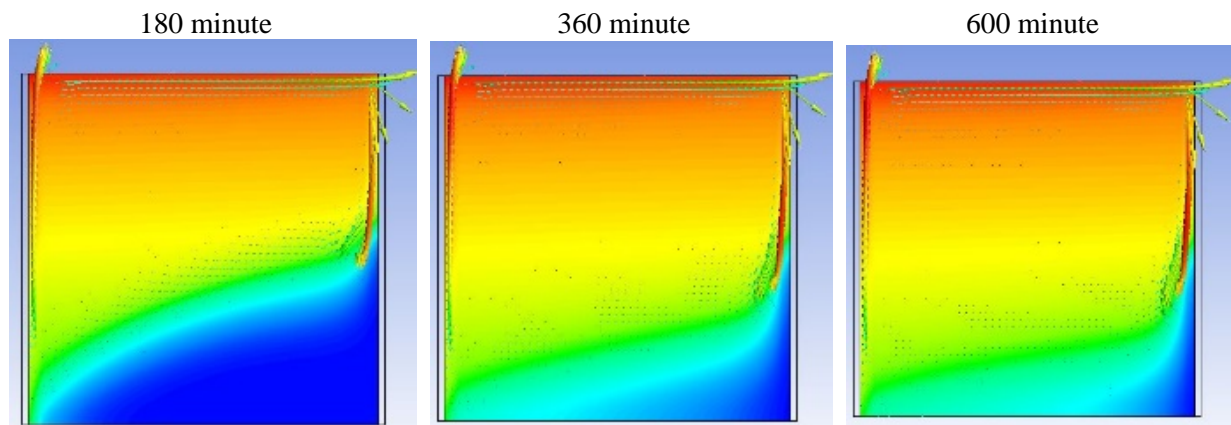


Figure 4. The velocity vector inside the liquid form of the paraffin wax which was resulted from the natural convection occurring in the liquid zone.

Can also be seen in Figure 3, besides paraffin wax, there are also conductor cables from thermocouples which were used to measure paraffin temperatures in various positions. According to the data available at [3], there were nine thermocouples attached to the paraffin container. Because of the relatively small size container (10 cm x 10 cm x 10 cm), the effect of placing the thermocouples could be significant. The effect of the installation of the thermocouples certainly not only affects the heat transfer process, but also the flow that occurs in natural convection events in the liquid part of paraffin wax.

Furthermore, the heat source in the experiment was held at a constant temperature of 90°C by using $\pm 2^\circ\text{C}$ hysteresis loop. This means that in reality the temperature is not constant, but oscillates between 88°C and 92°C. This of course will affect the heat entering the paraffin wax container. Additionally the heat source which temperature was kept constant was water. Regarding the placement of the heating element which was only in one position in the heat source container, the water would also experience natural convection so it needed to be an interval until the temperature can be uniformly constant at 90°C.

4. Conclusions

A model for investigating the melting process of paraffin wax which is used as thermal energy storage, was developed in the ANSYS FLUENT simulation software environment, and then carried out and the results were reviewed by comparing them with the results of previous experiments.

The conclusions that can be drawn from this study are:

- The melting of paraffin wax in the simulation happened relatively faster than in the actual experiment, due to the construction of the paraffin wax container, which required that the front part of the container not to be isolated for the purpose of data collection.
- As a result of the cube-shaped container, paraffin wax remains in the lower right corner of the container.
- The effect of placing thermocouples in paraffin wax container, which when compared to the relatively small size of the container, can be significant. This certainly needs further investigation.
- The choice of heat source and how to keep the temperature constant also need to be investigated further.

By looking at these results, the use of PCM as cold storage in solar photovoltaic air conditioning system is worth considering, as a backup or even as a replacement for the battery storage system that has been used so far.

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