Energy storage using NaOH phase change material for solar thermal application at constant heat flux

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Abstract. There is a mismatch between energy demand by consumers and supply from the sun. Therefore, we store Solar Energy in the phase change material (PCM) for storage energy. We used medium temperature range salt, Sodium hydroxide (NaOH), melting temperature at 591 K and heat of fusion 160 kJ/kg. We did the numerical simulation using COMSOL Multiphysics®, we kept radially variable surface flux at the bottom of the container. Linearly variable flux at the centre is 78 kW/m² and 18 kW/m² at the periphery. For numerical analysis, we used 3D enthalpy based model. We found that the bulk temperature of NaOH reaches about 800 K after 6 hours and total energy stored by the PCM is about 21 MJ. This amount of energy is very useful for domestic and small industrial process.

Keywords: Heat flux, Phase change material, Enthalpy based model, Numerical simulation.

1. Introduction

Solar energy has the potential to meet the energy requirements of domestic and industrial processes, but there is a time mismatch between solar energy supply and energy demand by the process. In this case, thermal energy storage allows the use of solar energy without the presence of solar radiation. Application of solar thermal energy with the industrial process will eliminate CO₂ emissions and fossil fuel consumption. However, the industry has problems to use solar energy due to ample space requirement. Phase change material (PCM) can resolve this issue and can supply heat energy at a constant rate for different thermal applications. Work reported on PCM heat storage by various authors is listed in table 1.
Table 1. Summary of work done on latent heat storage by various authors.

| Methods                         | Procedure                | Reference |
|---------------------------------|--------------------------|-----------|
| 1D enthalpy                     | Gauss-Seidel/Experimental | [1]       |
| 1D and 2D enthalpy              | Analytical               | [2]       |
| 2D fixed-grid enthalpy          | Finite volume approach   | [3]       |
| 2D fixed-grid enthalpy          | Gauss-Seidel iteration   | [4]       |
| -                               | Experimental             | [5]       |
| Review                          | -                        | [6]       |
| -                               | Experimental             | [7]       |

There are many PCM available for thermal applications but among all the PCM, NaOH is medium-temperature range PCM having cost-effective, and good heat storage capacity. Therefore, NaOH is chosen as area of the present work.

2. Mathematical Model

The heat transfers in container and PCM are assumed to be transient and three-dimensional. Body forces and convection are neglected. The container and PCM interface are uniform. Purely conductive and radiative heat transfer is allowed for all domains. For modelling, a three-dimensional heat transfer 3-D enthalpy based model has been used. Many authors have used enthalpy based model in 1D or 2D [1-4]. In this work, we have used 3D enthalpy model in which all three dimensions are considered for simulation.

Thermophysical property of the container and phase change material which is used during numerical simulation is listed in table 2.

Table 2. Thermophysical property of the container and PCM.

| Thermophysical property of Material | Density $\rho$ (kg/m$^3$) | Specific heat $c_p$ (kJ/kg-K) | Thermal conductivity $k$ (W/m$^2$-K) | Heat of fusion $\lambda$ (kJ/kg) | Melting temperature $T_m$ (K) |
|------------------------------------|-----------------------------|--------------------------------|-------------------------------------|--------------------------------|-----------------------------|
| Stainless steel (Polished)         | 7609                        | 0.59                           | 23                                  | -                              | 1740                        |
| NaOH [8]                           | 2130-1780                   | 2.01-2.09                      | 0.92-0.7                            | 160                            | 591                         |

2.1 Governing equation

The governing equations are:

$$\rho \frac{\partial H}{\partial t} + \nabla \cdot \mathbf{q} = \dot{Q}$$  \hspace{1cm} (1)

Where $\mathbf{q} = -k \nabla T$

For solid container

$$H = c_p T$$ \hspace{1cm} (2)

For Solid-phase PCM

$$H = c_p T : (T \leq T_m - \varepsilon)$$ \hspace{1cm} (3)

$$H = c_p T + \frac{\lambda}{2 \varepsilon} (T - T_m + \varepsilon) : (T_m - \varepsilon \leq T \leq T_m + \varepsilon)$$ \hspace{1cm} (4)

For Liquid phase PCM
\[ H = c_p T + \lambda : (T \geq T_m + \varepsilon) \]  

Nondimensional Stefan number (Ste)

\[ Ste = \frac{c_p(T_m - \varepsilon - T_b)}{\lambda} \]  

Melt fraction (\(\Phi\))

\[ \Phi = (1 - Ste) \]  

where \(\rho\) (kg/m\(^3\)) is density, \(c_p\) (kJ/kg-K) is specific heat capacity, \(H\) (kJ/kg) is specific enthalpy, \(k\) (W/m-K) is thermal conductivity, \(Q\) (W/m\(^3\)) is volumetric heat generation rate, \(T_b\) (K) is bulk temperature of PCM, \(T_m\) (K) is melting temperature, \(Ste\) is Stefan number, \(\varepsilon\) (K) is transition interval between solid to the liquid phase \([9]\), \(\Phi\) is solid-phase PCM, \(\lambda\) (kJ/kg) is the heat of fusion.

2.2 Boundary layout and grid generation

3-D enthalpy based model is computed using COMSOL 5.3a Multiphysics®. The simulation domain and grid generation are shown in figure 1 and 2 respectively. Various assumptions have been taken for the simulation setup.

- The solid container and PCM interface is uniform.
- The solid-liquid interface of PCM is progressed uniformly.
- Transport properties of the solid-liquid phases of the PCM are negligible.
- Super-heating and sub-cooling effects are neglected.
- Clearance effect between PCM and container are neglected
- The backward differentiation formula (BDF) is used for numerical simulation.

![Figure 1. Simulation domain of Container and PCM.](image)

![Figure 2. Grid generation of Container and PCM.](image)

2.3 Grid independence test and validation

Three different sets of grids are generated using the mesh generation module. First set of grids 44004, the second set of grids 88106 and third set of grids 176012 are taken for simulation. Grid independence test of temperature at the center vs. time shown in figure 3. Grid set of 88106 and 176012 show identical temperature vs. time distribution at the center of the PCM. Therefore, an optimal set of grid 88106 is used for further computation.
The present computational model is validated with the results of Siyabi et al. [10]. Figure 4 shows the validation of the present work with the benchmark. The temperature variation vs time shows good agreement of the present simulation setup with the published benchmark results.

![Figure 3. Grid independence test of present work concerning temperature vs. time at the center of the PCM.](image)

![Figure 4. Validation of this work with Siyabi et al (2018) [10].](image)

3. Results and discussions

Stainless steel polished container [9] having the outer radius of 16.7 cm, the height of 16.2 cm, and thickness 10 mm are filled with a NaOH phase change material (PCM). Mass of the PCM is selected based on receiver volumetric capacity and density of PCM. Radially variable constant inward heat flux is taken for the bottom surface, and all surface is exposed at a constant surface emissivity of 0.1 for radiation heat transfer. Heat flux on the receiver surface is shown in Table 3.

| R (m)   | Heat flux q₀ (kW/m²) | R (m)   | Heat flux q₀ (kW/m²) |
|--------|----------------------|--------|----------------------|
| 0.003  | 78.70                | 0.970  | 55.74                |
| 0.026  | 73.38                | 0.115  | 49.65                |
| 0.048  | 68.36                | 0.138  | 44.03                |
| 0.067  | 63.34                | 0.154  | 35.96                |
| 0.087  | 58.63                | 0.166  | 18.02                |

Initial and boundary condition:
when \( t \leq 0 \), \( T = 295 \) K; and when \( t > 0 \), \( q = q₀ \).

Transverse temperature contour of NaOH at 2\(^{nd}\), 4\(^{th}\) and 6\(^{th}\) hour is shown in figure 5. The temperature at bottom surfaces gradually increases from 850 K to 1025 K and temperature at the top surfaces increases from 370 K to 460 K. Figure 6 shows the temperature contour on a horizontal plane at the top, middle and bottom surface of NaOH at 6\(^{th}\) hour. At the bottom surface temperature at the center is high in comparison with the periphery but in case of middle and top surface temperature at the center is low in comparison with the periphery. This is due to heat flux at the center of the receiver is high at the bottom surface but in case of middle and top surface temperature is dominating inward direction due to container periphery.
Figure 5. The temperature contour of NaOH PCM along a vertical plane at 2\textsuperscript{nd}, 4\textsuperscript{th} and 6\textsuperscript{th} hours.

Figure 6. The temperature contour of NaOH along a horizontal plane at 6\textsuperscript{th} hour on the top, middle and bottom surface of PCM.

The temperature distribution profile of NaOH along diameter at middle of PCM is shown in figure 7. Initially, the temperature inside the complete domain is 295 K and gradually temperature increases. Temperature gradient at the periphery is high and at the center is negligible but after some time the temperature gradient at center starts increasing. Figure 8 shows the temperature distribution profile of NaOH along diameter at the top, middle and bottom surfaces of PCM at 6\textsuperscript{th} hour. From figure 8 it is clear that temperature at the bottom surface is high at the center, and gradually decreases up to periphery, but for the top and the middle plane temperature at the center is higher and it reduces towards the periphery.
Figure 7. The temperature distribution profile of NaOH along diameter at middle of PCM after different time intervals.

Figure 8. The temperature distribution profile of NaOH along diameter at the bottom, middle and top surface of PCM at 6th hour.

The bulk temperature and total energy storage by PCM is calculated using volumetric integration at each time intervals shown in equation 8.

$$\langle \psi \rangle = \frac{1}{\Delta V} \sum_{k=1}^{n} \int_{V} \psi(x, y, z, t) dV$$  \hspace{1cm} (8)

where $\psi$ is a function, $\langle \psi \rangle$ is average of function, $\Delta V$ is control volume, $k = 1 \text{ to } n$ is time interval, $(x, y, z)$ is spatial and $t$ is time coordinate. Figure 9 shows the bulk temperature of NaOH phase change material. From figure 9 it is clear that as time increases, bulk temperature of the PCM increases. Initially upto 3rd hour, bulk temperature gradient with time is higher but after 3rd hour temperature gradient is slightly less, it shows that after 3rd hour melting starts. Figure 10 shows total energy storage by NaOH PCM. From figure 10 it is clear that total energy stored by the NaOH phase change material is about 21 MJ.

Figure 9. Bulk temperature of NaOH, PCM at a constant heat flux

Figure 10. The total energy stored by NaOH, PCM at constant heat flux.

4. Conclusions

The temperature of the bottom surface reaches about 1050 K and top surface about 550 K. The huge temperature gradient is because of incomplete melting of the PCM. The bulk temperature of NaOH reaches
about 800 K at 6th hours and total energy stored by the PCM is about 21 MJ. This amount of energy is very useful for domestic and small industrial process.

5. References

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