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# Modeling of Solidification of CCHH ($CaCl_2$, $6H_2O$) in a Shell-and-Tube PCM based Heat Storage Unit

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**Abstract**

Phase Change Material (PCM) based thermal energy storage plays a great role in the era of energy storage due to its high energy storage density and constant phase change temperature. In the present work, solidification behavior of CCHH has been studied numerically in a shell-and-tube PCM based heat storage unit. The enthalpy based 2-D numerical model for shell and tube PCM heat exchanger unit has been considered to study the solidification characteristics. The numerical model has been validated using experiments measuring the temperature variation with time at different locations in the numerical domain of PCM. The predicted isotherm plots clearly show the temperature distribution in the domain during solidification. The melt fraction plots with time are plotted to find out the solid and liquid fraction of the PCM in the numerical domain. The stream function plots with time reflect the solid and liquid zones in the numerical domain during solidification. A close agreement of numerical and experimental study of the solidification behavior of CCHH has been observed in the present study which improves in design of such devices.

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*Keywords:* Phase change material; enthalpy based 2-D numerical model; heat storage unit; solidification.

## 1. Introduction

In recent year, a lot of research works on energy storage and its methodologies are going on worldwide due to energy crisis and environmental pollution. Thermal energy storage plays a greater role in the era of energy storage. The PCMs (Phase change Materials) based thermal energy storages are worked based on different parameters during

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melting and solidification process. Due to the high energy storage density and constant phase change temperature, phase change thermal energy storage (PCTES) has gradually become one of the preferred thermal energy storage systems over the last three decades. In the performance analysis, numerous researchers have intensively studied phase change materials (PCMs) as thermal energy storage because of their high thermal energy densities per unit volume and their availability in different fields of engineering with wide temperature ranges. PCMs store the energy in the form of latent heat during phase change and this energy is being used afterwards for different and several purposes like cooling of buildings, storing of medicines and beverages, cooling of electronic devices, domestic hot water, heating and cooling systems, electronic products, drying technology, waste heat recovery, refrigeration and cold storage [1]. Phase Change Materials (PCMs) are used to store and release thermal energy during the process of melting & freezing (changing from one phase to another). When such a material freezes, it releases large amounts of energy in the form of latent heat of fusion. Conversely, when the material is melted, an equal amount of energy is absorbed from the immediate environment as it changes from solid to liquid. This property of PCMs are used in a number of ways, such as thermal energy storages.

In the last few decades many researchers are contributing in the field of energy storage using PCMs in various capacities. Ismail et al. [2] reported numerical and experimental analysis on finned tubes using finite difference method. The number of fins, fin length, fin thickness, the degree of super heat and the aspect ratio of the annular spacing were found to influence the time for complete solidification, solidified mass fraction and the total stored energy. Trp A. [3] investigated the effect of forced convection considered between the HTF (Heat Transfer fluid) and the wall numerically and experimentally with shell and tube heat exchanger in transient form to study the thermal behavior of the latent heat storage during the charging and discharging process. Later on Trp et al. [4] investigated the influence of operating conditions and geometric parameters on heat transfer in water-paraffin shell-and-tube latent thermal energy storage in transient form. The numerical analysis has been done to visualize the influence of several HTF and operating conditions and several geometric considerations. Dutta et al. [5] did experimental and numerical studies on the heat transfer in a horizontal concentric as well as eccentric annulus containing Phase change Material (paraffin wax) with variable heat flux. The finite volume method (FVM) and semi implicit is formulated to find the progress of the melting front in the melting region. Al-Abidi et al. [6] worked on internal and external fin heat transfer technique for latent heat storage in a triplex heat exchanger where the PCM is in between the HTF flow region. The HTF is surrounded the PCM internally and externally. In the simulation the pure conduction and pure convection have been considered. Wang et al. [7] numerically studied the heat charging and discharging characteristics of a shell-and-tube phase change heat storage unit. The discharging process needs shorter time than the charging represented in their work. The work also incorporated the mass flow rate of the HTF and the phenomenon in different temperature for the PCM is n-octane. The effects of increasing the inlet temperature of the heat transfer fluid (HTF) on the charging and discharging processes of the PCM has been discussed. Lorente et al. [8] investigated phase change heat storage in an enclosure with vertical pipe in the center analytically and numerically. In the present work a physical system has been considered to study the transport phenomenon during solidification of PCM solution and a numerical solution method (Finite Volume Method) has been used to solve the governing equations. The solution method has been framed and coded in the 'FORTRAN' programming tool. The developed code has been validated with the experiments after successive grid independency test.

## 2. Model Formulation

The present model is based on a 2-D rectangular cavity to investigate the transport phenomena during solidification of the above PCM shown in Fig. 1. The solidification phenomenon of the CCHH ($CaCl_2$, $6H_2O$) in a cylindrical annulus axi-symmetrically heated at constant temperature from the left face of the rectangular cavity has been considered with the tube fitted with fin. Initially, the PCM is assumed at ambient temperature above the melting temperature. In order to create thermal convection in the cavity, the left face or the left wall is maintained at constant temperature ($T_c$) below the melting temperature ($T_{melt}$) when other walls (right side wall, the top side, bottom side) of the cavity are assumed to adiabatic. The present boundary condition develops a thermal gradient ($\Delta T/H$) along the length of the cavity. The solidification begins from the left face due to thermal cooling. During solidification a Rayleigh-Bernard convection is developed in the transition zone (solid-liquid phase) which indicates a sudden temperature fall in the PCM. The fin configuration added a heat addition and as well as subtraction from the top wall and the bottom wall also. The system data and the thermo-physical properties used for the simulation are given in Table 1 and Table 2, respectively.

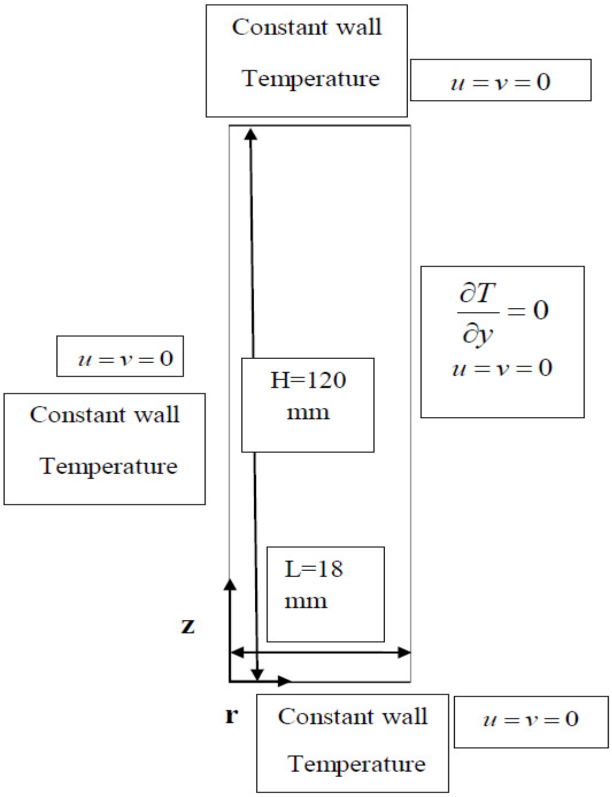


Fig. 1.Schematic of the problem domain with fin.

Table 1. System data for the model

| | |
|---|---|
| Cavity Height(H) | 120mm |
| Cavity Length(L) | 18mm |
| Solidification: | |
| Left wall temperature($T_H$) | 20°C |
| Initial temperature(Tint) | 40°C |

Table 2 Material properties used in the model

| Material | Density ($kg/m^3$) | | Thermal Conductivity (W/m-K) | | Specific Heat (J/kg-k) | | Melting point (°C) | | Latent Heat J/kg-k |
|---|---|---|---|---|---|---|---|---|---|
| | Solid | Liquid | Solid | Liquid | Solid | Liquid | Lower | Upper | |
| Calcium Chloride hexahydrate, | 1710 | 1710 | 1.088 | 0.539 | 1460 | 2130 | 29.7 | 29.9 | 187.4 |
| Copper | 8954 | | 386 | | 383 | | | | |

In developing the conduction and convection model for the thermal energy storage unit, the following assumptions are made.

- The flow is considered as laminar and unsteady.
- The PCM is assumed as Newtonian and incompressible.
- The effect of natural convection in the liquid phase of PCM is taken into account. The solid phase is free from internal stresses and no shrinkage during solidification.
- Heat transfer is considered only from the left side, top and bottom walls.

**Governing Equations**

Based on the approximations, the single domain model is represented below.
The continuity equation is given as

$$\frac{\partial(\rho)}{\partial t}+\nabla.(\rho \mathrm{U})= 0 \tag{1}$$

The momentum conservation equations are given as

$$\frac{\partial(\rho u)}{\partial t}+u\frac{\partial(\rho u)}{\partial r}+v\frac{\partial(\rho u)}{\partial z}=-\frac{\partial p}{\partial r}+\nabla.(\mu\nabla u)+S_u \tag{2a}$$

$$\frac{\partial(\rho v)}{\partial t}+u\frac{\partial(\rho v)}{\partial r}+v\frac{\partial(\rho v)}{\partial z}=-\frac{\partial p}{\partial z}+\nabla.(\mu\nabla v)+S_v+\rho g\beta(T-T_{ref}) \tag{2b}$$

In the equations (2a , 2b), the source terms $S_u$ *and* $S_v$ offer additional frictional resistance toward the fluid flow [9].
The energy conservation equation is given as

$$\frac{\partial(\rho c_p T)}{\partial t}+u\frac{\partial(\rho c_p T)}{\partial r}+v\frac{\partial(\rho c_p T)}{\partial z}=\nabla.(k\nabla T)+S_h \tag{3a}$$

where $S_h$ is a source term, represents evolution of the latent heat during solidification by the PCM. The corresponding latent heat source term ($S_h$) is given as

$$S_h=-\left\{\frac{\partial}{\partial t}(\rho f_l \Delta H)+\nabla.(\rho u \Delta H)\right\} \tag{3b}$$

where, $\Delta H$ is the latent enthalpy content in a cell, calculated based on the enthalpy update scheme.

$$\Delta H=0 \text{ when, } T<T_{melt} \tag{3c}$$

$$=L \quad \text{when, } T>T_{melt} \tag{3d}$$

In the above equations (1-3b) volume average properties are calculated as

$$\rho=f_l\,\rho_l+f_s\,\rho_s \tag{4a}$$

$$k=f_l\,k_l+f_s\,k_s \tag{4b}$$

$$c_p=f_l\,c_{p_l}+f_s\,c_{p_s} \tag{4c}$$

where, $\rho$ is the volume average density, and $f_l$ and $f_s$ are the liquid and solid fractions of the PCM, respectively.
The set of governing equations (1- 3) is simulated effectively with appropriate boundary conditions. The boundary conditions are given as

*Top face*(y = H):

The top surface of the PCM is subjected to an adiabatic wall with no heat transfer. Corresponding temperature of the top surface is the temperature of the atmosphere is shown in Fig. 1

$$\frac{\partial u}{\partial z}=0 \text{ and } u=v=0 \tag{5a}$$

*Bottom face* (y = 0): the bottom wall the experimental setup considers the atmospheric temperature and the wall is considered as an adiabatic condition.

$$\frac{\partial u}{\partial z} = 0 \text{ , } u = v = 0 \tag{5b}$$

*Left face* (x = 0):
The heat transfer fluid (HTF) is flowing from the left face of the numerical model.

$$-k\frac{\partial T}{\partial r} = h_r\left(T_{HTF} - T_r\right)$$

*Right faces* (x= L):
The boundary conditions for both left and right surfaces are

$$\frac{\partial T}{\partial x} = 0 \text{ and } u = v = 0 \tag{5c}$$

## 3. Solving Methodology

Discretization of different equation are performed considering the power law scheme of second order accuracy described by Patankar [11].The enthalpy update scheme evaluates the latent heat content of each computational cell based on the temperature predicted from the each iteration within a time step is expressed as follows[9]:

$$\left[\Delta H_P\right]_{n+1} = \left[\Delta H\right]_n + \frac{a_P}{a_P^0}\lambda\left(\left[h_P\right]_n - cF^{-1}\left[\Delta H_P\right]_n\right) \tag{6}$$

where $a_P^0 = \rho\Delta V / \Delta t$ and $a_p$ are the coefficient of discretized energy equation, $\Delta V$ is volume of a computational cell, $h_p$ is the sensible enthalpy at the nodal point *P*, and $F^{-1}$ is the inverse of the latent heat function. In the case of isothermal phase change process, the Eq.6 is modified by Chakraborty and Dutta [12]and used in the present work.

## 4. Model Validation with Experimental Results

After successful grid independent test, the developed model has been validated with the experimental results performed in the Heat Power Laboratory in the Department of Mechanical Engineering of Jadavpur University, Kolkata. The schematic diagram of the experimental setup of shell and tube PCM based heat storage are shown in Fig. 2. The model predicted temporal variation with time has been validated with the experimental results.

Experimental setup consists of the following components:

1. Control unit of temperature of HTF with flow control ( Constant temperature bath)
2. Transparent borosilicate glass tube.
3. PCM storage unit.
4. Data acquisition system.
5. Copper tube and the fitted circular fins.

Other parts include piping, stand and insulation material etc.

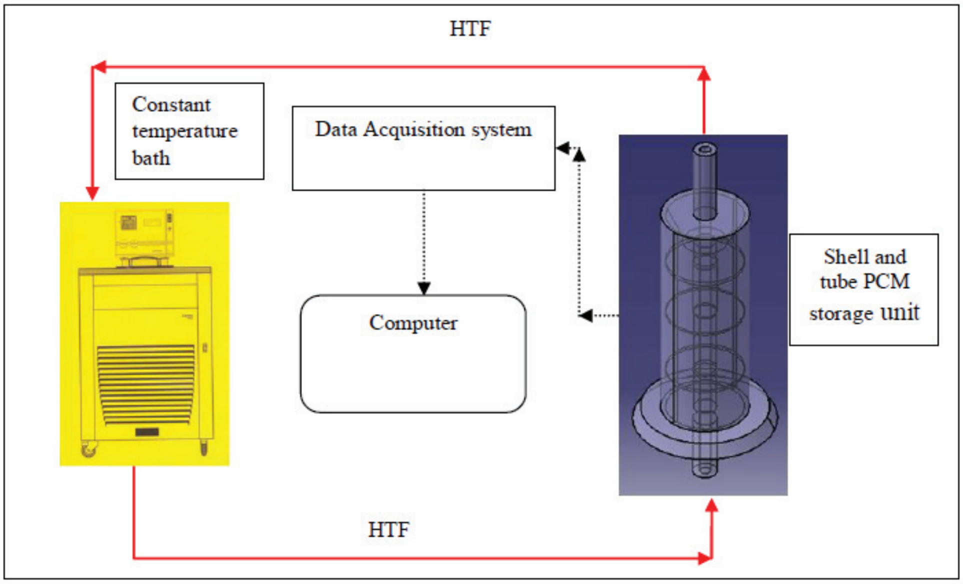


Fig.2 Experimental set up of shell and tube PCM based heat storage

Multiple sets of experimental data have been used to show the repeatability of the results. Though, there is a slight variation of temperature which is due to the variation in the position of the thermocouple within the PCMs. The experimental plots of temperature variation of thermocouples at different location are showing a good agreement with the numerical data generated from the numerical model shown in Fig. 3. It shows that rate of increase of temperature is very fast during sub-cooling and shows close prediction of the numerical results with the experimental results during solidification.

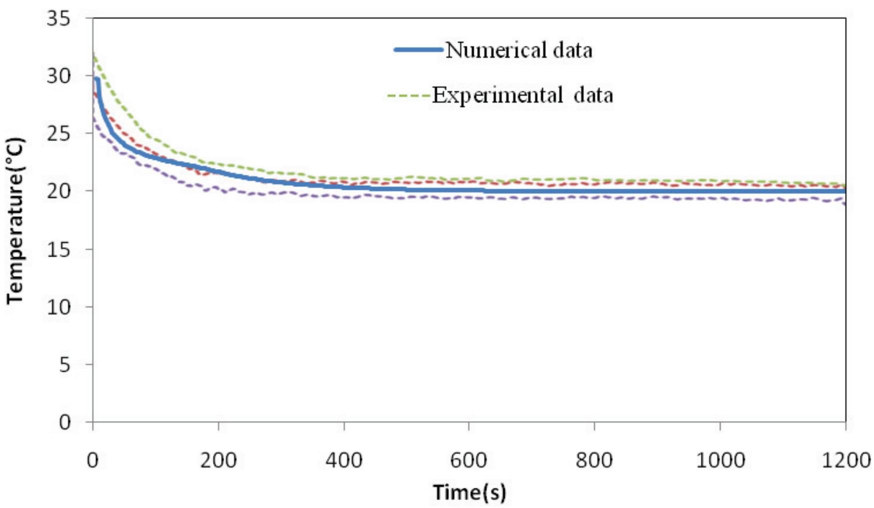


Fig. 3 Variation of temperature with time during solidification of calcium chloride hexahydrate with fin configuration

## 5. Results and Discussion

After successful validation of the developed model, isothermal plots and melt fraction plots during solidification of Calcium Chloride Hexahydrate ($CaCl_2$, $6H_2O$) at 20°C have been depicted in the Fig. 4(a,b).

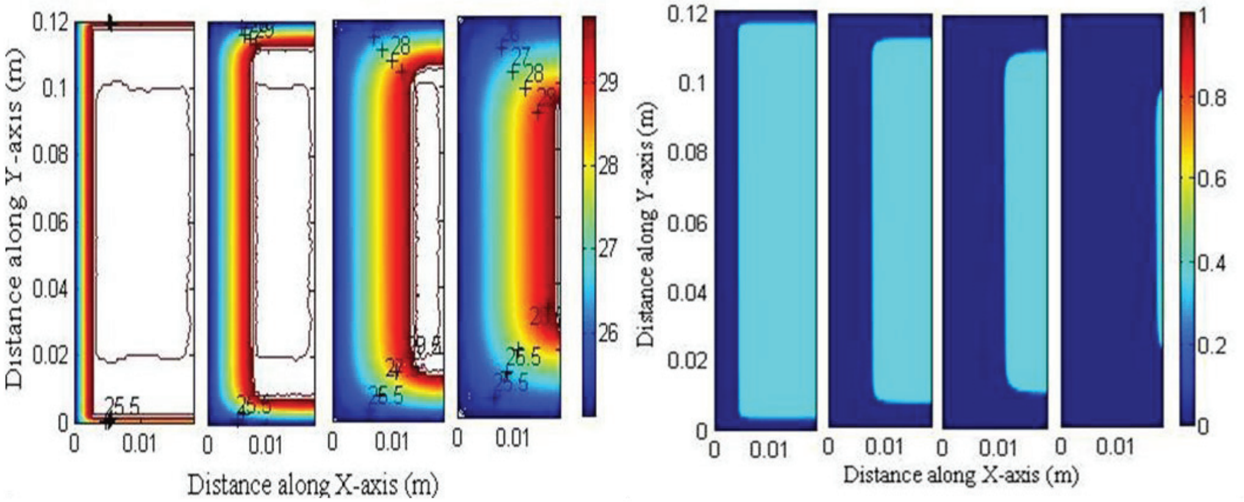


Fig. 4(a) Isotherm plot at T=20°C, t=30; 100; 200; 500sec and 4(b) Melt fraction at T=20°C, t=30; 60; 200; 500sec.

The Fig. 4(a) shows the isotherm plots in the numerical domain to show the solidification characteristics at 20°C constant temperature is chosen with a specified molten PCM temperature T=40°C. In case of normal solidification i.e. the heat extraction only from the left wall. The solidified layer forms vertically along the wall surface. The temperature gradient is acute and the solidified layer forms layer by layer along the left wall. The value of the isotherms is plotted with time. Due to fin arrangement, the PCM solidified along the three surfaces. Similar observations have been made from the melt fraction plots shown in Fig. 4(b).

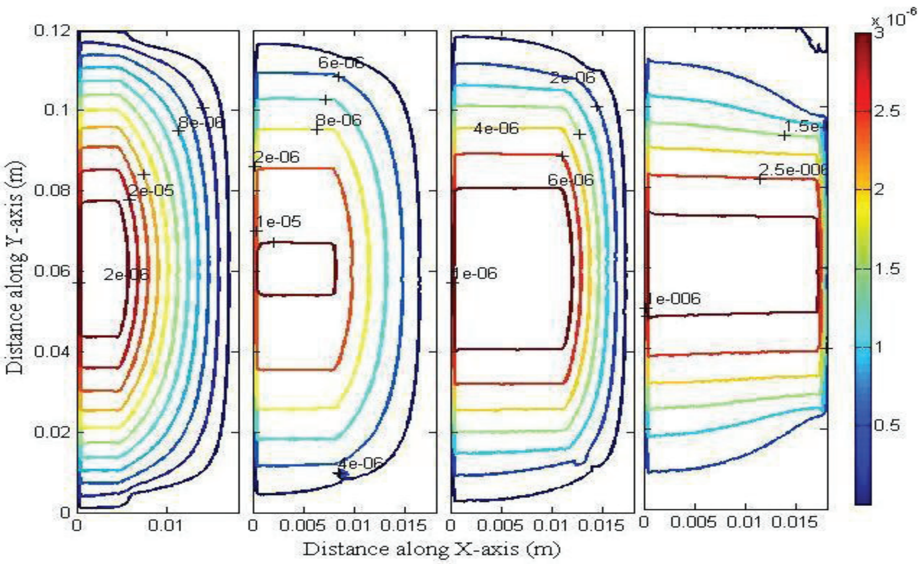


Fig.5. Stream function plot at T=20°C, t=30; 100; 200; 500sec.

Stream function plots during solidification of Calcium Chloride Hexahydrate ($CaCl_2$, $6H_2O$) at T 20°C has been shown in Fig. 5. In the case of solidification at the initial time t=0, the whole cavity is liquid and the strength of the stream function is maximum. The stream functions are shown with different time at different temperature. As the solidification starts the PCM along the wall starting solidified and the strength of the stream function decrease.

## 6. Conclusion

In the present work, solidification behavior of CCHH has been studied numerically in a shell-and-tube PCM based heat storage unit. The enthalpy based 2D numerical model of a shell and tube PCM heat exchanger unit has been developed to study the solidification characteristics. The numerical model has been validated using experimental data during solidification by temporal variation with time at different locations in the numerical domain of PCM. The isotherm plots clearly show the temperature distribution in the domain during solidification. The melt fraction plot at different time has been obtained to find out the solid or liquid quantity of the PCM in the numerical domain. The stream function plots with different time reflect the solid and liquid zones in the numerical domain during solidification at different time.


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