CFD Analysis of Latent Thermal Energy Storage for Erythritol Phase Change Material

Rajeev Ranjan[1], Aseem C. Tiwari[2]
[1]*Research Scholar, Dept. of Mechanical Engineering, University Institute of Technology, RGPV, Bhopal, Madhya Pradesh, India*
[2]*Professor and Head of Department, Dept. of Mechanical Engineering, University Institute of Technology, RGPV, Bhopal, Madhya Pradesh, India*

***Abstract* - Aimed to provide models for determining Latent Thermal Energy Storage (LTES) devices with help of PCMs, based on their operating conditions, thermo physical properties of materials and geometric parameters. The models are developed considering fluid dynamics and heat transfer involved in melting and solidification of PCMs. Parameters like container's diameter, temperature of inlet and velocity are varied to determine the melting and solidification time for the erithritol PCM. Along with this analytical correlation find between charging and discharging time' of storage device.**

***Index Terms* - TES (Thermal Energy Storage), PCM (Phase Change Material), LTES (Latent Thermal Energy Storage), HTF (Heat Transfer Fluid), CHP (Combined Heat and Power)**

I.INTRODUCTION

Phase change materials (PCM) are substance which releases and absorb energy at phase transition to utilize useful heat and cooling. The energy absorbed or released by phase transition for solid to liquid or vice-versa. The heat of fusion is much higher than the sensible heat. By melting and solidifying at the phase change temperature of PCM is capable of storing and releasing large amount of energy compared to sensible heat storage.

Phase change material is classified into several parts including type of thermo physical property chemical properties and others. The energy storage within PCMs, occurs from solid-solid, liquid-solid, solid-liquid, solid-gas, and liquid-gas phase changes. Even though liquid gas phase changes have a higher heat of transformation than the solid-liquid counterparts, they prove to be impractical for thermal storage since, large volumes or high pressure are required to store materials in their gas phase. Solid-Solid phase changes have relatively low heat of transformation and are slow processes. Thus, solid-liquid and liquid-solid are more practical for TES. Some types of PCM materials are Hygroscopic Materials can absorb and release water with change in temperature. Several construction materials are naturally hygroscopic such as, clay, wool insulation, and others the process can be segregated as,

- Condensation (gas to liquid): $\Delta H < 0$; enthalpy decreases.
- Evaporation (liquid to gas): $\Delta H > 0$; enthalpy increases [1]

Organic materials are typically derived from bio-based compounds, Paraffin waxes (CnHn+2), carbohydrates, lipid derived compounds, and others. E.g. alkanes, waxes, or paraffins. Within organic materials, there is a class called PCMs made up of molecular alloys, formed by alkane-based alloys which have the advantage of being thermo-adjustable, which means they allow alterations to the phase change temperature through their composition. Inorganic materials primarily consist of salt hydrates and eutectic mixtures. These materials are noted for their multiple applications in Solar Energy Storage.

Several organic and inorganic PCMs melt with a high heat of fusion in the moderate melting temperature range of (100 to 200°C). For their utilization as effective LTES materials, PCMs must possess certain desirable thermodynamic, kinetic, chemical, technical, and economic characteristics [1]. Following are some of the criteria considered in evaluating PCMs for LTES.

THERMODYNAMIC CRITERIA

Melting Temperature is in the desired operating temperature range of PCM. Having High Latent Heat of Fusion per unit volume so able to store much energy. Also having High Specific heat capacity, so that significant sensible TES can occur. Having High Density, so that less volume is occupied by the material. Materials having High Thermal Conductivity, so that small temperature differences are needed for charging and discharging the storage. Small Volume changes on phase transformation, so that a simple containment and heat exchanger can be used.

KINETIC CRITERIA

Super cooling is a major problem associated with salt hydrates as PCMs is the fact that they tend to be supercool considerably. The reason for the high degree of super cooling is the rate of nucleation (of crystals from the melt) or the rate of growth of nuclei (or both) is very slow, which reduces the advantage of the material for heat storage. Thus, little or no supercoiling is desirable, i.e. the melt should crystallize at its freezing point [1]. Super cooling can often be mitigated by adding nucleating materials. Some success has been attained by using additives with crystal structure like. The nucleating agents have certain characteristics like insoluble in water at all temperatures, having melting point higher than the highest temperature reached by the energy storage material in the storage cycle, not form solid solutions with the salt hydrate, not chemically react with the hydrate, and others.

TECHNICAL CRITERIA

Certain technical criteria should be observed for effective storage of PCMs like compactness, compatibility, viability, reliability, design simplicity, and others.

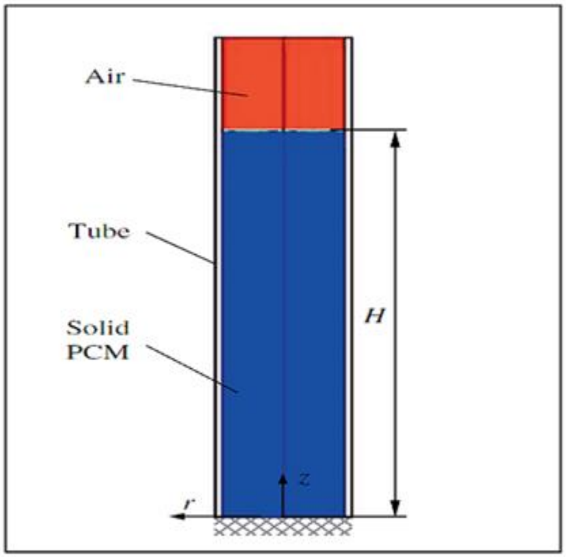
ECONOMIC CRITERIA

Economic Criteria like commercial availability and low cost are important for the PCMs. These prove to be important considerations for development of storage devices, since the scale of energy storage would depend on the respective application. When carefully evaluated, PCMs have the potential to significantly reduce electric demand and expenditure.

II. NUMERICAL SIMULATION AND CASE VALIDATION

In 2010, Shmueli H. et al. [2] conducted numerical and experimental analysis of a PCM in a vertical cylindrical tube. They also investigated effect of mushy zone constant 'C', on melting in a vertical cylindrical tube, using the solidification/melting model of the commercial CFD software Fluent. Vertical cylindrical tubes of 3 cm and 4 cm in diameter, with the wall temperatures of 10 and 30°C above mean melting temperature of the PCM, were considered for their experimental and numerical investigation. Following figure shows the interface of PCM exposed to air at 17 cm from the base, the total height of the tube being 20 cm.

For the numerical model, properties of PCM are based on a commercially available PCM, Rubitherm GmBH (RT27), with a melting temperature interval of 299.15 – 301.15K (26-28°C) with the entire system being at an initial temperature of 295.15 K (22°C). It is assumed, both solid and liquid phases are homogeneous and isotropic, and the process of melting is axisymmetric. The molten PCMs and the air are incompressible Newtonian fluids, and laminar flow is assumed in both. A temperature dependent expression is used to describe the density of air given as,



$\rho = 1.2 \times 10-5T2 - 0.001134T + 3.4978$ (3.1)

The governing equations used for the PCM-air are,

- Continuity

$D\alpha n/Dt = 0$ (3.2)

- Momentum

$$\rho \frac{D\vec{V}}{Dt} = -\nabla p + \mu \nabla^2 \vec{V} + \rho \vec{g} + \vec{S} \qquad (3.3)$$

- Energy

$$\rho \frac{Dh}{Dt} = k\nabla^2 T \qquad (3.4)$$

where ρ is the density, k is the thermal conductivity, μ is the dynamic viscosity, S→ is the momentum source term, V→ is the velocity vector, T is the temperature, and h is the specific enthalpy. The specific enthalpy is defined as a sum of the sensible enthalpy,

$$h_s = h_{ref} + \int_{T_{ref}}^{T} C_p dT \qquad (3.5)$$

The change in enthalpy due to phase change 'γ_L', where, 'h_{ref}' is the reference enthalpy at the reference temperature 'T_{ref}', 'C_p' is the specific heat, 'L' is the specific enthalpy of melting (latent heat of the material), and γ is the liquid fraction during the phase change which occur over a range of temperatures $T_s < T < T_l$, where 'T_s' and 'T_l' are the 'solidus' and 'liquids' temperatures respectively, defined by,

$$\gamma = \begin{cases} 0 & if\ T < Ts \\ 1 & if\ T > Tl \\ \frac{T-Ts}{Tl-Ts} & if\ Ts < T < Tl \end{cases} \qquad (3.6)$$

The source term S→ in the momentum equation is given by,

$$\vec{S} = -A(\gamma)\vec{V} \qquad (3.7)$$

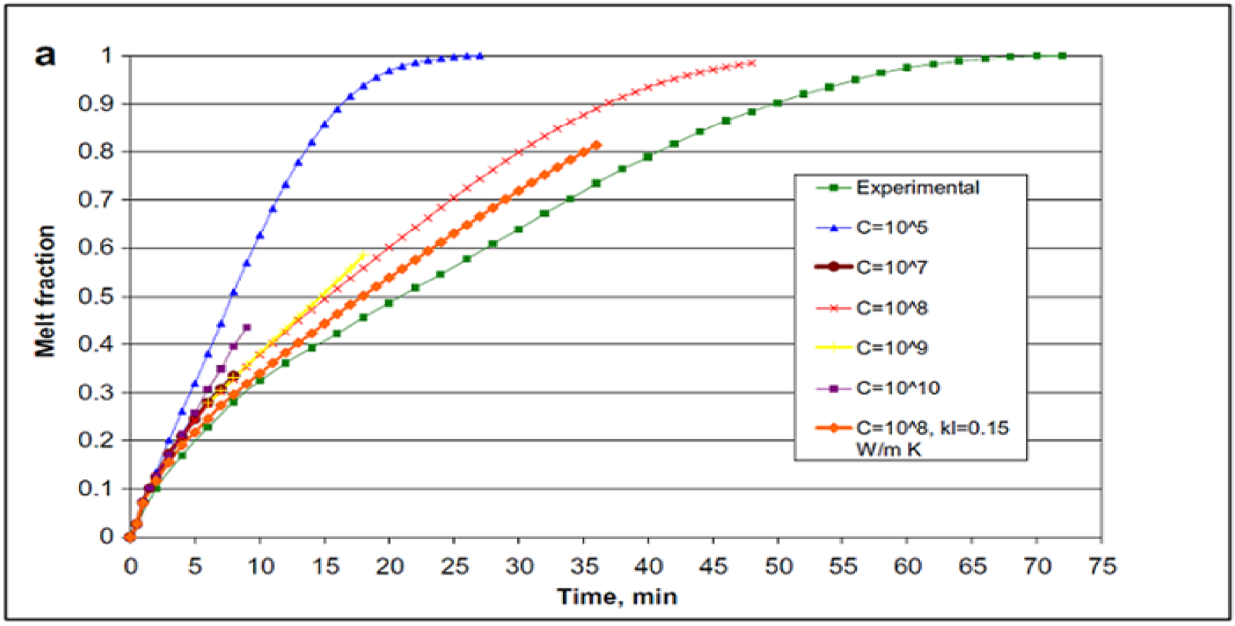
Where A(γ) is the "porosity function", which makes the momentum equation mimic Carman-Kozeny equations for flow in porous media,

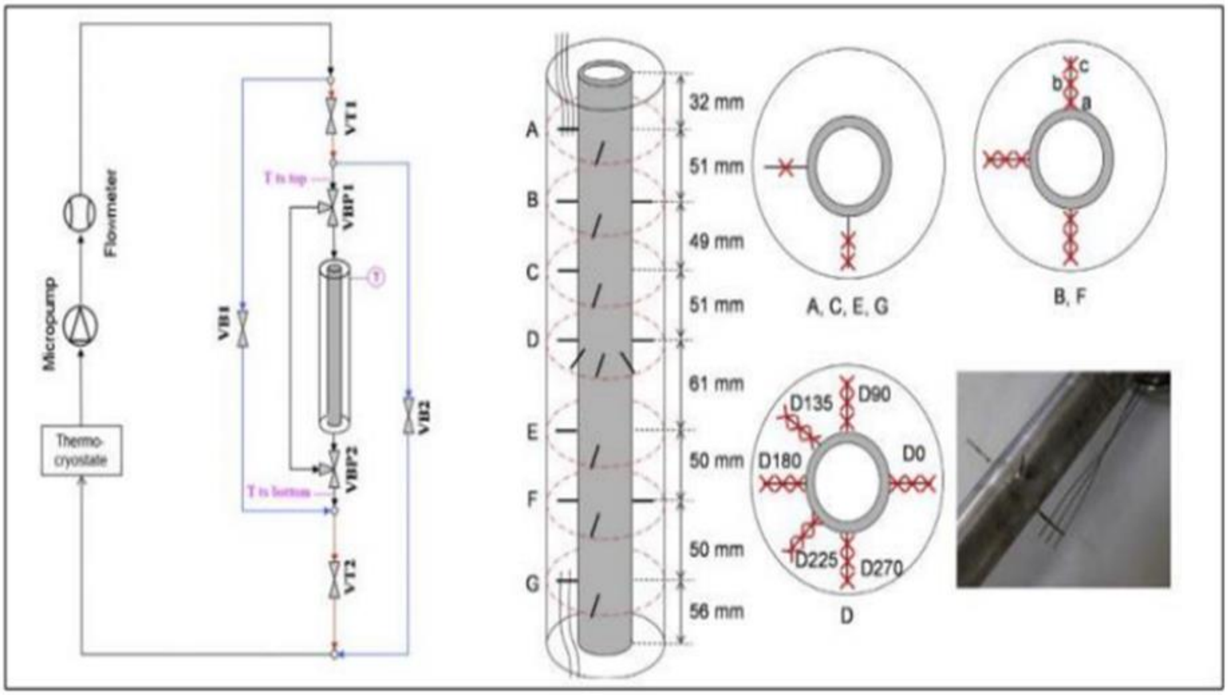
$$A(\gamma) = C(1-\gamma^2)/(\gamma^3+\epsilon) \qquad (3.8)$$

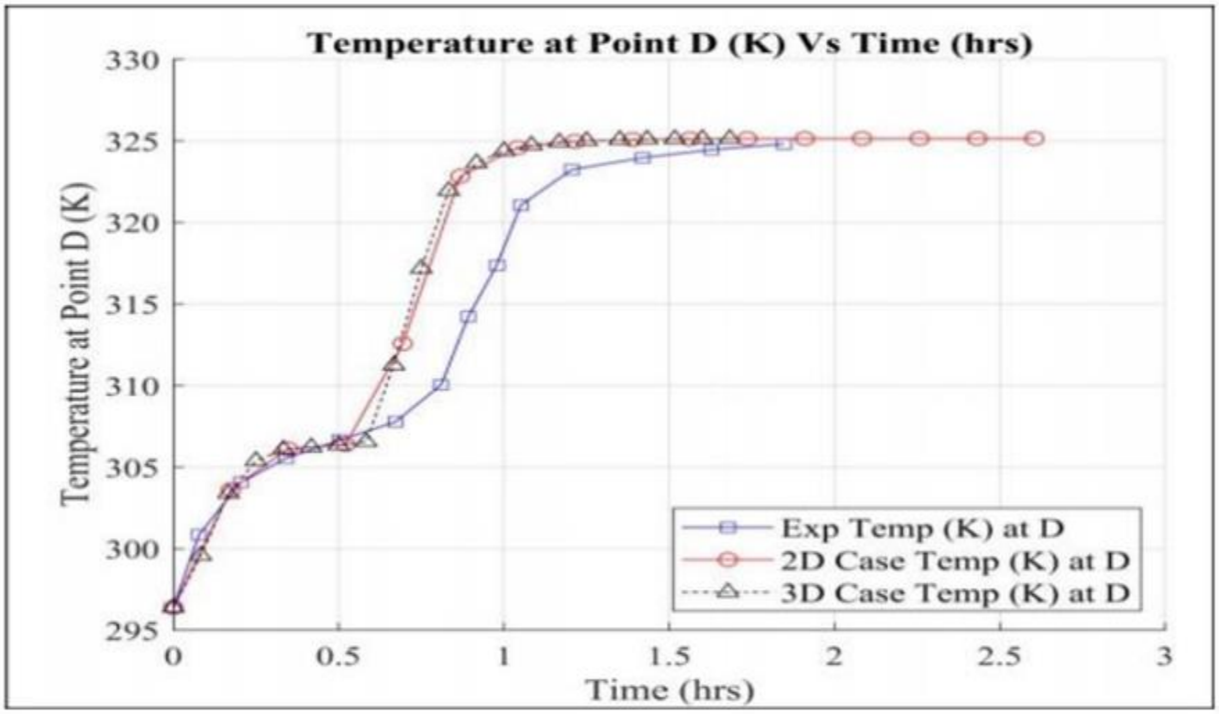
Where $\epsilon = 0.001$ is a small computational constant is used to avoid, division by zero, and where 'C' is the mushy zone constant [2]. The Fluent manual describes the mushy zone constant as the measure of amplitude of damping, if higher value of this, the steeper will be transition velocity of material, to zero as it solidifies. As the values increase causes oscillate the solution. The results for the model configuration with tube diameter of 4 cm, height of phase change material in the tube being 17 cm, and the wall temperature 10 K above the mean melting temperature of the PCM, have been studied for the purpose of this project. The effect of varying 'C' on the melting of PCM, between 10^5 and 10^{10} was investigated by Shmueli et al. [2] to obtain comparable results to the experimental results, as can be seen in the figure.

EXPERIMENTAL MODEL

which considers the melting of PCM in a vertical cylinder was experimentally and numerically investigated by Longeon et al. [3], for the melting of paraffin RT35 with a melting temperature of 308.15 K (35°C) provided by Rubitherm. The experimental setup is composed of a test-section, several instrumentation devices, and a Heat Transfer Fluid (HTF) Control Loop. The configuration explored injection of a Heat Transfer Fluid (HTF) in an inner tube. The experimental loop and thermocouple positions

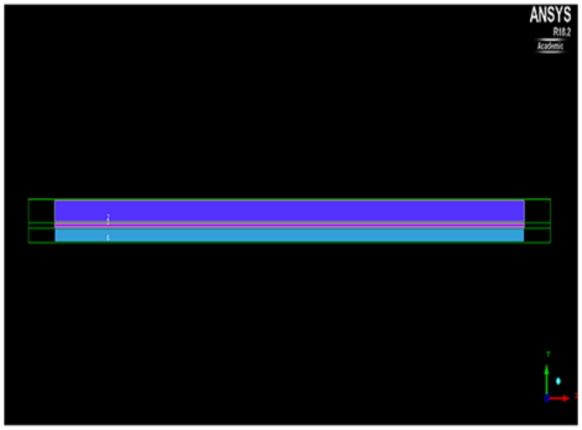


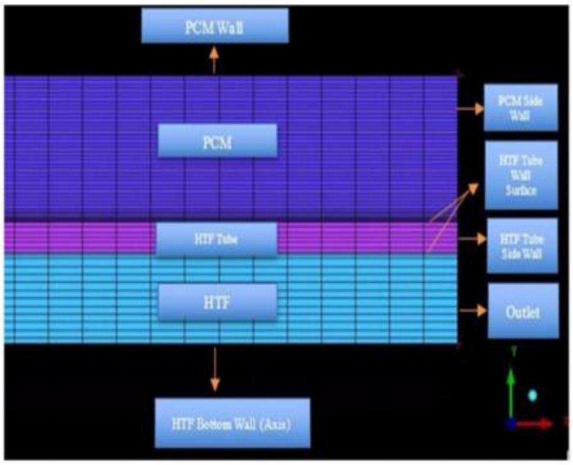




III. METHODOLOGY

Ansies simulations of the melting process were conducted using the commercial CFD software Fluent. The experimental setup was modeled with a 2-D axisymmetric geometry and a 3-D symmetric geometry. In both cases the flow is in +X direction for the HTF in the inner tube of annular geometry, the outer annulus containing the PCM. Also, gravity is defined along -X direction in the solver. Both the meshes were created by use of ANSYS





ICEM CFD software. Multi Block-Grid was created for both types of meshes. For the 2-D mesh the bottom wall parallel to X-axis is chosen as the axis of symmetry as can be seen in Figure. A mesh with 5k nodes for 2-D case was utilized, with element size. For the 3-D mesh a partial 'O-Grid' or 'C-Grid' blocking strategy was implemented for individual zones as can be seen in Figure. Both the meshes have same number of nodes along the axis of the annulus and the diameter. This enables a direct comparison between the two cases to check for any changes in the solution associated with the mesh type

BOUNDARY CONDITIONS

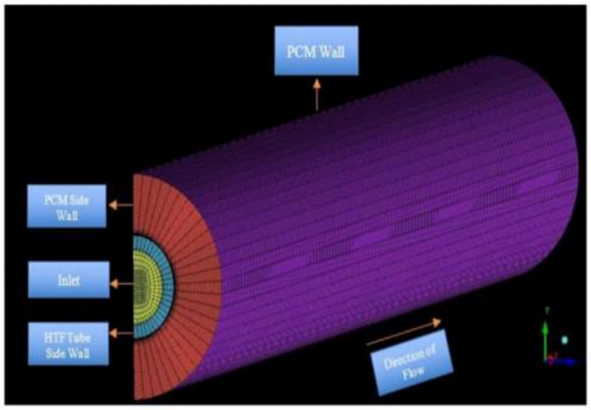
2-D CASE

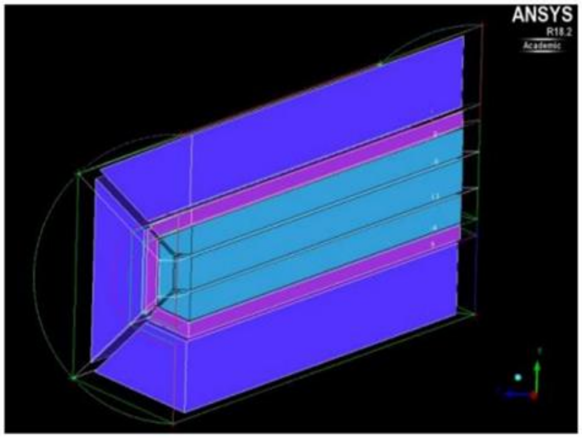
The 2-D Case was modeled using certain specific boundary conditions for the different zones in the geometry. The inlet zone is defined with velocity-inlet boundary condition with 0.01m/s and 326.15 K, whereas the outlet is defined with a pressure-outlet boundary condition, with a backflow temperature of 308.15 K. The bottom HTF wall parallel to X-axis is defined with the axis boundary condition. The inner and outer surfaces of the HTF-Tube are defined with coupled-wall boundary condition. The PCM side and outer walls are defined with adiabatic wall conditions.

2-D Mesh Zones

3-D CASE The 3-D Case was defined with same boundary conditions for the inlet and outlet zones, as that of the respective zones in the 2-D case. The symmetric walls of each domain, i.e. HTF, HTF Tube, and PCM domains, are defined as symmetric walls. The inner and outer surfaces of the HTF-Tube are defined with coupled-wall boundary condition. The side walls of HTF-Tube and PCM domains, along with the outer wall of the PCM domain, are defined with adiabatic wall boundary conditions

3-D Mesh Zones





To simulate the conditions of heat storage/transfer, for the moderate temperature 100 to 210°C (212 to 410 F) by-product heat produced by CHPs, the organic sugar-based alcohol Erythritol is chosen as the PCMs.

The properties of erythritol are given in Table.

Property	Value	Variation with Temp		Unit
Density (ρ)	1480	-		kg/m^3
Thermal Expansion Coefficient (β)	0.001014	-	-	1/K
Latent Heat Capacity (L)	339800	-	-	J/kg
Temperature Solidus (T_s)	389.85	-	-	K
Temperature Liquidus (T_l)	391.85	-	-	K
Specific Heat Capacity (Cp)	-	293.15 K	1380	J/kgK
	-	391.85 K	2760	
Thermal Conductivity (k)		293.15K	0.733	W/mK
		391.85 K	0.326	
Dynamic Viscosity (μ)	0.01	-	-	kg/ms

The HTF chosen for the new design is a dow-corning 550 fluid. Properties for both these fluids were specified by Parry et al [4]. An experimental setup created to model TES with a Shell-and-Tube Heat Exchanger using erythritol, was also numerically validated by Parry et al [4]. This is chosen due to the considerations for its common availability as an industry supply fluid and relatively low cost. The properties of the HTF can be seen in the Table below

Property	Value	Unit
Density(ρ)	1065	Kg/m^3
Specific Heat Capacity(C_p)	396	j/kgK
Thermal Conductivity(K)	0.1465	W/mK
Dynamic Viscosity(μ)	0.133125	Kg/ms

NUMERICAL MODEL

The HTF and PCM domains are modeled separately, where effect of variations in parameters are observed on the melting and time taken for complete melting in the PCM domain. Commercial CFD software Fluent is utilized to simulate the flow conditions and heat transfer.

Mesh domains were developed using the ANSYS ICEM CFD software for both the cases as discussed in Section Axisymmetric meshes for the 2-D cases and symmetric meshes for their 3-D counterparts were created with the same number of nodes and growth ratios for the simulations. For the initial simulations, to study the effect of inlet conditions on the time taken for complete melting, cases with 2-D axisymmetric mesh were developed as mentioned above.

Natural Convection is taken into consideration, by utilizing the Boussinesq approximation for the density of material RT35. The model incorporating Boussinesq approximation as described in Fluent User's Guide [5], treats the density as a constant in all solved equations, except in the buoyancy term of momentum equation, given by,

$$(\rho - \rho_0)g \approx -\rho\beta(T - T_0)g \quad (3.9)$$

where, ρ_0 is the constant density, T_0 is the operating temperature, and β is the thermal expansion coefficient. The Boussinesq approximation is used for eliminating ρ from the buoyancy term as given below,

$$\rho = \rho_0(1 - \beta\Delta T) \quad (3.10)$$

The approximation is valid if the changes in actual density are small, specifically, the Boussinesq approximation is valid when,

$$\beta(T - T_0) \ll 1 \quad (3.11)$$

Reynolds no

$$Re=\frac{\rho htf \times Vi \times Di,htf}{\mu} \quad (3.12)$$

R_e	V_i(m/s)
1020	8.5
1530	12.75
2040	17

VARIATIONS IN INLET TEMPERATURE

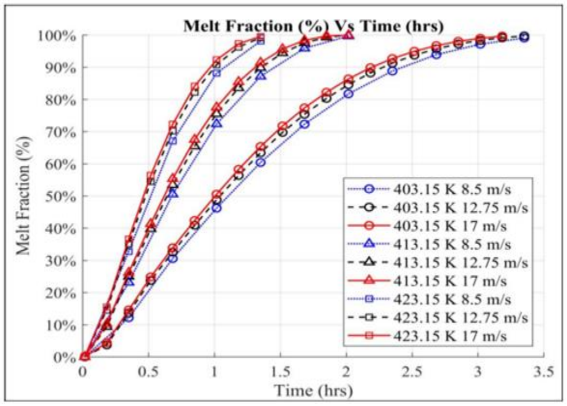
The variations in inlet temperature 'T_i', were also studied along with variation in V_i. Since, the melting interval of PCM is 116.7 to 118.7°C (389.85 to 391.85 K), three values for T_i were considered in the increment of approx. 10 K from 403.15 K, as shown in Table. This facilitates a comparative study of the inlet temperatures above the mean melting temperature of the PCM. In turn, this comparison gives us 9 combinations of T_i and V_i, which aides in further understanding of the significance of inlet conditions on the TES with PCM.

Results and Comparison

T_i/V_i	8.5 m/s	12.75 m/s	17 m/s
403.15 K	3.51	3.45	3.30
413.15 K	2.10	1.97	1.90
423.15 K	1.55	1.47	1.42

Results for the time taken for complete melting can be seen in Figure. From the distribution it is evident that the time taken for melting decreases as Ti increases. Comparatively, the time required for melting does not increase as significantly with increase in velocity. The time for completing melting for each combination can be seen in Table. The maximum time taken was observed for lowest Ti and Vi values i.e. 403.15 K and 8.5 m/s, whereas the minimum time taken for complete melting was for the highest values of Ti and Vi i.e. 423.15 K and 17 m/s.

Variations in time for complete melting with varying Ti and Vi



SOLIDIFICATION

The discharging process of the LTES device is considered by the solidification of PCM, as heat is extracted from the completely melted PCM in the container by passing a colder fluid through the inner tube. To have consistency with the melting process, variations in Vi were limited by the Re in order to have laminar flow in the inner tube (Re<2,300). The variations in Ti were considered below the mean melting temperature, which along with the variations in Vi, which provide nine more combinations as shown in Table below. It was observed that with decrease in Ti the time taken for solidification decreases proportionally. Also, the time taken for solidification decreases with increase in Vi, due to heat being carried away by the colder fluid faster at higher Vi. In order to obtain comparative results, the cases were initialized with 423.15 K as the initial temperature for HTF Tube and PCM domains

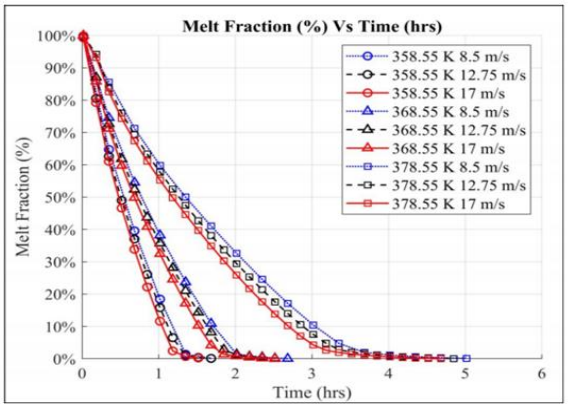


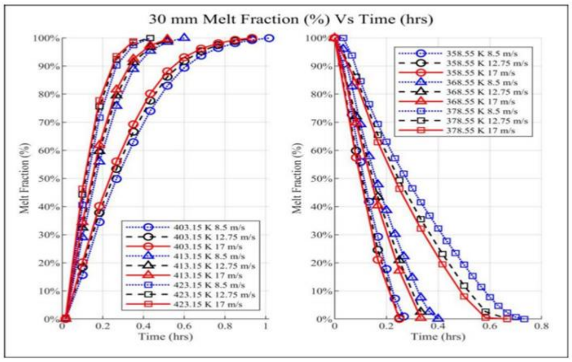
Table for complete solidification time with varying Ti and Vi

T_i/V_i	8.5 m/s	12.75 m/s	17 m/s
358.55 K	1.78	1.75	1.67
368.55 K	2.73	2.67	2.52
378.55 K	5.18	4.97	4.70

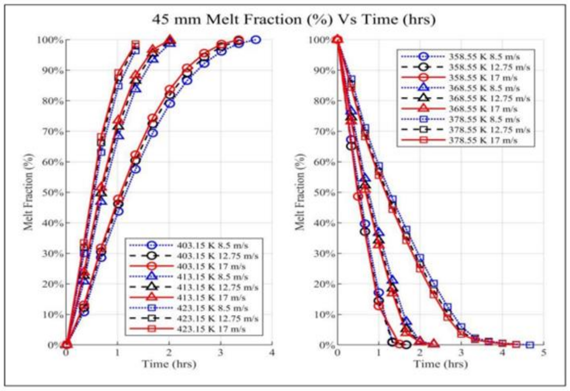
MELTING AND SOLIDIFICATION WITH CHANGE IN DIAMETER

Since the comparisons with 3-D simulations revealed negligible errors, 2-D cases were chosen for further analysis. Along with changes in diameter, simulations were carried out with variations in inlet temperature and velocity considering the values as described. This provides a complete set of results for all 3 diameters as can be seen in Figures below.

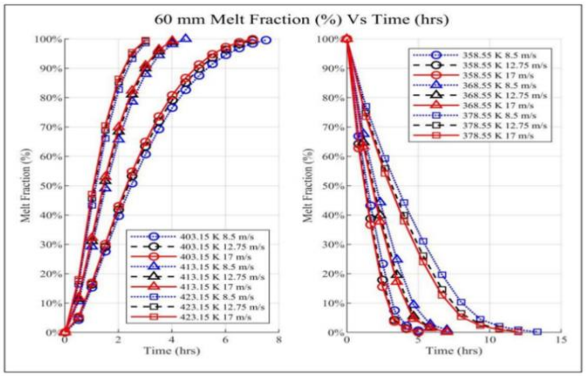
Time vs melt fraction graph for complete melting and solidification with varying Ti and Vi, for 30mm Diameter



Time vs melt fraction graph for complete melting and solidification with varying Ti and Vi, for 45mm Diameter



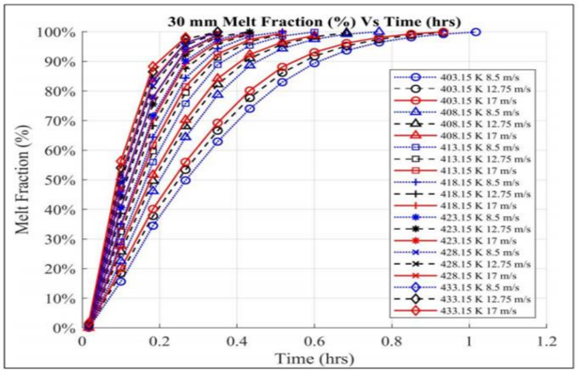
Time vs melt fraction graph for complete melting and solidification with varying Ti and Vi, for 60mm Diameter



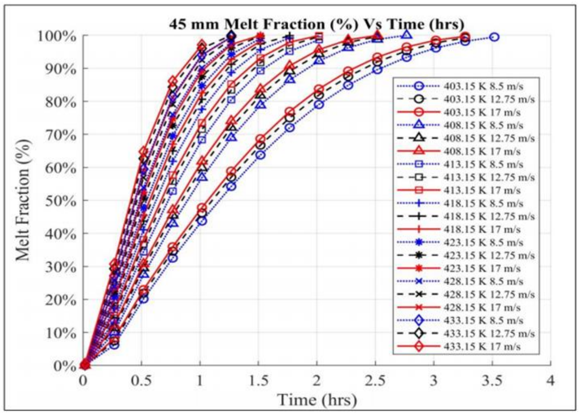
FURTHER VARIATIONS IN ‘Ti’

Since the ‘Ti’ was varied with an increment of 10 K from 403.15 K, we obtained a total of 27 cases considering the simultaneous change in velocities and diameters. To obtain an analytical correlation the inlet temperature was varied further within this range with increments of 5 K, in order to obtain a more inclusive dataset to determine the variations in time taken for melting, as can be seen in the Figures.

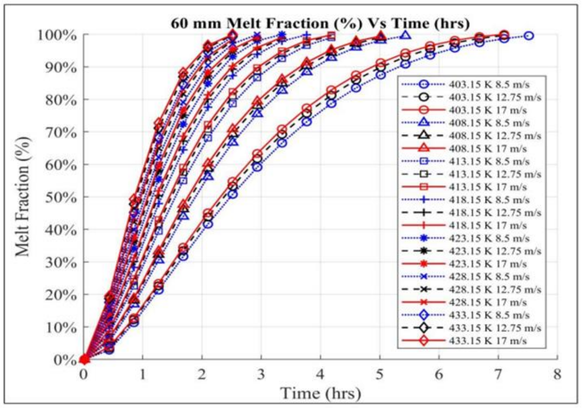
30 mm Diameter – Time Taken for Melting with 5 K Increment in Ti



45 mm Diameter – Time Taken for Melting with 5 K increment in Ti



60 mm Diameter – Time Taken for Melting with 5 K increment in Ti



RESULTS AND DISCUSSION

VARIATION IN TIME TAKEN FOR MELTING AND SOLIDIFICATION

1. The time taken for melting decreases with increase in ‘Ti’, since more heat is available for storage due to higher temperature difference in the initial temperature of HTF and the initial temperature of PCM. This holds true for time taken for solidification as well, i.e. the time taken for solidification decreases for lower ‘Ti’ values.
2. The time taken for melting or solidification decreases with increase in ‘Vi’, since the heat transfer is accelerated with increase in inlet velocity. During solidification, heat rejected by the PCM is accelerated with increase in inlet velocity.
3. The time take for melting and solidification increases significantly with increase in diameter for the same set of inlet conditions. The volume

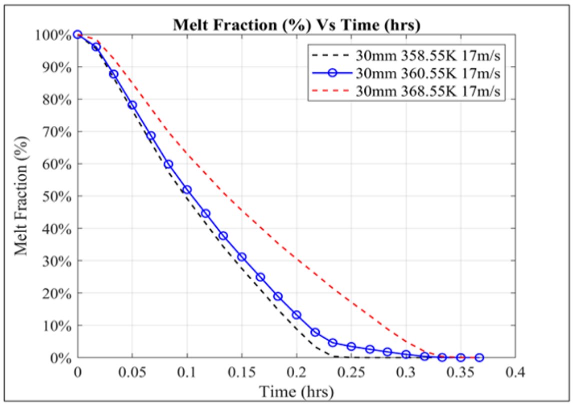
of PCM stored increases proportionally to the square of the diameter which requires more time for melting or solidification.

4. The difference in 3-D and 2-D simulations was observed to be negligible, for the axisymmetric model considerations, which effectively indicates that 2-D cases are adequate to model the melting and solidification processes for vertical annular cylinders.

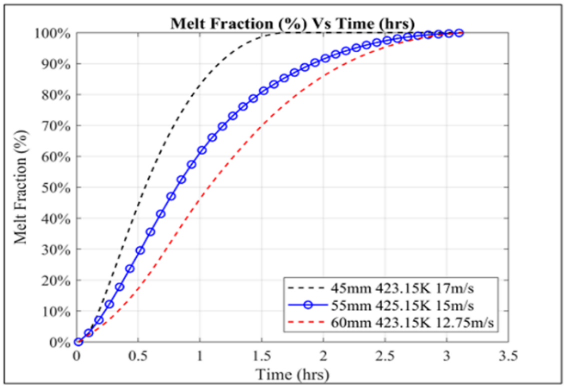
6.2 INTERPOLATION MODEL RESULTS

Different cases were considered to determine the values of melt fraction, or the amount of PCM melted, with variations in ‘(Do)pcm’, ‘Ti’, and ‘Vi’. The model can predict the required amount of time for charging or discharging, with variations in any of the parameters. Some of the cases tested have been shown in the figures below.

Case A: ((Do)pcm = 30 mm), (Ti = 360.55 K), and (Vi = 17 m/s)



Case B: ((Do)pcm = 55 mm), (Ti = 425.15 K), and (Vi = 15 m/s) Case B results for melting or charging



Case C: ((Do)pcm = 60 mm), (Ti = 375.55 K), and (Vi = 10 m/s) Case C results for solidification or discharging.

IV. CONCLUSION

After performing this experiment on melting and solidification of Erythritol PCMs with variations in operating conditions and geometric parameters able to analyse that time taken for melting decreases as Ti increases. Comparatively, the time taken for melting does not increase as significantly with increase in velocity and vice versa for solidification. Able to validate finite Volume simulations against experimental results, using CFD software Fluent 18.2, to understand the significance of variations in parameters, the dynamics of phase change behavior, and heat transfer involved in the phase change process. Along with this, the developed a method to predict performance of LTES devices over defined time periods, by developing models with MATLAB interpolation techniques and commercial simulation software ANSYS archive.

REFRENCES

[1] I. Dincer and M. A. Rosen, “Thermal energy storage,” Building Services Engineering Research & Technology, 2011.

[2] H. Shmueli, G. Ziskind, and R. Letan, “Melting in a vertical cylindrical tube: Numerical investigation and comparison with experiments,” Int. J. Heat Mass Transf., vol. 53, no. 19–20, pp. 4082–4091, May 2010.

[3] M. Longeon, A. Soupart, J. F. Fourmigué, A. Bruch, and P. Marty, “Experimental and numerical study of annular PCM storage in the presence of natural convection,” Appl. Energy, vol. 112, pp. 175–184, Jun. 2013.

[4] A. J. Parry, P. C. Eames, and F. B. Agyenim, “Modeling of thermal energy storage shell-and-tube heat exchanger,” Heat Transf. Eng., vol. 35, no. 1, pp. 1–14, 2014.

[5] ANSYS, “ANSYS Fluent User’s Guide,” vol. 15317, Nov. 2013.