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EXPERIMENTAL AND NUMERICAL STUDY ON THE MELTING BEHAVIOUR OF A PHASE CHANGE MATERIAL IN BUOYANCY DRIVEN FLOWS

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Abstract. In the present work, a thorough experimental and numerical study is performed to understand the melting behaviour of phase change materials (PCMs) in buoyancy driven flows. Paraffin (Rubitherm® RT35) is used as PCM which occupies 90% of the capsule volume and the rest is occupied by air. In the experimental trials, one of the side walls is heated to a constant temperature above the liquidus temperature of PCM and all other walls are insulated. The influence of different temperatures at the heated wall on the transport of melt-fraction is investigated by monitoring the melt-front at different time intervals. The experimental results are compared with the numerical model which is developed in OpenFOAM® framework. The paraffin-air multiphase system is solved using a volume of fluid (VOF) approach with phase-fraction based interface capturing. The fixed grid mathematical model based on enthalpy-porosity is employed to capture the transport of melt-fraction. A new treatment to enthalpy equation overcomes the necessity to iteratively solve for the coupled enthalpy and melt-fraction fields, thereby reducing the computational cost. The melt-front captured by the numerical model for different time intervals are compared with the experimental results and are found to be in excellent agreement.

1 INTRODUCTION

The phenomena of melting and solidification inherently occur in various industrial processes like casting, forming and production of metals and glass [1]. In some other applications like latent heat thermal storage devices in solar power stations and buildings, melting and solidification are utilized to store energy [2]. Quite often, the processes/systems involve more than one fluid making a systematic study through experiments or numerical methods more complex and challenging. Nonetheless, the study of melting and solidification phenomena give greater control over the processes and help to achieve optimization and higher efficiency. Hence in the current study, a numerical model to accurately pre-

dict the transport of melt-front in multiphase systems is developed and validated with experiments.

Current numerical models to predict the melt-front can be categorized into two groups: deforming and fixed grid schemes [3]. Deforming grid method requires continuous update of spatial discretization to track the melt front, which introduces programming and modelling complexities at higher computational costs. On the other hand fixed grid method tracks the melt-front through the enthalpy distribution, which is mathematically simpler to implement. Voller et al. [4] was the first to introduce the enthalpy method for fixed grids. Brent et al. [5] extended the enthalpy method to include porosity sink term disabling velocities in solid region. Voller and Swaminathan [6, 7] implemented a general enthalpy-porosity method to iteratively update the melt-fraction from temperature. Samarkii et al. [8] studied phase change with both fixed and deforming grid methods, outlining the advantages and disadvantages of both methods. Hu and Argyropoulos [9] and Basu and Date [10] reviewed in detail various improvements to the enthalpy-porosity method carried out by numerous researchers which addressed certain shortcomings of the fixed grid approach.

Assis et al. [11] performed a numerical and experimental study of melting of phase change material (PCM) enclosed in a spherical geometry with air on the top. The numerical simulations were performed using a commercial computational fluid dynamics (CFD) code ANSYS FLUENT 6.0 with the enthalpy-porosity method of Voller and Swaminathan [6]. The interface between air and PCM was solved using volume of fluid (VOF) approach. Numerical treatment of the change in density is not clearly stated in the paper and an axis of symmetry was assumed for simulation purposes. Shmueli et al. [12] conducted a detailed numerical study of the influence of the mushy zone constant on the transport of melt-interface in a vertical tube containing air above PCM. The modelling approach was similar to Assiss et al. [11] and a commercial CFD code ANSYS FLUENT 6.2 was employed for simulation purposes. Rösler and Brüggemann [13] studied PCM melting in Shell-and-Tube type geometry where the discontinuous enthalpy function was approximated to a continuous error function, thus eliminating the necessity to iteratively solve for melt fraction.

In 2013, Kim et al. [14] numerically modelled PCM melting enhanced by deformation of a liquid-gas interface. Volume of fluid technique was employed to track the liquid-gas interface and enthalpy-porosity method to track the melt-front. The study was undertaken using commercial CFD code FLUENT 12.0 and simulations were carried out for a 2-dimensional geometry. Galione et al. [15, 16] studied melting of n-Octadecane enclosed inside a spherical capsule using fixed grid phase-change model with variable material properties. Richter et al. [17] numerically simulated solidification in mould filling using VOF and enthalpy-porosity method. A cut-off parameter for Darcy porosity constant was modelled to make a more robust algorithm. Kozak und Ziskind [2] incorporated close-contact melting to their single fluid phase change model which fully captures the bulk solid motion that may occur during melting. The bulk solid motion is calculated by solving a detailed force balance equation in addition to enthalpy-porosity equations. Kasibhatla et al. [18] developed a variable viscosity model for single fluid system to simulate the effects

of settling of the solid phase.

From the above literature review, it is evident that very few studies [11, 12, 14, 17] are available for melting problems in multiphase systems. And almost all studies employ iterative techniques to solve the coupled enthalpy and melt-fraction fields. In the present work, a detailed numerical modelling in a multiphase framework is implemented to predict the behaviour of melting in buoyancy driven flows. Volume of fluid approach with phase-fraction based interface capturing is employed to solve the multiphase system and melting is modelled with enthalpy-porosity method. A numerical treatment to the enthalpy-porosity method is implemented to eliminate the requirement to solve the coupled enthalpy and melt-fraction fields iteratively. The numerical model is validated with several experiments conducted using paraffin RT35 from Rubitherm®, as PCM fluid and air as the secondary fluid.

2 EXPERIMENTAL SET-UP

An experimental set-up was designed and built in order to investigate the melting process of a phase change material (PCM). Figure 1 shows the schematic of the experimental set-up. Plexiglass material is used to build the capsule with dimensions 100 mm x 100 mm x 100 mm and is filled with PCM material. An aluminium heating plate of 16 mm thickness is fixed on the inner side of the left wall of the plexiglass capsule. A temperature controller is connected to the heater to maintain a constant temperature during the experimental trials. All walls are insulated using a polystyrol material which is then surrounded by air, except for the front wall which is open for images of the melt front to be taken. A DSLR camera (Nikon D5200) mounted on a tripod and equipped with a timer function is set up at a good distance from the front wall of the capsule to capture sharp and focused images. The timer is set to 300s interval and for a total duration of 70 minutes, which is the duration of the experimental trials. Paraffin RT35 from Rubitherm® is used as PCM which is filled up to 90% of the volume of the capsule. The height of the paraffin is measured before the start of each experimental trial. The temperature controller is set to a constant temperature at the start of each trial. Experiment trials are conducted for heating temperatures of 44 °C, 47 °C and 50 °C. The images are analysed using a plot digitizer tool[1] to mark the solid-melt interface of the paraffin.

3 MATHEMATICAL MODEL

The detailed mathematical model to solve melting problems in multiphase framework is outlined in this section. For the mathematical modelling, the following assumptions are considered:

1. Both fluids are considered immiscible with a sharp interface.

2. Air is treated as an incompressible fluid and Boussinesq approximation is made for PCM.

[1] http://arohatgi.info/WebPlotDigitizer/app

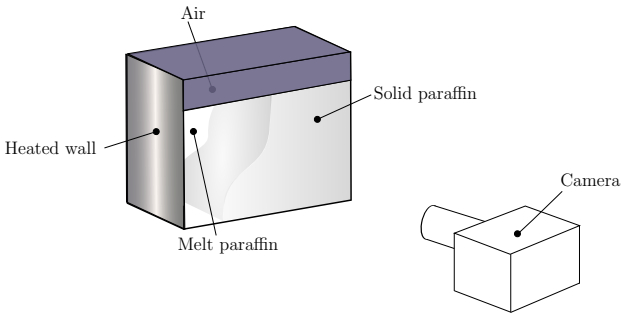


Figure 1: Schematic of the experimental set-up

3. Laminar flow conditions for both fluids.

4. Viscous heating and kinetic energy terms are neglected.

5. Material properties of both fluids are independent of temperature.

6. Surface tension effects are neglected.

With the above mentioned assumptions, the paraffin-air two phase system is described using the volume of fluid (VOF) approach, which is a fixed grid phase-fraction based interface capturing method. In this approach, a marker function called phase-fraction α is defined to locate the interface between the fluids. For example, in a two fluid system, a phase-fraction of 1 in a cell denotes fluid 1, a phase-fraction of 0 denotes fluid 2. All cells having a phase-fraction between 0 and 1 contains the interface. More on the numerical model can be found in [19]. The conservation equations for the paraffin-air system are :

Continuity:

$$\frac{\partial(\alpha_1)}{\partial t} + \frac{\partial(\alpha_1 u_i)}{\partial x_i} = 0 \tag{1}$$

Momentum:

$$\frac{\partial(\rho u_i)}{\partial t} + \frac{\partial(\rho u_i u_j)}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j}\left[\mu\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)\right] + S_D \tag{2}$$

Energy:

$$\frac{\partial(\rho h)}{\partial t} + \frac{\partial(\rho u_i h)}{\partial x_i} = \frac{\partial}{\partial x_i}\left(k\frac{\partial T}{\partial x_i}\right) \tag{3}$$

where u_i, ρ, μ and k are the velocity components, mixture density, dynamic viscosity and thermal conductivity, respectively. The phase-fraction α is defined as:

$$\alpha = \begin{cases} 0 & = \text{air} \\ 0 < \alpha < 1 & = \text{cell contains interface} \\ 1 & = \text{paraffin} \end{cases} \tag{4}$$

In the phase-change region inside the capsule, enthalpy-porosity approach is employed. The specific enthalpy h, of the mixture is defined as:

$$h = C_p T + \alpha \gamma L \tag{5}$$

where C_p is the mixture specific heat capacity and L is the latent heat of melting of the PCM material. The liquid fraction γ is purely dependent on the temperature T and is modelled as a step function with a linear behaviour between the solidus and the liquidus temperature, T_s and T_l, respectively as shown below:

$$\gamma = \begin{cases} 0 & if \quad T < T_s \\ \frac{T - T_s}{T_l - T_s} & if \quad T_s \leq T \leq T_s \\ 1 & if \quad T > T_l \end{cases} \tag{6}$$

Applying equation 6 to equation 3, we obtain the energy conservation equation in terms of temperature T, as shown below:

$$\frac{\partial(\rho T)}{\partial t} + \frac{\partial(\rho u_i T)}{\partial x_i} = \frac{\partial}{\partial x_i}\left(\frac{k}{C_p}\frac{\partial T}{\partial x_i}\right) - \alpha_1 \frac{L}{C_p}\left[\frac{\partial(\rho\gamma)}{\partial t} + \frac{\partial(\rho u_j \gamma)}{\partial x_j}\right] \tag{7}$$

The effect of solidification on momentum transport is taken into account by the Darcy-type source term S_D, in equation 8. The pressure gradient inside the mushy zone is coupled to the permeability using the modelling of Kozeny–Carman equation [3]. With the restriction of the Kozeny–Carman equation to be applicable in PCM region only, the source term S_D can be expressed as:

$$S_D = \alpha\ C \frac{(1-\gamma)^2}{\gamma^3 + \epsilon} u_i \tag{8}$$

where C is a large constant to describe the behaviour of the flow in the mushy zone. The term ϵ is a small numerical constant to avoid division by zero. The source term S_D dominates all other terms in the momentum equation when the melt fraction is 0 and thereby switches off all velocities in the solid region. On the other hand, when the melt fraction is 1, the source term vanishes.

Applying the mixture approach in the framework of the continuum model, the physical properties are determined as

$$\phi = \alpha(\gamma\phi_{melt} + (1-\gamma)\phi_{solid}) + (1-\alpha)\phi_{air} \tag{9}$$

where, ϕ can be substituted for μ, C_p and k, the mixture dynamic viscosity, specific heat capacity and thermal conductivity, respectively. For density, the Boussinesq approximation is applied to PCM region and air is assumed to be incompressible. With the aforementioned assumptions, the mixture density is defined as:

$$\rho = \alpha\left(\gamma\rho_{melt}(1-\beta(T-T_l)) + (1-\gamma)\rho_{solid}\right) + (1-\alpha)\rho_{air} \tag{10}$$

where β is the thermal coefficient of volume expansion of PCM.

The melt fraction and energy equations are coupled in a non-linear fashion requiring the enthalpy-porosity method to solve for both equations in a separate sub-cycle [6, 17]. The iterative process can sometimes be computationally exhaustive. To overcome this iterative process, a numerical treatment is implemented with a switch function f. The function checks whether the temperature in the cell is between the solidus and liquidus temperature or outside. Depending on the temperature range, the melt fraction transport is switched on and off. The function is described below:

$$f = \begin{cases} 1 & if \quad T_s \leq T \leq T_s \\ 0 & if \quad T > T_l \text{ or } T < T_s \end{cases} \tag{11}$$

With the function f, an implicit update of melt-fraction is implemented similar to the one described by Voller and Swaminathan [6]. This approach eliminates the necessity to iterate between the energy equation and melt-fraction update, thereby reducing the computational time significantly.

The introduced mathematical model is implemented in OpenFOAM® 4.0, an open source computational fluid dynamics (CFD) software. The convective terms in the conservation equation for momentum and energy are discretized with second order schemes. PIMPLE algorithm, which combines PISO and SIMPLE algorithms, is used to solve the pressure-velocity coupled Navier–Stokes equation. The transport equation for phase-fraction is solved using MULES (Multidimensional Universal Limiter with Explicit Solution) [20]. The convergence criteria for mass, momentum and energy equations are set by the normalized residual values less than 10^{-10}. Grid independence study is done by comparing results of three grids with cell lengths of $1.5cm$, $1cm$ and $0.75cm$. The numerical results show that the relative errors of melt fraction are less than 4% between the grid with $1cm$ and $0.75cm$ cell length. A study of the influence of time step on the numerical results are undertaken with time step sizes of 10^{-2}s, 10^{-3}s and 10^{-4}s. The relative errors of melt fraction are found to be less than 2% between the time step size of 10^{-3}s and 10^{-4}s. Therefore a grid with $1cm$ cell length and a time step size of 10^{-3}s is considered for all simulations.

4 RESULTS AND DISCUSSION

In this section, the numerical results of the paraffin-air melting are presented along with the influence of different heating temperatures on the melt transport. Additionally a validation of the implicit numerical treatment to update the melt fraction which is discussed in the previous section is presented.

For the validation of the implicit melt-fraction update using the numerical treatment through the switch function (equation 11), the experiments of Gau and Viskanta [21] are considered. In the experiments, Gallium with a melting point of 29.78 °C and a latent heat of melting of 80 160 J/kg was used as PCM. The density, dynamic viscosity, thermal conductivity, specific heat capacity and volumetric thermal expansion coefficient of liquid Gallium are considered as $6093\,\mathrm{kg/m^3}$, $0.001\,81\,\mathrm{Pa\,s}$, $32\,\mathrm{W/(m\,K)}$, $381.5\,\mathrm{J/(kg\,K)}$ and $1.2 \times 10^{-4}/\mathrm{K}$, respectively. The schematic of the experimental set-up is depicted in figure 2a and the comparison of the simulation results with the experiment in figure 2b. The melt fronts of the simulation are in excellent agreement with the experimental result, thus validating the enthalpy-porosity method with implicit numerical treatment.

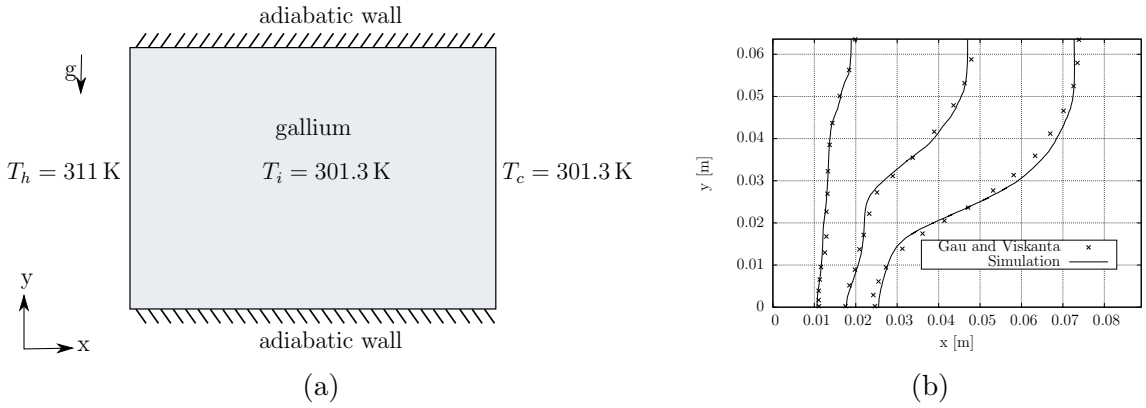


Figure 2: Validation of computational model: (a) schematic of Gallium experiments performed by Gau and Viskanta [21], (b) Melt-front comparison between simulation and experiments of Gau and Viskanta [21].

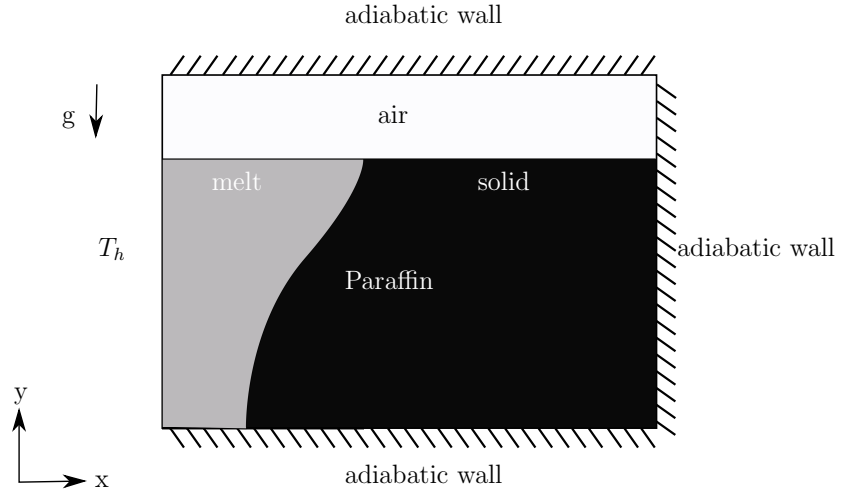


Figure 3: Schematic of the computational domain.

Density (ρ)	780 kg/m^3
Specific heat capacity (C_p)	2000 J/(kg K)
Dynamic viscosity (μ)	0.0247 Pa s
Thermal conductivity (κ)	0.2 W/(m K)
Latent heat of fusion (L)	160 000 J/kg
Solidus temperature (T_s)	34 °C
Liquidus temperature (T_l)	35 °C
Volumetric thermal expansion coefficient of melt (β)	0.001/K

Table 1: Physical properties of Rubitherm® RT35.

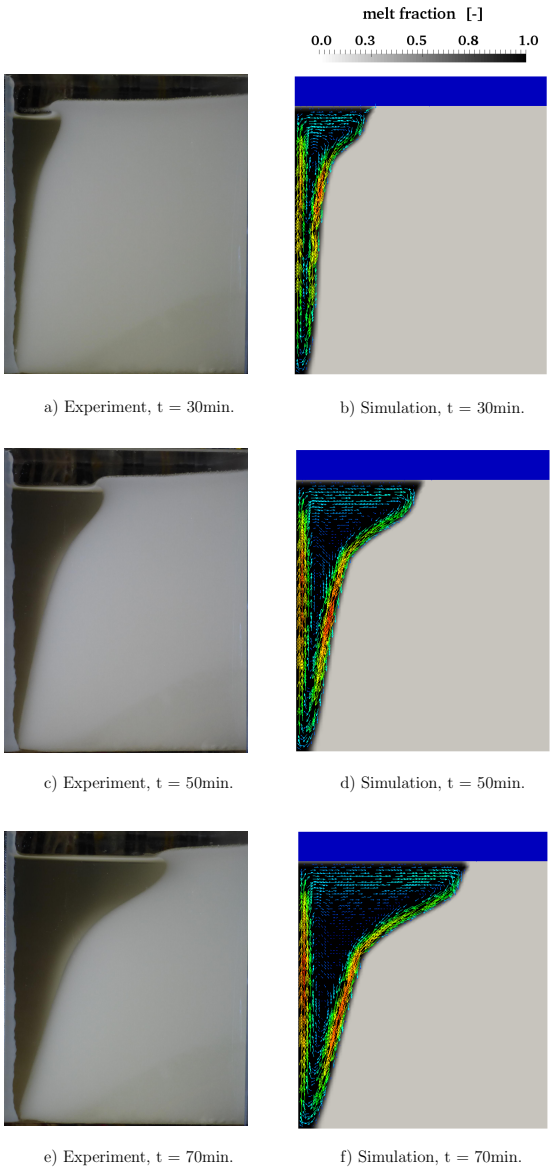
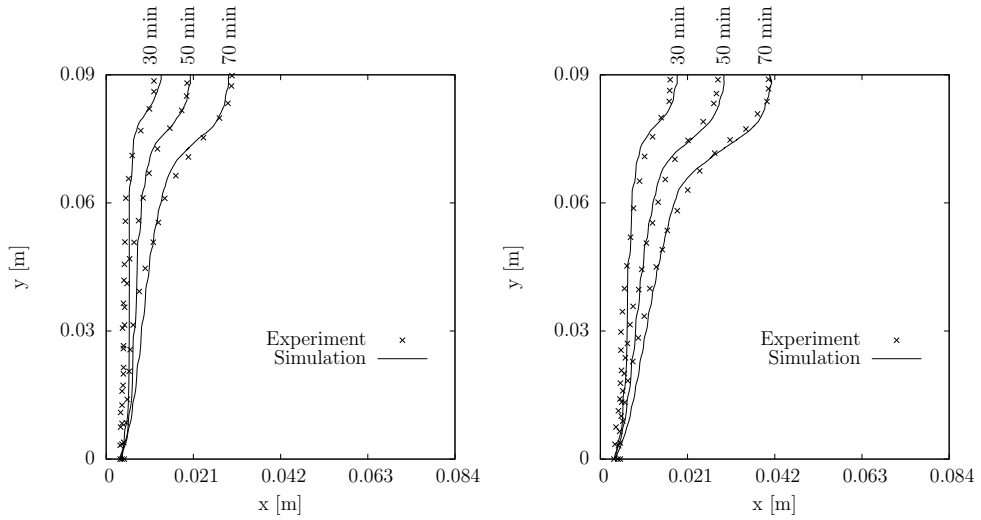
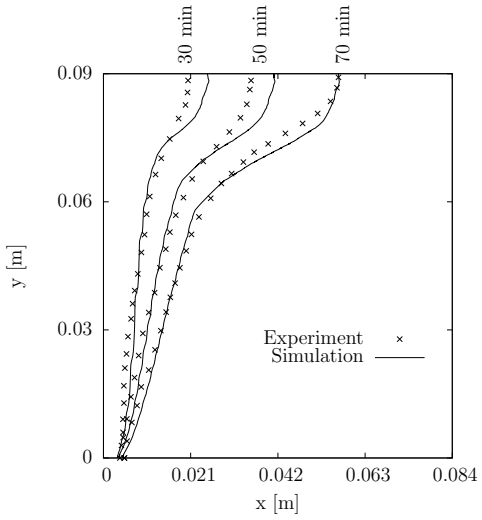


Figure 4: Comparison of the melt-front position ($T_h = 50\,°C$) at different time intervals between experiment (a, c, e) and simulation (b, d, f) with velocity vector plots.

The above validated enthalpy-porosity model with numerical treatment is implemented in a multiphase framework and simulations are carried out for the paraffin-air system. The schematic of the numerical domain can be seen in figure 3. The left wall of the domain is set to a fixed temperature and all other walls are considered to be perfectly adiabatic. In order to reduce the computational effort, all simulations are carried out with 2D assumption. The physical properties of the paraffin, Rubitherm® RT35 are listed in table 1. The mushy zone constant (C) is considered as 1×10^5 [11]. The density, dynamic viscosity, thermal conductivity and specific heat capacity of air are considered to be $1.177\,\mathrm{kg/m^3}$, $1.83 \times 10^{-5}\,\mathrm{Pa\,s}$, $0.0258\,\mathrm{W/(m\,K)}$ and $1006\,\mathrm{J/(kg\,K)}$, respectively.



(a) $T_h = 44\,^{\circ}\mathrm{C}$ (b) $T_h = 47\,^{\circ}\mathrm{C}$



(c) $T_h = 50\,^{\circ}\mathrm{C}$

Figure 5: Comparison of melt-fronts between experiments and simulations at different time intervals for a) $T_h = 44\,^{\circ}\mathrm{C}$, b) $T_h = 47\,^{\circ}\mathrm{C}$ and c) $T_h = 50\,^{\circ}\mathrm{C}$.

Figure 4 shows a comparison of the position of melt-fronts between experiment and simulations. The left wall here is maintained at a constant 50 °C and the initial temperature of the paraffin is set to 23 °C which was measured before the start of the experiment. At time $t = 30min$, the transport of melt front through buoyancy can be seen, though the effect of heat transport through conduction dominates at initial stages. With increased melting, the convective transport through buoyancy increases which is evident at $t = 50min$ and $70min$ in figure 4. The melt-front predicted by numerical simulations at all time intervals are qualitatively in excellent agreement with the experimental results.

A comparison of melt fronts between experiments and simulations for $T_h = 44\,°C$, $T_h = 47\,°C$ and $T_h = 50\,°C$ is shown in figure 5. The solid-melt interface from experiments are extracted using the digitizer tool mentioned earlier. For all the cases, the comparison is done for the time intervals of $t = 30min, 50min$ and $70min$. For temperatures $T_h = 44\,°C$ and $T_h = 47\,°C$, the melt front of experiments and simulations can be seen to overlap on each other. For $T_h = 50\,°C$, the numerical results can been seen to slightly over estimate the melt front close to the paraffin-air interface for the time intervals $t = 30min$ and $t = 50min$. But the melt-front prediction of the simulation for $t = 70min$ coincides to a very good extent with the experiments, particularly close to the paraffin-air interface. A possible explanation for the deviation seen at $t = 30min$ and $t = 50min$ for the case of $T_h = 50\,°C$ can be the incompressible fluid assumption for air. The consideration of physical properties of paraffin to be temperature independent, especially viscosity, can be another reason for the slight difference in melt-front prediction. Overall the melting model for multiphase paraffin-air system is shown to be in excellent agreement with the experiments.

5 CONCLUSIONS

The transport of melt-front in buoyancy driven multiphase system is systematically studied through experiments and numerical simulations. Paraffin RT35 from Rubitherm® is considered as the phase change material which is filled up to 90% of the capsule volume and the rest is occupied by air. Experiments are conducted for three different constant heating temperatures, $T_h = 44\,°C$, $47\,°C$ and $50\,°C$. The experimental results are compared with the numerical simulations modelled using the combined volume of fluid approach for paraffin-air multiphase system and enthalpy-porosity method for melting of paraffin. An implicit numerical treatment for melt-fraction update is implemented which reduces the computational cost significantly. The numerical results are seen to be in excellent agreement, qualitatively and quantitatively with the experiments, thus validating our mathematical model to predict melting/solidification phenomenon in multiphase flows.

In the next step, the numerical model is planned to be extended to include temperature variable physical properties for all phases. Additionally, modelling of air as a compressible fluid to successfully simulate the effect of volume changes on melt transport is planned.

6 ACKNOWLEDGEMENT

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