Revisiting tin melting for phase change model verification

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Abstract. Model verification is necessary before numerical models can be applied to produce meaningful results. For solid-liquid phase change modelling involving convection, pure gallium and tin melting have been widely used as reference for verification. It was later found that contrasting observations have been reported on the flow structure of both metals in the liquid region during the phase change process. Some researchers have reported monocellular while others reported multicellular structures in past works. In this work, tin melting problem was revisited by extending the results to flow structure visualization with Line Integral Convolution (LIC) plots to confirm the flow structure for tin melting thus pure metals in general. Enthalpy-porosity formulation coupled with Finite-Volume Method (FVM) was used to solve the set of governing equations which represented the problem at Prandtl Number = 0.02, Stefan Number = 0.01 and Rayleigh Number = 2.5×10^5. The location of solid-liquid interface and LIC plots at different times were presented. At initial state, the solid-liquid interface was closely similar for all grid sizes but as time progresses, finer grids provided improved solutions as expected. Reasonable fine grid size must be selected for solid-liquid phase change models to ensure complete physics of the problems are captured and eventually yield acceptable numerical results. The LIC plots confirmed that the flow structure is multicellular. Future phase change models referring to pure metal melting problem for verification should obtain similar flow structure to be considered acceptable.

1. Introduction

Phase change processes occur daily in our lives. It can either be solid-liquid, liquid-gas or solid-gas depending on the processes involved in a particular application. Solid-liquid phase change is widely investigated because it involves various engineering applications such as Phase Change Material (PCM) charging/discharging for heat storage/removal [1], material casting for customized manufacturing and deformation of materials by thermal processing [2]. Most studies on this phase change process applies numerical models to enable various conditions with different parameters to be investigated. These phase change models must be verified before it can be applied to produce meaningful results.

Since the past 30 years, pure metal melting has been used for solid-liquid phase change model verification. In the earliest experimental work by Gau and Viskanta [3], gallium was melted in a

rectangular cavity at various aspect ratios driven by vertical isothermal hot wall. Later, Brent et. al. [4] obtained good agreement with this work by solving the similar problem numerically. Next, in another experimental work by Wolff and Viskanta [5], tin was melted in the same geometry. Since then, these works have been used for model verification purposes by various numerical studies involving solid-liquid phase change with convection where a number of researchers chose to refer gallium [4, 6-9] while others opted for tin [9-15].

Several researchers argued that the observations and findings on the general flow structure of pure metals during melting for these early works were not consistent. Dantzig [6] and Stella [8] argued that the nature of the flow structure in the liquid region was different for gallium during melting process. They found out that the flow structure should be multicellular which was in contrast to monocellular as mentioned by Brent et. al. [4]. As for tin, Ho and Chu [10] obtained monocellular structure while some others [11-13] supported the argument that the flow structure should be indeed multicellular.

Alexiades et. al [16] and Hannoun et. al [17] have tried to explain grid selection and discretization schemes as the possible reasons for these discrepancies while Cerimele et. al [7] have raised concern on the method applied during the early experiment conducted. These works agreed that the flow structure in the liquid region for pure metal melting must be multicellular. Later, a reference solution for such problem have been suggested [18]. Most of these mentioned works have used streamlines to visualize the flow structure in the domain. However in this study, tin melting was revisited by extending the flow structure visualization with Line Integral Convolution (LIC) plots.

2. Problem Physics and Numerical Model

2.1. Computational Domain

The computational domain is described below in Figure 1:
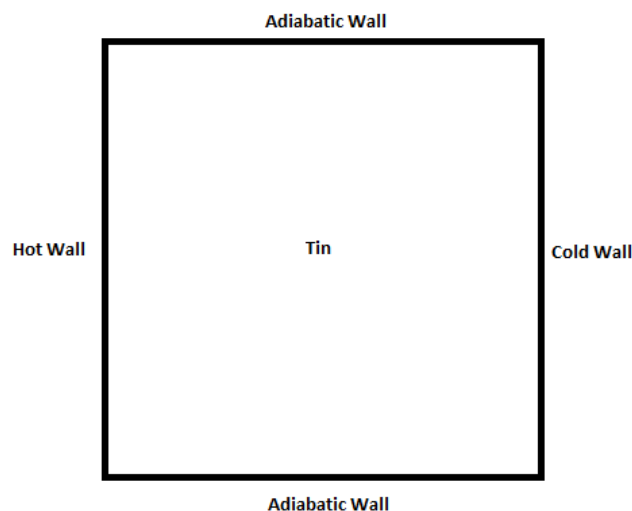

Figure 1. Computational Domain.

For this case of tin melting, two-dimensional computational domain with two horizontal adiabatic walls and two vertical isothermal walls were considered. The tin was initially in a solid state at T_m (no undercooling) and the left vertical wall set at a higher temperature, T_{hot} while the right vertical wall maintained at a lower temperature, T_{cold}. The temperature difference will eventually melt the tin and a liquid region will start to exist on the left side of cavity initiating convective effect due to buoyancy presence. This liquid region will replace the solid region as time progresses and the cellular cell will grow until the solid completely liquefies. Parameters for tin are given in Table 1. PIMPLE algorithm [19] which is a combination of Semi-Implicit Method for Pressure Linked Equation (SIMPLE) and

Pressure-Implicit of Split Operations (PISO) was used to solve the set of governing equations which represent the problem in OpenFOAM. Modifications were made to 'buoyantBoussinesqPimpleFoam' which is an existing solver in OpenFOAM to replicate the physics of the problem. In this work, the dimensionless numbers set were Prandtl Number = 0.02, Stefan Number = 0.01 and Rayleigh Number = 2.5 x 10^5.

Table 1. Tin Parameters for Simulation [18].

Density, ρ	7500 kg/m^3
Thermal Conductivity, k	60 W/m.K
Thermal expansion coefficient, β	2.67 x 10^{-4}
Melting Temperature, T_m	505 K
Hot Wall Temperature, T_{hot}	508 K
Cold Wall Temperature, T_{cold}	505 K
Domain dimension (Height x Width)	10 cm x 10 cm
Latent heat of fusion, L	60000 J/kg
Dynamic Viscosity, μ	6 x 10^{-3}kg/m.s
Specific heat capacity, C_p	200 J/kg.K

2.2. Enthalpy-Porosity Formulation

By assuming that the substance undergoing solid-liquid phase change is Newtonian and incompressible, system of equations for natural convection coupled with phase change can be used to simulate the problem by applying enthalpy-porosity formulation. The continuity, momentum and energy conservation equations are written as follows:

Continuity equation:

$$\nabla.(u) = 0 \tag{1}$$

Momentum equation:

$$\frac{\partial(\rho u)}{\partial t} + (\rho u.\nabla)u = \nabla.(\mu\nabla u) - \nabla p - C\frac{(1-\varepsilon)^2}{\varepsilon^3+b}u + \rho\beta g(T - T_{ref}) \tag{2}$$

Energy equation:

$$\frac{\partial(\rho C_p T)}{\partial t} + \nabla.(\rho C_p uT) = \nabla.(k\nabla T) - \frac{\partial[\rho\varepsilon L]}{\partial t} \tag{3}$$

Value of C depends on the morphology of the porous media while b is a small computational constant to avoid division by zero. Value of ε represents the porosity or liquid fraction of each cell. Since the phenomena is natural convection in the liquid region, buoyancy is represented by Boussinesq approximation in y-direction momentum equation. The latent heat source term is the volumetric latent heat rate of change of in the energy equation. The governing equations were discretized by Finite Volume Method (FVM). This is explained in detail in previous work [20].

3. Result and Discussion

3.1. Solid-Liquid Interface

The solid-liquid interface were compared with the reference solution for phase change with convection by Hannoun [18]. The results at different grids 100x100, 200x200 and 400x400 were compared at different times as shown in Figure 2. At initial state, the solid-liquid interface was closely similar for all grid sizes. At 100s, the interface is a straight vertical line and identical for all grids although coarser grid produces less accurate line. As time progresses, finer grids resulted in smoother line and improved accuracy. However, further finer grid than 400x400 provided insignificant improvement on result accuracy. Therefore, 400x400 grid was applied for further simulations.
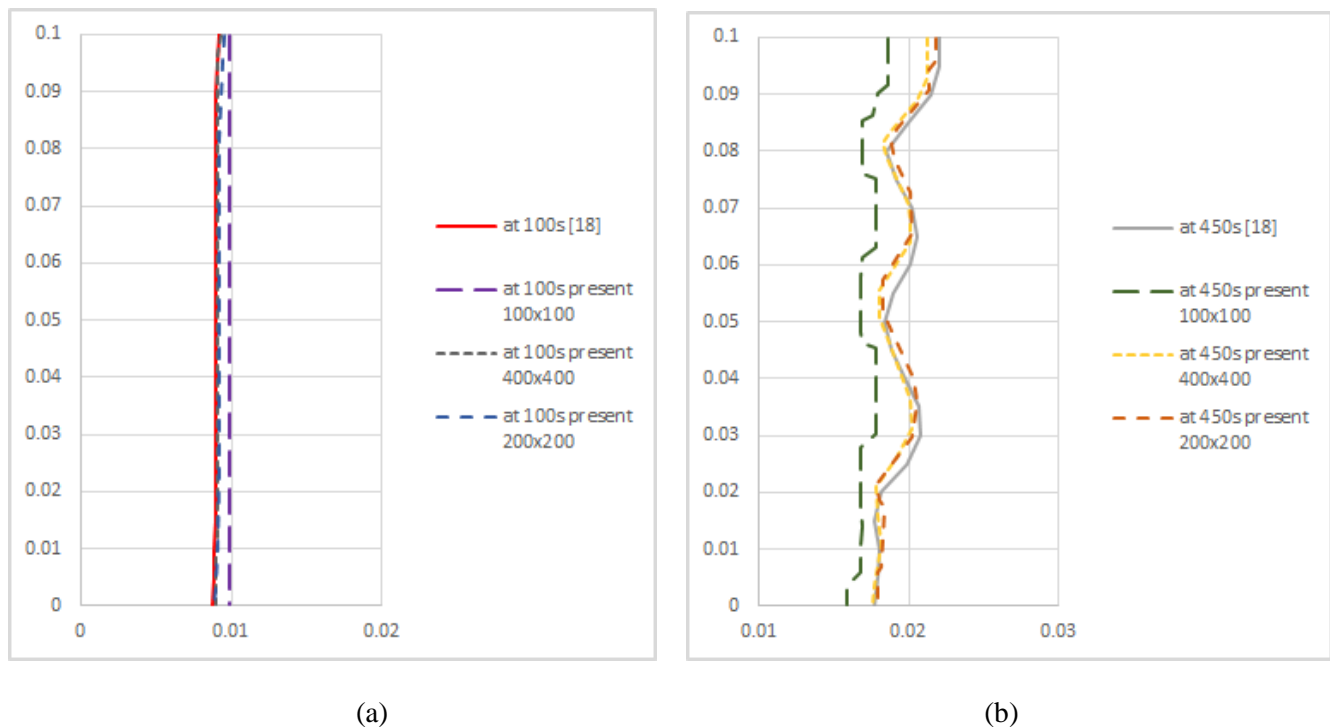

(a)   (b)

Figure 2. Solid-liquid interface location for tin melting at (a) 100s and (b) 450s using different grids.

Observation at 100s indicates that during the early part of melting process, conduction still dominates the heat transfer mechanism. At 450s, the interface line becomes wavy and protruding bumps becomes obvious indicating more dominant presence of convection as time progresses.

The location of solid-liquid interface at different times 100s, 200s and 450s are shown in Figure 3. As melting progresses, the interface moves from left to right as expected. The comparison with reference solution indicated very good agreement.

3.2. Flow Structure in Liquid Region

Next, the LIC plots of liquid region flow structure at different times were shown in Figure 4. The number of protruding bumps with respect to solid-liquid interface mentioned earlier indicates the number of cellular rolls present as shown in the flow structures at 250s, 400s and 600s. The flow structures were found to be always multicellular although the smaller rolls eventually merge to form larger rolls as time progresses.
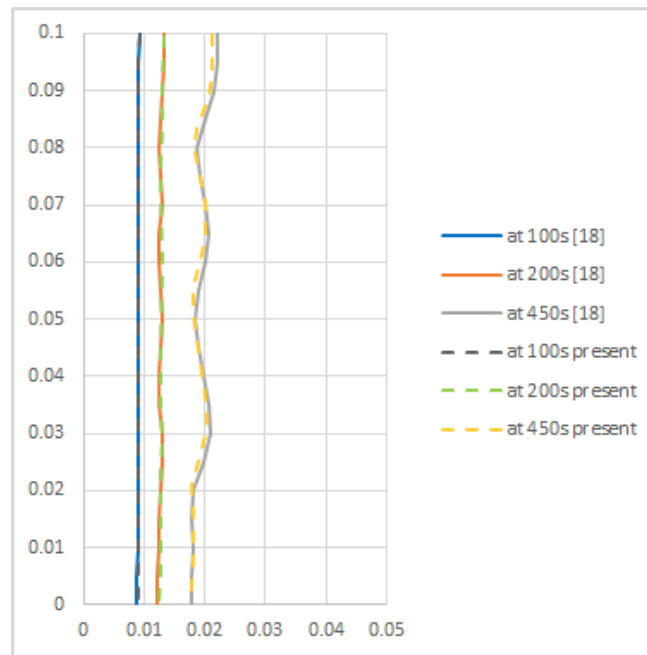
Figure 3. Solid-liquid interface location for tin melting at different times using 400x400 grid.
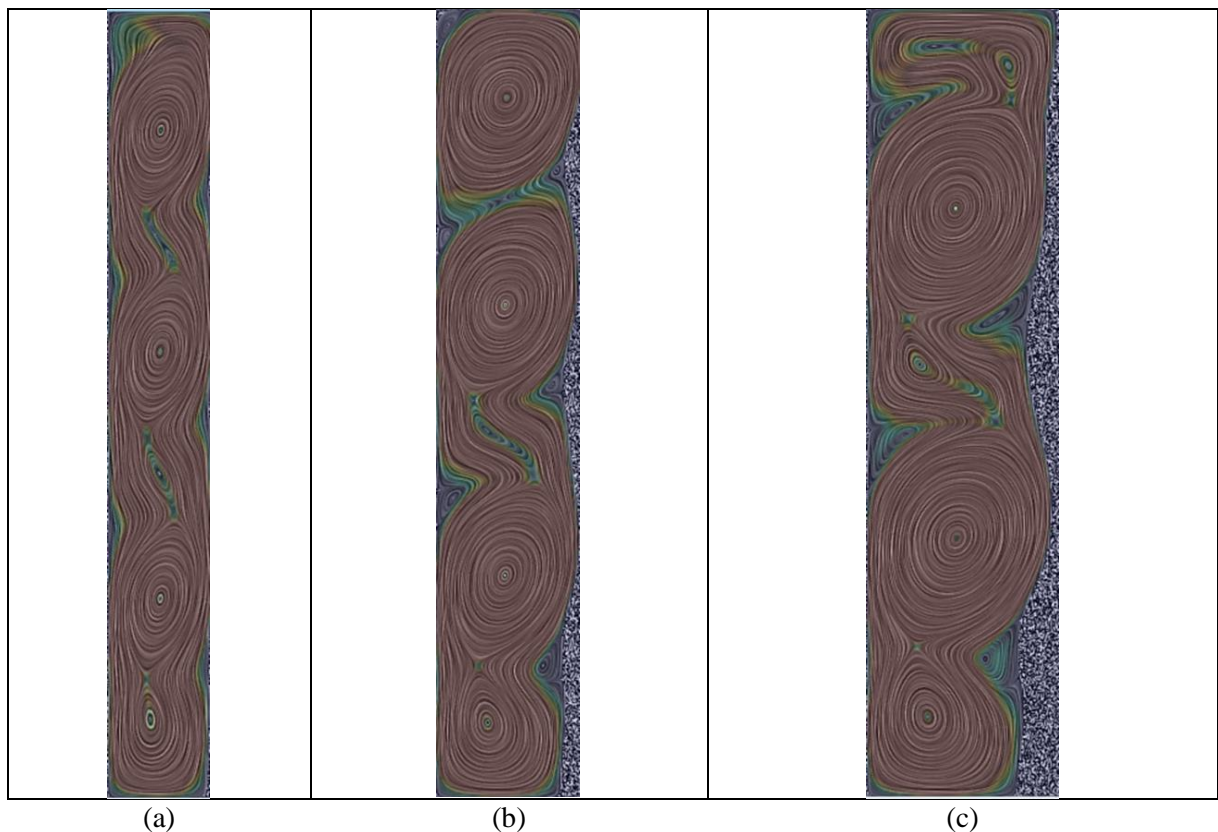

| (a) | (b) | (c) |

Figure 4. Flow structure at (a) 250s, (b) 400s and (c) 600s.

4. Conclusion

The LIC plots confirmed that the flow structure of tin and pure metal in general is multicellular as opposed to the findings (monocellular) of some other researchers . Reasonable fine grid size must be selected for solid-liquid phase change models to ensure complete physics of the problems are captured

and eventually yield acceptable numerical results. Future phase change models referring to pure metal melting problem for verification should obtain similar flow structure to be considered acceptable.

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