OPENFOAM SIMULATIONS OF ISOTHERMAL PHASE-CHANGE IN THE ABSENCE AND PRESENCE OF SHRINKAGE

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Introduction

Solidification and melting of metals are phase-change phenomena, which take place at a single temperature for pure metals, or at a range of temperatures for metal alloys. In this work, we focused only on phase-change of pure metals, i.e. isothermal phase change. Most metals have higher density in the solid phase than in the liquid phase. Therefore, during their solidification, their overall volume shrinks. This phenomenon is refereed to macro-shrinkage.

In this paper, we present our most recent results in simulating phase-change problems using OpenFOAM. We have studied two different problems involving isothermal phase change. The first one is a benchmark melting problem of pure gallium, and the second one is a solidification simulation of pure aluminium in the presence of macro-shrinkage.

Isothermal Melting Models

The model that we used to simulate the isothermal melting problem consists of continuity and energy equations, whose details can be found elsewhere [1], and the energy equation reads

$$\rho_0 c_p \frac{\partial T}{\partial t} + \rho_0 c_p \nabla \cdot (\boldsymbol{v} T) = \nabla \cdot (k \nabla T) + S_h \tag{1}$$

where ρ_0, c_p, T, $\boldsymbol{v}$, and k are the density, specific heat, temperature, liquid velocity, and thermal conductivity, respectively. The last term, S_h, represents the latent heat release due to melting. We have explored two different methods to calculate S_h. In the first method, which is referred to as the linear method, S_h is calculated as

$$S_h = -\rho_0 L_f \frac{\partial g_l}{\partial t} \tag{2}$$

where L_f is the latent heat and g_l is the liquid fraction. We define $g_l = 1$ in cells filled solely with liquid, and $g_l = 0$ in cells filled solely with solid. The liquid fraction is calculated from

$$\begin{aligned} T < T_f \quad &: \quad g_l = 0 \\ T > T_f \quad &: \quad g_l = g_l^n + \alpha \frac{c_p}{L_f}(T - T_f) \end{aligned} \tag{3}$$

where T_f and g_l^n are the melting point of a pure material and the most recent liquid fraction, respectively. In the second method, which is referred to as the error-function method developed by Rösler and Brüggemann [2], S_h is calculated as

$$S_h = -\rho_0 L_f \frac{4 \exp\left\{ -\left[\frac{4(T - T_m)}{T_l - T_s} \right]^2 \right\}}{(T_l - T_s)} \left(\frac{\partial T}{\partial t} + \boldsymbol{v} \cdot \nabla T \right) \tag{4}$$

where T_l and T_s are liquidus and solidus temperatures and T_m is the arithmetic mean between T_l and T_s.

Macro-Shrinkage Model

To simulate isothermal solidification in the presence of macro-shrinkage, we used the following model. The continuity equation reads

$$\nabla \cdot \boldsymbol{v} = S_s \tag{5}$$

where S_S is the shrinkage source and is calculated from

$$S_s^{i+1} = S_s^i - \left[\frac{\partial (\alpha_1 \rho_0)}{\partial t} + \nabla \cdot (\rho_0 \boldsymbol{v}) \right] \tag{6}$$

where α_1 is the volume fraction of melt. The advection equation of volume fraction (VOF method) is expressed as

$$\frac{\partial \alpha_1}{\partial t} + \nabla \cdot (\alpha_1 \boldsymbol{v}) + \nabla \cdot \left[(1 - \alpha_1) \alpha_1 \boldsymbol{v}_r \right] = S_s \tag{7}$$

where $\boldsymbol{v}_r$ is relative velocity.

Implementation

To simulate the above model in OpenFOAM we used buoyantBoussinesqPimpleFoam solver. The linear method is already implemented in OpenFOAM as solidificationMeltingSource fvOption. In this study, we implemented the error-function method by hard-coding equation (4) into the energy equation of buoyantBoussinesqPimpleFoam.

In the simulations, if solidificationMeltingSource is used with the original form of buoyantBoussinesqPimpleFoam, the solution algorithm is as follows: First, equation (1) is solved for a new temperature field using the liquid fraction field from the *previous* time step; and then, equation (4) is used to update the liquid fraction field. Here, we propose a revision to this solution algorithm by adding an inner iteration loop to repeat solving equations (1) and (4) at every time step until the solid fraction and temperature fields converge, i.e. don't change with further iterations. Our revision improves the computational efficiency of the algorithm as it allows one to use significantly larger time steps.

The details about the implementation of multiphase flow are in Yamamoto *et al.* [3]. Steep density variation around the melting point causes macro-shrinkage. We also validate the shrinkage model, while it is not implemented in OpenFOAM originally. In addition to the above model, the advection equation of liquid fraction with source term have to be solved. OpenFOAM originally provides a solver for multiphase flow as *interFoam*. This macro-shrinkage solver is developed by combining *interFoam* and *buoyantBoussinesqPimpleFoam* based on Bounds *et al.* [4].

Problem Statement

We have studied two different problems involving isothermal phase-change. The first problem is a benchmark problem for melting of pure Gallium [5]. The schematic of the problem is shown in Figure 1(a). It consists of a rectangular cavity initially filled with pure Gallium. The cavity is heated from the left wall and is insulated from the top and bottom. The temperature of the right wall is equal to the initial temperature. The initial and boundary conditions are also shown in the figure. The width and height of the cavity are 8.89 and 6.35 cm, respectively. The material properties were taken from Bounds *at al.* [5].

The second problem is a test case for solidification of pure aluminium in the presence of macro-shrinkage. The schematic of the problem is shown in Figure 3. It consists of a cavity partially filled with pure aluminium melt at 943 K in temperature. The solidification of two ingots of different aspect ratios were simulated. The width and height of ingot cavity for the first and second cases are 10 and 5 mm (aspect ratio of 2) and 40 and 5 mm (aspect ratio of 8), respectively. The physical properties were taken from Leitner *at al.* [6].

Results and Discussion

Simulation results for the melting problem are shown in Figure 2, where snapshots of the temperature field (colour) along with the velocity vectors (the black arrows) and the melting front (the while line) are plotted at: (a) 240, (b) 480, (c) 960, and (d) 1200 seconds after the start of melting. In the figure, the top and bottom rows show the results obtained using the linear and error-function methods, i.e. equations **Error! Reference source not found.** and **Error! Reference source not found.**, respectively. Predictions of the two models, including temperature distributions, flow patterns, and the locations

of the melting front are very similar. This provides confidence in the accuracy of these results. Due to the upwards thermal buoyancy forces the hot liquid Gallium moves upwards which results in higher temperatures, and consequently faster melting at the upper parts of the cavity.

For the macro-shrinkage problem, simulation results are shown in Figure 3 where snapshots of the temperature field (colour) along with the melting front (the white line) and the liquid-melt interface (the black line) are shown for the low and high aspect ratio ingots at the top and bottom rows, respectively, at 0.1 and 2.5 seconds after the start of solidification. For the low aspect ratio ingot, i.e. the top row, the size of the shrinkage cavity is small relative to the overall size of the ingot; while, for the high aspect ratio ingot, i.e. the bottom row, the size of this cavity is large relative to the overall size of the ingot. The calculation results qualitatively express the generally observed experimental results. More detailed simulations, including quantitative comparisons with the available experimental data are ongoing.

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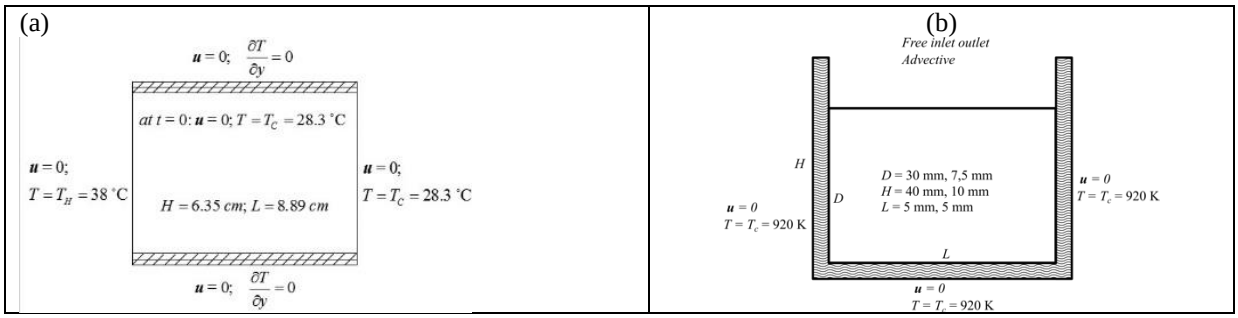
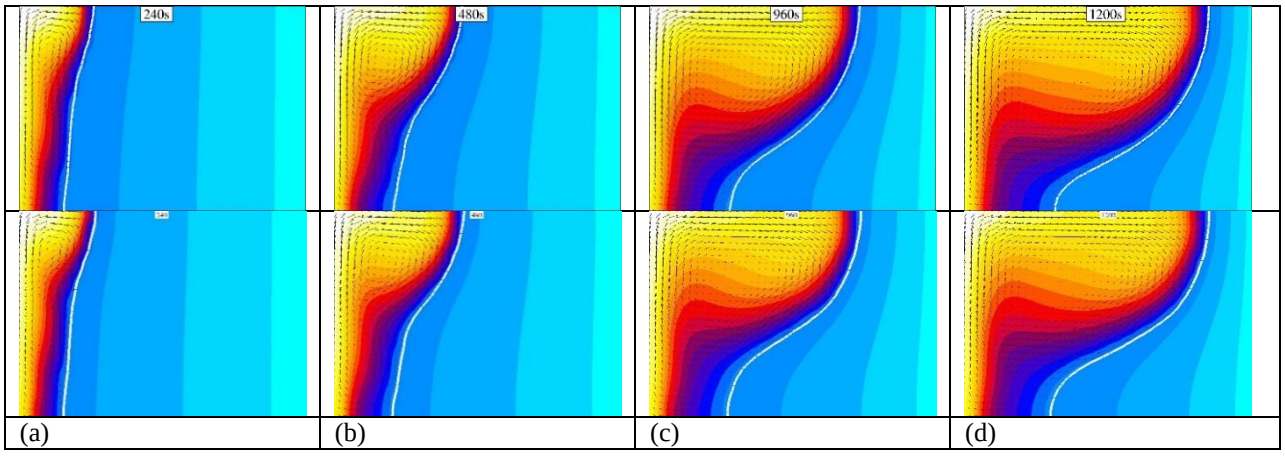


Figure 1: Schematics of the benchmark melting experiment (a) and the macro-shrinkage test problem simulated in this study (b)



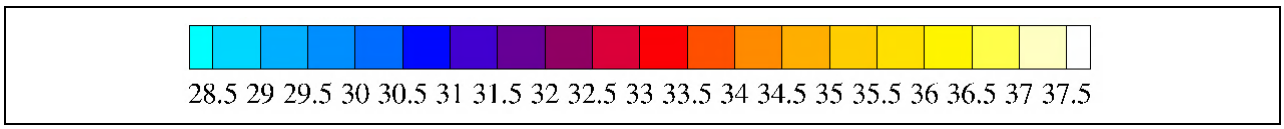


Figure 2: Snapshots after the start of melting obtained using the linear model (top row) and the error-function model (bottom row) at (a) 240, (b) 480, (c) 960, and (d) 1200 s. Each snapshot shows the temperature field (colour map), the velocity field (black arrows), and the melting front (white line)

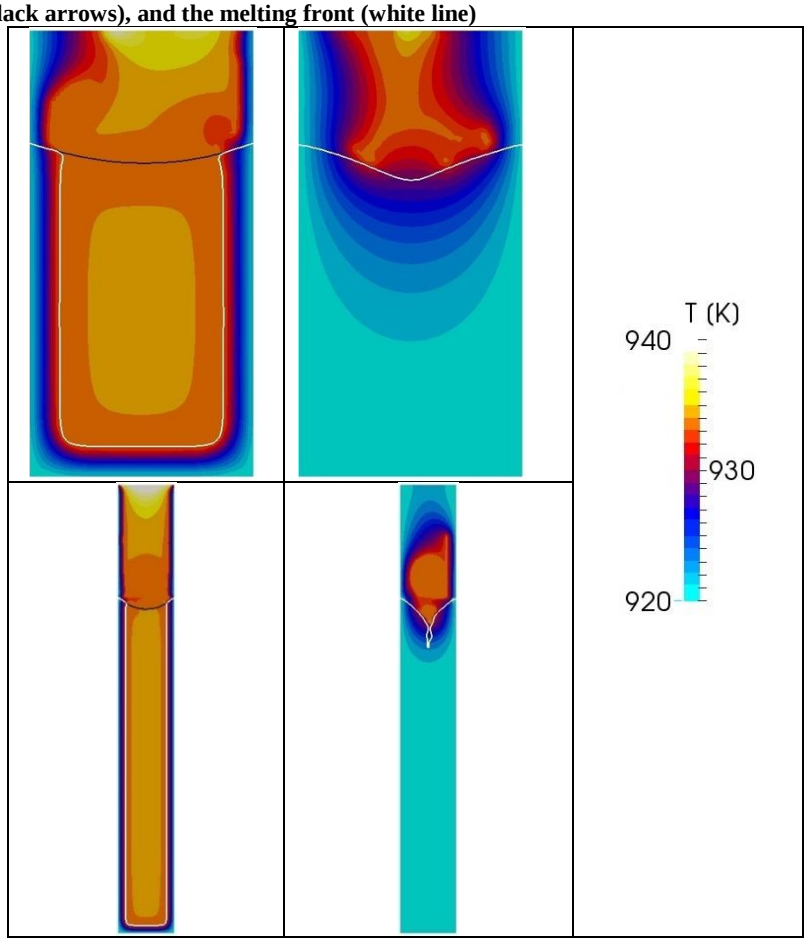


Figure 3: Snapshots after the start of solidification of the 10x5 mm ingot (top) and of the 40x5 mm ingot (bottom) at 0.1 (left) and 2.5 s (right). Each snapshot shows the temperature field (colour map), the solidification front (white line), and the liquid-melt interface (black line).