A 2D Numerical Simulation of Binary Alloy Solidification: Effect of Mesh Resolution on Formation of Channel Segregates

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Abstract. Mesh refinement is crucial for capturing the complex phenomena that governs the formation of channel segregates during binary alloy solidification. In this article, the influence of mesh size on the formation of channel segregates during the solidification of Sn-5wt%Pb alloy is numerically investigated. A solver is developed in OpenFOAM for solving the coupled transport equations of mass, momentum, energy and species. Subsequently, the simulations are performed for different mesh sizes to predict the flow field, temperature, species and solid fraction distribution including the morphology of channel segregates. From this study, it is observed that the mesh size significantly affects the morphology and the strength of channel segregates. For very fine mesh size, having sufficient number of grid point along their width, the formed channels are more continuous and the flow inside channels is resolved.

1. Introduction

Channel segregates causes the severe defects in the alloy cast products because they result in severe compositional and structural heterogeneities in the final product that cannot be eliminated by any manufacturing process [1]. These channels appear as narrow, long and highly solute-concentrated tracks oriented in some specific direction [1]. The characteristic length of these channels can alter the mechanical properties and the quality of solidifying cast product [1]. The channel segregates are generally formed due to the instabilities in the interdendritic fluid flow that arise near to the liquid-mushy interface during solidification [2]. These instabilities depend on the drag on interdendritic fluid flow in the mushy zone [1-3]. The permeability of the mushy zone varies over a range for the mapped value of liquid fraction from 1 to 0 [4]. It makes the calculated permeability vulnerable to the small liquid fraction change in mushy region that might result into inaccurate capturing of the channel segregates. Consequently, it becomes essential to choose a good mesh size to resolve it. There are very few article [1, 4] that discussed the influence of good mesh resolution. Therefore, an effort needs to be made to understand the role of mesh resolution in the formation of channel segregates during the solidification of binary alloys.

In this article, a 2D computational study is performed to investigate the influence of mesh size on the morphology of the channel segregates during solidification of Sn-5wt%Pb alloy. For this purpose, a solver is developed using a finite volume based OpenFOAM CFD platform. The solver predicts the evolution of flow field, temperature, species and solid fraction distribution including the morphology of the channel segregates. The simulations are performed for various mesh sizes which vary to a large scale. The results for the solute segregation and channel morphology are compared and presented.
2. Mathematical modelling

A fixed-grid continuum formulation approach is used to model the associated transport phenomena during solidification of binary alloy [4]. Only a brief discussion of model is presented here, more details can be found elsewhere [4]. The governing equations are shown in Table 1.

| Table 1. Governing equations [4]. |
|----------------------------------|
| **Mass conservation** | \( \nabla \cdot \vec{u} = 0 \) | (1) |
| **Momentum conservation** | \( \frac{\partial (\rho \vec{u})}{\partial t} + \nabla \cdot (\rho \vec{u} \vec{u}) = -\nabla p + \nabla \cdot (\mu \nabla \vec{u}) - \frac{\mu}{K} \vec{u} + \rho g \beta_T (T - T_{ref}) + \beta_C (C_l - C_{ref}) \) | (2) |
| **Energy conservation** | \( \frac{\partial (\rho c_p T)}{\partial t} + \nabla \cdot (\rho c_p \vec{u} T) = \nabla \cdot (k \nabla T) - \frac{\partial (\rho f_t L)}{\partial t} \) | (3) |
| **Species conservation** | \( \frac{\partial (\rho C)}{\partial t} + \nabla \cdot (\rho \vec{u} C) = \nabla \cdot (\rho f_t D_t \nabla C) + \nabla \cdot [\rho D^t \nabla (C_l - C)] - \nabla \cdot [\rho \vec{u} (C_l - C)] \) | (4) |

**Symbols**

- \( C \) Concentration
- \( k \) Thermal conductivity
- \( \rho \) Density
- \( c_p \) Specific heat capacity
- \( K \) Permeability
- \( \beta_T \) Thermal expansion coefficient
- \( \beta_C \) Solutal expansion coefficient
- \( d \) Dendritic arm spacing
- \( L \) Latent heat of fusion
- \( D \) Solutal diffusivity
- \( p \) Dynamic pressure
- \( f \) Mass fraction
- \( T \) Temperature
- \( l \) Liquid
- \( \vec{g} \) Gravity
- \( \vec{u} \) Continuum velocity vector
- \( \text{ref} \) Reference

The enthalpy-porosity scheme is used to update liquid fraction in the computation cell and Scheil’s model is used to capture the solute redistribution [4]. A transient incompressible solver is developed in OpenFOAM to model fluid flow, heat transfer and species transport along with solidification phase change. The governing equations are discretized using the finite volume approach. PIMPLE (PISO+SIMPLE) algorithm is used for the pressure-velocity coupling.

3. Computational domain and numerical validation

To study the influence of mesh size on formation of channel segregates, the solidification study of Sn-5wt%Pb is carried out in 2D rectangular cavity (0.1 m × 0.06 m) as shown in Fig. 1(a). The cavity is cooled from the left side and the remaining three sides are thermally insulated. The problem is chosen as per well-known experiments of Hebditch and Hunt [6]. The thermophysical properties of Sn-5wt%Pb alloy used in the simulation are reported elsewhere [2,4]. The developed solver is validated with the experimental and numerical results reported in literature for solidification of Pb-48wt%Sn alloy [5,6]. Figure 1(b) shows the variations of relative concentration of Sn (%) as a function of distance to cold
boundary (at cavity height of $Y = 5\, \text{mm}$) at the end of solidification. The predictions obtained from the present simulation are found to be in excellent agreement with the reported results (see Fig. 1(b)).

![Diagram](image)

**Figure 1.** (a) Computational domain considered, (b) Numerical validation of developed solver.

4. Results and discussion

The segregation maps in relevant region of the cavity (in which channels are formed) are shown in Fig. 2 at $t = 400\, \text{s}$ to illustrate the influence of different mesh sizes on channel segregates. From Fig. 2, it can be seen that the mesh resolution significantly affects the morphology of channel segregates. Simulations with a very fine mesh size show that all the channel segregates formed are interconnected with the horizontal channel at the bottom. Furthermore, the shape, size, inclination and location of the channels are modified. The reason for this transformation is that the channel segregates are the outcome of local transport phenomena at mesoscopic scale (mushy zone scale). The attendant transport phenomena are captured more accurately with finer meshes which appears to have a crucial impact on the predictions. From the present simulations, it is observed that 7-6 control volumes (CVs) along the width of channel segregates are sufficient to resolve the flow in channels and to predict their morphology and locations.
Figure 2. Channel segregates formed at $t = 400$ s for different grids of (a) 50×50, (b) 100×100, (c) 150×150, (d) 200×200, (e) 300×300, (f) 400×400, (g) 500×500, (h) 600×600.

To show the effect of mesh size on quantitate prediction of macrosegregation, the global segregation index ($GSI$) is computed [2]. The global segregation index ($GSI$) is defined as follows:

$$GSI = \frac{1}{C_0} \frac{1}{V_{\text{domain}}} \iiint_{V_{\text{domain}}} (C - C_0)^2 dV \right]^{1/2}$$

Figure 3 shows the transient evolution of $GSI$ for different mesh sizes. It is observed that the extent of global macrosegregation increases with increase in number of grids because of change in the morphology of channel segregates. Further, the deviation in the predicted $GSI$ for grids of 400×400 and 600×600 is ~ 1%. However, the morphology and locations of the channel segregates formed differs to
a large extent. Therefore, it becomes crucial to choose a sufficient mesh resolution for obtaining the grid independent solution and accurate prediction of channel segregates.

![Figure 3. Transient evolution of global segregation index, GSI (%) for different mesh size of 50×50, 100×100, 150×150, 200×200, 300×300, 400×400, 500×500, and 600×600.](image)

5. Conclusion
From this study, it can be concluded that the mesh refinement is very crucial for capturing the complex transport phenomena during the formation of channel segregates which further affects their morphology and orientations to a large extent. Simulations with finer mesh size shown that all the channel segregates formed are interconnected with the horizontal channel at the bottom. For the present case, it is noticed that the grid size of 500×500 (~7 CVs along the width of channel segregates) are sufficient to resolve the flow in the channels and to obtain the grid independent solution. However, these predictions need detailed comparison with the results acquired from controlled experiments.

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