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Modelling macrosegregation modification in dc casting of aluminium alloys in sheet ingots accounting for inlet melt flow, equiaxed grain morphology and transport

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Abstract. Macrosegregation is a severe defect present in direct-chill (DC) cast aluminium ingots and billets. In the recent years, experimental studies were conducted to modify and to an extent optimize macrosegregation formation by modifying the inlet melt flow. Due to several limitations, the grain settling behavior and corresponding liquid flow pattern is difficult to analyze using experiments. Simulations on the other hand can provide this insight. However, conducting 2D sheet ingot simulations, as has been previously done, provides an incomplete description of flow pattern. To avoid this and as a first qualitative study, full scale 3D sheet ingot simulation results with two different inlets are presented in this paper. A simplified three-phase multiscale solidification model accounting for solidification shrinkage, natural convection and equiaxed grain growth and transport is used to conduct this study. We show that modification of inlet flow results in modification of grain settling and eventually leading to modification of macrosegregation. The impact of grain morphology is also additionally analyzed.

1. Introduction

The root cause of irregularity in solute content at the scale of the cast product, referred to as macrosegregation, lies in the relative movement between the solid and liquid phases [1]. This relative movement can manifest in many forms in DC casting of aluminium alloys: solidification shrinkage, natural and forced convection, equiaxed grain transport and thermal deformation of the mushy zone. Of these, movement of solute lean equiaxed grains is considered to be a major cause of negative segregation at the center of the ingot [2]. Recent experimental work on Al-4.5wt%Cu sheet ingots by Wagstaff and Allanore [3, 4] focussed on modifying and to an extent eliminating negative segregation by introducing a vertical jet at the center of the ingot. This vertical jet resulted in resuspension of the grains leading to macrosegregation modification. Insight into the complex flow pattern of the solid and liquid phase is not possible using experimental methods and can be gained using numerical simulations. At the same time, sheet ingots have an asymmetric geometry and using 2D simulations, as has been done by several researchers [5–8], provides an incomplete description of the flow phenomena. The flow becomes even more complex with the introduction of the inlet jet. To avoid this problem, 3D simulations of sheet ingots needs to be conducted.

3D simulations are computationally expensive, especially keeping in mind the multiphase, multiscale solidification process. To have realistic simulation time, coarse meshes need to be used. But Al-4.5wt%Cu used by Wagstaff and Allanore [3,4] has a thin mushy zone and its reasonably accurate numerical resolution might increase the computational cost to prohibitive level. Pakanati *et al.* [8]



recently conducted numerical study and showed that Al-4.5wt%Cu and Al-8.375wt%Zn show similar macrosegregation behaviour in 2D sheet ingots. Al-8.375wt%Zn has a thick mushy zone and its accurate resolution is possible with coarse mesh. Taking all these aspects into account, in the current paper we qualitatively study the impact of inlet flow on macrosegregation formation and modification for Al-8.375wt%Zn in a sheet ingot. We modify the inlet flow by considering a simplified open inlet and an inlet with a vertical jet. Consequently we analyze the interaction of the inlet melt flow with equiaxed grains resulting in their resuspension and macrosegregation modification. Additional influence of the grain morphology on macrosegregation formation is also discussed. This study is conducted using the simplified three-phase, multiscale solidification model proposed by Tveito *et al.* [9].

2. Numerical model

The simplified three-phase, multiscale numerical model of equiaxed solidification, proposed by Tveito *et al.* [9], is based on the volume-averaging approach of Wang and Beckermann [10] and employs the operator splitting algorithm proposed by Založnik and Combeau [11]. For a detailed description of the model the reader is referred to these papers. Only the main features are described here. The Euler-Euler volume averaged model has two parts – macroscopic transport and microscopic growth. The macroscopic transport accounts for solute and heat transfer coupled with liquid flow induced by solidification shrinkage and thermosolutal convection. The densities of liquid and solid are assumed to be constant but different and the Boussinesq approximation is used for the liquid density in the buoyancy term accounting for thermal and solutal effects. For the solid phase, the flow pattern depends on envelope fraction (g_{env}). For envelope fractions smaller than the packing fraction (g_{pack} , a model parameter) the solid (equiaxed) grains are freely floating. The interfacial drag term C_D is modeled in the same manner as in [12] for spherical particles but by considering the envelope fraction instead of the solid fraction. The measure of grain morphology can be obtained by taking the ratio of the solid fraction and the envelope fraction, called as the internal solid fraction: $g_{intern} = g_s/g_{env}$. The grain is globular as the g_{intern} approaches 1 and is dendritic if $g_{intern} \ll 1$. For envelope fractions greater than the packing fraction, grains are assumed to form a rigid porous solid matrix moving with the casting velocity, \vec{V}_{cast} . The interfacial drag in the porous medium is modeled by a Darcy term, where the hydrodynamic permeability is calculated by the Kozeny Carman relation, using a the characteristic size of the porous structure, l_{KC} .

The microscopic part is treated locally within each volume element. The model accounts for finite diffusion in both solid and liquid phases and local thermal equilibrium is assumed. Nucleation of grains is assumed to occur on grain-refiner (inoculant) particles. According to the athermal nucleation theory of Greer *et al.* [13], the critical undercooling for free growth of a grain on an inoculant particle of diameter d is given by $\Delta T_c = 4\Gamma_{GT}/d$ where Γ_{GT} is the Gibbs-Thompson coefficient. The number of activated particles then depends on the size distribution of the particle population, which can be represented by an exponential distribution density function. This representation holds for the largest particles, which are activated at small undercoolings and therefore successful as nuclei. This size distribution is then discretized into m classes of inoculants. Each class i is represented by a volumetric population density, N_{nuc}^i , and a critical undercooling, ΔT_c^i . When the local undercooling reaches the critical undercooling of class i , its local inoculant density, N_{nuc}^i , is instantaneously added to the grain density, N_g , and N_{nuc}^i becomes locally zero.

3. Problem description

The current study is conducted on the DC cast ingot used in [7]. The ingot geometry with dimensions is illustrated in figure 1(a). We can reduce the computational domain to a quarter of the ingot (represented in red) due to symmetry. We consider two types of inlet: a simplified open inlet where liquid metal enters the domain from the top surface (figure 1(b)) and an inlet with a vertical jet directed towards the center of the ingot (figure 1(c)). The jet is constructed by reducing the inlet to a 30 mm x 30 mm orifice (marked in black in figure 1(c)). From here on, the simplified open inlet is referred to as Inlet 1 and the inlet with vertical jet is referred to as Inlet 2. The liquid metal is assumed to enter the domain at casting temperature T_{cast} , nominal solute concentration C_o and inoculant density N_{nuc}^i . The inlet velocity is

calculated from the global mass balance. The solidified metal is assumed to leave the domain from the bottom with a predefined casting velocity \vec{V}_{cast} of 60 mm/min. The heat is extracted by primary cooling through the mold and by secondary cooling directly to the falling water film flowing over the ingot surface. Primary cooling consists of three zones: meniscus, mold, and air gap. The boundary conditions are specified in [7]. The heat transfer coefficient due to secondary cooling is modelled using Weckmann and Niessen [14]. A binary Al-8.375%Zn alloy is used, similar to Založnik *et al.* [7] emulating the AA7449 alloy. The thermal and physical properties (including packing fraction 0.3) are also obtained from [7]. The inoculation data is taken from [8].

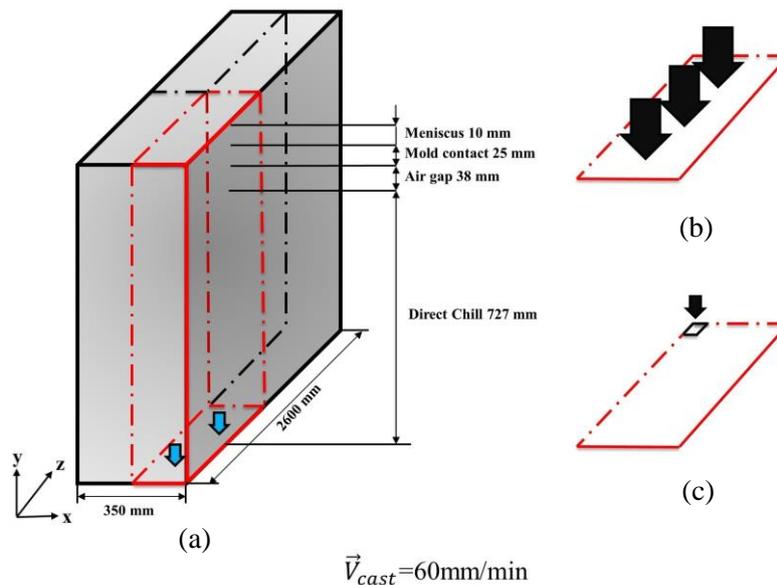


Figure 1. (a) The full isometric view of the sheet ingot. Symmetry axes is represented by dashed lines. The quarter of ingot marked in red is the simulation domain. (b) Simplified open inlet (Inlet 1) and (c) inlet with vertical jet at the center of the ingot (Inlet 2).

The transport equations are solved with a Finite Volume Method and the SIMPLE-algorithm for staggered grid is used for pressure-velocity coupling. The convective terms are discretized with a first-order upwind scheme and for time discretization a fully implicit first-order scheme is used. For all simulations a structured grid of 524,288 cells ($N_x \times N_y \times N_z = 32 \times 128 \times 128$) is employed. A constant time step of 5 ms is used and the calculations are run until steady state is reached.

4. Results and discussion

All studied cases are summarized in table 1. A total of four cases (1-4) based on the inlet mechanism and grain growth model are considered. Globular morphology is imposed ($g_{env} = g_s$) for Case 1 and Case 3. Grain morphology is simulated for Case 2 and 4. All the cases have the same transport mechanisms: shrinkage induced flow, natural convection and equiaxed grain motion. Case 3 and Case 4 additionally have forced convection due to the inlet jet.

The macrosegregation contour along the horizontal x-z plane for all the cases are shown in figure 2. The main features of the contours are discussed starting with Case 1. Negative segregation along the ingot width in z-direction is due to settling of solute lean grains and shrinkage induced flow. However, the formation of concentrated negative segregation region (marked in red) can be explained by taking a look at figure 3. An isosurface of packing fraction is overplotted with solid grains trajectory along the inclined mushy zone in the x-y plane (black arrows) and z-y plane (white arrow). The region marked in red in figure 2 for Case 1 has grains arriving from both the x and z direction. For the other parts of the ingot, the grain settling is predominantly along the x-direction. This additional contribution results in

more grains settling in that region, leading to more pronounced negative segregation. This can be further corroborated by examining figure 4, where the grain densities along the x-z plane are plotted for Case 1 and 3. For Case 1, the region marked in red shows high grain density, which corresponds to the negative segregation zone marked in red for Case 1 in figure 2.

Table 1. Simulation Cases.

Description	Case
Inlet 1 – Globular Grain Growth Model	1
Inlet 1 – Dendritic Grain Growth Model	2
Inlet 2 – Globular Grain Growth Model	3
Inlet 2 – Dendritic Grain Growth Model	4

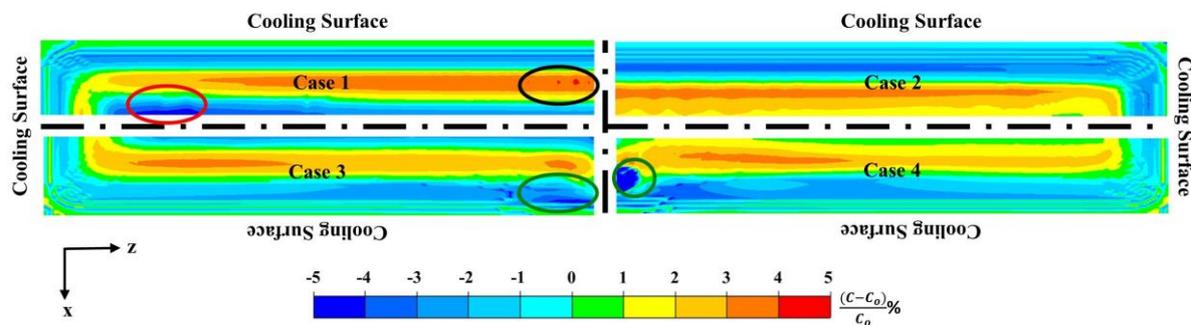


Figure 2. Relative macrosegregation contour plots along the horizontal x-z plane for all the cases. Only quarter ingot plots for each case are shown and the cooling sides are marked. The central axes are also marked.

The region marked in black for Case 1 in figure 2 shows more pronounced positive segregation. In fact, if we observe along the ingot width, the intensity of positive segregation gradually increases and peaks at the center of the ingot. This asymmetric positive segregation is due to the combination of the thermal-solutal convection and grain motion and can be explained using the illustration in figure 5. A 2D sheet ingot with packing front and relative liquid velocity flow loop in the x-y plane is shown in figure 5(a). Due to the grain settling towards the center of the ingot, solute rich liquid is expelled up and enriches the slurry region. The solute rich liquid is carried into the liquid pool and towards the mid-section of the ingot resulting in positive segregation [7]. In 3D, apart from the flow loop in the x-y plane (light grey to black), there is contribution from the z-y plane (red) and are illustrated with the packing front isosurface in figure 5(b) and figure 5(c), respectively. Similar to the 2D model, grain settling along the x-y plane expulses solute rich liquid up. The additional driving force along the z-y plane pushes this solute rich liquid towards the ingot center. Hence, the extent of enrichment varies along the z-direction. At the position of the light grey loop in figure 5(b), lower amount of solute enrichment can be observed. As we move further and reach the position where the black flow loop is marked, more enriched solute is available due to the driving force from z-y plane. This results in the enriched region marked in black for Case 1 in figure 2. The isometric view of the quarter ingot is shown in figure 6. The flow vectors for relative liquid velocity in black and solid settling velocity in red are marked. Due to the uniform open inlet, the inlet flow has little to no influence on the grain settling. This can be observed from the consistent settling of solid grains along the ingot width.

For Case 2, we have dendritic grains and the macrosegregation contour along the horizontal plane is shown in figure 2. As mentioned in the previous section, due to dendritic nature of the grains, slightly positive segregation is observed along the ingot width. Similar to Case 1, we also see solute accumulation towards the ingot center for Case 2. The mechanisms through which macrosegregation formation remains the same for Case 1 and 2 but the intensity of segregation is different to due the

presence of dendritic grains. This indicates that for a given inlet, macrosegregation depends on the morphology of the equiaxed grains, an inference previously reported in [9, 15].

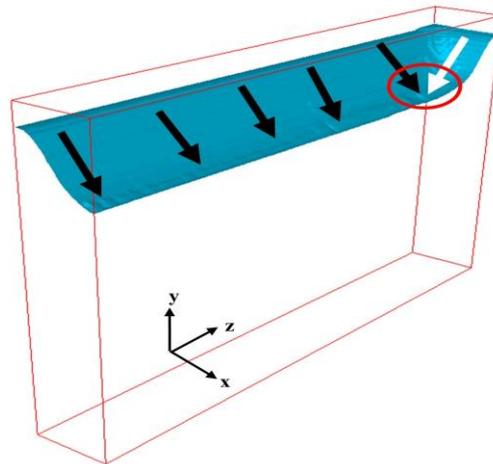


Figure 3. Illustration of Case 1 isosurface of solid fraction at the packing fraction. The black and white arrows indicate the solid grains trajectory in the x-y plane and z-y plane.

With the introduction of inlet jet in Case 3, macrosegregation is modified when compared with Case 1 for the same globular morphology. The inlet jet is known to create a flow loop which could potentially wash away solute along the inclined mushy zone. In figure 2, we can see this clearly in the region marked in green. In addition to this, the asymmetric negative and positive segregation observed in Case 1 is not present and an almost uniform distribution of segregation can be observed. The inlet flow results in redistribution of the grains and this can be seen in figure 4 for Case 3 and when we compare with Case 1, near uniform grain density can be seen along the ingot width. The interaction of the inlet flow with grain settling can be seen in the isometric view of the quarter ingot in figure 7. Similar to Case 1, the relative liquid velocity vectors are marked in black and the solid settling velocity vectors are marked red. The inlet jet ploughs through the mushy zone in the central part of the ingot, creating a small crater. In this region, there is no grain motion (unlike Case 1 in figure 6) as the inlet jet acts like a barrier and resuspends the grains away from the center of the ingot. This is the central theme of the research done by Wagstaff and Allanore [3, 4, 18]. The pushing of the grains from the center of the ingot can be clearly seen by the solid velocity vectors (red) in figure 7. Especially along the z-y plane, the grains are moving away from the center. Along the x-y plane, some degree of resuspension is seen as a fraction of grains have managed to override the inlet jet and settle towards the center. This is a consequence of having a relatively weak inlet jet. Stronger inlet jets can cause stronger barriers resulting in complete resuspension of the grains. However, the important aspect to be noted is the recirculation of the grains due to the inlet jet and the corresponding modification of macrosegregation.

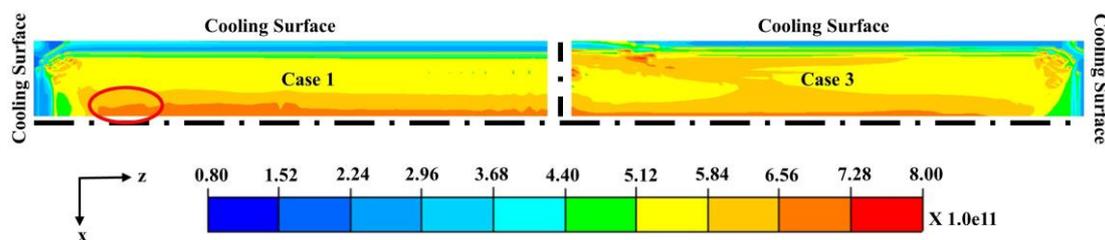


Figure 4. Grain density contours on the horizontal x-z plane for Case 1 and Case 3.

Solving of grain morphology and inlet jet requires proper treatment of the mushy zone due to the strong gradients in the velocity and envelope fraction along the inclined mushy zone. Since this work employs a relatively coarser mesh, it is possible that the island of negative segregation for Case 4, marked in green in figure 2, is caused due to numerical issues. However, solute wash up due to strong forced convection is nothing new in DC cast process [18]. The extent of solute depletion can depend on

the morphology of the grain, as discussed in the previous section. Compared to Case 2 with the same dendritic morphology ($g_{intern} \sim 0.5$), macrosegregation in Case 4 is different due to the presence of the inlet jet. Compared with Case 3 with the same inlet jet, macrosegregation in Case 4 is again different due to the presence of dendritic grains in the latter case. This comparison establishes that inlet jet can modify macrosegregation by resuspension and recirculation of the grains. The extent of modification further depends on the morphology of the grain: globular or dendritic.

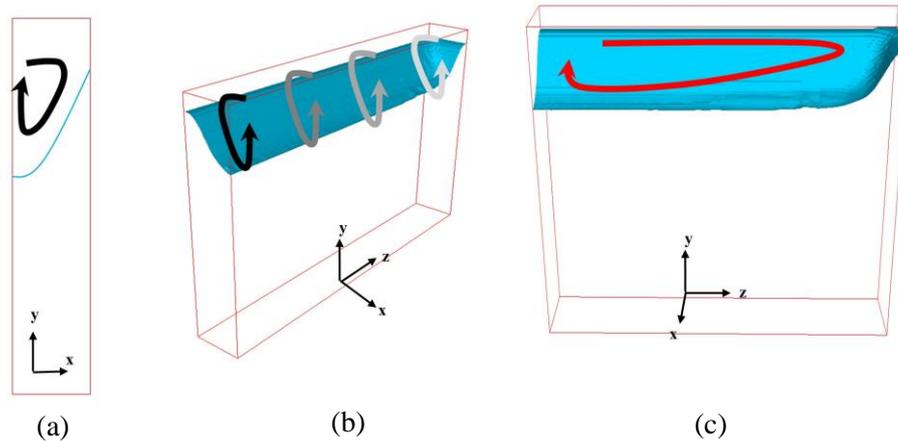


Figure 5. Illustration of the relative liquid velocity for (a) a 2D sheet ingot model and (b) & (c) a quarter of the 3D sheet ingot model.

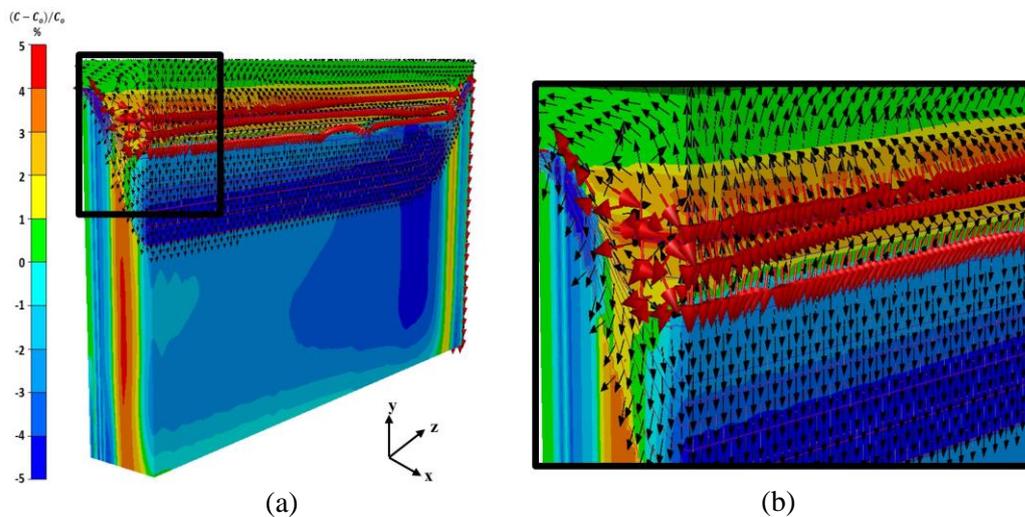


Figure 6. Isometric view of Case 1 plotted with solid fraction isolines, relative macrosegregation contours, relative liquid velocity vectors in black and solid settling velocities in red. (a) Full quarter ingot and the region marked in black square is enlarged in (b).

As previously mentioned, this study is to qualitatively complement the work done by Wagstaff and Allanore [3,4] where an Al-4.5wt%Cu alloy is used. Owing to numerical issues, this study is conducted using Al-8.375wt%Zn alloy which has a thick mushy zone. However, Pakanati *et al.* [8] indicated that both the alloys behave similarly when it comes to the interplay of various transport mechanisms. A direct comparison of these simulation cases with experiment is not possible as the ingot size and casting conditions are different. Nonetheless, this study provides a first qualitative study in this direction.

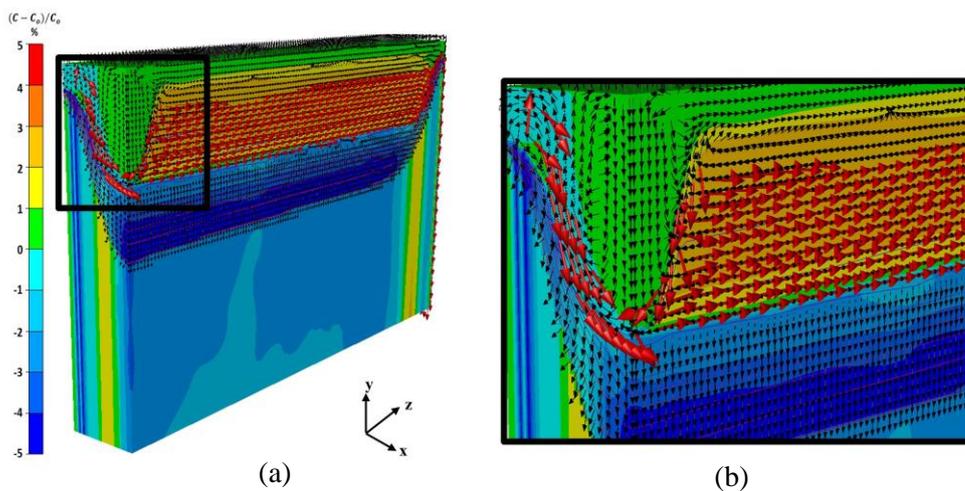


Figure 7. Isometric view of Case 3 plotted with solid fraction isolines, relative macrosegregation contours, relative liquid velocity vectors in black and solid settling velocities in red. (a) Full quarter ingot and the region marked in black square is enlarged in (b).

5. Conclusions

Modification of macrosegregation in DC casting by modification of the inlet melt flow has been analyzed in the current study. By using a simplified three-phase multi-scale solidification model, we have also analyzed the extent of the modification by accounting for both globular and dendritic grain morphology. The interaction of the inlet melt flow and the solid grains has been discussed by using visual representation of the flow, something that is not possible in experimental studies. The current model is sensitive enough to study macrosegregation modification and maybe optimization for future studies. Since this is a qualitative study, focus should also be brought on complementing the experimental work done on macrosegregation modification. Direct comparison with experiment is feasible only if we are able to keep the error induced due to mesh resolution, especially in the mushy zone, to minimum. Constructing uniform fine grids is an option but for 3D cases, it can result in prohibitive computational time. It can be avoided by using mesh adaptation to locally resolve the mushy zone. This could be the focus of future work.

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