A Generalized Approach for Macroscopic Modelling of Solidification of Ternary Alloys with Dendritic Arm Coarsening

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A generalized macroscopic two-dimensional mathematical model has been developed to simulate the transport phenomena occurring during the solidification of ternary alloy systems. The model is based on a fixed-grid enthalpy based control volume approach and is capable of capturing the effects of dendritic arm coarsening on the transport characteristics of the solidification process. Microscopic features pertaining to complex thermo-solutal transport mechanisms and dendritic arm coarsening are numerically modelled through a novel formulation of latent enthalpy evolution, consistent with the phase change morphology of general multi-component alloy systems. Numerical simulations are performed for ternary steel alloy and the resulting convection and macrosegregation patterns are analyzed. It is observed that dendritic arm coarsening leads to an increased effective permeability of the mushy region resulting in an enhanced macrosegregation. The numerical results are also tested against experimental results reported in the literature, and very good agreement is found in this regard.

KEY WORDS: solidification; numerical modeling; fluid flow; macrosegregation; dendrite arm.

1. Introduction

In recent years, significant efforts have been devoted towards development of macroscopic models to study transport phenomena occurring during the phase change process pertaining to the solidification of multicomponent alloys.1–4) There exists various techniques for macroscopic modeling of alloy solidification,5–7) however the most popular method is ‘enthalpy-porosity’ approach.8) This method eliminates the need of explicit tracking the solidification fronts, by modelling the entire macro-domain with a single set of volume-averaged continuum conservation equations. In this approach, latent enthalpy of a phase changing cell is related to the local porosity, which in turn, prescribes a frictional resistance on account of solidified phase distribution within the problem domain. This simplifies the numerical modelling requirements of a phase-change process considerably, by establishing a direct interlinkage between fluid flow, heat transfer and change of phase.

Due to the relatively simple phase-change characteristics of binary alloys, most of the enthalpy-based macroscopic models of alloy solidification have classically dealt with binary systems. Voller and co-workers9) initially applied this formulation for modelling mushy zone phase change problems, followed by more advanced numerical studies for complicated cases of alloy solidification problems.10–12) It can be noted here that prediction of solidification behaviour of such system would effectively require a more detailed assessment of the nature of solute redistribution and the associated phase equilibrium relationships. While the above mentioned studies contributed significantly towards understanding of physical phenomena involved in solidification of multicomponent alloys, a systematic study towards the development of enthalpy-based thermodynamically-consistent generalized simulation strategies for multicomponent alloy solidification has largely been ignored. In particular, macroscopic model for multicomponent systems, which can represent pertinent microscopic issues within the macroscopic framework in a metallurgically consistent manner is yet to be found in the literature. Typical microscopic issues include the morphology of the mushy region offering flow resistance, non-equilibrium solidification, macrosegregation, dendritic arm coarsening etc.

In the present work, a general mathematical procedure to formulate enthalpy-porosity based phase change modelling of a ternary alloy system is developed with effective representation of situations related to dendritic arm coarsening occurring during the solidification process. Towards this, suitable numerical schemes are devised to prescribe the permeability of the mushy zone as a function of the coarsening kinetics. In addition, a novel algorithm is developed that can effectively update the nodal latent heat on every iteration, consistent with the metallurgy of the dendritic arm coarsening. The model is capable of quantifying the effects of dendritic arm coarsening on macroscopic transport of momentum, heat and solute during solidification. As a demonstration of the numerical model developed in this study, solidification of three-element steel alloy is simulated and the resulting flow and macrosegregation patterns are analysed.
2. Mathematical Modelling

2.1. Governing Equations

The physical situation considered here is a two-dimensional rectangular mould containing a ternary metal alloy, initially in the molten state. The left boundary of the rectangular domain is subjected to a prescribed heat transfer coefficient (heat loss), whereas all other boundaries are kept insulated. Therefore the melt starts solidifying from the left vertical boundary and proceeds unidirectionally. The solid phase is assumed to be rigid and stationary, and fluid flow is two-dimensional and laminar. The problem domain is shown schematically in Fig. 1, describing the initial and boundary conditions.

Following a fixed-grid continuum formulation with a single-domain approach, the equations governing conservation of mass, momentum, energy and species concentration appropriate to the present ternary system can be written as follows

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{u}) = 0 \quad \text{.......................... (1)}
\]

\[
\frac{\partial (\rho \vec{u})}{\partial t} + \nabla \cdot (\rho \vec{u} \otimes \vec{u}) = -\nabla p + \nabla \cdot \left( \mu \nabla \vec{u} \right) + \rho \vec{f} + \nabla \cdot \left( \rho \vec{g} \right) + \rho \vec{J} \quad \text{.......................... (2)}
\]

Equations (1) and (2) are continuity equation and momentum equation respectively.

Here \( \rho, \vec{u}, \mu, p, K \) are the density, velocity, effective viscosity, pressure and permeability respectively, and the subscript \( i \) denotes the liquid phase.

The buoyancy source term, \( S_b \), appearing in Eq. (2), includes both thermal and solutal effects, and is given by the differences between local and initial values of temperature and liquid solute concentrations, respectively. Considering the effect of three components for the case of a ternary alloy, the buoyancy term in Eq. (2) can be written as:

\[
S_b = \rho g [ \beta_f (T - T_0) + \beta_1 (C_1 - C_{i0}) + \beta_2 (C_2 - C_{i0}) ] \quad \text{.......................... (3)}
\]

Here, \( \beta_f \) and \( \beta_i \) are the thermal volumetric coefficient of expansion and solutal volumetric coefficient of expansion respectively, \( T_0 \) is the initial temperature in the domain and \( C_{i0} \) is the initial solute concentration. Subscript ‘1’ and ‘2’ refer to element 1 and element 2 respectively.

The species conservation equation is given as follows:

\[
\frac{\partial (\rho C_i)}{\partial t} + \nabla \cdot (\rho \vec{u} C_i) = \nabla \cdot (\mu \nabla C_i) + \rho \vec{f}_i + \rho \vec{g}_i C_i + \rho \vec{J}_i \quad \text{.......................... (4)}
\]

where,

\[
S_b = -\left[ \frac{\partial}{\partial t} (\rho f_i \Delta H) + \nabla \cdot (\rho \vec{u} \Delta H) \right] \quad \text{.......................... (5)}
\]

here, \( f_i \) denotes mass fraction, and subscripts \( f \) and \( s \) refer to liquid and solid phases respectively. \( T \) is the temperature, \( c_p \) is the specific heat, and \( k \) is the thermal conductivity.

The source term, \( S_b \), is a consequence of latent heat evolution during the solidification process, and is related to the liquid mass fraction of a computational cell as; \( f_i = \Delta H/L \), where \( L \) is the latent heat of freezing and \( \Delta H \) is the latent enthalpy content of the computational cell under consideration.

The species conservation equation is given as follows:

\[
\frac{\partial}{\partial t} [\rho C_{mix}] + \nabla \cdot (\rho \vec{u} C_{mix}) = \nabla \cdot (\mu \nabla C_{mix}) + \rho \vec{f}_{mix} + \rho \vec{g}_{mix} C_{mix} \quad \text{.......................... (6)}
\]

Here, \( C_{mix} \) is the mixture composition, \( g \) is the volume fraction and \( D \) is the mass diffusion coefficient. \( C_i \) are species concentration in the liquid and solid respectively.

The term \( \rho C_{mix} \) appearing in Eq. (6) is evaluated as

\[
\rho C_{mix} = \rho g_1 C_1 + \rho g_2 C_2 + \rho C_3 \quad \text{.......................... (7)}
\]

It needs to be mentioned here that for the present case of a ternary alloy system, two independent species transport equations need to be essentially invoked; one equation for each constituent species. A major challenge in this regard would be to postulate a thermodynamically-consistent scheme that eventually relates the evolution of latent enthalpy with the local temperature, phase fraction distribution and composition of the constituent species that are obtained as solutions of the above equations. To achieve this purpose, a novel enthalpy updating strategy is proposed here (to be elaborated in the subsequent sub-section), which plays the pivotal role towards successful implementation of the present numerical scheme.

Furthermore, solute diffusion in the solid state is expressed as

\[
\frac{\partial (\rho f_i C_i)}{\partial t} = C_s \frac{\partial (\rho f_i)}{\partial t} + \frac{36 \rho D_i}{\lambda_2^2} (C_i^* - C_i) \quad \text{.......................... (8)}
\]

where the superscript * denotes values at the solid/liquid interface, and \( \lambda_2 \) is the secondary dendritic arm spacing. Assuming local equilibrium at the interface, the following relationships can be written for the two phase region

\[
C_j = \left( \frac{T - T_melt}{m_l} \right) \quad \text{.......................... (9)}
\]

\[
C_i^* = k_p C_i \quad \text{.......................... (10)}
\]

In Eq. (9), \( m_l \) is the slope of the liquidus line of the phase diagram.

The effective viscosity \( \mu \) is calculated as

\[
\mu = \mu_i \left[ 1 - \left( \frac{F_{ai} g_i}{0.3} \right)^2 \right] \quad \text{.......................... (11)}
\]
Here, the function $F_n$ is given by

$$F_n = 0.5 - \frac{1}{\pi} \tan^{-1} \left[ 100 \left( g_n - g_{2n} \right) \right] \quad \text{........... (12)}$$

In above equation, $g_{cr}$ is a critical solid fraction as described in the literature.\(^9\)

Accordingly, the permeability $K$ is assumed to vary as a function of liquid fraction\(^{14}\)

$$K = \frac{\lambda_2^3 f_i^3}{180 \left( 1 - f_i \right)^2 \left( 1 - F_n \right)} \quad \text{........... (13)}$$

In the above equation (Eq. (13)), permeability $K$ is a function of the porosity of the mushy zone, which is characterized by a coherent dendritic network in the molten metal matrix. In the enthalpy-porosity approach, porosity is modeled as the volume fraction of liquid in a computational cell, which, in turn, depends on the latent enthalpy content $\Delta H$ of the control volume under consideration during the phase change process. In a physical sense, $K$ describes the friction between the solid and the liquid, as determined from the fraction of liquid and the microstructural morphology. This is in accordance with the physical situation prevailing during the columnar solidification of alloys. In a typical columnar structure, the interdendritic paths are long enough to support the backflow of melt through the solid-liquid mixed zone.\(^{15}\) Due to dendritic arm coarsening, the solid-liquid interface moves in the microscopic length scale with progress in solidification. The coarsening occurs by remelting of some of the secondary dendritic arms during solidification.\(^{15}\) This gives rise to a localized fluid flow that would effectively determine the final macrosegregation, apart from the effects of multicomponent thermosolutal convection. Hence, it is important to link the permeability of the mushy zone with the kinetics of dendritic arm coarsening. Eq. (13) specifically accomplished this task, in which the secondary dendritic arm spacing $\lambda_2$ is a variable during the evolution of the solidification process.

### 2.2. Boundary Conditions

The boundary conditions consistent with the above set of differential equations as well as the physical problem depicted in Fig. 1 are as follows:

(a) Left wall: $u = 0, v = 0, -k \frac{\partial T}{\partial x} = h (T_s - T)$,

$$\partial (C_{i,j})_2 / \partial x = 0, \partial (C_{i,j})_1 / \partial x = 0$$

(b) Right wall: $u = 0, v = 0, \frac{\partial T}{\partial x} = 0, \partial (C_{i,j})_1 / \partial x = \partial (C_{i,j})_2 / \partial x = 0$

(c) Top wall: $u = 0, v = 0, \frac{\partial T}{\partial x} = 0, \partial (C_{i,j})_1 / \partial y = 0$,

$$\partial (C_{i,j})_2 / \partial y = 0$$

(d) Bottom wall: $u = 0, v = 0, \frac{\partial T}{\partial x} = 0, \partial (C_{i,j})_1 / \partial y = 0$,

$$\partial (C_{i,j})_2 / \partial y = 0$$

Here, $u$ and $v$ are velocity components along $x$-axis and $y$-axis respectively, $h$ is the convective heat transfer coefficient. Subscript ‘1’ and ‘2’ refer to element 1 and 2 respectively.

The initial conditions appropriate to the physical situation are as:

$$At \ t = 0, u = 0, T = T_s, (C_{i,j})_1 = (C_{i,j})_2 = (C_{i,j})_2$$

### 3. Numerical Modelling

The coupled governing differential equations for fluid flow, heat transfer and mass transfer are discretized using a fully time-implicit finite volume methodology.\(^{16}\) The fluid flow equations are solved using a pressure based primitive variable formulation according to the SIMPLER algorithm.\(^{16}\) Convection-diffusion terms in the discretized governing equations are modelled by employing a power-law differencing scheme zone.\(^{16}\) The above algorithm is appropriately extended for incorporating new features pertaining to dendritic arm coarsening, which distinguish the present model from the existing two-dimensional macroscopic models describing non-equilibrium solidification situations of multicomponent alloys. These new features are described below.

#### 3.1. Modelling of Mushy Zone Permeability

It may be mentioned here that the mushy zone is assumed to be a saturated porous medium that offers frictional resistance toward fluid flow in that region. Permeability of the mushy zone is an important parameter which needs to be prescribed in accordance with the morphology of the phase-changing domain. In the present context, the theory developed by Mortenson\(^{17}\) is adopted to calculate the secondary dendritic arm spacing at representative control point locations $i,j$ at every time step,

$$\left( \lambda_2 \right)_{ij}^3 = \frac{27 \Gamma D \mu}{4} \left( 1 - \left( k_p \right)_{ij} \right) \left( 1 - \left( g_{cr} \right)_{ij} \right) \left( 1 - \left( 1 - \left( g_{cr} \right)_{ij} \right) \right)^2 \left( T_{melt} - T_{ij} \right) \left( \lambda_{2,0} \right)_{ij}^3 + \left( \lambda_{2,0} \right)_{ij}^3 \quad \text{............... (14)}$$

where $\lambda_{2,0}$ is the secondary dendrite arm spacing corresponding to the previous time level and $\Gamma$ is the Gibbs-Thomson coefficient. It can be noted that such temporal updating of $\lambda_2$ is carried out only within the range $0.07 < g_s < 0.9$. For $g_s > 0.9$, the secondary dendrite arm spacing is assumed to be $3 \mu m^{13}$ as an initial choice for the present situation. The partition coefficient value can be varied according to requirements in the present numerical scheme. The integral can be evaluated by following numerical integration method.

The enthalpy-porosity source term for the control volume $i,j$ is given as

$$S = S_e + S_p u_p, \quad S_e = 0, \quad S_p = -\mu / K \quad \text{........ (15)}$$

where $\mu$ is described by Eq. (11) and $K$ varies according to $\left( \lambda_2 \right)_{ij}$ as per Eq. (13).

#### 3.2. Numerical Scheme for Enthalpy Update

The general form of the enthalpy updating expression given by Brent et al.\(^5\) is first written as follows:

$$\left[ \Delta H_p \right]_{n+1} = \left[ \Delta H_p \right]_n + \frac{\partial}{\partial t} \left[ \Delta H_p \right]_n - c \rho F^{-1} \left[ \Delta H_p \right]_n \quad \text{........ (16)}$$
where $\Delta H_f$ is the latent heat content of the computational cell surrounding the grid point $P$, $h$ is the sensible enthalpy, $c_p$ is the specific heat, $\lambda$ is a relaxation factor, $n$ is the iteration level, $a_0$ and $a_0^i$ are the coefficients of the infinite volume discretization equation, and $F^{-1}$ is the inverse of the latent heat function. It is to be noted here that in the above equation, $F^{-1}$ needs to be devised consistently with the microscopic physics pertaining to the dendritic arm coarsening phenomena in ternary metal alloy solidification, so that physically meaningful results can be obtained from the specific solidification model.

Considering the condition of local thermodynamic equilibrium, the liquids surface in the phase diagram can be used to specify a relationship between the liquid concentrations and the temperature. In a functional form, this is expressed as

$$T = T\left[\{C_i\}_i, \{C_o\}_o\right] \quad \text{..... (17)}$$

where $N + 1$ is the total number of species present in the alloy system. In a dilute ternary alloy system ($i = 2$), assuming linearized phase diagrams of the constituent binaries, a relationship between the temperature and liquid concentrations of the solutes along the liquidus surface can be written as

$$T = T_m + m_1(C_i) + m_2(C_i) \quad \text{..... (18)}$$

where $m_1$ and $m_2$ are the liquidus slopes of element 1 and element 2 respectively, and are given as

$$(m_i) = \left(\frac{\partial T}{\partial C_i}\right) \quad \text{..... (19)}$$

In Eq. (18), $T_m$ represents the melting temperature of the pure solvent, which happens to be an important input to the thermodynamic calculation database. Further, the equations describing the relationship between the concentrations and liquid fraction in a ternary system can be given as

$$\left(\frac{C_i}{C_o}\right) = (1 - y_i f_i) \frac{x_i}{\gamma_i}, \quad \text{for component } i \quad \text{..... (20)}$$

Here, $f_i$ is the mass fraction of the solid, $y_i = 1 - 2\gamma k_{yi}^e$, and $x_i = 1 - k_{yi}^e$, where $k_{yi}^e$ is the equilibrium partition coefficient for each solute ‘i’ and is given as $C_{ei} = k_{yi}^e C_i$. $\gamma$ is the back diffusion parameter and represents the degree of back diffusion in the dendritic solid. In case of zero back diffusion (i.e., $\gamma = 0$), the Scheil model becomes applicable, and in case of complete back diffusion (i.e., $\gamma = 1$), the lever rule holds. A microscopically-consistent estimate of the parameter $\gamma$ for more general situations, can be obtained as

$$\gamma = 2\alpha[1 - e^{-1/2\alpha} - e^{-1/2\alpha}] \quad \text{..... (21)}$$

where $\alpha = \frac{D_l l_s}{l_t^2}$ is the Fourier diffusion number, $D_l$ is the diffusion coefficient in the solid, $l_s$ is the solidification length scale (typically, of the order of secondary dendritic arm spacing), and $l_t$ is the local solidification time scale.

Now, from Eq. (20) in Eq. (18), one can arrive at an expression that relates $T$ with $f_i$, as

$$T = T_m + \sum_{i=1}^{N} \left[ m_i'(C_i) (1 - y_i) + m_i'(C_o) y_i f_i \right] \quad \text{..... (22)}$$

It needs to be noted here that Eq. (14) is valid for a general $N + 1$ component alloy system, with $N = 2$ representing the special case of a ternary alloy system.

In order to obtain the latent heat function ($F$), the latent enthalpy ($\Delta H$) is related with the phase-changing temperature, through the sensible enthalpy ($h$), as

$$h = F^{-1}(\Delta H) \quad \text{..... (23)}$$

where $h$ can be written as ($c_p T$). From Eqs. (22) and (23), an expression for the inverse of the latent heat function, corresponding to the case of multi-component alloy solidification systems, can be obtained as

$$F^{-1}(\Delta H) = T_m + \phi \quad \text{..... (24)}$$

where $\phi$ is given by

$$\phi = \sum_{i=1}^{N} \left[ m_i'(C_i) (1 - y_i) + m_i'(C_o) y_i f_i \right] \quad \text{..... (25)}$$

In order to ensure that the resultant liquid fraction conforms to the microscopic features of dendritic arm coarsening, additional microscopic issues must be considered. At this stage, condition of locally constant cooling rate is assumed, which is valid for a variety of practical applications such as directional solidification and crystal growth.

For such cases, the liquid mass fraction ($f_i$) can be expressed as

$$f_i = 1 - \frac{1 - \theta}{1 - k_p} + \frac{k_p}{(1 - k_p)^2} \theta^{-\gamma/k_p} \left(\frac{1}{\theta - 1}\right)^n \times F\left(\theta : k_p, n\right) \quad \text{..... (26)}$$

where

$$F\left(\theta : k_p, n\right) = \int_{\xi = 1}^{\theta^{-1}} e^{(2k_p - 1)/k_p} (\xi - 1)^{1/k_p} d\xi \quad \text{..... (27)}$$

Here $n$ represents an experimentally determined coarsening exponent, often specified in the range of 0.29–0.35. It may be noted here that the above case reduces to the specific case of Scheil’s equation when $n = 0$. However, irrespective of the value of $n$, the updated latent heat from Eq. (23) must yield a liquid fraction consistent with expression (26). Therefore, in order to obtain a metallurgically consistent solution for the above set of equations, the following steps are sequentially performed:

Step 1: Determine $C_i(i, j)$ from the latest iteration, using the macroscopic species conservation Eq. (6)

Step 2: Evaluate the integral in expression (27)

Step 3: Evaluate $f(i, j)$ using Eq. (26), indicated as $f_0(i, j)$

Step 4: Obtain $f(i, j)$ from Eq. (23), indicated as $f_2(i, j)$

Step 5: Update $f_i$ as

$$f_i(i, j) = f_2(i, j) + \alpha_i \text{sign} \left[ \left( T\left[\{C_i\}_i, \{C_o\}_o\right] \right) \left(\frac{C_i}{C_o}\right) \right]$$

where $\alpha$ is a relaxation factor.

The algorithm for correction of the liquid fraction basically attempts to neutralize the difference between values predicted by Eqs. (23) and (26), respectively. In order to ensure smooth convergence for solution, value of $\lambda_1$ is kept low ($\sim 0.05–0.1$).
Step 6: Solve for $u(i, j)$, $v(i, j)$, and $T(i, j)$, using the updated values of liquid fraction during next iteration within the same time-step. The fluid flow equations are solved using a pressure based primitive variable formulation according to the SIMPLER algorithm. The process described above is repeated until convergence is achieved. Once the convergence check is satisfied, simulation is advanced to the next time step and continued until the domain solidifies completely.

4. Results and Discussion

For the purpose of illustration of the present numerical model, simulations are performed for the case of a three element (Fe-0.08wt%C-0.1wt%Mn) steel alloy with iron, carbon and manganese as the constituent elements. The liquidus temperature of the ternary steel alloy system for the present case is 1805 K, while the melt initially is at a uniform temperature of 1830 K inside the domain. The heat transfer coefficient ($h_l$) at the left wall is taken as 125 W/m$^2$.K. Table 1 summarizes the species-dependent thermodynamic characteristics, as adopted in the present work. The relevant thermophysical properties for steel are listed in Table 2. Different grid sizes (40 × 40, 60 × 60 and 100 × 100) are used for the resolution of the computational domain of size (0.1 m × 0.1 m) to check for grid independence. It is found that a further refinement in grid spacing does not alter the numerical predictions appreciably.

Figure 2 shows the convection pattern for the ternary (Fe-0.08wt%C-0.1wt%Mn) system, at time, $t = 80$ s after commencement of solidification. Once the left vertical wall of the rectangular mould is subjected to cooling, thermal gradients establish flow in the melt, with thermal buoyancy forces governing the transport processes at the initial stages. Consequently, the cold fluid descends along the interface and takes a counterclockwise turn near the bottom of the cavity, as can be observed from the streamlines in Fig. 2. As solidification progresses, the rejected solute being lighter (for both carbon and manganese) than the bulk fluid, tends to reduce the density of fluid in the mushy zone and drive the fluid in the upward direction. However, in the present situation, the relative strength of solutal buoyancy is smaller than the thermal buoyancy, and therefore the flow field is dominated by the thermal buoyancy effect. Presence of a minor vortex near the bottom corner of the cavity is due to the local solutal gradient build-up around the region.

Figure 3 shows the flow pattern at a later stage ($t = 160$ s) of flow development. Due to the effect of directional heat transfer in the present case, flow is observed to progress in a longitudinal direction. Effect of localized solutal convection is negligible in the present case.

Figure 4 depicts the composition variation of carbon along the longitudinal (x-axis) direction at different time intervals during the solidification of the present alloy system. For the purpose of comparison, results from the present model are plotted along with those without coarsening considerations. Figures 4(a)–4(b) shows the composition varia-
tion at $t = 60 \text{ s}$ and $t = 180 \text{ s}$, and at a vertical location $y = 0.05 \text{ m}$. A sharp increase in solute concentration is noticed at the vicinity of the interface between mushy region and liquid region, because of the rejection of solute during solidification. Due to the thermal buoyancy effect, the rejected solute is carried downward along the interface leading to a composition variation in the vertical direction. The effect of dendrite arm coarsening is to decrease the frictional resistance towards fluid flow in the mushy region. This leads to an enhanced convective flow which transports the rejected solute in the bulk flow resulting in composition variation in the bulk portion of the domain. Since models considering fixed dendritic arm spacing are unable to capture the enhanced advective field, results from such model predicts almost homogeneous composition in the bulk portion of the domain with a flatter curve. Similar behavior is also observed for the composition variation for manganese.

The macrosegregation level of the constituent elements (carbon and manganese) during solidification is shown in Fig. 5. The figure plots the average redistribution of the components integrated over the whole volume of the casting as a function of time. In Fig. 5, macrosegregation effects are quantified as follows:

$$M(i) = \left[ \frac{1}{V} \left( \frac{C_{\text{mix}}}{C_{\text{eq}}^i} - 1 \right)^2 \right]^{1/2}$$  \hspace{1cm} (29)

where the subscript ‘$i$’ denotes solute element under concern.

4.1. Comparison with Experimental Results

In order to assess the quantitative predictive capabilities of the present model, a comparative study between experimental results reported in the literature and the corresponding outcomes from the present study is performed. Towards this, simulation results from the present model are compared with the experimental data corresponding to unidirectional solidification of an Al8.1wt%-Cu3wt%-Si ternary alloy system in a vertical water-cooled mold growth. Figure 6 shows the numerically predicted temperature values and the corresponding experimental data,23 at two different vertical locations within the mold. Model predictions considering dendrite arm coarsening and without coarsening are shown in the figure. Results of the present model are found to match well with the experimental results. Further, the simulated macrosegregation level of copper has been compared with experimental observations in Fig. 7, and good agreement is observed. In both the cases (Figs. 6–7), the experimental results are more accurately predicted by the present model than by existing ones. This is due to the fact that models considering fixed
increased permeability of the mushy zone, which in turn also indicate that the dendritic coarsening leads to an increased convective heat transfer coefficient for the constituent elements (carbon, manganese) are qualitatively similar, with macrosegregation patterns for the constituent elements studied. From the simulation results, it is observed that the macroscopic transport of mass, momentum, heat and solute is analyzed using a fixed-grid enthalpy-based mathematical model, and the mushy zone is modeled according to the coarsening kinetics of dendrite arms. Solidification for ternary steel alloy is numerically modeled according to the coarsening kinetics of dendrite arm spacing are unable to capture the enhanced advective field which has a very important bearing on the overall solidification transport and macrosegregation behavior.

5. Conclusions

In the present work, a macroscopic numerical model is developed which is capable of capturing the effects of secondary dendritic arm coarsening on the multicomponent solidification process. The macroscopic transport of mass, momentum, heat and solute is analyzed using a fixed-grid enthalpy-based mathematical model, and the mushy zone is modeled according to the coarsening kinetics of dendrite arms. Solidification for ternary steel alloy is numerically simulated and the resulting flow and macrosegregation patterns are studied. From the simulation results, it is observed that the macrosegregation patterns for the constituent elements (carbon, manganese) are qualitatively similar, with the severity of segregation dependent on the partition coefficient of the respective constituents. Numerical predictions also indicate that the dendritic coarsening leads to an increased permeability of the mushy zone, which in turn results in a more pronounced macrosegregation. Results from the present model are also compared with the experimental measurements reported in the literature and very good agreements are observed.

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Nomenclature

- $c$: specific heat
- $C$: species concentration
- $D$: mass diffusion coefficient of species
- $f$: mass fraction
- $g$: volume fraction
- $h$: specific enthalpy
- $h_c$: convective heat transfer coefficient
- $\Delta H$: latent enthalpy
- $K$: permeability
- $L$: latent heat
- $T$: temperature
- $\bar{u}$: velocity vector
- $u$: axial component of velocity
- $v$: radial component of velocity
- $\mu$: dynamic viscosity
- $\rho$: density
- $\Gamma$: Gibbs-Thomson coefficient

Subscripts

- $i$: initial
- $f$: final
- $g$: gas
- $l$: liquid
- $s$: solid
- $\text{mix}$: mixture

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