Two-Phase Modeling of Macrosegregation in a 231 t Steel Ingot

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The formation of macrosegregation in the steel ingots is a multiphase/multiscale flow phenomenon inherently. It still remains a challenge to simulate the macrosegregation in the large steel ingots. The objective of this work is to validate a two phase model by measuring the macrosegregation in a 231 t steel ingot. The model incorporates the descriptions of heat transfer, melt convection, solute transport, and the solid movement on the system scale with microscopic relations for grain nucleation and growth. The model simulates the solidification process by solving the conservation equations of mass, momentum, energy and species for both the liquid and solid phases. Besides, simulations are performed to investigate the influence of the critical solid volume fraction \( g_{\text{sc}} \) on the final macrosegregation pattern which was characterized by experimental measurements. It is indicated that the typical macrosegregation patterns encountered in a large steel ingot, including a positively segregated zone in the hot top and a negatively segregated zone in the bottom part of the ingot, are well reproduced with the current two phase model. Comparison of the simulation results and the measurements is made. It is demonstrated that the critical solid volume fraction \( g_{\text{sc}} \) is an important factor for the final macrosegregation pattern.

KEY WORDS: macrosegregation; steel ingots; two-phase model; critical solid fraction.

1. Introduction

Large steel ingots are typically used for key components such as steam turbine rotors, pressure vessels and mill rolls in the power, petrochemical, metallurgy and other heavy industries. It is important to improve the quality of the steel ingots. Macrosegregation, the macroscopic species inhomogeneous distribution, is the main defect in steel ingots. The feeding flow, thermosolutal convection, solid movement and deformation of the solid network are considered as the main reasons responsible for the formation of macrosegregation.\(^1\) Since the first model was proposed by Flemings and coworkers,\(^2\) various models have been developed to investigate the formation the macrosegregation by different methods.\(^3\)–\(^10\) However, only a few efforts have been made to predict the macrosegregation in industrial steel ingots due to the complexity and the great computation resource. The continuum model or volume averaged model, which apply one set of conservation equations for the solidification system, are widely applied due to its convenience. Combeau and coworkers\(^11\) adopted a volume-averaged model to investigate the formation of macrosegregation in a 65 t ingot. Beckermann \( et \) al.\(^12\) applied a volume-averaged model to a steel ingot of 43 ton. The mathematical equations are solved by the finite element method (FEM) to predict the macrosegregation in a 3.3 t steel ingot in the research of Bellet and coworkers.\(^13\) Li and coworkers\(^14\) applied the mixture model to predict the macrosegregation in a 360 t ingot. The multiphase models, solving multi-set of conservation equations for different phases, have been developed to predict macrosegregation in steel ingots recently. The effects of the motion and the morphology of equiaxed grains on macrosegregation have been investigated in a 3.3 t ingot using a two-phase model by Combeau and coworkers.\(^6\) Li \( et \) al.\(^15\) developed a two phase model to predict macrosegregation in a 53 t ingot, and comparisons were made between the predictions and measurements. Ludwig\(^6\) applied a sophisticated three-phase model to predict the macrosegregation in a 2.45 t ingot.

In this paper, the two phase model developed by the authors\(^15\) has been adopted to model the macrosegregation in a 231 t steel ingot. The simulation results are compared with the measurements in the plant. Moreover, different cases are conducted to investigate the effects of the critical solid fraction on the formation of macrosegregation.

2. Model Description

The macroscopic phenomena of heat transfer, fluid flow, solute transfer and solid movement, and the microscopic phenomena of grains nucleation and growth are coupled into the recently developed two-phase model. The conservation equations are solved both for the liquid and solid phase, linked by the interfacial balance, using the finite volume method (FVM). The mathematical model is summarized in Table 1, and complementary relations are listed in Table 2. In the Tables 1 and 2, \( t \) is the time, \( g \) is the volume fraction, \( \rho \) is the density, \( \Gamma \) is the interfacial phase change rate, \( u \) is the velocity, \( p \) is the pressure, \( \mu \) is the viscosity, \( g \) is the...
Table 1. Mathematical equations of the two-phase model.

| Equation                                      | Description                                                                 |
|-----------------------------------------------|------------------------------------------------------------------------------|
| \[
\frac{\partial}{\partial t} (g, \rho_t) + \nabla \cdot (g, \rho_t u_t) = \Gamma_t
\] | Mass conservation                                                           |
| \[
\frac{\partial}{\partial t} (g, \rho_s) + \nabla \cdot (g, \rho_s u_s) = -\Gamma_s
\] | Momentum conservation                                                       |
| \[
\frac{\partial}{\partial t} (g, \rho_t C_t) + \nabla \cdot (g, \rho_t u_t C_t) = \frac{S_p D_p}{\psi_s} (C_i^* - C_t) + C_t \Gamma_t
\] | Species conservation                                                        |
| \[
\frac{\partial}{\partial t} (g, \rho_s C_s) + \nabla \cdot (g, \rho_s u_s C_s) = -\frac{S_p D_p}{\psi_s} (C_i^* - C_s) + C_s \Gamma_s
\] | Energy conservation                                                         |
| \[
\frac{S_p D_p}{\psi_s} (C_i^* - C_t) + C_t \Gamma_t + \frac{S_p D_p}{\psi_s} (C_i^* - C_s) - C_s \Gamma_s = 0
\] | Interfacial species balance                                                 |

Table 2. Complementary relations.

| Property                      | Equation                                                                 |
|-------------------------------|--------------------------------------------------------------------------|
| Grain density                 | \[\frac{\partial}{\partial t} n + \nabla \cdot (n u) = N\]                |
| Nucleation model              | \[N = \frac{d\Delta T}{dt} \frac{n_{\text{se}}}{\sqrt{2\pi \Delta T_s^2}}\] |
| Interfacial solute diffusion lengths | \[\delta_s = \frac{d_s}{10}, \delta_l = \frac{d_l}{2}\]             |
| Microstructural dimensions   | \[d_i = \sqrt{\frac{2g_s}{f(n)}} \]                                    |
| Solid viscosity               | \[\mu_s = \frac{\rho_s}{g_s} [(1 - g_s) (|u_s| - (1 - g_s))]\]           |

Gravity, \( \beta \) is the drag force coefficient between the solid and liquid, \( C \) is the concentration, \( S \) is the interfacial area concentration, \( D \) is the mass diffusivity, \( T \) is the temperature, \( L \) is the latent heat, \( n \) is the grain density, and \( V \) is the grain nucleation rate. The subscripts "s" and "l" refer to solid phase and liquid phase, respectively. As for "sl", it means the solid-liquid interface. The two-phase model takes the thermosolutal convection, solid movement, and formation of the primary shrinkage cavity into consideration. The computation of shrinkage follows the methods in literatures.\(^ {12,15}\) The total shrinkage volume during each time step equals to the sum contraction of all elements. When the total shrinkage volume is larger than the volume of one element, corresponding elements are treated as empty. The deformation of the solid network is ignored, which was solved by the FEM in literatures.\(^ {13,18}\) Compared with the FVM, the FEM is believed to be more effective and also more complicated as for the consideration of deformation.

Here, the flow model is highlighted. According to Gidaspow model,\(^ {19}\) the drag force between solid and liquid in different situations are considered. The Wen and Yu model is employed in the low solid fraction area. This situation corresponds to a slurry regime in which the solid can move with the liquid flow. The Ergun model is applied for the situation of high solid fraction, and it is similar to porous medium flow where only the liquid can flow through the fixed solid skeleton. The critical solid fraction \( g_{sc} \) has been used as the distinguish criterion. The model of the interfacial drag coefficient is summarized in Eq. (1). In the equation, \( C_0 \) is a resistance coefficient related to the flow Reynolds number,\(^ {19}\) \( d_p \) is the diameter of the solid grain. It can be concluded from the model that the bigger \( g_{sc} \) is, the easier the slurry is to form and the greater chance for the solid does have to move.

\[
\beta = \left\{ \begin{array}{ll}
\frac{3}{4} C_D \frac{g_s g_t \beta_l}{d_p} |u_s - u_l|^{2.65} & \text{for} \quad g_s \leq g_{sc} \\
150 \frac{g_s^2 \mu_s}{g_t d_p^2} + 1.75 \frac{\rho_s \beta_l}{d_p} |u_s - u_l| & \text{for} \quad g_s > g_{sc}
\end{array} \right.
\]  

3. Results and Discussion

The two-phase model was applied to a 231 ton steel ingot, which was cast and measured by the steel plant of CITIC Heavy Industries Co., Ltd. The dimensions of the ingot system are illustrated in Fig. 1. The steel concentration was simplified as Fe-0.205 wt.% C. The molten metal was top poured at the temperature of 1570°C in a cast-iron mould with insulation sleeve. After teeming, a layer of exothermic powder was overlaid. The complete solidification time for this ingot was approximately 45 hours. Carbon concentration was measured in the longitudinal section at the bottom. Due to the symmetry along the centerline axis of mould, a 2-D simulation was conducted for 1/2 ingot. Considering the accuracy and computation time, a grid system consisting of 9126 cells was used with mesh size of 40 mm×40 mm. The time step was 0.05 s initially, and then it was adjusted to 0.5 s gradually. The critical solid fraction \( g_{sc} \) adopted was 0.20. The properties of the steel ingot and mold materials

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used are listed in Tables 3 and 4. The initial temperature for the mold, sleeve, and power are 25°C, 25°C, and 1500°C respectively. The boundary conditions are listed in Table 5.

The time evolution of solidification sequence is shown in Fig. 2. For the early stage as shown in Fig. 2(a), the solidification firstly takes place near the cold mould wall. The nucleation of the equiaxed grains is initially formed. These grains descend along the columnar surface and settles in the bottom of the ingot, which inducing a downward melt flow. Considering the solute partition effects \( k_p = \frac{c_s}{c_l} = 0.34 < 1 \), these solidified grains are solute depleted. Then a bottom negative segregation forms initially. At the middle stage as shown in Figs. 2(b) and 2(c), the thermosolutal convection dominates and induces a clockwise flow, descending to the center and ascending at the surface of the ingot. At the late stage as shown in Fig. 2(d), the solute-rich melt begins to solidify, which forms a positive segregation at the ingot top. It has to be pointed out that the some low carbon spot is formed near the rim of the ingot. This could be caused by the use of orthogonal computational mesh grids which are unable to describe the inclination of the ingot precisely.

Figure 3 shows the predicted final macrosegregation pattern of carbon in the fully solidified ingot. As shown in Fig. 3, a cone shaped negative segregation zone is observed at the bottom, while a positive segregation zone is at the hot top of ingot.

### Table 3. Thermophysical properties of the materials used in present simulation.

| Material   | Density/(kg·m⁻³) | Thermal Conductivity/W·m⁻¹·K⁻¹ | Specific heat at constant pressure/J·kg⁻¹·K⁻¹ |
|------------|------------------|--------------------------------|-----------------------------------------------|
| Steel      | 6990             | 39.3                           | 500                                           |
| Mold       | 7000             | 26.3                           | 540                                           |
| Sleeve     | 185              | 1.4                            | 1040                                          |
| Powder     | 260              | 0.6                            | 1040                                          |
| Air        | 1.5              | 0.042                          | 1092                                          |

### Table 4. The steel parameters used in the present simulations.

| Property                  | Value          |
|---------------------------|----------------|
| Melting temperature \( T_m/°C \) | 1532           |
| Liquidus slope \( m_l/(K\cdot wt.%⁻¹) \) | -80.45         |
| Partition Coefficient \( k_p \) | 0.314          |
| Latent Heat \( L/(J·kg⁻¹) \) | 2.71×10⁵       |
| Liquid viscosity \( \mu_l/(kg·m⁻¹·s⁻¹) \) | 4.2×10⁻⁵       |
| Liquid solute diffusion coefficient \( D_l/(m²·s⁻¹) \) | 2×10⁻⁸         |
| Solid solute diffusion coefficient \( D_s/(m²·s⁻¹) \) | 5.187×10⁻¹²    |

### Table 5. Thermal boundary conditions.

| Interface                        | Heat Transfer Coefficient/W·m⁻²·K⁻¹ |
|----------------------------------|-------------------------------------|
| Interface between the steel and the mold | h=1 000 W·m⁻²·K⁻¹                   |
| Interface between the steel and the sleeve | h=400 W·m⁻²·K⁻¹                    |
| Interface between the steel and the power | h=1 000 W·m⁻²·K⁻¹                   |
| Interface between the mold and the sleeve | h=1 000 W·m⁻²·K⁻¹                   |
| Interface between the mold and the outside air | h=140 W·m⁻²·K⁻¹                    |
| Interface between the sleeve and the power | h=1 000 W·m⁻²·K⁻¹                   |
| Interface between the sleeve and the outside air | h=10 W·m⁻²·K⁻¹                     |
| Interface between the powder and the outside air | h=40 W·m⁻²·K⁻¹                     |

Figure 4 present the comparisons of the predicted and measured macrosegregation along the transverse sections at different heights above the bottom face of the ingot. The positions of the transverse sections are shown in Fig. 1, and the heights over the bottom are 150 mm, 250 mm, and 350 mm for section A, section B, and section C respectively. Considering the huge cost of fully dissection, only the ingot bottom was sectioned and analyzed while the main body of the ingot still enters the following forging process. The quantitative chemical measurements were conducted by the

![Fig. 1. Schematic of the ingot system.](image)

![Fig. 4. Comparisons between measured and predicted segregations in (b) section A, (c) section B, (d) section C.](image)
infrared spectrometry method. As shown in Fig. 4, the overall carbon segregation is negative at these sections. From the center to the ingot surface, the measured carbon concentrations exhibit a tendency of increasing. The predictions are generally in agreements with this tendency, and the small increasing margin descends with the height from the bottom face of the ingot. However, some of the carbon concentrations at the sections are underestimated in the simulations compared with the measurements. The uncertainties in the thermophysical data, two-dimensional simplification of geometry, or measurements errors are the possible reasons contributing to these discrepancies. Future experiments should be designed and performed considering more details to provide a sound basis for assessing the model predictions.

In order to investigate the effect of the critical solid frac-

![Fig. 2. Predicted solidification sequence of 231 ton ingot. Left: solid volume fraction; Right: macrosegregation and liquid velocity. (a) 1.5 h, (b) 10 h, (c) 20 h, (d) 30 h.](image)

![Fig. 3. Predicted final macrosegregation of the ingot.](image)

![Fig. 5. The predicted final macrosegregations with different critical solid fraction: (a) $g_s=0.1$; (b) $g_s=0.3$.](image)

![Fig. 6. Time evolutions of the solid fraction and segregation at the point P with different critical solid fractions.](image)

![Fig. 7. Time evolutions of the solid vertical velocity at the point P with different critical solid fractions during 1.0 h–1.5 h.](image)
tion (gsc), other two cases with different critical solid fractions are studied i.e., gsc=0.1, and gsc=0.3, respectively. The predicted final macrosegregations are shown in Fig. 5. It is shown that the bigger critical solid fraction, the more negative segregation is at the ingot bottom.

Figure 6 shows the predicted evolutions of solid fraction and segregation at the point P, located in the bottom part (0.4 m above the bottom face) along the ingot centerline as shown in Fig. 1. When the point P is far from the solid-liquid interface during the initial solidification stage, the point P remains in the liquid region. With the solute redistribution effect, the solute concentration at the point P starts to increase and the segregations at P become slightly positive. At this stage, the solid fraction and segregation profiles at P with different gsc are almost the same. When the solid-liquid interface approaches P (about 1.0 h), the early solidified solid grains with depleted solute concentration, start to sink and get accumulated around P. Then segregations at P decrease instantly and become negative. At this stage (about 1.0 h–1.5 h), the curves of solid fraction and segregation start to separate for the different gsc.

The vertical velocity of the solid phase at the point P during solidification of 1.0 h–1.5 h is shown in Fig. 7. As analyzed above, the solid movements are affected by the thermosolutal convection and grains settlement. As for the point P located in solid-liquid interface at the ingot bottom, the convection brings the solid grains upward and the settlement moves the solid grains downward. The competition of these two effects is shown from the curves with fluctuations in the Fig. 7. The convection prevails at the beginning, and then the settlement does the domination. Due to the different gsc, different degrees of settlements have formed. As analyzed in the flow model, the bigger the critical solid fraction is, the easier the flurry flow is to occur. This trend can also be validated from Fig. 7. The vertical solid velocity reduces to zero at 1.20 h for gsc=0.1, while the others do at 1.34 h and 1.48 h for gsc=0.2 and gsc=0.3, respectively. Therefore, more grains tend to settle in the bottom for gsc=0.3 compared with the other two cases. With the development of solid-liquid interface, the balance of solid grains settlement and melt convection has been formed which corresponds to the zero vertical velocity in Fig. 7. With the balance, the profiles of solid fraction and segregation keep constant in Fig. 6. When the interface moves far from the point P, the melt convection becomes weak. Then the solid fraction starts to increase instantly. At the same time, the negative segregation degrees at P have been induced by the solute diffusion in the solid phase. Therefore, it gets the conclusion that the critical solid fraction does matters to the modeling of solid movements. It should be cautious to choose the value of the critical solid fraction to predict the formation of macrosegregation.

4. Conclusions

A two-phase model considering the transport phenomena both for the liquid and solid phase has been applied to investigate the macrosegregation formation in a 231 ton steel ingot. A positive segregation is located in the top and a negative segregation is at the bottom for the prediction results. The predictions are compared with measurements at bottom sections of the ingot. It is shown a good tendency of agreement. Moreover, different simulations have been conducted to investigate the effects of the critical solid fraction. The solid movements are combination results of melt convection and grains settlement. The greater the critical solid fraction, the more easily the solid dendrites get accumulated in the bottom, and the more serious negative segregation it will get at the bottom of the ingot. An appropriate value of the critical solid fraction should be chosen to simulate the formation of macrosegregation in consideration of the solid movements. Further simulation research, as well as more detailed experimental results even for a fully dissected steel ingot, is required to achieve a better agreement between the measurements and predictions, which is also favorable to the better understanding of the macrosegregation.

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