Numerical study of influence of inclusion movement on channel segregation in Fe- 0.21 wt% C- 0.1 wt% S alloy

D R Liu, Z P Yang, Q Y Sun, L P Wang, and B X Ma
School of Materials Science and Engineering, Harbin University of Science and Technology, No.4 Lin Yuan Road, Xiang Fang District, Harbin 150040, China
E-mail: anacylake@126.com

Abstract. A two-dimensional continuum model on solute and heat transport, and fluid flow is developed to numerically investigate the influence of inclusion movement on the development of channel segregation. A trajectory model is used to track the moving path of inclusion particles. Inclusion movement affects the flow field in simulation by means of interfacial friction coefficient. Simulations are performed on the Hebditch-Hunt casting. A parametric study is carried out to study the effects of with and without inclusions, and diameter ($5 \times 10^{-6}$ m, $10 \times 10^{-6}$ m, $20 \times 10^{-6}$ m and $40 \times 10^{-6}$ m) of inclusions on channel segregation. It is found that the channel segregation is strengthened with the consideration of inclusion movement. Compared to other diameters, inclusions with diameter $20 \times 10^{-6}$ m are found to enhance the channel segregation. This is because the larger inclusions ($40 \times 10^{-6}$ m) present a faster floating velocity that reduces the interaction time between inclusion upward movement and the development of solidification front, and then lessens the disturbance to solidification front that is important to the initialization of channel segregation. The upward movement of smaller inclusions ($5 \times 10^{-6}$ m and $10 \times 10^{-6}$ m) cannot greatly increase the upward velocity of fluid flow. Therefore, the formation of channel segregation is less affected.

1. Introduction
One particularly striking macrosegregation form during solidification of casting is channel segregation which is considered to be the most harmful defect, due to the fact that it cannot be removed in the manufacturing process [1]. Channel segregation typically occurs in alloys experiencing a slow solidification rate. They are finger-like A-shape or V-shape segregation bands [2]. Those bands are characterized to have a higher segregation than that of the nearby solid regions. Elements with the low melting point cluster here, corresponding to detrimental properties [2].

In order to deeply understand the fundamental origins of channel segregation, numerical modelling of channel segregation during solidification of metallic alloy has received great interest. Flemings believed that local dissolution characterized as a decrease of solid fraction and the resulting flow instability lead to channel segregates [3]. A series of research work of Založnik and Combeau showed that channel segregation stems from a perturbation to the advancement of the mushy zone front induced by the interdendritic liquid [1,4]. The local dissolution (decrease of solid fraction) does not necessarily occur to initiate a channel segregate. Li et al. developed a two-phase columnar solidification model and numerically investigated the formation of channel segregation [5, 6]. The simulations have justified that Rayleigh number is a qualitative indicator for characterizing the origin of channel segregates. Our previous work investigated the influence of increasing the initial
concentration of sulphur on the formation of channel segregation during solidification of iron-carbon-sulphur ternary system [7]. Simulations showed that channel segregation occurs accompanied by the local dissolution at the mushy zone front, when a high initial concentration of sulphur is considered. For a low initial concentration, however, the local dissolution does not necessarily induce channel segregation.

Although a lot of work has been done to understand channel segregation formation, the influence of inclusion transport has not been considered until now. Inclusions exist as a kind of impurity in the casting process, whose movement was believed to affect the flow field and then change the segregation pattern [8]. Thus the goal of this study is to analyze the impact of inclusion motion on the channel segregation. Parametric studies regarding different inclusion sizes are performed, in some degree, to quantify the conditions necessary for inclusions to strength channel segregation.

2. Model description

The model for the solidification of ternary alloys is an extension of the model for binary alloys developed by Pardeshi and Voller [9]. A set of equations of conservation of mass, energy and solute concentration is solved in conjunction with the momentum equation. A Boussinesq approximation is used to account for buoyancy driven flow. The mushy zone is treated as a porous medium of variable porosity. The multiple species on the transport phenomena manifests itself through some coupled effects [10]; the differences in the solutal expansion coefficients for the elements in the liquid phase, and the differences in the partition coefficients for the elements as well as the effects of the various species on the liquidus temperature. The continuum mixture model is used as a starting point for the simulation of macrosegregation.

The trajectory model is employed to investigate inclusion movement [11]. In order to simplify the computation of inclusion moving, a few assumptions are made; (1) inclusions are spherical, (2) every inclusion is considered to move independently and collision between inclusions is not included, (3) once inclusions reach the casting walls, they will be captured and stop moving.

The translational motion of one inclusion of velocity, \( v_{sx} \) and \( v_{sy} \), diameter, \( d \), and density, \( \rho_i \), can be described using Newton's law [11]:

\[
\frac{dv_{sy}}{dt} = -\frac{3}{4} \frac{\rho_l}{\rho_i d} (v_{sy} - v_y) |v_{sy} - v_y| C_D + \left(1 - \frac{\rho_l}{\rho_i}\right) g
\]

\[
\frac{dv_{sx}}{dt} = -\frac{3}{4} \frac{\rho_l}{\rho_i d} (v_{sx} - v_y) |v_{sx} - v_y| C_D
\]

(1)

where \( v_y \) and \( \rho_l \) are the velocity and density of the liquid, respectively; \( C_D \) is a drag coefficient; \( g \) is the gravitational acceleration; and \( t \) is time. The first term on the right-hand side of equation (1) is the drag force exerted by the liquid, and the second is the buoyancy force.

The movement of inclusions in the molten metal is assumed to affect the flow streamlines. The interfacial friction coefficient is calculated by the Gidaspow correlation [12]:

\[
K_{ix} = \frac{3}{4} C_D \frac{F_s f_i \rho_l}{d} |v_{sx} - v_{ix}| f_i^{-2.65}
\]

(3)
where $K_\alpha$ is the interphase friction coefficient; $f_l$ the volume fraction of liquid; $F_i$ the volume fraction of inclusion in the mesh. When the local volume fraction of solid exceeds 0.2, the inclusion is thought to be captured by the dendritic network and the velocity is abruptly set to zero.

The general governing conservation equation is discretized using a finite volume method. A staggered grid is employed for the discretization of the momentum equation. A power law scheme is adopted to estimate the convection-diffusion flux at the control volume faces. Equations (1) and (2) are discretized implicitly. The movement of inclusions does not step into the pressure correction equation. The resolution of the velocity-pressure coupling is performed by the single-phase solution algorithm SIMPLER.

3. Results and discussion
The model for simulating macrosegregation was verified using a numerical benchmark proposed by Založnik et al. [13]. The test was concerned with solidification of a binary Sn-5wt%Pb alloy in a Hebditch-Hunt casting. Full details of validation concerning mesosegregation and macrosegregation patterns are available in a published article [7]. The test with an acceptable outcome gives us confidence that the self-developed computer codes are reasonable for the following analysis. In the present contribution, the previously verified model is extended to include the inclusion movement.

The study configuration in [7] is used in this research. A Hebditch-Hunt casting is a two-dimensional rectangular mould cavity of 0.06 m height and 0.1 m width. The mould cavity is thermally insulated on the left, top and bottom walls and chilled by water at the right wall. The coolant temperature keeps constant at 25 °C. For the following simulations, uniform grids $100 \times 60$ with grid size 0.001 m are employed. The model alloy is Fe-0.21 wt% C-0.1 wt% S. The 500 inclusions are initially introduced into the liquid at random positions. Inclusions have the same diameter and their size will not change during solidification. Main thermophysical properties and boundary conditions used in the computations are listed in Table 1 [13]. In order to study the impact of inclusion movement on the channel segregation formation, two cases are defined. The main characteristics are given in Table 2. The first case is used as the reference case. For Case 2, the movement of inclusions is switched off. For Case 3 and Case 4, the influences of inclusion size on channel segregation are investigated.

| Density (kg m$^{-3}$) | Fe - 0.21 C - 0.1 S | Inclusion |
|-----------------------|---------------------|-----------|
| 6910.0                | 3640.0              |           |
| Binary partition coefficient (C) | 0.169 | — |
| Binary partition coefficient (S) | 0.024 | — |
| Liquidus slope (C, °C wt%$^{-1}$) | -118.41 | — |
| Liquidus slope (S, °C wt%$^{-1}$) | -30.4 | — |
| Thermal expansion coefficient (K$^{-1}$) | $6.0 \times 10^{-5}$ | — |
| Solutal expansion coefficient (C, wt%$^{-1}$) | 0.011 | — |
| Solutal expansion coefficient (S, wt%$^{-1}$) | 0.0123 | — |
| Secondary dendrite arm spacing (m) | $500 \times 10^{-6}$ | — |
| Coolant temperature (°C) | 25 | — |
| Heat transfer coefficient at the chill (W m$^{-2}$ s$^{-1}$) | 20 | — |
### Table 2. Cases definition

|        | Inclusion movement | Diameter (m) |
|--------|------------------|--------------|
| Case 1 | Yes              | $20 \times 10^{-6}$ |
| Case 2 | No               | —            |
| Case 3 | Yes              | $5 \times 10^{-6}$ |
| Case 4 | Yes              | $10 \times 10^{-6}$ |
| Case 5 | Yes              | $40 \times 10^{-6}$ |

#### 3.1. Influence of inclusion movement (comparison between Case 1 and Case 2)

Comparisons between simulated macrosegregation maps in Case 1 and Case 2 are shown in figure 1. Only the distribution of carbon concentration is presented. The global macrosegregation pattern of sulphur is very similar to that of carbon, as the two elements both have partition coefficients smaller than 1 and show the same sign in the solutal expansion coefficients. Their corresponding thermal expansion coefficients are small enough ensuring that the effects of solutal buoyancy outweigh the effects of thermal buoyancy.

![Figure 1](image)

**Figure 1.** Maps of macrosegregation of carbon in (a) Case 1 and (b) Case 2.

The channel segregation (solute-rich strip) is intensive in Case 1. Since inclusions have a lower density than that of liquid, they tend to float to the top of the casting cavity. 51 inclusions among 500 inclusions are randomly chosen. The moving trajectories are illustrated in figure 2. With diameter $20 \times 10^{-6}$ m, all these inclusions float up within 100 s and finally are captured by the top boundary of casting. The more penetrated channels are the direct consequence of a relatively higher velocity induced by inclusion movement at the initial stage of solidification (figure 3a). For the melt solidifying from liquidus temperature (zero superheat), a porous mushy zone quickly forms and the solutal buoyancy plays a dominant role from the onset of solidification. The solutal configuration creates an upward flow in the melt at the cooled side across the phase changing front and a downward flow in the bulk liquid. At some locations, the upward fluid flow ahead of the solidification front is subject to drag forces from the floating inclusions. Such stronger upward flow easily triggers instability at the solidification front in the regions where it leaves the mushy zone. Such instability that the continuously advancing solidification front faces leads to channel segregation [4].
Figure 2. Moving trajectories of 51 inclusions randomly selected among the 500 inclusions.

Figure 3. Flow field and iso-fractions of solid at different times: (a) Case 1 and (b) Case 2

When comparing figure 3a and figure 3b, we can see that without inclusion movement (Case 2), during solidification, the flow field is clearly structured as a counter-clockwise cell and the magnitude of fluid flow is relatively weak. The oscillations on iso-fractions of solid are less pronounced. It is why figure 1b shows segregated channels of low intensity.
3.2. Influence of inclusion size

The formation of mesosegregation when changing inclusion diameters is illustrated in figure 4. The intensity of channel segregation is low in Case 5 with a larger inclusion size \((40 \times 10^{-6} \text{ m})\), figure 4 d). Compared with Case 5, segregated channels with a stronger intensity in Case 1 deeply diffuse into the mushy zone \((20 \times 10^{-6} \text{ m})\), figure 4 c). The degree of channel segregation is comparable in Case 3 and Case 4 (figures 4a and b). According to Stokes law, the larger the inclusions, the faster the floating velocity. The quick upward movement of large inclusions slightly coincides with the development of solidification front. The up-movement of inclusions cannot greatly strengthen the upward flow velocity of interdendritic liquid. Therefore, the perturbation from the interdendritic fluid flow is reduced. In comparison with large inclusions, small inclusions \((5 \times 10^{-6} \text{ m and } 10 \times 10^{-6} \text{ m})\) are more easily entrained by the fluid flow. They do not present a strong tendency of floating up. Under such condition, the channel segregates are, on some degree, suppressed.

Figure 4. Maps of macrosegregation of carbon: (a) Case 3, (b) Case 4, (c) Case 1, (d) Case 5.

4. Conclusion

A mathematical model was developed to simulate the transport of inclusions and the formation of mesosegregation. Inclusion motion has an impact on increasing the intensity of channel segregation. A relatively serious channel segregation is found in the case with inclusion movement and with inclusion diameter \(20 \times 10^{-6} \text{ m}\). With increasing the size to \(40 \times 10^{-6} \text{ m}\) or decreasing the size to \(5 \times 10^{-6} \text{ m}\), the degree of channel segregation is reduced. All the above simulations are performed with melt superheat zero. With inclusion movement, the parametric study indicates that there exists a relatively small window of initial conditions that result in a serious channel segregation. Although the calculations provide some insight into the impact of inclusion movement on channel segregation, an experimental validation is needed for model improvement.
Acknowledgements
Authors acknowledge financial supports from the National Natural Science Foundation of China (Grant No. 51101045) and from the Research and Development and Application of Technology Project for young researcher of Harbin (Grant No. 2014RFQXJ026).

References
[1] Combeau H, Založnik M, Hans S, Richy PE 2009 Metall. Mater. Trans. B 40 289
[2] Bennon W D, Incropera FP 1987 Metall. Trans. B 18 611
[3] Flemings M C 2000 ISIJ Int. 40 833
[4] Založnik M, Combeau H 2010 Int. J.Therm. Sci. 49 1500
[5] Li J, Wu M, Hao J, Ludwig A 2012 Comput. Mater. Sci. 55 407
[6] Li J, Wu M, Hao J, Kharicha A, Ludwig A 2012 Comput. Mater. Sci. 55 419
[7] Liu DR, Kang X H, Li D Z 2012 IOP Conf. Ser. Mater. Sci. Eng. 33 012093
[8] Li D, Chen X, Fu P, Ma X, Liu H, Chen Y, Luan Y, Li Y 2013 Mat. Sci. Submitted http://arxiv.org/pdf/1308.3344.pdf
[9] Pardeshi R, Voller V R, Singh A K, Dutta P 2008 Int. J. Heat Mass Transfer 46 1115
[10] Schneider MC, Beckermann C 1995 Metall. Mater. Trans. A 26 2373
[11] Gu J P, Beckermann C, Giamei A F 1997 Metall. Mater. Trans. A 28 1533
[12] Li W, Shen B, Shen H, Liu B 2012 IOP Conf. Ser. Mater. Sci. Eng. 33 012090
[13] Založnik M, Kumar A, Combeau H 2010 Comput. Mater. Sci. 48 11