



## Modeling diffusion-governed solidification of ternary alloys – Part 2: Macroscopic transport phenomena and macrosegregation



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### ABSTRACT

Part 1 of this two-part investigation presented a multiphase solidification model incorporating the finite diffusion kinetics and ternary phase diagram with the macroscopic transport phenomena (Wu et al., 2013). In Part 2, the importance of proper treatment of the finite diffusion kinetics in the calculation of macrosegregation is addressed. Calculations for a two-dimensional (2D) square casting ( $50 \times 50 \text{ mm}^2$ ) of Fe–0.45 wt.%C–1.06 wt.%Mn considering thermo-solutal convection and crystal sedimentation are performed. The modeling result indicates that the infinite liquid mixing kinetics as assumed by classical models (e.g., the Gulliver–Scheil or lever rule), which cannot properly consider the solute enrichment of the interdendritic or inter-granular melt at the early stage of solidification, might lead to an erroneous estimation of the macrosegregation. To confirm this statement, further theoretical and experimental evaluations are desired. The pattern and intensity of the flow and crystal sedimentation are dependent on the crystal morphologies (columnar or equiaxed); hence, the potential error of the calculated macrosegregation caused by the assumed growth kinetics depends on the crystal morphology. Finally, an illustrative simulation of an engineering 2.45-ton steel ingot is performed, and the results are compared with experimental results. This example demonstrates the model applicability for engineering castings regarding both the calculation efficiency and functionality.

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### 1. Introduction

Part 1 of this two-part investigation presented a multiphase solidification model that incorporated the finite diffusion kinetics and ternary phase diagram with the macroscopic transport phenomena [1], and this model was used to analyze the solidification of a ternary alloy (Fe–0.45 wt.%C–1.06 wt.%Mn) for cases without flow. The finite diffusion kinetics in both the liquid and solid were observed to play an important role in the formation of the microsegregation and solidification path, especially at the initial stage of solidification. Under normal casting conditions (where the cooling rate is not too high), the finite diffusion in the solid was recognized as an important phenomenon governing the solidification path [2]; however, the importance of finite diffusion in the liquid has not been paid sufficient attention because for most technical alloys, the diffusion coefficient of the liquid is 2 to 3 orders of magnitude larger than that of the solid. Researchers normally believe that the liquid can be treated as infinite mixing; hence, models

such as the lever rule, Gulliver–Scheil, Brody–Flemings [3], and Clyne–Kurz [4] are valid for analyzing the solidification path. In Part 1, we compared the solidification paths ( $T - f_s$  curve and path of  $(c_{\ell, \text{Mn}}, c_{\ell, \text{C}})$ , etc.) predicted by the models considering different liquid diffusion kinetics and observed that with the assumption of infinite-mixing in the liquid (Gulliver–Scheil or lever rule), it was not possible to model the initial solidification stage adequately [1]. In ternary (or multicomponent) systems, the diffusion of each individual element in the liquid plays an even more important role. Due to the large difference between the two solute elements (C and Mn) in the diffusion coefficient, partition coefficient, and liquidus slope, there is initially almost no enrichment of Mn in the liquid, while the liquid concentration of C is progressively enriched. The difference between the equilibrium concentration ( $c_{\ell, i}^*$ ) and volume-averaged concentration ( $c_{\ell, i}$ ) of the interdendritic or inter-granular melt is significant at the initial stage of solidification. The assumption of  $c_{\ell, i}^* = c_{\ell, i}$  by the infinite liquid mixing kinetics does not apply at this initial stage. This phenomenon has actually been recognized for decades [2,5–7]; however, the numerical treatment of the finite diffusion kinetics and its importance in the calculation of macrosegregation have not been systematically investigated.

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It is understood that macrosegregation occurs due to relative motion between the liquid and solid, resulting from different interdendritic/inter-granular flow and crystal sedimentation phenomena [8,9]. The early stage of solidification appears to be the most critical for the formation of macrosegregation because the significant interdendritic/inter-granular flow and crystal sedimentation phenomena occur at this stage. At the late stage of solidification, as the dendrite network is developed in the deep mushy zone or the equiaxed crystals are densely packed, flow becomes less significant.

Most solidification models applicable for the calculation of macrosegregation are based on a predefined solidification path in accordance with the lever rule assumption [10–17], the Gulliver–Scheil assumption [15–23], or an assumption of infinite solute mixing in the liquid combined with finite solid back diffusion [24–28]. A comparison study (lever rule against Gulliver–Scheil) by Schneider and Beckermann [15] for the case of solidification considering only thermo-solutal convection indicated no significant difference in the calculation of macrosegregation. In contrast, a similar comparison by Sundarraj and Voller [28] for another case considering shrinkage-induced flow during solidification indicated a strong difference in the calculation of inverse segregation between the lever rule and Gulliver–Scheil. A common base of all of the aforementioned models is the assumption of infinite solute mixing in the liquid. Only limited studies have been performed [28–30] that have attempted to incorporate the finite diffusion kinetics in the liquid with the macrosegregation models; however, all of these studies were limited to the binary alloy system and made no distinction (or comparison) between cases of different crystal morphologies (columnar, equiaxed, and mixed columnar–equiaxed).

The first volume-average-based model incorporating diffusion growth kinetics, which considers the multiphase nature, was developed by Beckermann et al. [31,32]. This model was recently extended by the current authors to include the mixed columnar–equiaxed solidification for ternary alloys [1]. The morphology of the growing crystals is simplified: a cylinder for columnar and a sphere for equiaxed, such that the diffusion-governed growth kinetics around and inside the growing crystals can be solved analytically. The main advantage of this simplification is to enhance the calculation efficiency, as the computational cost of most macrosegregation models is very high.

Models including both diffusion growth kinetics and dendritic morphology are also available. Significant advances were made with the contributions of Rappaz and Thevoz [5,6] who proposed a micro–macro solute diffusion model for equiaxed dendritic solidification. Following this work, Wang and Beckermann [33–35] suggested a multiphase approach encompassing either equiaxed or columnar solidification, in which a volume-averaging method was used to model multiphase transport phenomena including flow and grain sedimentation. Recently, Ciobanas and Fautrelle [36,37] proposed an ensemble-averaged multiphase Eulerian model for mixed columnar–equiaxed solidification, although convection and grain sedimentation were not considered. Rappaz and Boettinger [7] extended the model of Rappaz and Thevoz to consider the ternary alloy, and the model was used to analyze the effect of various diffusion coefficients of the solute elements on the solidification path. Building upon the major features of these works, an expanded model (for binary alloys), which encompasses mixed equiaxed–columnar solidification, convection, and grain sedimentation and tracks the evolution of dendritic morphologies has been presented by the current authors [38–41]. Although some trials were made using such a model for calculating macrosegregation [42], the high calculation cost has prevented the model from being applied recently for calculations of engineering castings.

Additionally, some morphological parameters describing the crystal envelope need to be determined and validated in advance.

In the current paper (Part 2), parameter studies on the same 2D square casting ( $50 \times 50 \text{ mm}^2$ ) of Fe–0.45 wt.%C–1.06 wt.%Mn as described in Part 1 [1] are performed, and melt flow and crystal sedimentation are considered. The study examines the liquid diffusion kinetics (finite diffusion against infinite diffusion) and its effect on the formation of macrosegregation.

## 2. Numerical model and simulation settings

A mixed columnar–equiaxed solidification model was presented previously [43,44], and this model was extended to consider ternary alloys [1,45,46]. The key features of the model include:

1. Three phases are considered: liquid ( $\ell$ ), equiaxed ( $e$ ), and columnar ( $c$ ). These phases are quantified by their volume fractions:  $f_\ell$ ,  $f_e$ , and  $f_c$ , respectively. Simple crystal morphologies are assumed: spheres for equiaxed (globular) grains and cylinders for columnar (cellular) dendrite trunks.
2. The solidification (mass transfer) rate is calculated by considering the growth of the equiaxed crystals and columnar trunks based on the finite diffusion-governed growth kinetics. Thermodynamic equilibrium is primarily assumed at the solid–liquid interface, and solute partitioning occurs at the interface during solidification.  $c_{\ell,i}^*$ ,  $c_{e,i}^*$  and  $c_{c,i}^*$  represent the thermodynamic equilibrium concentrations at the interface. The volume-averaged concentrations of different phases are numerically solved:  $c_{\ell,i}$ ,  $c_{e,i}$ ,  $c_{c,i}$ , where  $i = A$  or  $B$ , representing different solute elements. The growth velocity of the crystal is derived based on a Stefan problem at the interface by solving the diffusion fields around and inside the crystals (cylinder or sphere) analytically [1]. The concentration differences ( $c_{\ell,i}^* - c_{\ell,i}$ ), ( $c_{e,i}^* - c_{e,i}$ ) and ( $c_{c,i}^* - c_{c,i}$ ) are driving forces for the diffusion and hence driving forces for crystal growth.
3. The origin of equiaxed crystals is modeled according to a continuous heterogeneous nucleation law originally developed by Oldfield [47]. This approach is based on the assumption of many potential nucleation sites in the parent melt. The nucleation sites belong to different families. Each family can only be activated as newly nucleated grains when a corresponding undercooling  $\Delta T$  is achieved. The undercooling  $\Delta T$  serves as the only driving force for nucleation. A Gaussian distribution is used to describe the statistical outcome of all the families of the nucleation sites.
4. No nucleation of columnar trunks is modeled. The origin of the columnar trunks is assumed to start from the mold wall, and the columnar tip front is tracked explicitly. The columnar tip front grows in the direction closest to the temperature gradient with a growth velocity,  $v_{\text{tip}}^c$ , determined by the LGK (Lipton–Glicksman–Kurz) model [2,43,48].
5. As mentioned above (Point 2), thermodynamic equilibrium solute partitioning occurs at the interface during solidification. However, for the condition of a very high cooling rate (or when the liquid diffusion coefficient of a solute element is very small), the thermodynamic equilibrium condition at the liquid/solid interface could be violated, and a solute-trapping phenomenon would occur [2,49]. The partition coefficient is no longer constant but falls in a range between the thermodynamic equilibrium partition coefficient  $k_i$  and 1, depending on the growth velocity. In the current model, the growth velocity dependent partition coefficient is not considered. Therefore, a simple approach is introduced to consider the 'solute trapping'. When the solid-side equilibrium concentration  $c_{e,i}^*$  or  $c_{c,i}^*$  becomes

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