Menghuai Wu*, Abdellah Kharicha and Andreas Ludwig Discussion on Modeling Capability for Macrosegregation

DOI 10.1515/htmp-2016-0133 Received June 28, 2016; accepted December 23, 2016

Abstract: Macrosegregation originates from the solute partitioning at the liquid-solid interface and the relative motion between liquid and solid phases during solidification of metal alloys. A suitable macrosegregation model should incorporate solidification thermodynamics, crystal growth kinetics, multiphase computational fluid and even thermal-structural mechanics. dynamics, No current model includes all those phenomena, hence leading to assumptions having to be made. This paper discusses some modeling assumptions regarding the treatment of (1) diffusion kinetics of crystal growth, (2) crystal dendritic morphology and (3) solidification shrinkage. Theoretical analyses based on test calculations were made. We find that some previous models, which oversimplified some of the aspects mentioned above for the purpose of computational efficiency, can only be applied to study macrosegregation qualitatively. They lead to significant error estimations of macrosegregation. When the quantitative accuracy for macrosegregation is of primary importance, the multiphase-based models with an appropriate treatment of these aspects, despite the sophisticated computational requirements, are recommended.

Keywords: macrosegregation, solidification, crystal growth, heat and mass transfer, porosity, diffusion kinetics

Introduction

Macrosegregation of alloy castings is caused by microsegregation and relative motion between liquid and solid phases during solidification [1–4]. As categorized in Figure 1, solute partitioning at the solid-liquid interface induces the compositional difference between solid and liquid phases, and diffusion-governed crystal growth kinetics plays an important role in the formation of microsegregation. The liquid/solid relative motion can be induced by the flow, the crystal sedimentation, or the deformation of a dendritic network of crystals in the liquid-solid two-phase region. Causes for the flow can be different, e. g. thermo-solutal buoyancy, shrinkage, etc. A suitable macrosegregation model should consider the aforementioned phenomena by incorporating solidification thermodynamics, crystal growth kinetics, multiphase fluid mechanics, and even thermal-structural mechanics. No current model can include all those phenomena; therefore assumptions are a practical necessity.

Different solidification models were proposed for calculating macrosegregation in alloy castings. Some of those models are simple and computationally efficient, incorporating only one mixture-continuum phase and simplified growth kinetics [5–7]; others are relatively complex and costly, incorporating the nature of multiphase/multiphysics [8-21]. Although plenty of experimental evaluation efforts have been made, it is still difficult to judge the validity of some model assumptions, merely based on the claimed agreements between calculation and experiments. This is because there are too many other uncertain variables, such as process parameters and physical properties that may influence the modeling result. Comprehensive reviews of this topic can be found elsewhere [3-4]. This article discusses some model assumptions, many of which stemming from previous models, and their validity for modeling macrosegregation quantitatively. Those assumptions are: (1) diffusion kinetics of crystal growth; (2) crystal dendritic morphology; (3) solidification shrinkage.

Diffusion-governed crystal growth kinetics

The early continuum model for macrosegregation did not consider the diffusion-governed crystal growth kinetics explicitly [5, 6]. Furthermore it assumed that the alloy

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(microsegregation $\begin{cases} \text{solute partition (thermodynamics)} \\ \frac{1}{2} & \text{solute partition (thermodynamics)} \end{cases}$



Figure 1: Origin of macrosegregation.

solidification follows a predefined solidification path, i.e. the evolution of solid phase and the concentrations in the solid and liquid states are a function of temperature. In the solidification mushy zone, the interdendritic melt is assumed to have completely mixed, and the solute in the solid phase is either completely mixed due to strong back diffusion (following the assumption of lever rule), or no back diffusion (following the assumption Gulliver-Scheil). It is known that complete mixing of interdendritic melt is a good assumption for the deep mushy region where the volume fraction of solid is large, but it is an unrealistic assumption for the primary dendrite tip region where the volume fraction of solid is small [22, 23], as schematically shown in Figure 2. A solute diffusion profile around the growing crystal initially forms for the columnar dendrite tip region, and the volume-averaged concentration in the interdendritic melt, $\langle c_{\ell} \rangle$, is significantly different from the thermodynamic equilibrium concentration, c_{ℓ}^{\star} , which applies only at the liquid-solid interface. For simplicity, $\langle c_{\ell} \rangle$ will be written as c_{ℓ} . It is only in the tip region, where the relative motion by flow is significant because of the high permeability. Therefore, the macrosegregation model based on the assumption of the lever rule or the Gulliver-

Scheil equation would potentially cause quantitative errors.

In order to demonstrate the significance of the diffusion-governed growth kinetics in macrosegregation, a 2D test case was calculated: a square casting $(50 \times 50 \text{ mm}^2)$ of a ternary alloy (Fe-0.45 wt. %C-1.06 wt. %Mn). The liquid melt with an initial temperature of 1,777 K is cooled from all sides of the boundary with a constant heat transfer coefficient (300 W \cdot m⁻² \cdot K⁻¹) and a constant ambient temperature of 373 K. The crystal morphology during solidification is purely globular (spherical). The nucleation parameters are: maximum crystal number density $n_{\text{max}} = 2.0 \times 10^9 \text{ m}^3$, undercooling for maximum nucleation rate $\Delta T_{\rm N}$ = 5 K, and Gaussian distribution width ΔT_{σ} = 2 K. There is no solidification shrinkage. Flow is induced by sedimentation of equiaxed crystals and thermo-solutal buoyancy of the melt. A volume-averaged two-phase model [8] was used. Both melt (liquid phase) and equiaxed crystals (solid phase) are treated as separated and interpenetrating continua. The liquid and solid phases have different velocities, but they are coupled through the drag forces. The Boussinesq approach is employed to consider the buoyancy force for the crystal



Figure 2: Schematic of the solute distribution field in the dendrite tip region.

sedimentation. Other settings for the simulation and thermal physical properties are given in references [24, 25]. A diffusion-governed solidification model [17, 21] was used to calculate the solidification rate. As shown in Figure 2(b), the solute partitioning during crystal growth causes pile-up of the solute in the liquid region at the solid-liquid interface. In turn, the solute pile-up slows down the crystal growth rate. Actually, the final growth rate of the crystal can be determined by solving a Stefan problem analytically [21]. The solute partitioning at the solid-liquid interface is balanced by the solute diffusions in both the liquid and solid phase regions. The diffusion lengths, l_{ℓ} and l_{s} , are related to the radius of the spherical grain, R. The diffusion coefficients of carbon in both liquid and solid are 2.0×10^{-8} and $1.0 \times 10^{-9} \text{ m}^2 \cdot \text{s}^{-1}$, respectively; the diffusion coefficients of manganese in liquid and solid are 4. 0×10^{-9} and $1.2 \times 10^{-13} \text{ m}^2 \cdot \text{s}^{-1}$. Three calculations for this test case were made: I) with the consideration of diffusion-governed growth kinetics, II) with the assumption of Gulliver-Scheil, III) with the assumption of the lever rule. For the latter two cases, the diffusion coefficients in liquid are increased to an enormous value $(10^{-6} \text{ m}^2 \cdot \text{s}^{-1})$, to mimic the complete mixing; the diffusion coefficients for the solid are either very large (lever rule) or zero (Gulliver-Scheil).

Final macrosegregation patterns of the casting with the three calculations are compared in Figure 3. The distribution of c_i^{index} are evaluated, where c_i^{index} is the so-called segregation index which is calculated as $(c_{\min,i} - c_{0,i})/c_{0,i}$. $c_{\min,i}$, is the mixture concentration of the co-existing primary solid and liquid (or rest eutectic at the end of solidification) phases. The complexity of the crystal sedimentation during solidification induces negative segregation in the middle and lower bottom region, and the solute-enriched melt is pushed upwards to the top surface and side-wall regions. Detailed analysis of the formation of such segregation patterns was performed elsewhere [24, 25].

As the global flow/sedimentation patterns of all three calculations are quite similar, their macrosegregation patterns exhibit certain qualitative similarities. However, large differences in segregation intensity were observed. The c_{i}^{index} distribution range ($c_{i,max}^{index} - c_{i,min}^{index}$) increase significantly in the order of I, II, III. Calculations based on Gulliver-Scheil or the lever rule overestimate the macrosegregation dramatically. The reason is that the solute enrichment in the interdendritic melt is overestimated by



Figure 3: Comparison of c_i^{index} distributions in a 2D casting by assuming different growth kinetics: (a) I for diffusion-governed kinetics; (b) II for Gulliver-Scheil; and (c) III for lever rule. The crystal morphology during solidification is purely globular. The upper row is for C, and the bottom row is for Mn. The segregation patterns are shown in the same color scale, and the segregation variation ranges are given for each figure individually.

the assumption of the Gulliver-Scheil or lever rule. Here it is worth mentioning that in another case, i. e. columnar solidification under thermo-solutal convection, the assumption of Gulliver-Scheil <u>and</u> lever rule overestimates meso-segregates [25, 26].

Crystal morphology

In steel ingots sedimentation of the equiaxed crystals causes a cone-shaped negative segregation zone in the bottom region. If the dendritic morphology of the equiaxed crystals is simplified as being globular, the severity of the bottom-negative segregation is overestimated [17, 27, 28]. A reasonable modeling approach is to treat the equiaxed dendrite as a porous object, which is enclosed in a so-called *envelope* [10, 12, 14, 19]. Inside the *envelope*, there are interdendritic melt and solid dendrite. The volume fraction of solid inside the envelope, f_{si} ,

which can be calculated or presumed, defines how globular (massive) the crystal is. The shape of the envelope can be diverse [20], but it can be modeled as a volume equivalent sphere, as described by a set of geometrical (morphological) parameters.

As summarized in Table 1, the influence of the crystal morphology on the macrosegregation comes from 4 aspects. First, the dendritic morphology influences the crystal packing behavior. Globular crystals ($f_{\rm si}$ ~1.0) are prone to being more densely packed than dendritic crystals ($f_{\rm si}$ <1.0), leading to more severe negative segregation. Second, dendritic crystals can more easily block the columnar tip front, causing the columnar to equiaxed transition (CET), as opposed to the globular grains. The macrosegregation mechanism during columnar solidification differs from that during equiaxed solidification. A further effect of dendritic crystals is that the solute-entrapped interdendritic melt would be prone to move with the dendrite, hence reducing the sedimentation-induced macrosegregation. Finally, hydrodynamic

Table 1: Comparison of morphological features between dendritic and globular crystals.



interaction (drag force) between the liquid melt <u>and</u> the crystals is morphology-dependent. The drag force for dendritic grains depends on numerous structural parameters [29, 30], e.g. internal porosity of dendritic grains (1– f_{si}), the interdendritic arm spacings λ_2 , the sphericity of the grain envelope φ_e , while the drag force for globular grain is mainly determined by the grain size and the solid volume fraction.

A 2.45 ton steel ingot (Fe -0.45 wt. %C) is simulated with a mixed columnar-equiaxed solidification model. Typically, a mixed structure of columnar and equiaxed is obtained in the as-cast ingot. Here, the involved phases, i. e. the melt (f_{ℓ}) , the growing columnar trunks (f_c) and the equiaxed crystals (f_e) , are treated as separate and interpenetrating continua. The columnar phase is considered stationary, while the flow of the melt and the motion of the equiaxed crystals are calculated explicitly. Other modeling features for the mixed columnar-equiaxed solidification can be found in previous publications [17, 31, 32]: growth of columnar dendrite trunks; nucleation, growth and sedimentation of equiaxed crystals; thermo-solutal convection of the melt; solute transport by both convection and crystal sedimentation; and the columnar-to-equiaxed transition (CET). The sedimentation of the equiaxed crystals in such ingots plays the most important role in the formation of the macrosegregation. In order to demonstrate the influence of the crystal dendritic morphology on the macrosegregation, three calculations were performed by assuming different internal porosities of dendrite for equiaxed crystals, i. e. different values offsi are used. In this particular case, by introducing the f_{si} , the relationship between the volume fraction of the crystal envelope (f_e^{Env}) and the volume fraction of solid (f_e) is established: $f_e^{Env} = f_e/f_{si}$. The modeling results are shown in Figure 4. By comparison with the model of globular grains ($f_{si} = 1$), the model of dendritic grains ($f_{si} = 0.7$) predicts the following: the larger the equiaxed zone, the smaller the negative segregation intensity in the equiaxed zone. The model assuming globular crystals overestimates the macrosegregation. A study for a 3.3 ton steel ingot was made by Zaloznik and Combeau, and the same conclusion was drawn [33].

Solidification shrinkage

Macrosegregation and shrinkage cavity/porosity are two concomitant casting defects [34, 35], as shown in Figure 5. Cavity or porosity is caused by the solidification



Figure 4: Influence of dendritic morphology on the macrosegregation. f_{si} is the volume fraction of solid inside the envelope of equiaxed dendrite. A 2.45 ton ingot is simulated. (a)-(c). Macrosegregation distribution in a vertical section. (d). Comparison of the centerline segregation profiles between simulations and experiment. Nucleation parameters: $n_{max} = 2.0 \times 10^9 \text{ m}^3$, $\Delta T_N = 5 \text{ K}$, and $\Delta T_\sigma = 2 \text{ K}$.

shrinkage, which is also a cause for the flow, hence for the formation of macrosegregation (Figure 1). <u>Actually</u>, the earliest theoretical model as suggested by Flemings for analyzing the so-called 'inverse segregation', was based on this mechanism [36]. The inverse segregation is caused by 'feeding' the solidification shrinkage in the deep *mush zone* with the solute-enriched interdendritic melt, leading to the increase of mixture concentration in the deep mush region. The problem is that most numerical models, which were previously applied for modeling engineering castings, can only treat macrosegregation and shrinkage separately. The interplay of both phenomena and the influence of the interplay on the macrosegregation are unknown.

A four-phase mixed columnar-equiaxed solidification model is used to investigate the influence of the solidification shrinkage $(\Delta \rho = \rho_s - \rho_\ell)$ on the macrosegregation. The four phases are: the liquid melt, the equiaxed phase, the columnar phase, and the covering liquid slag. The thermal-mechanical deformation of the ingot is ignored, but the introduction of $\Delta \rho$ leads to a domain change of the volume integral of all metal phases inside the ingot. The liquid slag on the top of the ingot appears to fill the volume change on the top of the ingot, hence leading to the formation of the shrinkage cavity. The slag phase belongs to an Eulerian phase, for which a full Navier-Stokes equation is to be solved. No mass and species transfer between the slag and the other three metal phases is required, but the treatment of the momentum and energy exchanges between them is crucial for the

formation of free surface and shrinkage cavity, which in turn influences the flow field and formation of segregation.

- The same 2.45 ton steel ingot is simulated.
- Three calculations are performed by assuming different solidification shrinkages, i. e. $\Delta \rho$ of them are varied.

The modeling results, together with the comparison with the experiment, are shown in Figure 6. Most notably, the solidification shrinkage is explicitly considered, but the thermo-solutal convection of liquid melt and the crystal sedimentation of equiaxed crystals have been modeled with Boussinesq approximation. This means that in all three cases, the shrinkage-induced cavities and the shrinkage-induced flows are different, but the strengths of the flow due to the thermo-solutal buoyancy, the crystal sedimentation and sedimentation-induced flows are almost identical.

Three important effects of the solidification shrinkage on the macrosegregation were observed. First, the formation of the top shrinkage cavity (pipe) adjusts the position of the concentrated positive segregation. With the increase of $\Delta \rho$, the shrinkage cavity grows and the region of concentrated positive segregation moves to a lower position. Second, the solidification shrinkage influences the multiphase flow in/near the columnar tip front, hence it acts upon the meso-segregates' intensity in the middle radius region of the ingot. When no solidification shrinkage is considered ($\Delta \rho = 0$, Figure 6



Figure 5: Macrosegregation and shrinkage cavity in a 2.45 ton steel ingot. (a) Numerical simulation result of c_{c}^{index} ; (b) Sulfur print in a vertical section of the as-cast ingot.



Figure 6: Influence of solidification shrinkage ($\Delta \rho = \rho_s - \rho_\ell$) on macrosegregation. (a)-(c). Macrosegregation distribution in a vertical section. (d). Comparison of the centerline segregation profiles between simulations and experiment. Nucleation parameters for equiaxed crystals: $n_{max} = 5.0 \times 10^9 \text{ m}^3$, $\Delta T_N = 9 \text{ K}$, and $\Delta T_\sigma = 2 \text{ K}$.

(c)), the thermo-solutal convection becomes unstable, together with the equiaxed sedimentation near the columnar tip region, which destabilizes the growth of the *mushy zone*, leading to the formation of streak-like meso-segregates [31]. In other cases, when the solidification shrinkage is taken into account, e.g. $\Delta \rho = 297 \text{ kg}/$ m^3 , Figure 6(a), the solidification shrinkage, i.e. the shrinkage-induced feeding flow, in the columnar solidification region tends to stabilize the flow in the columnar tip front region. The formation tendency of the meso-segregates markedly diminishes. Finally, the feeding flow in the casting center at the late stage of solidification can enhance the negative segregation (or reduce the positive segregation) along the centerline of the ingot. This effect can be verified by the Flemings' theory [2]. The difference of macrosegregation along the centerline as calculated by the three cases (Figure 6(d)) is quite large.

Summary and discussion

The modeling capability for macrosegregation has significantly improved in the last decades since computational multiphase fluid dynamics were introduced to treat the multiphase transport phenomena during solidification. Many numerical models have been proposed in the meantime. The continuum model, for its simplicity and calculation efficiency, has been successfully applied to realize a fundamental understanding of macrosegregation mechanisms. However, when the quantitative accuracy of a model is of interest, each model simplification/ assumption will be under scrutiny. The model assumptions regarding the treatment of the diffusion kinetics of crystal growth, crystal dendritic morphology and solidification shrinkage are discussed in this paper. The following conclusions have been drawn.

- The infinite (complete) mixing kinetics as assumed by the classical solidification model, e. g. Gulliver-Scheil or the lever rule – which cannot properly consider the solute distribution in the interdendritic or intergranularmelt at the early stage of crystal growth, leads to an error estimation of macrosegregation.
- 2) In order to model the crystal sedimentation induced macrosegregation, it is crucial to consider the crystal dendritic morphology. The dendritic morphology influences the crystal packing behavior; the blocking criterion for CET (columnar-to-equiaxed transition); the way to transport the interdendritic solute and the drag force between the crystal and the melt. Using a simplified globular morphology instead of real dendritic morphology leads to an overestimation of the sedimentation-induced macrosegregation intensity.
- 3) Ignoring the solidification shrinkage in ingot casting will lead to an error estimation in the position of the

concentrated positive segregation, the meso-segregates in the middle radius region, <u>and</u> the centerline segregation.

No single model is currently able to include all of the 'causes and effects' for macrosegregation, as summarized in Figure 1. The causes for the liquid-solid relative motion are manifold, but a specific casting process may be characterized by one or a few dominant flow phenomena. In this regard a process-oriented model was often considered as sufficient. For example, a continuum solidification model with thermo-solutal convection was used to investigate the formation mechanism of *freckles* [37], which occur typically during unidirectional solidification of super-alloys; a two-phase columnar solidification taking into consideration of the deformation of the mushy zone was used to investigate centerline segregation in continuously cast steel slabs [38]; a two-phase solidification model considering capillary force driven (Marangoni) convection was used to study the phase separation and macrosegregation of monotectic alloys [15]; a coupled Eulerian-Lagrangian approach was applied to study the channel segregates as induced by the motion of nonmetallic inclusions (NMI) in steel ingot [39].

Mesh (grid size) sensitivity is a further issue for modeling macrosegregation. Some details of the macrosegregation, e. g. meso-segregates or channel segregates, are still not solvable quantitatively, due to limited computational resources [40]. Therefore, the numerical studies on the channel segregates remain in a qualitative way to get onset conditions for channels according to some criterion functions [41] and to study the channel growth according to the flow-solidification interaction [42, 43]. <u>A</u> griddependency study is always required for such applications.The importance of reliable input data, e.g. physical properties and process parameters, for the macrosegregation calculation has not been discussed here.

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