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The effect of velocity based packing schemes on macrosegregation development in simulations of equiaxed solidification

A. Plotkowski*, M.J.M. Krane

Purdue Center for Metal Casting Research, School of Materials Engineering, Purdue University, 701 W. Stadium, West Lafayette, IN 47906, United States

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ABSTRACT

Simulations of equiaxed solidification must consider the advection of solid grains and their eventual coalescence into a rigid, permeable structure. Most models up to this point have used one of two similar treatments where this transition occurs at a uniform value for either the grain envelope fraction or the solid fraction. A major drawback of this approach is that it does not explicitly account for the effect of the local velocity field, which may either advect grains into the rigid solid or away from it. A simple velocity based model has been proposed in which the packing of a given control volume is based on the condition of its downstream neighbors. This velocity based packing scheme was implemented in a model for horizontal direct-chill casting, but its effects on the predicted solidification structure were not investigated in detail. The present study describes this and one modified approach in the context of a model of a cylindrical static casting of AA7050 and compares both to the standard constant packing fraction approach. A parametric study is performed to determine the effect of several model parameters, including the critical solid fraction, grid spacing, free floating particle size, and dendrite arm spacing, on the formation of macrosegregation. Avenues for future research are identified.

1. Introduction

During the solidification of metallic alloys, long range compositional variation, commonly termed macrosegregation, often develops and produces unwanted phases and non-uniform properties. Macrosegregation is a complex defect that depends on the thermo-solutal transport during the casting process and is subsequently a function of the alloy properties, boundary conditions, and system geometry. Due to the complicated and coupled nature of the equations that govern the transport phenomena during solidification, numerical models have long been used to gain a deeper understanding of casting processes, and, in particular, the development of macrosegregation. Early models focused on columnar microstructures but later efforts have modeled equiaxed solidification, which must take into account the transport of solid grains suspended within the liquid metal and their eventual coalescence into a rigid solid structure. This situation is particularly relevant to the grain refined castings commonplace in the wrought aluminum industry. One of the sub-models in these simulations that has a drastic effect on the solution is the manner in which the transition from a slurry of suspended solid particles to a permeable rigid mushy zone is treated.

* Corresponding author. Tel.: +1 6163505947.
E-mail address: plotkoal@gmail.com (A. Plotkowski).

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Ni and Beckermann [1] proposed a volume-averaged, two-phase model for transport phenomena in solidification processing which was later used to model equiaxed solidification in vertical direct chill casting of an Al–Cu alloy by Reddy and Beckermann [2]. The model considers the solid and liquid phases separately and couples them using a variety of interfacial transfer terms. It also requires some type of nucleation model, or as Reddy and Beckermann assume, some known number density of grains. They further assumed a globular grain morphology, and used a uniform and constant packing volume fraction of 0.637, which corresponds to the density of random close packed spheres [3], as the criteria for the coherency. The packing fraction is considered both constant and uniform throughout the domain, but for brevity, will be referred to as simply the constant packing fraction (CPF) approach.

Wang and Beckermann expanded the two-phase model to include the interdendritic liquid as a third phase, allowing for modeling of the grain envelope [4,5], which includes the solid and the liquid trapped between the dendrite arms. They used a set of morphological relationships [6] to determine the fraction solid and solid-liquid interfacial area inside the grain envelope. Further relationships were used to govern grain nucleation and growth, as well as flow partitioning between the inter- and extradendritic liquid. This model used a slight variation on the constant packing fraction in that it was applied to the grain volume fraction (including the solid particles and interdendritic liquid) rather than the solid volume fraction. The grain envelopes were assumed spherical, and packing occurred at a grain volume fraction of 0.637.

The models proposed by Beckermann's group include details of the liquid-solid interactions, including the mass transfer between phases, allowing better predictions of solid growth kinetics, while models based on the work of Vreeman et al. [7] assume that the state of the solid–liquid mixture can be determined uniquely from the instantaneous temperature and mixture composition. The tradeoff, however, is that multi-phase models are computationally more expensive than their mixture counterparts and that the necessary input parameters have a high degree of uncertainty. Vreeman et al. [7,8] devised a continuum model based on the work of Ni and Incropera [9,10] that casts the governing equations in a mixture form similar to that originally proposed by Bennon and Incropera [11,12]. Thus, a set of equations are solved for mixture velocity, enthalpy and composition rather than separate conservation equations for each phase, improving the computational efficiency of the model but losing some of the detail of the multi-phase approach. The grain morphology is not modeled explicitly, rather, the use of a packing fraction lower than 0.637 (in terms of volume fraction solid) implicitly defines a relationship between grain fraction and solid fraction for the entire domain. In this case, packing fractions between 0.15 and 0.30 were used for vertical direct chill casting of Al-4.5 wt%Cu and Al-6.0 wt%Mg alloys.

Other models have been developed based on the multi-phase approach of Beckermann's group [13,14] using as many as five phases [15,16] in which columnar and equiaxed grains, the interdendritic liquid in each type of solid structure, and the bulk liquid are considered separately in order to model the columnar to equiaxed transition. Mixture models similar to Vreeman's approach have also been used [17–21]. In all cases, some form of the constant packing fraction method was used. Various assumptions or models of the grain morphology have been implemented, but no effort has been made to address the validity of neglecting the effect of the flow field.

For either type of model, experimental data for the solid fraction at which dendrites coalesce is essential. Some experimental studies have been performed to determine this packing fraction, often termed the dendrite coherency point, using two different experimental approaches. Rheological methods test the shear strength of an alloy through the freezing range and the coherency point is marked by a sudden change in slope [22–25]. Alternatively, thermal analyses measure the temperature difference between two points, which exhibits a minimum at coherency due to the increased thermal transport in the solid [26,27]. Arnberg and coworkers performed a series of studies reporting measured coherency fraction for various aluminum alloys [26,28–30] which ranged widely, including very low packing fractions for silicon rich foundry alloys (0.06–0.10 for alloy B390) to higher values for Zn rich alloys (0.23–0.34 for alloy 713) and pure aluminum (0.53 for 99.99 wt% Al). This last value, measured in a metal which produces no dendrites, approaches the spherical assumption discussed above. Each result is for a particular solidification condition, alloy composition, and level of grain refinement, all of which may affect the dendrite morphology and number of equiaxed particles. Generally speaking, increased solute content [28] and cooling rate [26] tend to reduce the packing fraction by encouraging highly dendritic morphologies, while larger grain refiner additions [27] form a more globular microstructure and increase the packing fraction.

The primary disadvantage of the constant packing fraction method is that it does not explicitly consider the effect of the local velocity field on the likelihood of packing. Advection of solid particles indirectly influences the packing scheme by affecting the solid fraction field. However, particles are more likely to pack if their velocity is towards a packed interface, and less likely to attach when advected away from the interface (Fig. 1), an effect that is not considered in the constant packing fraction model, even in the multi-phase cases that consider the local grain morphology [6]. Vušanović and Krane [31] introduced a simple rule set to account for the velocity field by basing packing not on the condition of the numerical cell of interest, but on the condition of a neighboring cell in the downstream direction. They implemented this approach in a simulation of horizontal direct chill casting of aluminum using the transport model of Vreeman et al. [7], and compared the velocity based method to various constant packing fraction cases. However, they only looked at the new model under a single set of conditions. It is necessary to analyze the effects of the velocity-based model further in order to fully understand its differences from the constant packing fraction approach.

The purpose of this study is to more closely examine the behavior of two velocity-based packing schemes as a function of the various model parameters. The implementation of the packing scheme proposed by Vušanović and Krane [31] and a new variant are explained in detail in the context of a static casting simulation. These simulations are based on the formulation of Vreeman et al. [7] for a multicomponent aluminum alloy (AA7050), commonly cast industrially in a grain