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Study of the influence of mushy zone permeability laws on macro- and meso-segregations predictions

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ABSTRACT

In this article the influence of the mushy zone permeability on the prediction of macrosegregation and mesosegregation (e.g. channel type segregation) has been studied using three different permeability laws. The three permeability laws have similar permeability in the inner part of the mushy zone (low liquid fraction regions), however, in the outer part of the mushy zone (high liquid fraction regions) permeability differs significantly. Simulations are performed for the solidification of a Sn–Pb alloy in a two-dimensional rectangular cavity using the three permeability laws and the effects of differences in these laws in the outer part of the mushy zone on macro- and meso-segregation are studied. We notice a sensitivity of the predicted macro- and meso-segregation, and of the width and shape of the mushy zone to various permeability laws. The sensitivity of the prediction of mesosegregates is much stronger than that of macrosegregation predictions. The value of the microstructural parameter used in the permeability laws plays an important role on the intensity of the macrosegregation and the nature of channel segregates with regard to their number, length and orientation. It has been observed that the permeability in the outer part of the mushy zone plays a key role in the formation of channel segregates.

1. Introduction

Defects in metal casting processes depend critically on the permeability associated with interdendritic liquid flow in the mushy zone. Fluid flow in the mushy zone causes macrosegregation in castings by redistributing the segregated solute elements [1–5] and in some cases forms channel type segregates (a kind of mesosegregation) in the mushy zone [5–10]. The interdendritic fluid flow in the mushy region may cause perturbations of the growing columnar structure, causing instability of the growth front, which can lead to further instability of the segregation map and formation of channel segregates. The formation of channel segregates in castings represents a severe form of defect since the composition and crystalline structure of the solid within the channels differ significantly from those of the nearby solid regions. In casting they appear as long narrow trails aligned in some preferred direction, with solute concentration greater than that of the surrounding regions. The scale of channel segregates (referred to as mesosegregates in this article) can influence the homogenization of the ingot and its extent in the casting can severely influence the quality of ingots and their mechanical properties.

Macrosegregation was widely studied using models consisting of macroscopic models based on mixture theory or volume averaging, coupled to models of microsegregation. In the volume-averaged formulation, generally, the equations are established on a representative element volume (REV), small with respect to the extent of the mushy zone, but large compared to the dendrite arm spacing (DAS). The averaging method allows the use of a single set of equations in the whole domain (fully liquid, mushy zone and fully solid). The solution procedures of these macroscopic models involve the discretization of the macroscopic conservation equations based most often either on a finite volume formulation e.g., [1–5], or on a finite element formulation e.g., [5,11]. In these formulations, the mushy zone is considered as a saturated porous medium with varying permeability and the flow in the mushy zone is governed by the Darcy law. The permeability in the mushy zone, which for the simplest model is a function of the liquid fraction and the dendritic arm spacing (DAS), varies over a wide range of magnitude for a variation of liquid fraction from one to zero. The dependence of permeability on liquid fraction is highly nonlinear, thus a small variation in the liquid fraction can result in large variation of permeability which can significantly affect the flow in the mushy zone and hence the segregation pattern. For instance,

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Nomenclature

C	average mass fraction of solute (Pb), wt%
C_0	initial mass fraction of solute (Pb) in the alloy, wt%
c_p	specific heat, J kg^{-1} K^{-1}
d	representative size in the dendritic structure, m
g_l	volume fraction of liquid
g_s	volume fraction of solid
g	gravity vector, m s^{-2}
GM	global macrosegregation index
h	enthalpy, J kg^{-1}
k	thermal conductivity, W m^{-1} K^{-1}
K	permeability, m^2
L	latent heat of fusion, J kg^{-1}
m	liquidus slope, K wt%$^{-1}$
p	pressure, Pa
t	time, s
T	temperature, K
∇T	temperature gradient, K m^{-1}
v	superficial average velocity, m s^{-1}
v_l	intrinsic velocity of the liquid phase, m s^{-1}
V	volume, m^3
V_{domain}	volume of the computational domain, m^3
X, Y	coordinate axes, m

Greek symbols

β_T	thermal expansion coefficient, K^{-1}
β_c	solutal expansion coefficient, wt%$^{-1}$
μ	dynamic viscosity, kg m^{-1} s^{-1}
ρ	mass density, kg m^{-3}

Subscripts

0	reference
l	liquid
m	melting point for a pure substance
s	solid

Singh et al. [12] reported the effect of mush permeability on macrosegregation. They considered different permeability models and tried to find one that would provide the best fit to experimental results of Krane and Incropera [13]. However, their discussions were limited only to the macrosegregation and did not consider channel mesosegregations.

Within a volume-averaged solidification model the permeability is the principal parameter of the Darcy term, which describes the hydrodynamic drag of the porous mush in the averaged momentum balance equation. Models relating the permeability to the local liquid fraction and the DAS are generally used to calculate the permeability. Therefore, the mushy zone permeability model becomes one of the parameters that will have an essential effect on segregation profiles, as the permeability determines the intensity of the movements of interdendritic liquid [14–18], which finally causes segregations.

The determination of permeability for high liquid fractions ($\sim$1) is difficult, which presents a challenge for solidification modelling [19–26]. In the inner part of the mushy zone (lower liquid fractions ranging approximately from 0.2 to 0.7) various models of permeability are in general good agreement with the experimental values of directly measured permeabilities [21–23] or with permeabilities obtained from modeling of the flow on experimentally determined dendritic structures [19,24–28]. Clearly, no experimental data exists for liquid fractions higher than 0.7 [19–21]. To cover this range of liquid fractions, extrapolations are used, giving largely different permeabilities, sometimes by two orders of magnitude [21–23]. Alternatively, Bhat, Poirier et al. modeled the permeability by 2D fluid flow computations on artificial or experimental dendritic structures [24–26] going to liquid fractions of up to 0.93. They then provided extrapolations, for which they claimed to be valid up to $g_l = 0.99$ [29]. Other flow modeling studies [19,20,27,28] report permeabilities for a more limited range of liquid fractions, in all cases staying below 0.90, and mostly even lower. Uncertainties for the range $g_l > 0.90$ are thus high. Incidentally, this range is decisive for the formation of channel mesosegregations. To the authors' best knowledge, the effect of such differences in permeability in the outer part of the mushy zone on predictions of channel mesosegregations is not well studied in the literature.

The objective of this article is to investigate such effects, since the prediction of channel mesosegregations may depend on the permeability in the outer part of the mushy zone. In this respect, two important aspects of the numerical studies aimed at studying channel segregates using different permeability laws require special attention; (a) what permeability law is used in the numerical simulations and (b) how do these permeability laws influence the predictions of macro- and meso-segregation. In order to assess these aspects, simulations using three permeability laws are performed in the current study for solidification of a binary alloy in a side-cooled cavity. The different permeability laws are functions of local liquid fraction and a microstructural parameter used as a length scale to represent the microstructure. The article is organized as follows. We first introduce the various permeability laws used in simulations. These laws are used for prescribing the permeability in the Darcy term in the momentum conservation equation. Thereafter, we present simulation results for a 2D benchmark solidification case and discuss the effects of various permeability laws on the prediction of macro- and meso-segregation. The influence of the value of the microstructural parameters used in the permeability laws on the intensity of the macro-and meso-segregation is also assessed.

2. Mathematical modelling

2.1. Conservation equations

The conservation equations for mass, heat and solute are averaged over both liquid and solid phase (assuming columnar solidification with fixed solid phase, equal and constant solid and liquid densities, except in the buoyancy term, where the Boussinesq approximation is used, a linearized phase diagram with a constant liquidus slope and Scheil law for microsegregation) and are given as follows [5]:

$$\text{Mass conservation}: \ \nabla\cdot\mathbf{v} = \nabla\cdot(g_l\mathbf{v}_l) = 0 \tag{1}$$

$$\text{Energy conservation}: \ \rho\frac{\partial h}{\partial t} + \rho c_p \mathbf{v}\cdot\nabla T = \nabla\cdot(k\nabla T), \tag{2}$$

where the average enthalpy h, assuming constant and equal c_p for solid and liquid phase, is expressed as

$$h = g_s h_s + (1-g_s)h_l = c_p(T-T_0) + (1-g_s)L. \tag{3}$$