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Dendritic model for macrosegregation prediction of large scale castings

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ABSTRACT

A dendritic model with the consideration of heat transfer conservations, solute transfer conservations, melt convection, grain nucleation and growth, and the sedimentation of crystal was introduced to predict the macrosegregation of large scale casting. The model was validated by a Pb-5 wt.% Sn classic benchmark experiment and then used to predict the macrosegregation of a 3.3-ton industrial Fe-4.5 wt.% C ingot. Secondary dendrite arm spacing (SDAS) was considered in present model and SDAS was found plays an important role on liquid flow and affects final characteristic of segregation. The quasi A-segregation caused by the instability of interdendritic flow was presented in this study. A negative segregation zone under hot top was presented and the ingot size effect plays more important role than cooling conduction on the formation.

1. Introduction

Macrosegregation is a serious defect of metal castings, especially for large scale ingot castings. It causes non-uniform microstructure for downstream hot working process, and leads to deleterious properties in application. The formation of macrosegregation of castings was extensively investigated in the last half centuries. Hultgren (1973) suggested that the compositional heterogeneity occurs when the relative motion appears between liquid and solid phases during solidification. This motion normally caused by thermosolutal convection, floatation or sedimentation of free moving grains (Li et al., 2014b) or inclusion (Li et al., 2014a), shrinkage induced feeding flow, mechanical or other external stirring, deformation of solid skeleton, and some other reasons (Sang et al., 2010). Modeling this relative motion with mass, momentum, species and enthalpy transfer is a general method for macrosegregation prediction.

Several macrosegregation models were presented since the first mushy zone model of Fujii et al. (1979). After that, melt convection and grain sedimentation were further counted into the factors by Wang and Beckermann, 1996 in 1990s. Wu and Ludwig (2006) provided a model coupling mass, momentum, and energy with a three-phase (liquid phase, columnar phase, and equiaxed grain phase) process simulation in 2000s. This model successfully predicted the occurrence of the columnar-to-equiaxed transition (CET). Combeau et al. (2009) considered influence of the motion and the morphology of equiaxed grains in the macrosegregation formation of a 3.3-ton steel ingot but omitted the columnar phase effect. The predicted results are well consistent with the experimental results provided by Aubert & Duval (Les Ancizes, France). Li et al. (2012b) investigated the effects of pipe shrinkage on the final macrosegregation pattern of a 3.3-ton steel ingot using a two-phase model. In addition, Ha et al. (2003) presented the simulation of molten steel in continuous slab casting under electromagnetic field. They found that the electromagnetic can effectively damp detrimental local flows which may cause surface erosion and macrosegregation in steel products.

A reasonable result can be achieved through two-phase model, i.e., liquid and solid phases (Li et al., 2012b), or even three-phase mixed columnar-equiaxed model, i.e., liquid, columnar, and equiaxed phases (Li et al., 2014b), while in the most case, excessive segregation was lead to in the bottom equiaxed zone due to the assumption of globular equiaxed grain in above mentioned models. In those case, not only the grains were simply treated as equivalent spheres but also the influence of secondary dendrite arm spacing (SDAS) on the growth of grains and momentum exchange between dendritic grains and liquid was ignored. In order to further improve the accuracy of macrosegregation prediction, Ahmadein et al. (2015) presented a 5-phase model based on the study of Wu and Ludwig (2009a) and the model was applied to predict macrosegregation of a lab scale Al-4 wt.% Cu ingot. In this study, a dendritic model with the consideration of SDAS is pre-

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Nomenclature

c_0	Initial concentration (wt.%)
c_l, c_s	Species concentration (wt.%)
c_{ref}	Reference concentration (wt.%)
c_{mix}	Mix concentration (wt.%)
C_{ls}	Species exchange between liquid and solid ($kg\,m^{-3}\,s^{-1}$)
c_p^l, c_p^s	Specific heat ($J\,kg^{-1}\,K^{-1}$)
D_l, D_s	Diffusion coefficient ($m^2\,s_{-1}$)
d_s, d_{env}	Diameter of solid and envelop (m)
f_l, f_s, f_{env}	Volume fraction of liquid phase and solid phase (1)
f_{li}, f_{le}	Liquid fraction of interdendritic melt and extradendritic melt (1)
f_{si}	Ratio of solid phase to grain envelope (1)
H	Heat transfer coefficient ($W\,m^{-2}\,K^{-1}$)
H^*	Volume heat transfer coeff. between phases ($W\,m^{-3}\,K^{-1}$)
h_l, h_s	Enthalpy ($J\,kg^{-1}$)
$K_{ls} = -K_{sl}$	The drag force coefficient ($kg\,m^{-3}\,s^{-1}$)
k	Solute partitioning coefficient at the l/s interface (1)
k_l, k_s	Thermal conductivity ($W\,m^{-1}\,K^{-1}$)
$M_{ls} = -M_{sl}$	Net mass transfer rate between liquid phase and solid phase ($kg\,m^{-3}\,s^{-1}$)
m	Slope of the liquidius in phase diagram (K)
N_e	Grain production rate by nucleation ($m^{-3}\,s^{-1}$)
n	Grain number density (m^{-3})
p	Pressure ($N\,m^{-2}$)
$Q_{ls} = -Q_{sl}$	Energy transfer between liquid and solid phases ($J\,m^{-3}\,s^{-1}$)
S_s	Surface area concentration of solid phase (m^{-1})
S_{env}	Surface area concentration of envelope (m^{-1})
T	Temperature (K)
t	Time (s)
u_{l_x}, u_{l_y}	Liquid velocity in horizontal and vertical $m\,s^{-1}$
u_{s_x}, u_{s_y}	Solid velocity in horizontal and vertical $m\,s^{-1}$
v_{tip}	Dendrite tip velocity ($m\,s^{-1}$)
v_{Rs}	Grain growth velocity ($m\,s^{-1}$)
λ_2	Secondary dendrite arm spacing (m)

Subscripts

l	Liquid phase (melt)
s	Solid phase (solid skeleton)
env	Grain envelope (equiaxed dendritic grains)

sented and validated by lab scale Sn-5 wt.% Pb experiment, then the model is used to predict the macrosegregaton of a 3.3-ton large scale Fe-4.5 wt.% C ingot casting.

2. Model description

The present model is generally based on the fully coupled equiaxed model developed by Combeau et al. (2009). Conservation equations, sources and exchange terms, and some auxiliary equations are list in Table 1. The main assumptions of the model include:

- Two phases are considered in melt solidification, including liquid melt and equiaxed dendritic grains artificially covered by an envelope (f_{env}), which links the tips of the primary and secondary dendrite arms. The equiaxed dendritic grains consist of the solid skeleton and interdendritic liquid (Fig. 1). In present model, two "hydrodynamic" phases with the solid, denoted by f_s, and the liquid phase, denoted by f_l are taken into account. The liquid phase includes the extradendritic melt (f_{le}) and the interdendritic melt (f_{li}), so that $f_{le} + f_{li} = f_l$, and $fl + f_s = 1$.
- By equivalent an equivalent sphere (with the diameter of d_{env}) of the same volume as the actual crystal envelope is set. The area concentration of the envelope (S_{env}) is modeled by introducing a shape factor denoted by ϕ_e from Wang and Beckermann (1993). Accounting for the dendritic structure of grains, the area concentration of solid skeleton (S_s) is (in Table 1) determined by a function (Appolaire et al., 2008) related to SDAS and area concentration of envelope.
- A three-parameter heterogeneous nucleation method is employed to take into account the nucleation of equiaxed grains. The details of the nucleation method can be found in literatures of Ludwig and Wu (2002) and Wu and Ludwig (2006).
- The growth of envelope (v_{tip}) is based on Kurz et al. (1986) (KGT model). But the growth of the solid skeleton (v_{Rs}) is governed by solute diffusion; the concentration difference ($c_l^* - c_l$) in the interface of solid and liquid is the driving force for the growth of solid phase.
- Thermodynamic equilibrium is assumed at the solid–liquid interface, which means that the concentrations at the liquid–solid interface (c_{l^*}, c_{s^*}) are calculated from phase diagram. Volume-averaged concentrations of liquid (c_l) and solid (c_s) are calculated by solving species conservations, and the segregation is characterized by the concentration of the two-phase mixture (c_{mix}).
- Enthalpy equations for both phases are solved by energy conservations. A large volumetric inter-phase heat transfer coefficient H^* is artificially set to make the local thermal equilibrium. So, only one temperature representing all two phases in each volume element. The value of H^*, recommended by Wu and Ludwig (2007) shown in the Table 2 can fulfill the condition of the simulation convergence and temperature difference.
- The packing limit is set as 0.4 from Combeau et al. (2009) for grain envelope. Which means that when grain-volume fractions are smaller than packing limit ($f_{env} < 0.4$), the solid phase (f_s) is in the free-floating form, otherwise, the solid phase is fixed.
- A drag force model defined by Wang et al. (1995) and Wang and Beckermann (1996) is employed in this model for the calculation of solid/liquid interfacial drag force. The f_s, f_{si}, S_s, S_{env}, and ϕ_e are the necessary inputs, and the K_{ls}, drag force coefficient, is calculated from this model.
- Neither the solidification shrinkage nor fragment movement is considered in present model. Thermosolutal convection is modelled using the Boussinesq approach.

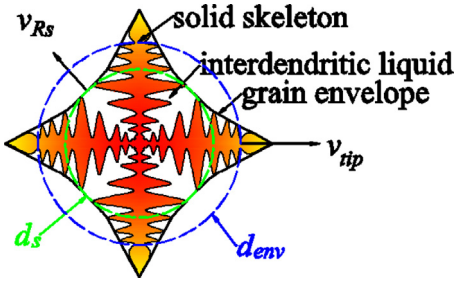

Fig. 1. Equiaxed dendritic morphology: a brief cross section of equiaxed dendritic grains.

All phases share the same pressure field, P. The conservation equations in Table 1 are numerically solved using a so-called phase coupled SIMPLE (PC-SIMPLE) algorithm. In this study, all calculations are fully implicit and run with a time step kept on the order of 10^{-2}. For each time step, up to 60 iterations may be necessary to reduce the residual values of momentum, volume fraction, species, and user-defined scalars below 10^{-5} and the enthalpy conserva-