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Modelling mixed columnar-equiaxed solidification with melt convection and grain sedimentation – Part II: Illustrative modelling results and parameter studies

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ABSTRACT

A volume-averaging multiphase solidification model was introduced in Part I. In Part II, illustrative simulations are made for two benchmarks, a unidirectional solidification benchmark and a cylindrical ingot casting, using a binary Al–Cu alloy. For the case of unidirectional solidification the competing growth of columnar and equiaxed structures, evolution of different phase regions, solute redistribution, and the influence of grain sedimentation and melt convection are analyzed in detail. The columnar-to-equiaxed transition (CET) is investigated, with important insights derived from the CET prediction. The new features of the model and its applicability to industrial-type castings are demonstrated with simulations of a cylindrical ingot casting. This is done in both a 2D axisymmetric and a full 3D geometric domain to demonstrate the ability of the model to produce consistent results. The main features of the model that are verified include tracking of the columnar primary dendrite tip, nucleation of equiaxed grains ahead of the columnar tip front, hydrodynamic and solutal interactions between the equiaxed and columnar structures, the columnar-to-equiaxed transition (CET), melt convection and grain sedimentation, and macrosegregation and the final macrostructure. With appropriate modelling parameters the typical columnar-equiaxed macrostructure observed in experiments can be reproduced. Uncertainties due to model parameters and assumptions are addressed and discussed.

1. Introduction

In the last century significant progress has been made in describing the formation of the mixed columnar-equiaxed macrostructure, however the ability to control and dictate the as-cast macrostructure in a casting or ingot remains a challenge for metallurgists and foundrymen. Modelling efforts of the previous decades [1–4] have elucidated many aspects of the interdependent phenomena in columnar-equiaxed solidification, but due to the complex interaction of the multiphase flow and grain sedimentation during solidification and constraint of computing resources, modelling mixed columnar-equiaxed solidification at the process scale has not been fully realized and remains a problem under much current investigation.

Significant advances in modelling of dendritic alloys 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 [7,8] suggested a multiphase approach encompassing either equiaxed or columnar solidification, in which a volume averaging method is used to model global multiphase transport phenomena including flow and grain sedimentation. Recently, Ciobanas and Fautrelle [9,10] proposed an ensemble-averaged multiphase Eulerian model for mixed columnar-equiaxed solidification, although convection and grain sedimentation were not taken into account. Building upon the major features of these works, an expanded model, which encompasses mixed equiaxed-columnar solidification, convection and grain sedimentation, and tracks the evolution of dendritic morphologies has been presented by the current authors and is demonstrated here.

As stated in Part I, a model for mixed columnar-equiaxed solidification should bridge the macro and micro length scales, encompass both dendritic and non-dendritic morphologies, track the columnar primary dendrite tip front (which separates the pure equiaxed solidification zone from the mixed columnar-equiaxed solidification zone), and simulate multiphase flow and grain sedimentation. To incorporate these phenomena into a single model a volume-averaging multiphase solidification model with five thermodynamic phase regions is proposed. These five phase regions include the solid dendrites and the interdendritic melt in equiaxed grains, the solid dendrites and the interdendritic melt in columnar trunks, and the extradendritic melt. For melt flow and grain sedimentation, three hydrodynamic phases are defined: equiaxed grains, composed of solid dendrites and interdendritic melt; columnar dendrite trunks, composed of solid dendrites and

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Nomenclature

c_0	initial (nominal) concentrations of alloy (wt.%)
c_E	eutectic concentration (wt.%)
c_ℓ, c_e, c_c	concentrations of hydrodynamic ℓ-, e-, or c-phases (wt.%)
$\bar{c}^c_{env}$	average concentration at columnar tree trunk envelope (wt.%)
$\bar{c}^e_{env}$	average concentration at equiaxed grain envelope (wt.%)
c^c_d, c^c_s	concentrations of interdendritic melt and solid dendrites in columnar tree trunk (wt.%)
c^e_d, c^e_s	concentrations of interdendritic melt and solid dendrites in equiaxed dendritic grain (wt.%)
c_{mix}	mix concentration (wt.%)
c^*_ℓ, c^*_s	equilibrium concentration at liquid–solid interface (wt.%)
$c_{p,\ell}$, $c_{p,s}$	specific heat of liquid and solid (J kg^{-1} K^{-1})
D_ℓ, D_s	diffusion coefficient in liquid or solid phase (m^2 s^{-1})
d^c	average diameter of columnar tree trunk (m)
d^e	average diameter of equiaxed grain diameter (m)
f_ℓ, f_e, f_c	volume fraction of hydrodynamic ℓ-, e-, or c-phases (1)
f^c_s, f^c_d	volume fraction of solid dendrites or interdendritic melt in columnar tree trunk referring to total volume (1)
f^e_s, f^e_d	volume fraction of solid dendrites or interdendritic melt in equiaxed grain referring to total volume (1)
f^{free}_c	critical volume fraction of columnar phase for entrapment of equiaxed grains (1)
$f_{e,CET}$	hard blocking criterion (Hunt model) (1)
f^{extra}_{Eu}	extradendritic eutectic phase (1)
$f^{intern}_{Eu,e}$, $f^{intern}_{Eu,c}$	interdendritic eutectic phases in equiaxed or columnar phase (1)
f^{total}_{Eu}	total eutectic phase (1)
g	gravity (m s^{-2})
G	temperature gradient at the columnar primary dendrite tip (K cm^{-1})
H_w	heat transfer coefficient at casting-chill interface (W m^{-2} K^{-1})
k	solute partitioning coefficient at the liquid–solid interface (1)
k_1	growth parameter in KGT model (m s^{-1} K^{-2})
k_2	growth parameter in KGT model (m s^{-1} K^{-3})
k_ℓ, k_e, k_c	thermal conductivity (W m^{-1} K^{-1})
L	latent heat (J kg^{-1})
l_ℓ	diffusion length around grain/trunk envelope (m)
m_ℓ	liquidus slope of binary phase diagram (K)
$M_{\ell e}(=-M_{e\ell})$	liquid-equiaxed net mass transfer rate (kg m^{-3} s^{-1})
$M_{\ell c}(=-M_{c\ell})$	liquid-columnar net mass transfer rate (kg m^{-3} s^{-1})
M^c_{ds}	interdendritic solidification rate in columnar trunk (kg m^{-3} s^{-1})
M^e_{ds}	interdendritic solidification rate in equiaxed grain (kg m^{-3} s^{-1})
n_{max}	maximum equiaxed grain density, or maximum available nucleation sites in heterogeneous nucleation law (m^{-3})
T_0	initial temperature (K)
T_f	melting point of pure metal (Al) (K)
T_L	liquidus temperature (K)
T_ℓ, T_e, T_c	temperatures of hydrodynamic ℓ-, e-, or c-phases (K)
T_E	temperature of eutectic reaction (K)
T_w	mould temperature (K)
ΔT	undercooling (K)
ΔT_c	undercooling at the columnar primary dendrite tip (K)
ΔT_N	undercooling for maximum grain production rate (K)
ΔT_σ	Gaussian distribution width of nucleation law (K)
$\vec{u}_\ell$, $\vec{u}_e$, $\vec{u}_c$	velocity vector of hydrodynamic ℓ-, e- or c-phase (m s^{-1})
v_{env}	growth velocity of the volume-equivalent envelope (m s^{-1})
$v^c_{tip'}$	growth velocity of columnar primary dendrite tip (m s^{-1})
α^c_d, α^c_s	volume fraction of interdendritic melt, solid dendrites inside the columnar tree trunks ($\alpha^c_d + \alpha^c_s$=1) (1)
α^e_d	volume fraction of interdendritic melt inside equiaxed grains (1)
α^e_s	volume fraction of solid inside equiaxed grains ($\alpha^e_d + \alpha^e_s$=1)
β_T	thermal expansion coefficient (K^{-1})
β_c	solutal expansion coefficient (1)
β_s	solidification volume shrinkage (1)
Φ^c_{circ}	circularity of the envelope of the columnar dendritic trunk (1)
Φ^c_{env}	shape factor of columnar dendrite trunk (1)
Φ^e_{env}	shape factor of equiaxed dendritic grain (1)
Φ^e_{sph}	sphericity of equiaxed grain envelope (1)
Γ	Gibbs–Thomson coefficient (m K)
λ_1	primary dendrite arm space of columnar tree trunk (m)
λ_2	secondary dendrite arm space (m)
μ_ℓ	viscosity (kg m^{-1} s^{-1})
ρ_ℓ, ρ_e, ρ_c	average densities of hydrodynamic ℓ-, e-, or c-phases (kg m^{-3})
$\rho^{ref}_\ell, \rho^{ref}_e$	reference densities of extradendritic melt and equiaxed phase (kg m^{-3})
ρ_s	density of pure solid dendrite (kg m^{-3})

interdendritic melt; and the extradendritic melt. As the columnar dendrite trunks generally move with a predefined velocity, only two set of momentum conservation equations are solved for the flow of the extradendritic melt and the movement of the equiaxed grains. The interdendritic melt inside the equiaxed grains is assumed to move with the equiaxed grains, and the interdendritic melt inside the columnar trunks moves with the columnar dendrite trunks.

A major focus area of research in mixed columnar-equiaxed solidification is the columnar-to-equiaxed transition (CET). Numerous previous investigations of the CET were carried out under a relatively simple condition/assumption, i.e. the unidirectional solidification. Hunt [11] based on a 1D analytical model has suggested that CET might occur when the volume fraction of equiaxed grains ahead of the columnar primary dendrite tip front exceeds a critical value of $f_{e,CET} = 0.49$, known as hard blocking mechanism. Based on this assumption he successfully established a CET map: a correlation of the columnar primary dendrite tip growth velocity $v^c_{tip'}$ with the local temperature gradient G at the moment when CET occurs. This CET map was later confirmed and further improved by including nucleation effects [12] and more precise growth kinetics and by incorporation of a multi-field system taking into account hard- and soft-blocking mechanisms [9,10,13–17]. Subsequent phase field and stochastic models have also confirmed the CET phenomenon in a unidirectional solidification configuration [18–20]. Indeed, phase field methods can provide almost all the necessary physical details of CET, though they are limited to domain scales at the microscopic level. In the mean time unidirectional solidification experiments were often accompanied to verify the above models or to help exploring new models. From the