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A four phase model for the macrosegregation and shrinkage cavity during solidification of steel ingot



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ABSTRACT

A four-phase mixed columnar-equiaxed solidification model is introduced to calculate the formation of macrosegregation and shrinkage cavity during solidification of steel ingot. The four phases are the liquid melt, the solidifying solid with columnar morphology, the solidifying solid with equiaxed morphology, and the gas phase (or covering liquid slag). Multiphase/multiphysics transport phenomena (mass, momentum, species and enthalpy) are solved with a volume-average approach. Solidification induced mass and species transfers among metal phases are considered according to the thermodynamics and diffusiongoverned crystal growth kinetics. The gas phase (or covering liquid slag) is only required to feed the shrinkage cavity and no mass/species exchange with other metal phases occurs. The following modeling results are obtained: the progress of columnar tip front and growth of columnar tree trunks, the nucleation and growth of equiaxed grains, the melt flow and equiaxed crystal sedimentation, the solute partitioning at the solid/liquid interface, the transport of the solute species and induced macrosegregation, the shrinkage cavity, the interaction or competition between growing columnar and equiaxed phases and the occurrence of columnar to equiaxed transition (CET). Those modeling capacities were verified by the calculation of a 10.5 tons steel ingot. The experimentally determined profile of the shrinkage cavity, Sulfur print and chemical analysis of macrosegregation of the ingot in a vertical section were also available. Satisfactory agreement was obtained between the simulation and experimental result. Finally, a new hypothesis for the initialization of A-segregates is proposed: the motion of equiaxed phase and its interaction with the melt flow in the vicinity of growing columnar tip front lead to formation of an A-shape segregation band starting from the ingot corner just above the columnar-to-equiaxed transition area. This A-segregation band might provide a favored location for the initialization of Asegregates. Further dedicated experiment should be carried out to verify it.

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1. Introduction

Macrosegregation and shrinkage cavity/porosity, Fig. 1(a) and (b) [1–4], are two concomitant casting defects resulting mainly from density variation during solidification. For decades they have been a focus of numerical modeling research in the field of casting and solidification. However, most numerical models can only treat segregation [5–9] and shrinkage

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Nomenclature

C C C	species concentration 1
cℓ,ce,cc	species concentration, 1
Cici	reference concentration, I
$C_{\ell}^*, C_{\mathrm{c}}^*, C_{\mathrm{e}}^*$	equilibrium concentration at interface, 1
$C_{\ell e}(=-C_{e\ell})$	species exchange between liquid and equiaxed, kg m ⁻³ s ⁻¹
$C_{\ell c}(=-C_{c\ell})$	species exchange between liquid and columnar, kg m ⁻³ s ⁻¹
C,	material constant in Eq. (28), $m(K/s)^{1/3}$
	mix concentration 1
-mix aindex	appropriate index %
mix	segregation index, %
$C_{\rm p}^{\ell}, C_{\rm p}^{\rm C}, C_{\rm p}^{\rm e}, C_{\rm p}^{\rm s}$	specific heat, J kg ⁻¹ K ⁻¹
D_ℓ , $D_s(D_e, D_c)$	diffusion coefficient, m ² s ⁻¹
d _e	equiaxed grain diameter, m
d _c	columnar trunk diameter, m
fe.fe.fc. fo	volume fraction of different phases, l
ffree	critical f_c for free moving equiaxed phase.
f ^c	equiaxed grain nacking limit 1
Je fEnv	volume fraction of equipyed grain envelope 1
Je f	fraction colid in equipyed grain envelope, 1
J _{si}	
g	gravity, m s ⁻²
$ec{g}_\ell'$	deduced gravity, m s ⁻²
G	temperature gradient, K m $^{-1}$
$h_1 \sim h_4$	heat transfer coefficient, W m $^{-2}$ K $^{-1}$
H^*_{ii}	volume heat transfer coeff. between phases, W m ⁻³ K ⁻¹
$h_{a}h_{b}h_{a}h_{a}h_{a}$	enthalny I kg ⁻¹
href href href href	reference enthalpy Ika^{-1}
\mathcal{U}_{ℓ} , \mathcal{U}_{e} , \mathcal{U}_{c} , \mathcal{U}_{g}	pormoshility of liquid in porous modium m ²
	drag coefficient between columnar and equipyed $\log m^{-3} c^{-1}$
$K_{ce}(=-K_{ec})$	drag coefficient between columnar and equiaxed, kg in 33^{-1}
$K_{\rm cg}(=-K_{\rm gc})$	drag coefficient between gas and columnar, kg m ⁻³ s ⁻¹
$K_{\rm eg}(=-K_{\rm ge})$	drag coefficient between gas and equiaxed, kg m^{-3} s ⁻¹
$K_{\ell c}(=-K_{c\ell})$	drag coefficient between liquid and columnar, kg m ⁻³ s ⁻¹
$K_{\ell e}(=-K_{e\ell})$	drag coefficient between liquid and equiaxed, kg m ^{-3} s ^{-1}
$K_{\ell q}(=-K_{q\ell})$	drag coefficient between liquid and gas, kg m ^{-3} s ^{-1}
k g g	solute partitioning coefficient at the ℓ/s interface.
Ke Ka Ka Ka	thermal conductivity. W m ^{-1} K ^{-1}
1	actual columnar length in tin cell m
I	latent heat $1k\sigma^{-1}$
	liquid equipped not mass transfer rate $k \alpha m^{-3} c^{-1}$
$M_{\ell e}(=-M_{e\ell})$	liquid columnar not mass transfer rate, kg m ⁻³ c ⁻¹
$M_{\ell c}(=-M_{c\ell})$	ilquid-columnar net mass transfer rate, kg m ² S
m	slope of liquidus in phase diagram, K
Ne	equiaxed grain production rate by nucleation, m ⁻³ s ⁻¹
n	equiaxed grain number density, m ⁻³
n _c	columnar trunk number density, m ⁻³
<i>n</i> _{max}	maximum equiaxed grain number density, m^{-3}
р	pressure, N m ⁻²
$\Delta P_{\rm cr}$	critical pressure drop for pore formation, $N m^{-2}$
$Q_{\ell e}(=-Q_{e\ell})$	total energy exchange between liquid and equiaxed, $Jm^{-3}s^{-1}$
$Q_{\ell 0}^{d}(=-Q_{0\ell}^{d})$	energy transfer between liquid and equiaxed phases, I m ⁻³ s ⁻¹
$O_{in}^{p}(=-O_{ni}^{p})$	energy exchange due to liquid-equiaxed phase change. $Im^{-3} s^{-1}$
$Q_{\ell e}(=-Q_{e\ell})$	total energy exchange between liquid and gas, $Im^{-3}s^{-1}$
$\zeta_{\ell}g(-Q)$	total energy exchange between liquid and columnar $Im^{-3}c^{-1}$
$Q_{\ell c}(=-Q_{c\ell})$	total energy exchange between inquit and columnal, jii ~ s
$Q_{\ell c}^{\dagger} (= -Q_{c\ell}^{\bullet})$	energy transfer between inquite and columnidit, $\int III = S^{-1}$
$Q_{\ell c}^{r}(=-Q_{c\ell}^{r})$	energy exchange due to inquid-columnar phase change, J m ⁻³ s ⁻¹
$Q_{ec}(=-Q_{ce})$	total energy exchange between equiaxed and columnar, $Jm^{-3}s^{-1}$
$Q_{ec}^{u}(=-Q_{ce}^{u})$	energy transfer between equiaxed and columnar, J m ⁻³ s ⁻¹
$Q_{cg}(=-Q_{gc})$	total energy exchange between gas and columnar, J m $^{-3}$ s $^{-1}$
$Q_{eg}(=-Q_{ge})$	total energy exchange between gas and equiaxed, $J m^{-3} s^{-1}$
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$R(R_{\rm e}, R_{\rm c})$	grain radius (equiaxed, columnar), m		
Re	also used for Reynold number in Eq. (23)–(25), l		
R _{f, e}	maximum radius of equiaxed grain, m		
R _{f, c}	maximum radius of columnar trunk, m		
R _{tip}	tip radius of columnar primary dendrite, m		
S_{A}^{c}, S_{A}^{e}	surface area of columnar (equiaxed) per volume, m^{-1}		
T, T_ℓ , T_e , T_c , T_g	temperature, K		
T _f	melting point of pure metal (Fe), K		
T ^{rer}	reference temperature for liquid density, K		
T _{ref}	reference temperature for enthalpy, K		
$T_{\text{liquidus}}, T_{\text{Eutectic}}$	liquidus, eutectic temperature, K		
T	cooling rate, K s ⁻¹		
ΔT	constitutional undercooling, K		
$\Delta T_{\rm N}$	undercooling for maximum grain production rate, K		
$\Delta T_{\rm tip}$	undercooling at the columnar dendrite tip, K		
ΔT_{σ}	Gaussian distribution width of nucleation law, K		
t	time, s		
Δt	time step, s		
$U_{\ell e}(=-U_{e\ell})$	local inquid-equiaxed momentum exchange due to drag force $\log m^{-2} c^{-2}$		
$\vec{U}_{\ell e} (= -\vec{U}_{e\ell})$	liquid-equiaxed momentum exchange due to phase change kg m ⁻² s ⁻²		
$\vec{U}_{\ell e} = \vec{U}_{e\ell}$	total liquid-columnar momentum exchange rate kg m ^{-2} s ^{-2}		
$\vec{U}_{\ell c}^{d}(=-\vec{U}_{c\ell}^{d})$	liquid-columnar momentum change due to drag force, kg m ⁻² s ⁻²		
$\vec{U}_{\ell c}^{\rm p}(=-\vec{U}_{c\ell}^{\rm p})$	liquid-columnar momentum exchange due to phase change, kg m ⁻² s ⁻²		
$\vec{U}_{\ell\sigma}^{(\ell)}(=-\vec{U}_{\sigma\ell}^{(\ell)})$	liquid–gas momentum exchange rate, kg m $^{-2}$ s $^{-2}$		
$\vec{U}_{c\sigma}(=-\vec{U}_{\sigma c})$	columnar–gas momentum exchange rate, kg m $^{-2}$ s $^{-2}$		
$\vec{U}_{eg}(=-\vec{U}_{ge})$	equiaxed-gas momentum exchange rate, kg m $^{-2}$ s $^{-2}$		
$\vec{u}_{\ell}, \vec{u}_{e}, \vec{u}_{c}, \vec{u}_{g}$	velocity vector, m s ⁻¹		
$v_{\rm Rc}, v_{\rm Re}$	growth speed in radius direction (columnar, equiaxed), m s ^{-1}		
v _{tip}	grain growth speed in tip direction, m s $^{-1}$		
$\beta_{\rm T}$	thermal expansion coefficient, K^{-1}		
β_{c}	solutal expansion coefficient, wt.% ⁻¹		
$\Phi^{e}_{imp}, \Phi^{c}_{imp}$	growth impingement factor (equiaxed, columnar), l		
λ_1	primary dendrite arm space, m		
$\rho_{\ell}, \rho_{\rm e}, \rho_{\rm c}, \rho_{\rm g}$	density, kg m ⁻³		
ρ_{ℓ}^{ref}	reference density, kg m ^{-3}		
ρ_{ℓ}^{p}	density for buoyancy force, kg m ⁻³		
ρ	mixture density of metal phases, kg m ⁻³		
$\Delta \rho$	solidification shrinkage, l		
= = = =	VISCOSITY, Kg m ⁻¹ S ⁻¹		
$ au_{c}, au_{e}, au_{g}$	stress-strain tensors, kg m ^{-1} s ^{-1}		
Subscripts			
l ℓ mark l	iquid		
e equiax	ed		
c colum	nar		
g gas phases			

[10–11] separately. No model is able to deal with them by incorporating multiphase transport phenomena with volume shrinkage, as schematically depicted in Fig. 1(c), although casting practices [1,12] and laboratory experiments [13–15] have provided clear evidence for the appearance of macrosegregation and shrinkage defects in a coupled manner. Based on a previous study [16], the influence of the solidification shrinkage on the macrosegregation comes from the following aspects: (1) formation of the top shrinkage cavity (pipe) adapts the position of the concentrated positive segregation; (2) the solidification shrinkage adapts the multiphase flow in/near the columnar tip front, hence influences the macrosegregation intensity in the middle radius region of the ingot; (3) feeding flow in the deep mushy zone at the late stage of solidification can enhance the negative segregation (or reduce the positive segregation) along the centerline of the ingot. A model capable of predicting the as-cast structure with consideration of formation of both shrinkage cavity and macrosegregation is greatly required.



Fig. 1. Schematic of the solidification process of an ingot casting, and accompanying macrosegregation and shrinkage phenomena. (a) Sulfur print of a 10.5-tons steel ingot with nominal composition of 0.30 wt%C [1]; (b) schematic description of the different types of macrosegregation and shrinkage defects; (c) schematic of the solidification process and phases involved.

According to the appearance of the shrinkage defects in the casting and the existing knowledge about their formation mechanisms, three types of shrinkage defects can be categorized [17]: (i) micro porosity or pores, (ii) open pipe-shrinkage or shrinkage cavity, and (iii) macro porosity. Micro porosity (i) occurs in the deep interdendritic mushy zone, where it is hard for the melt to feed the solidification shrinkage. When the shrinkage-induced pressure drop reaches a threshold, pores would initiate and grow in the interdendritic space. This kind of porosity was initially modeled analytically with the solution of the pressure drop in the mushy zone [18], then investigated with more advanced numerical method [19]. As the nucleation and growth of the micro pores are closely related to the gas content, rejection of the gas element by solidification becomes an important issue for the pore formation. Therefore, a diffusion-governed growth model was also proposed to analyze the pore growth kinetics [20]. One has to admit that the above-mentioned models, despite their sound physical basis, are mostly applied for theoretical investigation of the mechanisms of porosity formation, but it is difficult to use them for predicting the pore formation quantitatively. For simplicity, some criterion functions purely based on the thermal field, e.g. the Niyama criterion [21], were derived to predict the probability of occurrence of the shrinkage porosity and the most likely position of the shrinkage porosity in engineering castings. Later on, many researchers extended this idea by considering the effect of mush zone morphology and permeability [22]. Some successes were achieved, and those criterion functions were implemented in commercial software, e.g. ProCAST [23] and MAGMASOFT [24], to aid engineers to minimize the porosity in engineering castings. Open pipe-shrinkage or shrinkage cavity (ii) is that seen in the hot top region of the ingot of Fig. 1. The sinking of the melt level due to the accumulated volume shrinkage in the still-connected bulk melt region leads to the formation of a funnel-shape 'pipe'. Formation of the macro porosity (iii) inside the casting is similar to the open pipe shrinkage; the only difference is that it forms in a closed melt region which is disconnected (surrounded by the already-solidified region) from the open pipe shrinkage. Therefore, the numerical treatment of these two types of macroscopic shrinkage cavities is similar: calculation and relocation of the accumulated volume shrinkage based on thermal and gravity fields [25]. None of the aforementioned numerical models have considered the multiphase transport phenomena, and their interaction with the formation of macrosegregation is ignored.

Referring to Flemings [5] and Flemings and Nereo [26] the shrinkage-induced feeding flow in the interdendritic region leads to the reverse segregation. Actually, formation of almost all types of macrosegregation in castings is related to the density variation during solidification, i.e. the same cause for the formation of shrinkage defects. For example, the flow due to thermal-solutal buoyancy of melt can cause channel segregation (A-segregates) in steel ingots [27], freckles in unidirection-ally solidified casting components [28], centerline positive/negative (depending on flow pattern) segregation in steel ingots [5,29,30] and continuous castings [5,31]. Density change due to solidification shrinkage can lead to centerline segregation in continuous castings [27,32,33]. Sedimentation of equiaxed crystals due to the density difference between liquid and solid can lead to typical bottom cone-shape negative segregation in heavy ingots [27,30]. In order to model the aforementioned segregation, the ability to solve the multiphase transport phenomena of Fig. 1(c) is the key.

The authors have developed a 3-phase mixed columnar–equiaxed solidification model [34–36]. A further effort is to extend the previous model to treat the formation of the shrinkage cavity by including an additional gas (or covering slag) phase [16,37]. The final goal is to develop an Eulerian multiphase solidification model to calculate the shrinkage cavity/porosity and macrosegregation in industry ingots. Concept of the four-phase model was briefly introduced in a conference publication, and the model was tested for a 2.45 tons ingot with geometry of big-end-up [16]. Main novelties of the current paper are as follows. (1) All details of the model are described; (2) Calculations of a 10.5 tons ingot with geometry of big-end-down are made and verified against experimental result; (3) Based on the analysis of the modeling results a new hypothesis for the initiation of A-segregates is proposed.

Table 1

Mass:

Conservation equations of the four-phase solidification model.

wi

$$\frac{\partial}{\partial t}(f_{\ell}\rho_{\ell}) + \nabla \cdot \left(f_{\ell}\rho_{\ell}\bar{u}_{\ell}\right) = -M_{\ell e} - M_{\ell c},\tag{1}$$

$$\frac{\partial}{\partial t}(f_e\rho_e) + \nabla \cdot \left(f_e\rho_e \bar{u}_e\right) = M_{\ell e},\tag{2}$$

$$\frac{\partial}{\partial t}(f_c\rho_c) = M_{\ell c},\tag{3}$$

$$\frac{\partial}{\partial t}(f_{g}\rho_{g}) + \nabla \cdot \left(f_{g}\rho_{g}\bar{u}_{g}\right) = 0.$$
(4)

Momentum

$$\frac{\partial}{\partial t} \left(f_{\ell} \rho_{\ell} \vec{u}_{\ell} \right) + \nabla \cdot \left(f_{\ell} \rho_{\ell} \vec{u}_{\ell} \otimes \vec{u}_{\ell} \right) = -f_{\ell} \nabla p + \nabla \cdot \bar{\vec{\tau}}_{\ell} + f_{\ell} \rho_{\ell} \bar{g}_{\ell}' - \vec{U}_{\ell e} - \vec{U}_{\ell e} - \vec{U}_{\ell g}, \tag{5}$$

$$\begin{aligned} & \text{th}\ \bar{\bar{\tau}}_{\ell} = \mu_{\ell} f_{\ell} (\nabla \otimes \bar{u}_{\ell} + (\nabla \otimes \bar{u}_{\ell})^{-}), \ \bar{g}_{\ell} = \frac{\rho_{\ell}^{c} (1,c_{\ell}) - \rho_{\ell}^{c_{\ell}}}{\rho_{\ell}^{\text{ref}}} \ \bar{g}, \ \rho_{\ell}^{\text{b}} (T,c_{\ell}) = \rho_{\ell}^{\text{ref}} \cdot (1 + \beta_{\mathrm{T}} \cdot (T^{\text{ref}} - T_{\ell}) + \beta_{\mathrm{c}} \cdot (c^{\text{ref}} - c_{\ell})). \\ & \frac{\partial}{\partial t} \left(f_{\mathrm{e}} \rho_{\mathrm{e}} \bar{u}_{\mathrm{e}} \right) + \nabla \cdot \left(f_{\mathrm{e}} \rho_{\mathrm{e}} \bar{u}_{\mathrm{e}} \otimes \bar{u}_{\mathrm{e}} \right) = -f_{\mathrm{e}} \nabla p + \nabla \cdot \bar{\bar{\tau}}_{\mathrm{e}} + f_{\mathrm{e}} \rho_{\mathrm{e}} \bar{g} + \vec{U}_{\ell \mathrm{e}} + \vec{U}_{\mathrm{ce}} - \vec{U}_{\mathrm{eg}}, \end{aligned}$$
(6)

with
$$\overline{\overline{\tau}}_e = \mu_e f_e (\nabla \otimes \overline{u}_e + (\nabla \otimes \overline{u}_e)^T)$$
, μ_e equiaxed viscosity [40].

$$\frac{\partial}{\partial t} \left(f_{g} \rho_{g} \vec{u}_{g} \right) + \nabla \cdot \left(f_{g} \rho_{g} \vec{u}_{g} \otimes \vec{u}_{g} \right) = -f_{g} \nabla p + \nabla \cdot \tilde{\vec{t}}_{g} + f_{g} \rho_{g} \vec{g} + \vec{U}_{\ell g} + \vec{U}_{eg} + \vec{U}_{eg}, \tag{7}$$

with
$$\overline{\tilde{\tau}}_{g} = \mu_{g} f_{g} (\nabla \otimes \overline{u}_{g} + (\nabla \otimes \overline{u}_{g})^{T})$$

$$\frac{\partial}{\partial t}(f_{\ell}\rho_{\ell}c_{\ell}) + \nabla \cdot \left(f_{\ell}\rho_{\ell}\bar{u}_{\ell}c_{\ell}\right) = \nabla \cdot (f_{\ell}\rho_{\ell}D_{\ell}\nabla c_{\ell}) - C_{\ell c} - C_{\ell e},\tag{8}$$

$$\frac{\partial}{\partial t}(f_e\rho_e c_e) + \nabla \cdot \left(f_e\rho_e \bar{u}_e c_e\right) = \nabla \cdot (f_e\rho_e D_e \nabla c_e) + C_{\ell e},\tag{9}$$

$$\frac{\partial}{\partial t} (f_c \rho_c c_c) = \nabla \cdot (f_c \rho_c D_c \nabla c_c) + C_{\ell c}, \tag{10}$$

Enthalpy:

Species

$$\frac{\partial}{\partial t}(f_{\ell}\rho_{\ell}h_{\ell}) + \nabla \cdot \left(f_{\ell}\rho_{\ell}\vec{u}_{\ell}h_{\ell}\right) = \nabla \cdot (f_{\ell}k_{\ell}\nabla \cdot T_{\ell}) - Q_{\ell c} - Q_{\ell c} - Q_{\ell c},$$
(11)

$$\frac{\partial}{\partial t} \left(f_e \rho_e h_e \right) + \nabla \cdot \left(f_e \rho_e \bar{u}_e h_e \right) = \nabla \cdot \left(f_e k_e \nabla \cdot T_e \right) + Q_{\ell e} + Q_{ce} - Q_{eg}, \tag{12}$$

$$\frac{\partial}{\partial t}(f_c\rho_c h_c) = \nabla \cdot (f_c k_c \nabla \cdot T_c) + Q_{\ell c} - Q_{c e} - Q_{c g},$$
(13)

$$\frac{\partial}{\partial t} \left(f_{g} \rho_{g} h_{g} \right) + \nabla \cdot \left(f_{g} \rho_{g} \vec{u}_{g} h_{g} \right) = \nabla \cdot \left(f_{g} k_{g} \nabla \cdot T_{g} \right) + Q_{\ell g} + Q_{eg} + Q_{eg}, \tag{14}$$

with $h_{\ell} = \int_{T_{ref}}^{T_c} c_p^{\ell} dT + h_{\ell}^{ref}$, $h_e = \int_{T_{ref}}^{T_e} c_p^{e} dT + h_e^{ref}$, $h_c = \int_{T_{ref}}^{T_e} c_p^{e} dT + h_e^{ref}$, $h_g = \int_{T_{ref}}^{T_g} c_p^{g} dT + h_g^{ref}$, and the solidification latent heat $L = h_{\ell}^{ref} - h_e^{ref} = h_{\ell}^{ref} - h_c^{ref}$.

Equiaxed grains:

$$\frac{\partial}{\partial t}n + \nabla \cdot \left(\vec{u}_{e}n\right) = N_{e},\tag{15}$$

with
$$N_e = \frac{d(\Delta T)}{dt} \cdot \frac{n_{max}}{\sqrt{2\pi} \cdot \Delta T_{\sigma}} \cdot e^{-\frac{1}{2} \cdot \left(\frac{\Delta T - \Delta T_N}{\Delta T_{\sigma}}\right)^2}$$
, $\Delta T = T_f + mc_\ell - T_.$

2. Model

2.1. Description/assumptions

An Eulerian multiphase approach is used. Details of the three-phase mixed columnar–equiaxed solidification model were described previously [34–36]. With the additional gas phase the model is modified, and all conservation equations are sum-

Table 2

Interphase transfer (closure laws).

I. Mass transfer

$$M_{\ell e} = v_{R_e} \cdot \left(n \cdot \pi d_e^2\right) \cdot \rho_e \cdot \Phi_{\rm imp}^e,\tag{16}$$

With $v_{R_e} = \frac{D_\ell}{R_e(1-R_e/R_{f,e})} \cdot \frac{c_\ell^* - C_\ell}{c_\ell^* - C_e^*} + \frac{2D_s}{R_e} \cdot \frac{c_e^* - C_e}{c_\ell^* - C_e^*}$ and $\Phi_{imp}^e = f_\ell$.

$$M_{\ell c} = \begin{cases} \nu_{R_c} \cdot \left(\pi d_c / \lambda_1^2\right) \cdot \rho_c \cdot \Phi_{imp}^c & \text{for col. trunks without primary tips} \\ \left[\nu_{R_c} \cdot \left(\pi d_c \cdot l\right) + \nu_{tip} \cdot \left(\pi R_{tip}^2\right)\right] \cdot n_c \cdot \rho_c \cdot \Phi_{imp}^c & \text{for col. trunks with primary tips} \end{cases},$$
(17)

with $v_{R_c} = \frac{D_c}{R_c} \cdot \frac{c_1^2 - c_c}{c_l^2 - c_c} \cdot \ln^{-1}(\frac{R_{tc}}{R_c}) + \frac{2D_c}{R_c} \cdot \frac{c_c^2 - c_c}{c_l^2 - c_c^2}$, v_{tip} and R_{tip} are based on LGK model [41], and $\Phi_{tip}^c = \begin{cases} 1 & d_c \le \lambda_1 \\ 4f_\ell/(4 - \pi) & d_c > \lambda_1 \end{cases}$. II. Species transfer

$$C_{\ell e} = \begin{cases} k \cdot c_{\ell}^* \cdot M_{\ell e} + S_{\mathsf{A}}^e \cdot \rho_e \cdot \frac{D_s}{R_e/2} \cdot (c_e^* - c_e) & \text{for solidification} \\ c_e \cdot M_{\ell e} & \text{for melting} \end{cases},$$
(18)

$$C_{\ell c} = \begin{cases} k \cdot C_{\ell}^* \cdot M_{\ell c} + S_{\rm A}^{\rm c} \cdot \rho_{\rm c} \cdot \frac{D_{\rm s}}{R_{\rm c}/2} \cdot (c_{\rm c}^* - c_{\rm c}) & \text{for solidification} \\ c_{\rm c} \cdot M_{\ell \rm c} & \text{for melting} \end{cases},$$
(19)

III. Energy transfer

$$Q_{ij} = H_{ij}^* f_i f_j (T_i - T_j),$$
(20)

with *i*, *j* indicating interaction phases (ℓ , e, c, g).

A large volume heat exchange coefficient (10¹¹ [W m⁻³ K⁻¹]) is applied between each pair of metal phases (H_{te}^* , H_{tc}^* , H_{tc}^*), while a smaller volume heat exchange coefficient (10³ [W m⁻³ K⁻¹]) is applied between solid metal phase and gas phase (H_{eg}^* , H_{cg}^*), H_{tg}^* is modeled according to Ranz-Marshall [37,42].

IV. Momentum transfer

$$\vec{U}_{\ell e} = \vec{U}_{\ell e}^{\rm p} + \vec{U}_{\ell e}^{\rm d}, \quad \vec{U}_{\ell e}^{\rm p} = \vec{u}^* \cdot M_{\ell e}, \tag{21.a}$$
$$\vec{U}_{\ell e}^{\rm d} = K_{\ell e} \cdot \left(\vec{u}_{\ell} - \vec{u}_{e}\right), \tag{22.a}$$

$$\vec{u}^* = \begin{cases} \vec{u}_{\ell} & \text{(solidification)} \\ \vec{u}_e & \text{(re-melting)} \end{cases} \quad \text{where } K_{\ell e} \text{ refers to [43]}$$

$$\vec{U}_{\ell c} = \vec{U}_{\ell c}^{\text{P}} + \vec{U}_{\ell c}^{\text{d}}, \quad \vec{U}_{\ell c}^{\text{P}} = \vec{u}^* \cdot M_{\ell c}, \quad (21.b) \qquad \qquad \vec{U}_{\ell c}^{\text{d}} = K_{\ell c} \cdot \left(\vec{u}_{\ell} - \vec{u}_{c}\right), \quad (22.b)$$

$$\vec{U}_{eg} = \vec{U}_{eg}^{p} + \vec{U}_{eg}^{d}, \ \vec{U}_{eg}^{p} = 0,$$
 (21.e) $\vec{U}_{eg}^{d} = K_{eg} \cdot \left(\vec{u}_{e} - \vec{u}_{g}\right),$ (22.e)

$$\vec{U}_{cg} = \vec{U}_{cg}^{p} + \vec{U}_{cg}^{a}, \ \vec{U}_{cg}^{p} = 0, \qquad (21.f) \qquad \vec{U}_{cg}^{a} = K_{cg} \cdot \left(\vec{u}_{c} - \vec{u}_{g}\right), \qquad (22.f)$$

where $K_{\ell g}$, K_{eg} and K_{cg} refer to Table 3.

marized in Table 1. Closure laws for the conservation equations are given in Tables 2 and 3. A brief description of the model features and assumptions are as follows.

- Four phases (Fig. 1(c)) are defined: primary liquid (ℓ), solidifying equiaxed crystals (e), columnar tree trunks (c), and gas or covering slag phase (g). Their volume fractions (f_{ℓ} , f_{e} , f_{c} , f_{g}) sum up to one. The mass transport equations considering the mass transfer due to solidification ($M_{\ell e}$, $M_{\ell c}$) are solved by Eqs. (1)-(4).
- There is no mass transfer between gas (or covering slag) and other metal phases, and the gas phase is supposed to be immiscible with the metal phases, and to be sucked into the casting domain to feed the open pipe shrinkage. The

Table 3

Momentum exchange coefficients between metal and gas (or slag) phases.

Symmetric model is applied [45]:	$R_{ m e}= ho_{ m pg}ert ec{u}_{ m p}-ec{u}_{ m g}ert d_{ m pg}/\mu_{ m pg},$	(24)
$K_{\rm pg} = \frac{\rho_{\rm pg} R_{\rm e} C_D}{144 \tau_{\rm pg}} d_{\rm pg} A_{\rm pg}, \qquad (23)$	$C = \begin{cases} 27.6 & R_e \le 1 \\ 24.4 + 0.15 P (587) + P & 1 - P \le 103 \end{cases}$	(25)
where subscript 'p' indicates different	$C_{\rm D} = \begin{cases} 24(1+0.15K_{\rm e}^{3.000})/\kappa_{\rm e}, & 1 < \kappa_{\rm e} \le 10^{\circ}, \\ 0.44 & R_{\rm e} > 10^{3} \end{cases}$	(25)

where subscript 'p' indicates different metal phases: '*l*', 'e' or 'c'.

$$\tau_{\rm pg} = \rho_{\rm pg} d_{\rm pg}^2 / 18\mu_{\rm pg},\tag{26}$$

$$A_{\rm pg} = 6f_{\rm p}f_{\rm g}/d_{\rm pg},\tag{27}$$

 $\mu_{pg} = \min(\mu_p, \mu_g); \ \rho_{pg} = \min(\rho_p, \rho_g); \ d_{pg}: modeling \ parameter \ (diameters) \ as \ function \ of \ volume$ fractions of involving phases.

interface between gas and other phases is explicitly tracked with the isoline defined by $f_g = 0.5$. The microscopic porosity which might form in the deep inter-dendritic region is treated differently (Section 2.2).

- The primary liquid, equiaxed and gas phases are moving phases, for which the corresponding Navier-Stokes equations are solved by Eqs. (5)–(7) to get \vec{u}_{ℓ} , \vec{u}_{e} and \vec{u}_{g} , while $\vec{u}_{c} \equiv 0$.
- The liquid and solid phases have different densities, hence the solidification shrinkage due to phase change from liquid (ℓ) to solid (e and c) is explicitly calculated. However, the thermo-solutal convection of the liquid melt is modeled with Boussinesg approximation. This approximation means that the density of the liquid melt is treated as constant (independent on the concentration and temperature), and a source term for the thermo-solutal buoyancy force is added to the momentum conservation equation.
- Thermo-mechanical deformation of the ingot during solidification and subsequent cooling after solidification are not considered. It is assumed that the solidification shrinkage due to the density difference between liquid and solid only leads to the formation of shrinkage cavity, but does not lead to mechanical deformation.
- For binary alloys, three volume-averaged concentration fields (c_{ℓ}, c_{e}, c_{c}) are solved for the three metal phases, Eqs. (8)-(10). Thermodynamic equilibrium condition always applies at the liquid-solid interface, and solute partition occurs during solidification at the liquid-solid interface. For ternary alloys, three more species concentration fields for the second allov element in each phase should be solved [35].
- Enthalpy equations for all four phases are solved, Eqs. (11)-(14). Due to the fact of relatively large thermal diffusivity, we assume that only one temperature (T) represents average temperature of all the phases in each volume element. Therefore, empirical inter-phasic volume heat exchange coefficients are applied to balance the temperatures among the phases. Choice of those coefficients seems not to violate the energy conservations, but they have significant influence on the calculation efficiency (convergence behavior).
- A diffusion-governed growth kinetic is considered to calculate the solidification mass transfer ($M_{\ell e}, M_{\ell c}$), Eqs. (16) and (17). Simple crystal morphology is assumed: step-wise cylinder for columnar tree trunks, and sphere for equiaxed grains. The growth speed of the crystal is governed by the species diffusion in liquid melt around the cylinder (or sphere) and by the species back diffusion in the cylindrical (or spherical) crystal.
- To deal with the hydrodynamic interaction between phases properly, a simplified dendritic morphology for the equiaxed phase [38] is assumed, and a concept of "equiaxed grain envelope" is employed. A dendritic equiaxed crystal is described by the equiaxed grain envelope, which includes the solid 'dendrite' and the inter-dendritic melt. The ratio of the volume of solid 'dendrite' to the volume of the equiaxed grain envelope is predefined: f_{si} . Therefore, the volume fraction of equiaxed grain envelopes (f_e^{Env}) is related to the volume fraction of the net solid phase of equiaxed crystals (f_e) by $f_e^{\text{Env}} = f_e/f_{si}$.
- The columnar dendrite trunks are assumed to originate from the mold wall. Neither nucleation of columnar trunks nor equiaxed-to-columnar transition (ECT) is taken into account. The position of the columnar primary dendrite tips is explicitly tracked [34]. The growth of the columnar primary dendrite tips stops when the volume fraction of the equiaxed (envelope) phase (f_e^{Env}) reaches 0.49 (hard blocking criterion) in front of the primary columnar dendrite tips [39], then columnar-to-equiaxed transition (CET) occurs.
- The packing limit for crystals is set as 0.637 [40]. When the sum of the volume fraction of equiaxed envelopes (f_e^{Env}) and columnar phase (f_c) exceeds this limit, the solid crystals will form a rigid body.
- The hydrodynamic interaction between equiaxed and columnar phases is considered. The equiaxed crystals are trapped by the columnar dendrite trunk when the local volume fraction of the columnar phase (f_c) reaches a critical value of 0.2 [34], i.e. an infinitely large drag force is applied between both solid phases. Otherwise, no drag is considered between them.
- Heterogeneous nucleation and transport of the equiaxed crystals are considered, Eq. (15). Grain fragments brought into the mold during filling, further fragmentation of dendrites during solidification and the attachment of equiaxed grains into columnar tips (as a part of the columnar phase) are ignored.

- The size (d_e) and number density (n_e) of equiaxed grains and the diameter (d_c) of the columnar trunks are explicitly calculated, while a constant value for the primary arm spacing (λ_1) of columnar dendrites is predefined based on experimental data.
- The CFD software package, ANSYS FLUENT 15.4, is used to solve the transport equation system. It provides flexibility to include additional exchange and source terms, and even to modify the transport equations.

2.2. Simplified microscopic shrinkage porosity model

Microscopic shrinkage porosity is not explicitly modeled, but the Niyama criterion function [21], as modified by Carlson and Beckermann [22], is implemented. In this paper, we call it the CBN (Carlson–Beckermann–Niyama) criterion, Eq. (28). The possibility of occurrence of shrinkage porosity and the amount of pores (volume fraction of voids) decrease with the locally calculated value of CBN criterion. In other words, the smaller the CBN criterion function, the greater the probability that shrinkage porosity would occur, and the more pores would form.

$$CBN = C_{\lambda} \frac{G}{\dot{T}^{5/6}} \sqrt{\frac{\Delta P_{cr}}{\mu_{\ell} \Delta \rho \left(T_{\text{Liquidus}} - T_{\text{Eutectic}}\right)}},$$
(28)

where C_{λ} is a material constant, 1.44×10^{-4} [m(K/s)^{1/3}], being used for determining the secondary dendrite arm spacing; *G* and \dot{T} are the temperature gradient and cooling rate, which are evaluated at a critical temperature of T_{cr} (=0.1 · $T_{Liquidus}$ + 0.9 · $T_{Eutectic}$), assuming that $T_{Eutectic}$ corresponds to the end solidification; $\Delta \rho$ is the solidification shrinkage, $(\rho_s - \rho_\ell)/\rho_\ell$; ΔP_{cr} is the critical pressure drop when a pore-nucleus with a critical radius of r_{pore} in the deep mushy zone can overcome capillary force ($2\sigma/r_{pore}$) and metallostatic pressure (P_{static}) to grow. ΔP_{cr} is 1.01 × 10⁵ Pa for steel [22]. As no threshold of CBN for the occurrence of pores can be determined in advance, this criterion is in the current paper used only for qualitative evaluation of the occurrence probability of the microscopic shrinkage porosity.

Although the current Eulerian approach offers the possibility to calculate the interdendritic flow, it is extremely hard to solve the feeding flow in the deep mush near the end of solidification due to the convergence difficulty. Therefore, a so-called 'simplified porosity model' is introduced [32,33]. When the temperature drops below the critical temperature of T_{cr} , volume shrinkage by solidification is ignored, i.e. the solidification is assumed to occur without volume change. This treatment is made by assuming that the remaining melt in the deep mush solidifies as a solid-pore mixture with the mixture density equal to the liquid density.

3. Modeling result for a 10.5 tons ingot

3.1. Configuration

A 10.5 tons steel ingot with nominal composition Fe-0.3 wt%C-0.74 wt%Mn-0.13 wt%Si-0.017 wt%S-0.01 wt%P was cast in an octagonal chill mold [1]. The casting was sectioned vertically for Sulfur print, which showed shrinkage cavity and global segregation pattern (Fig. 1(a)). Additionally, 20 points of chemical analysis (drilling samples of a diameter of 10 mm) on the same vertical section were made to quantify the severity of the macrosegregation. A typical solidification time of a 10 tons ingot in a chill mold should take about 3 h.

The alloy is multicomponent, but in this paper we present results of an analysis for a simplified binary alloy (Fe-0.3 wt%C). The material properties of the alloy and covering liquid slag, and some important boundary conditions are summarized in Table 4 and Fig. 2. As no appropriate process conditions and parameters (mold geometry and mold material properties) for the simulation purpose were documented, the settings for the missing parameters are necessarily estimated. Actually, very few appropriate experimental studies on such parameters for steel ingots of such scale have ever been made historically. The thermal boundary condition is approximated as an 'effective heat transfer coefficient' between the ingot surface and the ambient temperature ($T_w = 300$ K). This means that the joint effects of the heat transfers at the casting-mold interface, through the mold thickness, and at the mold-ambient interface are included in one parameter, i.e. the effective heat transfer coefficient.

No mold filling is calculated, and the mold is assumed to be initially filled with liquid melt of 1782 K (above the liquidus 1781.015 K). This small superheat is assumed based on the fact that the most superheat is released during mold filling. A zero-gradient boundary condition is applied at the 'pressure inlet' for other quantities: temperature, concentrations. Nucleation parameters of equiaxed crystals [46] are: $n_{max} = 5.0 \times 10^9 \text{ m}^{-3}$, $\Delta T_N = 5.0 \text{ K}$, $\Delta T_{\sigma} = 2.0 \text{ K}$. A concept of "equiaxed grain envelope" is considered by assuming a certain amount of solid 'dendrite' in the grain envelope (f_{si}). This parameter is unknown in advance; hence a parameter study by varying it from 0.5 to 0.9 is performed. A value of 0.6 is found to be reasonable for this alloy (Section 4). Calculation with the 4-phase Eulerian model including gas (air) phase is extremely time consuming (demanding very small time step) due to the large density difference between gas and metal phases. Therefore, a covering slag (liquid), which is also used in praxis, is considered instead of gas phase. As schematically shown in Fig. 2 (right half), the liquid slag phase flows through the 'pressure inlet' into the calculation domain to feed the solidification shrinkage. Initially, the entire calculation domain is assumed to be filled with the liquid steel, i.e. ℓ -phase. However, in order to avoid numerical difficulty, a tiny volume fraction (10^{-6}) is assigned to other three phases, i.e. e-, c-, g-phases.

Table 4

Thermodynamic and physical properties of materials [16,46].

Steel		
Melting point of pure iron, T_f Liquidus slope, m Equilibrium partition coefficient k Melt density, ρ_{ℓ} Solid density, ρ_{e} , ρ_{c} Specific heat, c_{b}^{ℓ} , c_{5}^{e} , c_{7}^{e} Thermal conductivity, k_{ℓ} , k_{e} , k_{c} Latent heat, L Viscosity, μ_{ℓ} Thermal expansion coefficient, β_{T} Solutal expansion coefficient, β_{c} Primary dendritic arm spacing, λ_{1} Diffusion coefficient (liquid), D_{ℓ}	$\begin{array}{c} K \\ K \ (wt\%)^{-1} \\ - \\ kg \ m^{-3} \\ kg \ m^{-3} \\ J \ kg^{-1} \ K^{-1} \\ W \ m^{-1} \ K^{-1} \\ J \ kg^{-1} \\ I \ kg^{-1} \\ sg \ m^{-1} \ s^{-1} \\ m^{2} \ s^{-1} \\ m^{2} \ s^{-1} \end{array}$	$\begin{array}{c} 1805.15 \\ -80.45 \\ 0.36 \\ 7027 \\ 7324 \\ 500 \\ 34.0 \\ 2.71 \times 10^5 \\ 4.2 \times 10^{-3} \\ 1.07 \times 10^{-4} \\ 1.4 \times 10^{-2} \\ 1 \times 10^{-3} \\ 2.0 \times 10^{-8} \\ 1.0 \times 10^{-9} \end{array}$
Covering slag		
Viscosity, μ_g Density, ρ_g Specific heat, c_p^g Thermal conductivity, k_g	$\begin{array}{c} kg \ m^{-1} \ s^{-1} \\ kg \ m^{-3} \\ J \ kg^{-1} \ K^{-1} \\ W \ m^{-1} \ K^{-1} \end{array}$	0.01 2500 1815 4.0



Fig. 2. Configuration of the 10.5 tons ingot, and corresponding boundary conditions. The geometry is in 3D with an octagonal cross section, but here only a 2D vertical section is shown.

The ingot was simulated in full 3D, and was discretized into 0.24 million volume hexahedron elements (average mesh size of 18 mm). One calculation took 2.5 weeks on a SGI cluster with 12 cores of 3.5 GHz.

3.2. Solidification result

The solidification sequence is shown in Fig. 3. The global solidification process is mainly governed by heat transfer, and partially influenced by the motion of crystals. The cooling and solidification start from the mold wall. Columnar phase develops from the mold wall and grows towards the casting center. In the meantime equiaxed grains nucleate and grow in the vicinity of columnar tips, and compete with the growth of columnar phase. The equiaxed grains tend to sink and settle to the ingot bottom region. The melt is dragged downwards along the columnar tip front by the sinking grains, Fig. 3(I) and



Fig. 3. Solidification sequence at I, II, III, corresponding to 280, 1880 and 7900 s. Both f_c and f_e are shown in grey scale. The velocity of the melt (\vec{u}_{ℓ}) is shown together with f_c (a), while the velocity of the equiaxed crystals (\vec{u}_e) is shown with f_e (b). Some isolines of volume fraction of phases are marked, indicating the columnar tip front ($f_c = 10^{-3}$), equiaxed packing bound ($f_e = 0.38$), and the mushy region. At 7900 s, zoomed views of the velocities in the mushy region are shown.



Fig. 4. Final segregation distribution. The segregation index, $c_{\text{mix}}^{\text{index}} = 100 \times (c_{\text{mix}} - c_0)/c_0$, is used to evaluate the macrosegregation, where c_{mix} is the local mixture concentration among the existing metal phases (equiaxed, columnar and remaining eutectic), i.e. $c_{\text{mix}} = (f_\ell \rho_\ell c_\ell + f_e \rho_e c_e + f_c \rho_c c_c)/(f_\ell \rho_\ell + f_e \rho_e + f_c \rho_c c_c)$.

(II). The sinking grains together with the downward melt flow along the columnar tip front induce a rising melt flow in the middle of the ingot. In turn, this rising flow of the melt tends to bring the equiaxed phase into the ingot center region, Fig. 3(I-b) and (II-b), but most of the equiaxed phase will settle in the bottom of the ingot. Thermo-solutal convection contributes to the interdendritic flow and global melt flow in the bulk. Both \vec{u}_{ℓ} and \vec{u}_{e} fields are unstable and non-axisymmetric. As the flow of the melt and motion of the equiaxed grains are fully coupled with other transport phenomena (energy, species and mass), the instability of the flow patterns will directly influence the solidification sequence. Sedimentation of equiaxed crystals in the bottom region will cause the volume fraction of the equiaxed phase to increase quickly. As $f_e^{\text{Env}} (=f_e|f_{\text{si}})$ reaches the packing limit (0.637), the equiaxed crystals will form a rigid solid network and stop moving. Melt flow through the packed equiaxed crystals is still possible, but it will gradually slow down by the decreasing permeability with the further solidification. It is also seen in Fig. 3(II) that the progress of the columnar tip front, as indicated by the isoline of $f_c=10^{-3}$, is also stopped by the accumulation of equiaxed phase at the bottom. As $f_e^{\text{Env}} (=f_e|f_{\text{si}})$ in the lower part is high enough (larger than the so-called mechanical blocking limit of 0.49), the columnar-to-equiaxed transition (CET) occurs. In the upper part of the ingot, the columnar primary dendrite tips can continue to grow, as no sufficient equiaxed crystals exist in front of them.

At the late stage of solidification when the columnar tip fronts meet at the casting center, see inset figures of Fig. 3(III), a narrow 'V' shape of mushy zone develops. Both the motion of equiaxed crystals and the melt flow act in a same direction, i.e. towards the bottom of the mushy zone, because the solidification shrinkage in the bottom mushy region needs to be fed. The magnitude of velocities of both melt flow and crystal motion is quite small. The amount of the equiaxed phase is also quite small.

The flow and crystal sedimentation are the key for understanding the formation of macrosegregation, and they will be analyzed in Section 3.3. The final segregation pattern is shown in Fig. 4. A large concentrated positive segregation area just below the top shrinkage cavity is predicted. A cone-shape negative segregation zone is found in the bottom region, which coincides with the packed zone of equiaxed phase. A striking feature of the modeling result of Fig. 4 is the positive segregation pattern in the middle radius region and an A-shape segregation band in the vertical sections. This positive A-shape segregation band starts from the bottom corners, develops slightly above the packed equiaxed zone, and extends to the upper part of the ingot. If we compare this numerically-predicted A-shape segregation band with the lower part 'sedimentation induced A-segregates' of the experiment (Fig. 1(a)), we see that they form a similar pattern, but the channels of the A-segregates were observed in the upper part and near the middle-radius region, while the numerical simulation shows a dispersed positive segregation in the corresponding region. As we have learnt previously [36,46–49], to model channel segregation a high grid resolution (mesh size less than ~mm) is required. Here a relatively coarse grid (18 mm) is used for the calculation.

Note that the nucleation parameters, together with the equiaxed dendritic morphological parameter (f_{si}), are not available in advance. They are difficult to determine experimentally. Here a numerical parameter study was performed, targeting an experimentally reported segregation pattern (Fig. 1) [1]. The calculated segregation pattern (Fig. 4) agrees qualitatively with the experiment (Fig. 1(a)). A quantitative comparison of the segregation distribution along the centerline between simulation and experiment (Fig. 5) is made and a reasonable agreement is achieved as well. Further discussion is made in Section 4.



Fig. 5. Comparison of centerline segregation (c_{mix}^{index}) between simulation and experiment.



Fig. 6. Formation of shrinkage cavity. The volume as filled by metal phases $(\ell -, e_-, c_-)$ is shown in color, as scaled by f_ℓ (red for full liquid melt; blue for full solid). The volume between the initial and actual melt levels is filled with liquid slag, i.e. the formed shrinkage cavity. The velocity field of the slag phase (\tilde{u}_g) on a vertical symmetry plane is also shown. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

The formation of the shrinkage cavity is shown in Fig. 6. With the Eulerian approach, no sharp interface between the covering liquid slag and steel melt can be distinguished. The volume element which includes liquid slag-metal interface is occupied by both slag and metal phases whose volume fractions sum up to one. Therefore, the free surface, i.e. the interface between the covering liquid slag and metal phase, is recorded by the iso-surface of $f_g = 0.5$. With the progress of solidification, the forming cavity is continuously filled by the liquid slag from the 'pressure inlet'. The growth of solid shell at the top edge of the steel ingot and the gradual sink of the melt level lead to the formation of the funnel shape of cavity. The volume integral of the final (end solidification) shrinkage cavity is predicted to be 0.06 m^3 , i.e. 4.0% of the volume of the entire ingot ($V_0 = 1.5 \text{ m}^3$), which agrees with the solidification shrinkage rate of the alloy, ($\rho_s - \rho_\ell$)/ $\rho_s = 4.05\%$. The formation of the microscopic shrinkage porosity is calculated indirectly by the CBN criterion, i.e. a post-processing of the modeling result of the thermal field. The final distribution of the CBN criterion is shown in Fig. 7. The smallest CBN criterion



Fig. 7. CBN criterion for microscopic shrinkage porosity.

is located in the upper part of the casting centerline, indicating the possible position of shrinkage pores, which is confirmed by the as-cast ingot of Fig. 1(a).

3.3. Formation of macrosegregation

Formation of macrosegregation can be analyzed by the variation of the local mixture concentration c_{mix} . Combining mass and species conservation equations, we get:

$$\frac{\partial}{\partial t}\bar{\rho} = -\nabla \cdot \left(f_{\ell}\rho_{\ell}\bar{u}_{\ell}\right) - \nabla \cdot \left(f_{e}\rho_{e}\bar{u}_{e}\right),\tag{29}$$

$$\frac{\partial}{\partial t}(\bar{\rho}c_{\rm mix}) = -\nabla \cdot \left(f_{\ell}\rho_{\ell}\bar{u}_{\ell}c_{\ell}\right) - \nabla \cdot \left(f_{\rm e}\rho_{\rm e}\bar{u}_{\rm e}c_{\rm e}\right),\tag{30}$$

where $\bar{\rho}$ is the mixture density of metal phases $(f_{\ell}\rho_{\ell} + f_{e}\rho_{e} + f_{c}\rho_{c})$. With an approximation of $\bar{\rho} \approx \rho_{\ell} \approx \rho_{e} \approx \rho_{c}$, the Eq. (30) can be written as:

$$\frac{\partial}{\partial t} c_{\text{mix}} \approx (c_{\ell} - c_{e}) \nabla \cdot \left(f_{e} \vec{u}_{e} \right) - f_{\ell} \vec{u}_{\ell} \cdot \nabla c_{\ell} - f_{e} \vec{u}_{e} \cdot \nabla c_{e}.$$
(31)

The variation of c_{mix} is contributed by three terms, corresponding to three macrosegregation mechanisms during the mixed columnar-equiaxed solidification, as shown in Fig. 8.

The first term $(c_{\ell} - c_{e})\nabla \cdot (f_{e}\vec{u}_{e})$ describes the contribution of the accumulation or depletion of equiaxed phase due to motion of crystals. For an alloy element with its partition coefficient *k* less than one, $(c_{\ell} - c_{e})$ usually has a positive value. A positive value of $\nabla \cdot (f_{e}\vec{u}_{e})$ means the depletion of equiaxed phase, as shown in Fig. 8(I-a). More equiaxed phase leaves than enters the reference volume element, and the depletion of the equiaxed phase is fed by the liquid melt coming from its surroundings. In this case c_{mix} increases, and a positive segregation forms. In another words, the replacement of the solute-lean equiaxed phase by the solute-rich melt leads to the formation of positive macrosegregation. In the opposite case, a negative value of $\nabla \cdot (f_{e}\vec{u}_{e})$, i.e. accumulation of equiaxed phase due to motion of crystals and squeezing the liquid melt out of the reference volume element, as shown in Fig. 8(II-a), would lead to a decrease of c_{mix} , i.e. the negative segregation.

The second term $-f_{\ell}\vec{u}_{\ell} \cdot \nabla c_{\ell}$ describes the contribution of the interdendritic melt flow through the stationary mushy zone (columnar dendrite region or packed equiaxed network) to the formation of macrosegregation. Referring to a reference volume element, when the mass of solute being brought into the volume element by the flow is different from the mass of solute being brought out of the volume element, macrosegregation occurs. Normally, a liquid concentration gradient, ∇c_{ℓ} , exists in the growing mushy zone. As shown in Fig. 8(I-b), a positive value of the term $-f_{\ell}\vec{u}_{\ell} \cdot \nabla c_{\ell}$, i.e. the melt flows in the direction against the direction of ∇c_{ℓ} , leads to the formation of positive segregation. In the opposite case, as shown in Fig. 8(II-b), a negative value of the term $-f_{\ell}\vec{u}_{\ell} \cdot \nabla c_{\ell}$, i.e. the melt flows in the same direction of ∇c_{ℓ} , leads to the formation of negative segregation.

The third term $-f_e \vec{u}_e \cdot \nabla c_e$ describes the transport of equiaxed phase, which has a concentration gradient ∇c_e (equiaxed crystals entering the volume element have different concentration from those leaving the volume element). As shown in Fig. 8(I-c), the term $-f_e \vec{u}_e \cdot \nabla c_e$ has a positive value, i.e. the equiaxed crystals entering the reference volume element have higher concentration than those leaving the volume element, and hence it leads to the formation of positive segregation. In the opposite case, as shown in Fig. 8(II-c), the term $-f_e \vec{u}_e \cdot \nabla c_e$ has a negative value, leading to the formation of negative segregation.

The above theory is applied to study the macrosegregation in the steel ingot. As examples, two types of segregation are analyzed: one is the bottom negative segregation and the other is the A-shape segregation band in the lower part of the ingot. The evolution sequence of $c_{\text{mix}}^{\text{index}}$, $\partial c_{\text{mix}}/\partial t$, and the other three contributing terms of Eq. (31) is shown in Fig. 9.



Fig. 8. Schematic of macrosegregation mechanisms during mixed columnar-equiaxed solidification.





Fig. 9. Evolution of the macrosegregation near the bottom of the ingot in Zoom 1 (Fig. 4). (a) Segregation index $c_{mix}^{index} = 100 \times (c_{mix} - c_0)/c_0$ is shown with color scale, overlaid with vectors of the melt velocity (black) and the motion of equiaxed phase (white); (b) The variation of the mixture concentration $\partial c_{mix}/\partial t$; (c)-(e) Maps of three contributing terms $(c_{\ell} - c_e)\nabla \cdot (f_e u_e), -f_\ell u_\ell \cdot \nabla c_\ell, -f_e u_e \cdot \nabla c_e$. (b)-(e) share the same color scale (-5.0~+5.0×10⁻⁶ s⁻¹), and three isolines of phase fraction $(f_c = 10^{-3}, 0.5 \text{ and } f_e = 0.38)$ are also shown to indicate different phase regions. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

The bottom negative segregation (Fig. 9(a)) develops in the region near the equiaxed phase packing border, i.e. slightly above the isoline of $f_e = 0.38$ where $\partial c_{\text{mix}}/\partial t$ has negative value (Fig. 9(b)). It is mainly due to the contribution of the first term $(c_{\ell} - c_e)\nabla \cdot (f_e \hat{u}_e)$, as seen in Fig. 9(c), although the positive value of the second term $-f_{\ell}\hat{u}_{\ell} \cdot \nabla c_{\ell}$ (Fig. 9(d)) can partially compensate the first term. The contribution of the third term $-f_e \hat{u}_e \cdot \nabla c_e$ (Fig. 9(e)) is negligible. It can be concluded that accumulation of the equiaxed phase at the bottom region due to the crystal sedimentation is the main mechanism for the bottom negative segregation. With the progress of solidification, a cone-shape is developed, taking the shape of the sediment equiaxed zone.

The A-shape segregation band (Fig. 9(a)) develops in the columnar structure region between isolines of $f_c = 10^{-3}$ and 0.5, within the mushy zone and some distance above the bottom equiaxed packing border, as shown with the yellow mark (as pointed by white arrow) of the term $\partial c_{\text{mix}}/\partial t$ in Fig. 9(b). This yellow mark is the outcome of the competition between the first and the second terms, as seen in Fig. 9(c) of another yellow mark and in Fig. 9(d) of the blue mark. The contribution of the third term is negligible. Actually, the yellow mark of $\partial c_{mix}/\partial t$ in Fig. 9(b) comes from the balance of $(c_{\ell} - c_{e})\nabla \cdot (f_{e}\overline{u}_{e})$ and $-f_{\ell}\vec{u}_{\ell} \cdot \nabla c_{\ell}$, but the term $(c_{\ell} - c_{e})\nabla \cdot (f_{e}\vec{u}_{e})$ overwhelms the term of $-f_{\ell}\vec{u}_{\ell} \cdot \nabla c_{\ell}$. A positive value of $(c_{\ell} - c_{e})\nabla \cdot (f_{e}\vec{u}_{e})$, yellow mark in Fig. 9(c), means that the depletion of the equiaxed phase locally, and volume of the leaving equiaxed phase is compensated by the liquid melt. This effect may be difficult to observe from the velocity fields, as the variations of the melt flow and the velocity of equiaxed phase are quite small. The above analysis suggests that the formation of the A-shape segregation band is related to the motion of equiaxed phase: some equiaxed crystals leave or the motion of the equiaxed crystals accelerates at a certain region (the yellow mark as pointed by the white arrow). The above hypothesis is different from our previous knowledge about the formation of channel segregation in the case of pure columnar solidification (no equiaxed phase): the channel originates from the mush destabilization due to the melt flow at the columnar tip front and grows gradually due to the flow-solidification interaction in the mushy zone [47,48,50,51]. The current modeling results for the mixed columnar-equiaxed solidification imply that the motion of equiaxed phase may lead to the formation of an A-shape segregation band. Further discussions are made in following section.

4. Discussion

The ability of the three-phase mixed columnar-equiaxed model [34,35,38] to calculate macrosegregation has been progressively evaluated against ingots of different size [46,52,53] and benchmark castings in laboratory [47,48]. Ignorance of the formation of shrinkage cavity by the previous model was recognized as an error source for macrosegregation calculation. The extension of the three-phase model by considering an additional phase (gas or liquid slag phase) for the formation of shrinkage cavity is to overcome the above drawback, while the other features of the model were retained. Recently, we have investigated the influence of the solidification shrinkage on the formation of macrosegregation on a 2.45 tons ingot, and demonstrated the importance and the necessity to consider the effect of formation of the shrinkage cavity [16]. The calculated macrosegregation result approaches more closely to the reality when shrinkage is considered.

The calculation of the 10.5-tons steel ingot in the current paper for both shrinkage cavity and macrosegregation shows satisfied qualitative agreement with the experiment. The quantitative comparison of the centerline segregation between calculation and experiment shows also reasonable agreement. Actually, further calculations for 2.45, 3.3 and 25 tons steel ingots were made by using the same four-phase model, and similar agreement between simulations and experiments was obtained. For conciseness, simulation results of those ingots are not presented here.

The calculated shrinkage cavity in Fig. 7 is quite similar to that of the as-cast ingot of Fig. 1(a). The difference between them is that the experimental one is more 'V'-shaped and conic, while the calculated one looks rather parabolic. Reasons for this difference can be understood as follows. Firstly, the model for the treatment of the new phase (gas or liquid slag), especially regarding to its interactions with other metal phases, is not sufficiently precise. Secondly, the physical parameters for the shrinkage (density difference between liquid melt and solid phases, and density variation with the temperature and concentration) are not accurate. Thirdly, the thermal boundary condition, especially in the hot top region, is not properly described.

A concept of "equiaxed grain envelope" is employed to treat the dendritic morphology of equiaxed crystals. A parameter describing the solid fraction inside the grain envelope, f_{si} , is needed, but it is unknown in advance. In order to understand the sensitivity of the modeling result of macrosegregation to the pre-assumed f_{si} , a parameter study by varying f_{si} from 0.5 to 0.9 was made, and the segregation profiles along the centerline of the 10.5 tons ingot are plotted in Fig. 10. With the increase of f_{si} , equiaxed crystals are more massive inside the grain envelope; hence they are more densely packed in the bottom and the negative segregation in the bottom cone-shape equiaxed zone becomes more intensive. Another interesting finding is that f_{si} influences the global solidification sequence as well. It modifies the global structure distribution between columnar and equiaxed regions. When f_{si} is large enough, e.g. ≥ 0.7 , due to the enhanced sedimentation of equiaxed crystals and densely-packed equiaxed region in the bottom, a so-called mini-ingotism phenomenon [54] occurs in the upper part of the ingot. At the late stage of solidification in the upper part of the ingot (at the height of ca. 1.6 m) columnar tip fronts meet at the casting center before the lower part (at the height of ca. 1.4 m) is fully solidified. Further solidification of the lower part behaves like a mini-ingot. This kind phenomenon was investigated previously [46], and it induces a typical 'S'-shape segregation curve as what we see in Fig. 10 for the curves of $f_{si} = 0.7$ and 0.9. No such 'S'-shape curve, i.e. no mini-ingotism phenomenon, is seen for cases of $f_{si} = 0.5$ and 0.6. The experimental measurement of the centerline segregation



Fig. 10. Influence of f_{si} on the centerline macrosegregation distribution.

(6 points, being fitted by piecewise linear) is also shown in Fig. 10. One has to say that no calculated curve fits ideally to the experimental result. From the experimental curve, together with the Sulfur print of Fig. 1(a), there seems no clear evidence of mini-ingotism in this ingot. Therefore, a value of $f_{si} = 0.6$ is recommended for simulation of this ingot. Note that more enhanced models for dendritic solidification are also available [29,55,56], where f_{si} is explicitly calculated, but calculation costs are dramatically increased as additional interdendritic liquid phase must be considered. Therefore, they are not recommended for calculating industry ingots of such tonnage.

Notice that in Fig. 1(a) we marked the A-segregates in the lower part of the ingot as 'sedimentation induced Asegregates', which seems to appear differently from the A-segregates in the upper part of the ingot. The so-called 'sedimentation induced A-segregates' are thick positively segregation region, which started from the ingot corner and tended to appear in the form of a truncated hollow cone in parallel to the columnar-to-equiaxed transition area, while the A-segregates in the upper part of the ingot include many thin and curved channels (maybe laminar structure) of segregation and they are located in the middle radius region of the ingot where columnar structure dominates. Historically, different terms were used to describe the 'sedimentation induced A-segregates', e.g. rope-like A-segregates [57,58], streak-type inverted-V segregation [59], but they were generally classified as A-segregates without distinction from other type of A-segregates. We think that they occur by different mechanisms. The sedimentation induced A-segregates, corresponding to the A-shape segregation band (Fig. 4), are evidently induced by the motion/sedimentation of equiaxed crystals. As shown in Fig. 9, in the region just above the junction point between columnar tip front and the packed equiaxed zone, some equiaxed crystals leave the columnar tip front region (or the motion of equiaxed crystals accelerates), causing a positive value of the term $(c_{\ell} - c_{e})\nabla \cdot (f_{e}u_{e})$. A positive segregation band develops there gradually. Actually, in 1960s, Blank and Pickering [57] observed the rope-like A-segregates in steel ingots, and they described that "they (the rope-like A-segregates) occur more or less at the interface between the columnar and central equiaxed dendrites where it might be expected that dendrites can nucleate in metal ahead of the main columnar dendrite interface; many of the existing theories for the formation of A-segregates do not satisfactorily explain these features." Therefore, they inferred that the settling equiaxed dendrites along the columnar dendrite interface (tip front) leads to a small pointed accretions or piles of dendrites at the junction with the columnar dendrites, forming a gap between the piles of equiaxed dendrites and the columnar dendrites. The falling equiaxed dendrites drag the solute-enriched melt with them, and the solute-enriched melt will be entrapped in the columnar-equiaxed gap, forming the rope-like positive segregation zone. Almost at the same time, Ohno observed the similar phenomenon in his ammonium chloride water experiment [59]: "The equiaxed crystals settle in the center of the mold, and form a valley. The soluteconcentrated zone is trapped between the solid shell (columnar zone) and equiaxed zone. Because the connection between the solid shell and the equiaxed crystal zone is considered to be very weak, the equiaxed crystals zone can separate from the solid shell and can be pulled into the bulk liquid in the valley forming tears in the equiaxed crystal zone when the lower part of the equiaxed crystal zone settles. The tears finally form streak-type inverted-V segregation." The explanation of Blank and Pickering [57] and that of Ohno [59] are not the same as what we found in Fig. 9, but their works provided some clues that the formation of the A-shape segregation band, namely the sedimentation induced A-segregates, is related to the motion and sedimentation of equiaxed crystals.

Another fact from Fig. 1(a) is that some middle radius A-segregates (thin channels) are simply the extension of the sedimentation induced A-segregates. This is also observed in many other ingots [1,57]. It means that the crystal sedimentation induced A-shape segregation band presents a source of the A-segregates, or provides a favorite position to initialize the A-segregates in the middle radius region of the ingot. We still believe that most A-segregates in the middle radius region of the ingot originate from the mush destabilization in the columnar zone due to the thermo-solutal convection, but the A-shape segregation band might provide a favored location for the mush destabilization in the vicinity of the columnar tip front. Further dedicated experiment should be carried out to verify it.

Finally, it should be noted that the calculation cost increases with the number of phases as considered by the model and with the grid resolution (number of volume elements). The mesh size of 18 mm as used for the current ingot is rather coarse. Nevertheless, each calculation takes a very long time (2.5 weeks). As shown in Fig. 1(a), many channels of A-segregates in the upper part middle radius region of the ingot are seen from the real casting, but the simulation result (Fig. 4) shows only a dispersed positive segregation in the corresponding region. Obviously, fine details of A-segregates are missing by the model. Previous study [46] indicated that the number of the A-segregates, as calculated by the model, increases with the grid resolution. A grid size of order mm is required to resolve the channels. Unfortunately, due to the limitation of the current computer hardware we are not able to resolve the fine details of the A-segregates in such a heavy industry ingot.

5. Conclusion

This work has extended a previous 3-phase mixed columnar–equiaxed solidification model [34–36] to treat the formation of shrinkage cavity by including an additional phase, i.e. gas phase or covering liquid slag. An industry steel ingot (10.5 tons) was calculated to demonstrate key features of the new model. They are the progress of columnar tip front and growth of columnar tree trunks, the nucleation and growth of equiaxed grains, the melt flow and equiaxed crystal sedimentation, the transport of the solute species and induced macrosegregation, the shrinkage cavity, the interaction or competition between growing columnar and equiaxed phases and the occurrence of columnar to equiaxed transition (CET).

Experimental results for the 10.5 tons ingot were available: profile of the shrinkage cavity, Sulfur print and chemical analysis of a vertical section [1]. It is found that the calculated macrosegregation pattern, including top concentrated positive segregation zone below shrinkage cavity (pipe), bottom negative segregation zone, and A-shape segregation band, shows qualitative agreement with the Sulfur print. The quantitative comparison of the centerline segregation between calculation and experiment shows also reasonable agreement. Similar shape of shrinkage cavity (pipe) is calculated to that of experiment. The microscopic porosity, as modeled by CBN criterion [22], gives good indication for the potential occurrence of shrinkage pores as observed from experiment. Actually, ingots of 2.45, 3.3 and 25 tons were also calculated and compared with analyses of the as-cast ingots, and similar agreement was obtained. Those results will be presented in future.

One drawback of the model is the high calculation cost. As a compromise, a relatively coarse grid (\sim cm) was used. It allows calculating the global distribution pattern of macrosegregation, but it does not allow the resolution of their fine details. For example, we can only predict the sedimentation induced A-shape segregation band, but channels of A-segregates in the upper part and near the middle radius region of the ingot as observed from some experiments cannot be solved. Previous modeling works [47–49] on benchmark castings at the laboratory scale have demonstrated the ability for calculating the channel segregates by use of extreme fine grid (\sim mm). However, the use of such fine grid for heavy industry ingots is out of capacity of the current computer hardware.

Finally, a new hypothesis for the initialization of A-segregates is proposed: the motion of equiaxed phase and its interaction with the melt flow in the vicinity of growing columnar tip front lead to formation of an A-shape segregation band starting from the ingot corner just above the columnar-to-equiaxed transition area. This A-segregation band might provide a favored location for the initialization of A-segregates. Some works from the 1960s provided some clues to support this hypothesis, but further dedicated experiment should be carried out to verify it.

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