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Numerical model of solidification process in binary Al-Fe alloy under centrifugal casting①

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[Abstract] During the solidification process of binary Al-Fe alloy under centrifugal casting, the primary phase of Al_3Fe migrates along the radius because of the density difference between the primary phase and the liquid alloy. Therefore the temperature and concentration field are affected significantly by both the fluid flow and the solid phase migration. In order to take this factor into consideration, a two-phase flow numerical model has been established in column coordinate to depict the solidification process of Al-Fe alloy under centrifugal casting according to the feature that there exists the solid phase migration during the process. Thus the solidification process of Al-Fe alloy under centrifugal casting has been described much more pertinently.

[Key words] centrifugal casting; Al-Fe alloy; two phase flow; numerical model
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1 INTRODUCTION

The solidification process of binary Al-Fe alloy under centrifugal casting is controlled by the mass, momentum, heat and chemical species transportation. Therefore, it is an important means to know the microstructure and the segregation of binary Al-Fe alloy under centrifugal casting by numerical model that depicts the solidification process of binary Al-Fe alloy under centrifugal casting. At present, several models of the solidification of centrifugal cast have already been established. ZHANG et al[1] established a numerical model which described the heat transmission process of centrifugal SHS ceramics liner tube based on Fourier heat transmission equation. But this model only described the process separately and ignored the interaction among the three transmission processes. JIAO et al[2] put forward a comprehensive numerical model for the solidification process of electromagnetic centrifugal casting, which depicted the three transmission effects under the condition of fluid flow. However, during the solidification process, both solid and liquid phases exist simultaneously and heat transmission parameters vary with different phases, this model didn't consider these facts respectively. HAN et al[3] proposed a numerical model with a source item to describe the solidification process of electromagnetic centrifugal casting, which took the variation of the thermophysical property parameters with temperature into account. But the features that solid and liquid phases coexist during the solidification process have not been embodied yet. Further more, the species transmission process was ignored in these two models, which resulted in the ignorance of the effect of species transmission on the process of heat and momentum transmission. Moreover, the mass of molten metal per unit volume should vary with the phase transformation process, while this variation was neglected in the continuous equations of these models. From this point of view, the above models were not definite enough in depicting those solidification systems.

In addition, there is an important difference between the solidification process of Al-Fe alloy centrifugal casts and that of other centrifugal casts, that is, because the primary phase in Al-Fe alloy migrates along the radius due to the density difference between the primary phase and the liquid alloy[4~8], the distribution of temperature and composition is affected significantly in the solidification process owing to the solid phase migration. But the nucleation and growth of the primary phase and the viscosity of liquid alloy vary with temperature and composition, which reacts on the solid phase migration and alters the migration velocity. So the effect of solid phase migration on temperature and composition field during the solidification process should be considered in this numerical model. At the beginning of 1990s, Fanesan et al[9] and Ni et al[10] proposed two-phase flow numerical models successively. But during the solution of the models, the solid phase velocity was assumed to be zero or the same as that of the liquid phase due to the lack of solution premise, so the solid phase velocity has not been solved practically.

In this paper, the conservation equations controlling the mass, momentum, energy and species transportation process have been established in column coordinate system under the conditions of two

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phases flow according to the features of the solidification process in binary Al-Fe alloy under centrifugal casting. Besides those equations, an equation governing the solid phase migration has also been proposed, which enables the solution of solid phase velocity. Thereby, the solidification process in binary Al-Fe alloy under centrifugal casting has been described quantitatively.

2 METHEMATICAL MODEL

The experiment of Al-Fe alloy centrifugal casting has been performed on a vertical centrifugal casting machine. A numerical model is established according to the features of the solidification system. Assumptions invoked in the development of the numerical model include:

1) The liquid metal rotates at the same speed with the mold soon after it fills in the mold. That is to say, there is no relative movement among the mold, solid phase and liquid phase in the direction of θ, i.e. $v_{l\theta} = v_{s\theta} = v_\theta$. On this basic premise, the flow of liquid metal is only caused by the heat diffusion, the solid phase contraction and the agitation of solid phase migration.

2) During the solidification process, the effect of centrifugal force is more significant than that of gravity. Thus the vertical velocities of solid phase particles relative to that of liquid phase can be ignored. Then it is assumed that the velocities of solid phase particles and liquid metal in the direction of the axis are the same.

Since the centrifugal cast is in a cylindrical shape and is symmetrical about the rotation axis, thus investigation is focused on the transverse section of the casting along the rotation axis in a column coordinate system, which efficiently overcomes the intrinsic demerit of the former solidification simulation system in rectangular coordinate system that the result of subdivision is not symmetrical and the simulation results distorts partially[11]. During the solidification, the temperature fields of the mold and the casting are symmetrical about the rotation axis, therefore, the origin of the coordinate is set on the center of bottom of the solidification system.

A minute element is taken from the solidification system. The spatial dimension of the minute element is Δr, Δz, $\Delta\theta$. The volume of it is $\Delta r \cdot \Delta z \cdot r\Delta\theta$. The volume of minute element is large enough compared with the micro-interfacial structure, while it is much smaller than that of the whole solidification system.

2.1 Energy conservation equation

For every minute element the energy conservation equation can be expressed as

Heat increment of a minute element in Δt time = Net heat increment arising out of liquid phase flow + Net heat increment arising out of solid phase flow + Net heat increment arising out of heat diffusion + The release of latent heat

Therefore, the differential equation of heat transmission during the solidification can be expressed as

$$\begin{aligned}
&\frac{\partial}{\partial t}\left[(f_s\rho_s C_{ps} + f_l\rho_l C_{pl})T\right] + \\
&\frac{1}{r}\frac{\partial}{\partial r}\left[(f_s\rho_s v_{sr} C_{ps} + f_l\rho_l v_{lr} C_{pl})T\cdot r\right] + \\
&\frac{1}{r}\frac{\partial}{\partial\theta}\left[(f_s\rho_s v_\theta C_{ps} + f_l\rho_l v_\theta C_{pl})T\right] + \\
&\frac{\partial}{\partial z}\left[(f_s\rho_s v_{sz} C_{ps} + f_l\rho_l v_{lz} C_{pl})T\right] = \\
&\frac{1}{r}\frac{\partial}{\partial r}\left[(f_s\lambda_s + f_l\lambda_l)\frac{\partial T}{\partial r}\cdot r\right] + \\
&\frac{1}{r^2}\frac{\partial}{\partial\theta}\left[(f_s\lambda_s + f_l\lambda_l)\frac{\partial T}{\partial\theta}\right] + \\
&\frac{\partial}{\partial z}\left[(f_s\lambda_s + f_l\lambda_l)\frac{\partial T}{\partial z}\right] + L\cdot\frac{\partial(f_{ss}\rho_s)}{\partial t}
\end{aligned} \tag{1}$$

The boundaries among casting, sand mold and permanent mold are regarded as perfect boundaries, and respectively conform to the boundary condition equations shown below.

1) The boundary between sand mold and casting

$$\lambda_c\frac{\partial T}{\partial r} = \lambda_{san}\frac{\partial T}{\partial r} \tag{2}$$

where $\lambda_c = f_s\lambda_s + f_l\lambda_l$.

2) The boundary between sand and permanent mold

$$\lambda_{san}\frac{\partial T}{\partial r} = \lambda_{met}\frac{\partial T}{\partial r} \tag{3}$$

3) The boundary between permanent mold and casting

$$\lambda_c\frac{\partial T}{\partial r} = \lambda_{met}\frac{\partial T}{\partial r} \tag{4}$$

The heat in mold and casting surface which contacts with air eliminates primarily by convection and radiation. The heat conduction at these boundaries conforms to the equations shown below.

1) At the inner surface of casting

$$-\lambda_c\frac{\partial T}{\partial r} = h_1(T_{am} - T) + F\varepsilon_{Al}\sigma(T_{am}^4 - T^4) \tag{5}$$

2) At the outer surface of permanent mold

$$-q = h_2(T_{am} - T_m) + F\varepsilon_{Fe}\sigma(T_{am}^4 - T_m^4) \tag{6}$$

where it is presumed that $T_m\big|_{t=0} = T_0$ and that $T\big|_{t=0} = T_p$.

2.2 Species conservation equation

The conservation equation about the species transport process can be expressed as

The average composition increment of a minute element in Δt time =

Net species increment arising out of liquid phase flow +

Net species increment arising out of solid phase flow +

Net species increment arising out of solute diffusion

Thus the species conservation in the form of differential equation can be expressed as

$$\frac{\partial}{\partial t}(f_s\rho_s c_s + f_l\rho_l c_l) + \frac{1}{r}\frac{\partial}{\partial r}\left[r(f_s\rho_s v_{sr}c_s + f_l\rho_l v_{lr}c_l)\right] + \frac{1}{r}\frac{\partial}{\partial \theta}(f_s\rho_s v_{\theta}c_s + f_l\rho_l v_{\theta}c_l) + \frac{\partial}{\partial z}(f_s\rho_s v_{sz}c_s + f_l\rho_l v_{lz}c_l) = \frac{1}{r}\frac{\partial}{\partial r}\left[r\left(f_s\rho_s D_s\frac{\partial c_s}{\partial r} + f_l\rho_l D_l\frac{\partial c_l}{\partial r}\right)\right] + \frac{1}{r^2}\frac{\partial}{\partial \theta}\left[f_s\rho_s D_s\frac{\partial c_s}{\partial \theta} + f_l\rho_l D_l\frac{\partial c_l}{\partial \theta}\right] + \frac{\partial}{\partial z}\left[f_s\rho_s D_s\frac{\partial c_s}{\partial z} + f_l\rho_l D_l\frac{\partial c_l}{\partial z}\right] \quad (7)$$

Species transport during the solidification proceeds in an isolated system because there is no solute volatilization and physical chemistry reaction such as oxidization during the solidification of the alloy. In this case, the species transport density is zero at every boundary. The gravity segregation can be ignored because the liquid alloy is agitated before pouring. The initial state of species distribution can be regarded as uniform distribution, that is $c|_{t=0} = c_0$.

2.3 Solid phase migration equation

There are two forces acting on every solid phase particles during the solidification process in binary Al-Fe alloy under centrifugal casting. One is the dynamic force along the radius caused by centrifugal force field, the other is the viscous resistance coming from liquid phase during the motion of the particles. Therefore, according to Newton's second law, the solid phase migration equation can be expressed as follows[12]

$$\frac{4}{3}(\rho_s - \rho_l)\cdot\pi R_p^3\omega^2 r - 6\pi R_p v_{sr}\eta = \frac{4}{3}\frac{dv_{sr}}{dt}\cdot\rho_s\pi R_p^3 \quad (8)$$

where the equivalent radius of the particle $R_p = \sqrt[3]{3V_p/4\pi}$, where V_p is the volume of the solid phase particle.

2.4 Mass conservation equation

The exchange of mass between minute element and environment is mainly aroused by the fluid flow and solid phase migration. Thus the mass conservation equation can be expressed as

The mass increment of a minute element in Δt time =

Mass difference arising out of liquid phase flow +

Mass difference arising out of solid phase migration

Thus the mass conservation equation in the multi-phase region can be expressed as

$$\frac{\partial}{\partial t}(f_l\rho_l + f_s\rho_s) = -\frac{1}{r}\frac{\partial}{\partial r}\left[r(f_l\rho_l v_{lr} + f_s\rho_s v_{sr})\right] - \frac{1}{r}\frac{\partial}{\partial \theta}(f_l\rho_l v_{\theta} + f_s\rho_s v_{\theta}) - \frac{\partial}{\partial z}(f_l\rho_l v_{lz} + f_s\rho_s v_{sz}) \quad (9)$$

2.5 Momentum conservation equation

The momentum conservation equation of the solidification system can be expressed as

The momentum accumulation of a minute element in Δt time =

Momentum increment arising out of liquid phase flow +

Momentum increment arising out of solid phase migration +

Impulse arising out of the body force acting on the minute element +

Impulse arising out of the Darcy resistance acting on the minute element +

Impulse arising out of the surface force acting on the minute element

Thus the momentum conservation equation in a space coordinates system can be expressed as

1) In the direction of r

$$\frac{\partial}{\partial t}(f_l\rho_l v_{lr} + f_s\rho_s v_{sr}) + \frac{1}{r}\frac{\partial}{\partial r}\left[r(f_l\rho_l v_{lr}v_{lr} + f_s\rho_s v_{sr}v_{sr})\right] + \frac{1}{r}\frac{\partial}{\partial \theta}(f_l\rho_l v_{\theta}v_{lr} + f_s\rho_s v_{\theta}v_{sr}) + \frac{\partial}{\partial z}(f_l\rho_l v_{lz}v_{lr} + f_s\rho_s v_{sz}v_{sr}) = 4\pi^2 n^2 r(f_l\rho_l + f_s\rho_s) - \left[\frac{1}{r}\frac{\partial(r\tau_{rr})}{\partial r} + \frac{1}{r}\frac{\partial \tau_{\theta r}}{\partial \theta} + \frac{\partial \tau_{zr}}{\partial z}\right] -$$

$$\frac{\partial p}{\partial r} - \frac{\mu}{k_r} f_l^2 (v_{lr} - v_{sr}) \tag{10}$$

2) In the direction of θ

$$\frac{\partial}{\partial t}(f_l\rho_l v_\theta + f_s\rho_s v_\theta) + \frac{1}{r}\frac{\partial}{\partial r}\left[r(f_l\rho_l v_{lr}v_\theta + f_s\rho_s v_{sr}v_\theta)\right] + \frac{1}{r}\frac{\partial}{\partial\theta}\left[(f_l\rho_l + f_s\rho_s)v_\theta v_\theta\right] + \frac{\partial}{\partial z}\left[f_l\rho_l v_{lz}v_\theta + f_s\rho_s v_{sz}v_\theta\right] = -\left[\frac{1}{r}\frac{\partial(r\tau_{r\theta})}{\partial r} + \frac{1}{r}\frac{\partial\tau_{\theta\theta}}{\partial\theta} + \frac{\partial\tau_{z\theta}}{\partial z}\right] - \frac{1}{r}\frac{\partial p}{\partial\theta} \tag{11}$$

3) In the direction of z

$$\frac{\partial}{\partial t}(f_l\rho_l v_{lz} + f_s\rho_s v_{sz}) + \frac{1}{r}\frac{\partial}{\partial r}\left[r(f_l\rho_l v_{lr}v_{lz} + f_s\rho_s v_{sr}v_{sz})\right] + \frac{1}{r}\frac{\partial}{\partial\theta}(f_l\rho_l v_\theta v_{lz} + f_s\rho_s v_\theta v_{sz}) + \frac{\partial}{\partial z}(f_l\rho_l v_{lz}v_{lz} + f_s\rho_s v_{sz}v_{sz}) = -(f_l\rho_l g + f_s\rho_s g) - \left[\frac{1}{r}\frac{\partial(r\tau_{rz})}{\partial r} + \frac{1}{r}\frac{\partial\tau_{\theta z}}{\partial\theta} + \frac{\partial\tau_{zz}}{\partial z}\right] - \frac{\mu}{k_z} f_l^2(v_{lz} - v_{sz}) - \frac{\partial p}{\partial z} \tag{12}$$

where

$$\tau_{rr} = \mu\left\{\frac{2}{r}\frac{\partial(rf_l v_{lr})}{\partial r} - \frac{2}{3}\left[\frac{1}{r}\frac{\partial(rf_l v_{lr})}{\partial r} + \frac{1}{r}\frac{\partial(f_l v_\theta)}{\partial\theta} + \frac{\partial(f_l v_{lz})}{\partial z}\right]\right\} \tag{13}$$

$$\tau_{\theta\theta} = \mu\left\{\frac{2}{r}\frac{\partial(f_l v_\theta)}{\partial\theta} - \frac{2}{3}\left[\frac{1}{r}\frac{\partial(rf_l v_{lr})}{\partial r} + \frac{1}{r}\frac{\partial(f_l v_\theta)}{\partial\theta} + \frac{\partial(f_l v_{lz})}{\partial z}\right]\right\} \tag{14}$$

$$\tau_{zz} = \mu\left\{2\frac{\partial(f_l v_{lz})}{\partial z} - \frac{2}{3}\left[\frac{1}{r}\frac{\partial(rf_l v_{lr})}{\partial r} + \frac{1}{r}\frac{\partial(f_l v_\theta)}{\partial\theta} + \frac{\partial(f_l v_{lz})}{\partial z}\right]\right\} \tag{15}$$

$$\tau_{r\theta} = \tau_{\theta r} = \mu\left[\frac{1}{r}\frac{\partial(f_l v_{lr})}{\partial\theta} + \frac{1}{r}\frac{\partial(rf_l v_\theta)}{\partial r}\right] \tag{16}$$

$$\tau_{rz} = \tau_{zr} = \mu\left[\frac{\partial(f_l v_{lr})}{\partial z} + \frac{1}{r}\frac{\partial(rf_l v_{lz})}{\partial r}\right] \tag{17}$$

$$\tau_{\theta z} = \tau_{z\theta} = \mu\left[\frac{\partial(f_l v_\theta)}{\partial z} + \frac{1}{r}\frac{\partial(f_l v_{lz})}{\partial\theta}\right] \tag{18}$$

2.6 Equation governing variation of solid phase fraction caused by solid phase migration

The variation of solid phase fraction during the solidification caused by solid phase migration also follows the conservation principle. Thus the variation of solid phase in any minute element can be expressed as

Solid phase fraction increment of a minute element in Δt time = Solid phase fraction flowing into the minute element in Δt time - Solid phase fraction flowing out of the minute element in Δt time

Thus the equation governing the variation of solid phase fraction caused by solid phase migration can be expressed as

$$-\frac{\partial f_{se}}{\partial t} = \frac{1}{r}\frac{\partial(rf_s v_{sr})}{\partial r} + \frac{1}{r}\frac{\partial(f_s v_\theta)}{\partial\theta} + \frac{\partial(f_s v_{sz})}{\partial z} \tag{19}$$

2.7 Supplementary equations

During the solidification process of a casting, the increment of solid phase fraction in every minute element comes from the proceeding of solidification and the solid phase migration. Therefore

$$\Delta f_s = \Delta f_{ss} + \Delta f_{se} \tag{20}$$

where Δf_{ss} —Solid phase fraction increment caused by solidification, Δf_{se} —Solid phase fraction increment caused by solid phase migration.

The solute transport during the solidification is under the control of both diffusion and convection, therefore

$$c_s = c_l K_E (1 - f_s)^{K_E - 1} \tag{21}$$

where $K_E = \dfrac{k_0}{k_0 + (1 - k_0)\exp[-(R\delta/D_s)]}$.

where δ—The thickness of diffusion boundary layer, which is about 0.01 ~ 1 mm; R—Growth rate.

The solidification processes of Al-Fe binary alloys (Al-2%Fe, Al-5%Fe, Al-10%Fe) under centrifugal casting have been comprehensively simulated based on the above mathematical model. The simulation results are identical to the experiment results. These results will be reported in other papers.

3 CONCLUSIONS

A two-phase flow mathematical model, which depicts the three transportation phenomena, has been established according to the features of the solidification process of Al-Fe alloy under centrifugal casting. The mathematical model includes mass, momentum, species and energy conservation equations. The solid phase migration equation and the equation governing the variation of solid phase fraction caused by solid phase migration have been given, which solves the problem of the solution of solid phase velocity under the condition of two phases flow. Through solving all these equations simultaneously, the physical quantities during the solidification can be calculated and the solidification process is described in quantification.

NOMENCLATURE

ρ_s — Density of solid phase, kg/m^3;

ρ_l — Density of liquid metal, kg/m^3;

R_p — Equivalent radius of solid phase particle, m;
C_{ps} — Specific heat of solid phase, J/(kg·K);
C_{pl} — Specific heat of liquid metal, J/(kg·K);
m — Mass of solid phase patricle, kg;
ω — Mold rotation speed, rad/s;
η — Viscosity of liquid metal, Pa·s;
L — Latent heat, J/kg;
T — Temperature of casting, K;
T_p — Pouring temperature, K;
T_0 — Mold preheated temperature, K;
T_{am} — Ambient temperature, K;
v_{sz} — Axial velocity of solid phase particle, m/s;
v_{sr} — Radial velocity of solid phase particle, m/s;
v_{lz} — Axial velocity of liquid metal, m/s;
v_{lr} — Radial velocity of liquid metal, m/s;
v_θ — Circumferential velocity, m/s;
f_s — Volume fraction of solid phase;
f_l — Volume fraction of liquid phase;
F — View-factor;
ε — Emissivity;
σ — Boltzmann constant;
h — Coefficient of heat convection, W/(m^{-2}·K^{-4});
λ_l — Thermal conductivity of liquid phase, W/(m^2·K);
λ_s — Thermal conductivity of solid phase, W/(m^2·K);
λ_c — Thermal conductivity of the casting, W/(m^2·K);
λ_{san} — Thermal conductivity of sand mold, W/(m^2·K);
λ_{met} — Thermal conductivity of permanent mold, W/(m^2·K);
c_l —Concentration in liquid phase;
c_s —Concentration in solid phase;
D_s —Diffusion coefficient in solid phase;
D_l —Diffusion coefficient in liquid phase;
p —Pressure of liquid phase, Pa;
τ—Shear stress, Pa;
k —Permeability;
μ—Effective viscosity;
q —Specific heat transfer rate, W/m^2.

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