Numerical Simulation of Microstructure Evolution During Alloy Solidification by Using Cellular Automaton Method

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This paper presents two and three dimensional cellular automaton (CA) based models and derived coupling models to simulate micro-scale microstructure evolution during alloy solidification. The models adopt a local solutal equilibrium approach to calculate the kinetics of the solid/liquid (SL) interface evolution, which allows the reasonable calculation of crystal growth from the initial unstable stage to the steady-state stage without the need of a kinetic parameter. Dendrite morphologies with various crystallographic orientations and well developed side branches in two and three dimensions can be successfully simulated by the proposed models. In conjunction with the lattice Boltzmann method (LBM), adopted for numerically solving fluid flow and solutal transport, a coupling model was derived to simulate the solutal dendrite growth in the presence of melt convection. The 2D model was extended to the multiphase system for the simulation of divorced eutectic solidification of spheroidal graphite (SG) cast iron. The quantitative capabilities of the models are addressed by comparing simulations to analytical predictions and experimental data.

KEY WORDS: solidification; microstructure simulation; cellular automaton; lattice Boltzmann method.

1. Introduction

During the last two decades, considerable advances have been achieved in the numerical modeling of microstructure evolution in solidification. Simulation provides detailed information on the interactions between transport phenomena and phase transition, offers insights into the underlying physics of microstructure formation, and thus improves our fundamental understanding of the mechanisms of solidification. This will contribute to alloy design, the improvement of current solidification technologies, and the development of new processes.

The cellular automaton (CA) technique can handle complex topology changes in two and three dimensions. It has the attractive advantages such as simplicity of formulation and computational convenience when implemented to solve phase transition problems with an acceptable computational efficiency. It has, therefore, become a feasible approach for the modeling of microstructural evolution. Extensive efforts have been dedicated to develop various models based on the CA concept to simulate a wide variety of solidification microstructure features on the meso- and micro-scales.

The CA models were first developed for meso-scale modeling of grain growth. In 1993, Rappaz and Gandin published the classic paper to report their developed meso-scale CA model for the simulation of grain structure evolution during solidification. The model includes the physics of nucleation, growth kinetics, and crystallographic orientation. The mechanism of competitive dendrite growth is directly embedded in the CA algorithm. The model can perform the time-dependent simulation of typical equiaxed and columnar grain structures, and columnar-to-equiaxed transition (CET). Thereafter, a series of studies were reported on the simulations of grain structures formed in various casting processes by applying the meso-scale CA models. Since in the meso-scale CA models, the curvature effect and solute redistribution in solidification are not taken into account, and the dynamics of the moving SL interface is referenced only to the local temperature in the solidifying region, they are unable to describe the detailed dendrite features such as the side branches, microsegregation, and the formation of second phases (eutectic).

The work reported by Dilthey and Pavlik in 1998 marks the milestone of the CA approach for the simulation of dendritic morphology on a micro-scale. They developed a diffusion-controlled CA model for the simulation of solutal dendrites, in which the growth velocity is calculated from the complete solution of the transport equations for the solid and liquid phases, including the boundary condition of solute balance at the moving SL interface. Nastac further improved the model by incorporating the time-dependent solution of the heat transfer equation, enabling the simulation of constrained and unconstrained dendrite growth and of the columnar-to-equiaxed transition (CET). Since the velocity is calculated based on the sum of its x and y Cartesian components, the model suffers from the strong artificial anisotropy of the CA mesh.

Based on a similar methodology of the complete solution of the transport equations, Beltran-Sanchez and Stefanescu devoted their efforts to reduce the artificial anisotropy of CA square mesh and mesh dependency of CA simulation by improving the calculation of normal velocity
and trapping rules for new interface cells. The quantitative capabilities of the model were well addressed by validation of the simulation results with experimental data and the Lipton–Glicksman–Kurz (LGK) theory.

Lee and co-workers\(^{14,15}\) developed a CA-FD model in which the growth velocity is also determined by solving the solute conservation equation subject to the boundary conditions at the SL interface. The model adopts a modified decentered-square growth algorithm to generate various crystallographic orientations. Recently, the model was further developed by incorporating the solution of the Navier–Stokes equations to simulate the dendritic solidification under natural and forced convection in two and three dimensions.\(^{16}\)

The diffusion-controlled CA models\(^{10–16}\) with the assumption of solute conservation at the moving SL interface mentioned above have the merit of allowing the simulation of dendrite growth without the need of introducing a kinetic coefficient. Since the condition of solute conservation is only satisfied for steady-state growth, those CA models fail to reasonably calculate the growth velocity of the interface points undergoing unstable growth.

Building on an earlier micro-scale CA model, Zhu and Hong developed a micro-scale modified CA (MCA) model by incorporating the effects of the solute and the curvature undercoolings on the equilibrium temperature at the SL interface. The model was applied to simulate single and multi-dendritic growth in two and three dimensions.\(^{17,18}\) non-dendritic and globular microstructures formed in semisolid process,\(^{19}\) dendritic growth in the presence of forced melt convection,\(^{20,21}\) and microstructure formation in regular and irregular eutectic alloys\(^{22,23}\). The model was also extended to the ternary and quaternary alloy systems by coupling it with the thermodynamic and phase equilibrium calculation package PanEngine.\(^{24,25}\) In the MCA model, the kinetics of the moving SL interface is calculated from the analytical theories of dendrite growth or by the Gibbs–Thomson equation. In the former method, the velocity of the moving SL interface is calculated as a function of the local undercooling according to the analytical models that describe the steady-state growth of the dendrite tip. This approximation leads to mostly graphical morphologies providing only a qualitative understanding. For the latter approach, a kinetic coefficient must be properly determined for quantitative simulations.

Based on the previous efforts, Zhu and Stefanescu (ZS)\(^{26}\) proposed a solution of the kinetics of dendritic growth in the low Péclet number regime, which permits reasonable calculation of the velocity for both stable and unstable dendrite growth without the need of introducing a kinetic coefficient. The quantitative capabilities of the model were demonstrated by analytical and experimental validation. It is also able to reproduce realistic features for both equiaxed and columnar dendrites with a good computational efficiency. The model was extended to the three dimensions\(^{27}\) to the system including melt convection by incorporating the solution of the Navier–Stokes equations to simulate the dendritic solidification in two and three dimensions.\(^{16}\)

The model and the derived models. The extended multiphase model for the simulation of divorced eutectic microstructure is described in detail. Some simulation examples are presented to illustrate the capabilities of the proposed models.

2. Model Description and Numerical Algorithm

For the simulation of pure diffusive dendritic growth of binary alloys, the kinetics of dendritic growth is determined using a local composition equilibrium approach proposed by Zhu and Stefanescu (ZS).\(^{26}\) According to this approach, the evolution of the SL interface is calculated directly from the difference between the local equilibrium composition and the local actual liquid composition. The local equilibrium composition is calculated from the local temperature and weight mean curvature (\(wmc\)) that is incorporated with the effect of anisotropic surface energy, while the local actual liquid composition is obtained by numerically solving the solutal transport equation in the domain. This approach reasonably describes the dynamics of dendrite growth from the initial unstable stage to the steady-state stage without the need to introduce a kinetic parameter. To model convective dendritic growth with forced melt convection, the ZS approach for dendritic growth is incorporated with the kinetic-based lattice Boltzmann method (LBM) that describes transport phenomena by the evolution of distribution functions of moving pseudo-particles for numerically solving fluid flow and solute transport governed by both convection and diffusion. The details of the governing equations and numerical algorithms for the simulation of two dimensional (2D) and three dimensional (3D) diffusive dendritic growth and 2D convective dendritic growth can be found elsewhere.\(^{26–28}\) The model for 2D dendritic growth was extended to the multiphase system for the simulation of divorced eutectic solidification of SG cast iron. The governing equations and numerical algorithms to calculate the solute and temperature fields, the interface curvature, the crystallographic anisotropy, and the kinetics of the growth of primary austenite dendrite and SG are described subsequently.

The present model only considers the solidification of hypoeutectic SG cast iron, and the growth of SG in the liquid is ignored. It is assumed that the local equilibrium is maintained at the austenite/liquid (\(γ/L\)) and graphite/austenite (Gr/\(γ\)) interfaces. As the eutectic solidification proceeds, the growing austenite rejects solute at the \(γ/L\) interface according to, \(C_γ = kC_γ\) where \(k\) is the partition coefficient, and \(C_γ\) and \(C_L\) are the compositions of the austenite and liquid phases at the \(γ/L\) interface, respectively. On the other hand, the growing graphite absorbs solute at the Gr/\(γ\) interface. The graphite composition is \(C_{Gr} = 1\), and there is no diffusion in the graphite phase. Thus, solute diffusion is considered only in the liquid and austenite phases, and the interfaces. The governing equation for solute diffusion in the entire domain is given by

\[
\frac{\partial C}{\partial t} = \nabla \cdot (D \nabla C) + C_γ(1-k) \frac{\partial C}{\partial t} + (C_γ-C_{Gr}) \frac{\partial C_{Gr}}{\partial t}
\]

where \(C\) is the composition, \(D\) is the diffusivity, and the
The local composition equilibrium approach based on the ZS model is adopted to calculate the kinetics for the growth of primary austenite dendrite and SG. For the SG growing in austenite, the effect of curvature can be ignored. Thus, the equilibrium composition in austenite at the interface cell is evaluated with

\[ C^e_{\text{Gr}/\gamma} = C_{\gamma 0} + (T^* - T^e_{\text{Gr}/\gamma}) / m_{\text{SGr}} \]

where \( m_{\text{SGr}} \) is the solubility slope of graphite, \( T^* \) is the interface temperature, and \( T^e_{\text{Gr}/\gamma} \) is the equilibrium solidus temperature at the initial solid composition \( C^e_{\gamma 0} \). According to the equilibrium condition at the interface, during one time step interval, the increase in Gr fraction of an interface cell is calculated with

\[ \Delta f_{\text{Gr}} = G_{\text{Gr}} \cdot \left( C^e_{\text{Gr}/\gamma} - C_{\gamma 0} \right) / \left( C^e_{\text{Gr}/\gamma} - C_{\gamma 0} \right) \]

where \( G_{\text{Gr}} \) is a geometrical factor that must be used to eliminate the artificial anisotropy caused by the CA square grid and to produce the circular shape of SG. \( G_{\text{Gr}} \) is defined by:

\[ G_{\text{Gr}} = \min \left[ 1, \frac{1}{2} \left( \frac{4}{s_I} + \frac{1}{2} \sum_{m=1}^4 s_{II}^m \right) \right] \]

with \( s_I \) and \( s_{II} \) indicate the states of the nearest neighbor cells and the second-nearest neighbor cells, respectively. The geometrical factor defined by Eq. (4) is used to account for the fact that as the number of neighboring solid cells increases, the solidification rate of a cell increases. Equation (4) also reflects the consideration that the geometrical relation between cells is proportional to the cell spacing. The effect of the second-nearest neighbor cells is weaker than that of the nearest neighbors.

The interface equilibrium composition \( C^e_{\gamma 0} \) in Eq. (3) is calculated from Eq. (2) and determined by interface temperature. The graphite composition, \( C_{\gamma 0} \), is equal to one, and \( C^e_{\gamma 0} \) is the local actual composition obtained by solving Eq. (1). Thus, the kinetics of Gr growth in \( \gamma \) is controlled by carbon diffusion in the austenite.

For the primary austenite dendrite growth in the liquid, the interface equilibrium liquid composition, \( C^e_{\gamma/L} \), is calculated by

\[ C^e_{\gamma/L} = C_0 + (T^* - T^e_{\gamma/L}) / m_{\gamma/L} + \Gamma_{\gamma} \cdot K \cdot f_1(\varphi, \theta_0) / m_{\gamma/L} \]

where \( m_{\gamma/L} \) is the liquidus slope of the austenite, \( \Gamma_{\gamma} \) is the Gibbs–Thomson coefficient of the austenite, and \( K \) is the local interface curvature calculated using the counting-cell method. \[ f_1(\varphi, \theta_0) \] is a function accounting for the anisotropy of the surface tension and is calculated by

\[ f_1(\varphi, \theta_0) = 1 - 15\varepsilon \cos[4(\varphi - \theta_0)] \]

where \( \varepsilon \) is the degree of anisotropy of the surface energy, and the growth angle \( \varphi \) can be calculated from the gradient of the austenite fraction at the \( \gamma/L \) interface using the following equation:

\[ \varphi = \arccos \left( \frac{\partial f_j / \partial \varphi}{(\partial f_j / \partial \varphi)^2 + (\partial f_j / \partial \theta)^2} \right)^{1/2} \]

where \( f_j \) is the austenite fraction in the interface cell.

The model considers the anisotropy in both surface energy and interfacial kinetics for the growth of austenite dendrite. Thus, the increase in the fraction of austenite in an interface cell is evaluated with

\[ \Delta f_{\gamma} = f_2(\varphi, \theta_0) \cdot (C^e_{\gamma/L} - C_{\gamma/L}) / (\gamma/L(1 - k)) \]

where \( C^e_{\gamma/L} \) is the interface equilibrium composition calculated by Eq. (5), and \( C_{\gamma/L} \) is the local actual liquid composition obtained by numerically solving Eq. (1). \( \Gamma_{\gamma} \) is a geometrical factor related to the states of neighboring cells, defined by an equation similar to Eq. (4), where the graphite fraction \( f_{Gr} \) is substituted with the austenite fraction \( f_{\gamma} \). \[ f_2(\varphi, \theta_0) \] is a function that accounts for the kinetic anisotropy calculated by

\[ f_2(\varphi, \theta_0) = 1 + \delta_k \cos[4(\varphi - \theta_0)] \]

where \( \delta_k \) is the degree of the kinetic anisotropy.

Since the thermal diffusivity of Fe–C alloys is about three orders of magnitude larger than the solute diffusivity in the liquid, the kinetics for dendritic growth is assumed to be solute-transport controlled. For the sake of simplicity, the temperature field in the domain is, therefore, considered to be uniform and cooled down with a cooling rate. The cooling rate of the domain is calculated with

\[ \frac{\partial T}{\partial t} = - \dot{T} + \frac{L_{\gamma}}{\rho c_p} \cdot \frac{\partial f_{\gamma}}{\partial t} + \frac{L_{\text{Gr}}}{\rho c_p} \cdot \frac{\partial f_{\text{Gr}}}{\partial t} \]

where \( \dot{T} \) is an imposed cooling rate (heat extraction), \( \rho \) is the density of liquid, \( c_p \) is the specific heat of liquid, and \( L_{\gamma} \) and \( L_{\text{Gr}} \) are the latent heat of austenite and graphite, respectively.

3. Results and Discussion

3.1. Dendritic Growth in Two and Three Dimensions

Figure 1 presents the single dendrite morphology of a succinonitrile-acetone (SCN-0.4 mol% Ace) alloy simulated by the 2D ZS model, shown in the temperature field and the composition field, respectively. The dendrite was freely growing in an undercooled melt of \( \Delta T = 0.9 \) K. The calculation was performed on a domain of \( 600 \times 600 \) mesh with mesh size \( \Delta x = 0.5 \mu m \). The physical properties used for simulation were obtained from literature. As shown in Fig. 1, the thermal diffusion layer is wider than the solute diffusion layer. This is due to the fact that for this alloy system the thermal diffusivity is about two orders of magnitude larger than the solutal diffusivity.

The 2D ZS model was extended to three dimensions. The most difficult issue for this extension is the description of different crystallographic orientations in three dimensions. The extended 3D model calculates the 3D weight mean curvature (wmc) that is incorporated with the
anisotropy of surface tension based on the surface divergence of the Cahn–Hoffman $\xi$-vector. This approach for 3D wmc calculation is convenient to be implemented in the Cartesian coordinates and allows the simulation of 3D dendrites with various preferential crystallographic orientations in a straightforward manner.

The modeling of 3D single dendrite was performed for a Ni–5wt%Nb alloy. The physical properties of the alloy studied are: the liquidus slope $m_L = -7.5$ K/(wt%), the partition coefficient $k = 0.81$, the Gibbs–Thomson coefficient $\Gamma = 3.65 \times 10^{-7}$ m K, the solute diffusion coefficient in the liquid $D_s = 3.0 \times 10^{-9}$ m$^2$/s, and the solute diffusion coefficient in the solid $D_s = 1.0 \times 10^{-12}$ m$^2$/s. The calculations were carried out on a cubic domain of $250 \times 250 \times 250$ mesh with uniform mesh size $\Delta x = 0.8$ mm. Figure 2 presents the simulated dendrite morphologies for a Ni–5wt%Nb alloy at undercoolings of 2 K and 3.5 K. The degree of anisotropy of the surface energy, $\epsilon$, was taken as 0.02 and 0.04 for Figs. 2(a) and 2(b), respectively. It can be seen from Fig. 2(a) that low undercooling and small surface energy anisotropy yields the branchless needle dendrite. The 3D needle dendritic tip exhibits a nonaxisymmetric shape that is similar to the one simulated using the phase field model reported by Karma et al. On the other hand, with a higher undercooling and a larger value of $\epsilon$, the model reproduces realistic dendrite features observed experimentally, such as nonaxisymmetric paraboloid tip, the incubation length along the tip before generating secondary arms, and the well developed side branches with random spacing forming approximately perpendicular to the primary trunks.

Karma et al. performed the quantitative simulation of 3D single dendrite growth in pure substances. The shape of the steady-state needle dendrite tip is found to be nonaxisymmetric and deviates from a paraboloid in the fourfold symmetry mode for a cubic crystal. In addition, the finite shape away from the tip is well fitted by the power law $z = -\Delta x^2/3$ predicted by the microsolvability theory.

To investigate the steady-state morphology of the needle dendrite tip simulated by the present model, the transverse and longitudinal sections of the dendrite tip shown in Fig. 2(a) were examined. Considering the symmetrical nature of a tip, the Cartesian coordinates $(x, y, z)$ were transformed into cylindrical coordinates $(r, \phi, z)$. The length was rescaled with the tip radius. Figure 3 shows the transverse sections of a simulated dendritic tip. Each section is equally spaced along the $z$-direction by $10\Delta x$ ($\Delta x = 0.8$ mm) with the first plane of $3\Delta x$ from the tip, i.e., $z_i = z_{\text{tip}} - 3\Delta x$ $- 10\Delta x(i - 1)$, where $i = 1, \cdots, 8$. The open circles are the simulated points at the SL interface, where the solid fraction, $f_s$, equals 0.5, which is obtained by interpolating the solid fractions in the relevant interface cells. The solid lines indicate the shapes of the Fourier decomposition given by$^{30}$

$$r^2(\phi, z) = \sum_{n} A_n(z) \cos 4n\phi \quad \cdots \cdots \cdots \cdot(11)$$

where $r$ is the radial distance from the $z$-axis. As shown, the transverse section near the tip is close to a circular shape. However, it gradually deviates from the circular shape with increasing distance from the tip. This illustrates that the
shape close to the tip is nearly axisymmetric, whereas it deviates from an axisymmetric shape behind the tip. It also can be noted that the shapes from the simulation and the Fourier decomposition are almost superimposed, indicating that the nonaxisymmetric shape of dendrite tip deviates from a paraboloid with the fourfold symmetry mode for this cubic crystal.

Figure 4 presents the power law fit and the fourth-order polynomial fit to the longitudinal section of the fin contour ($\phi=0°$) in the region near the dendrite tip growing along the $z$-direction in Fig. 2(a). In the figure, the power law fit by $z = -\alpha s^\beta$ was performed with both $\alpha$ and $\beta$ as free parameters. The result shows that the fitted parameter $\beta$ equals 1.665, which is close to the theoretical value $5/3$ predicted by the microsolvability approach for nonaxisymmetric dendritic growth. As shown in Fig. 4, the power law fit is more accurate than the fourth-order polynomial fit.

The model was applied to simulate the formation of multi-equiaxed dendrites in alloy solidification under normal practical conditions. Figure 5 illustrates the evolution of multi-equiaxed dendritic growth of an Al–2wt%Cu alloy. Note that the model can reproduce realistic features of multi-dendritic growth with various crystallographic orientations, such as the development, coarsening, and competition of primary trunks and secondary arms, and the interactions among dendrites.

As for the 2D ZS model, the extended 3D model is also computationally efficient. For example, the calculation time for Fig. 5 is about 8 h on a PC with 2.93GHz Intel Pentium Dual-Core CPU.

### 3.2. Dendritic Growth with Melt Convection

Previously, the numerical studies on the interaction of dendritic growth and melt convection were mostly based on the methods of phase-field, level set, or cellular automaton incorporated with the solution of Navier–Stokes (NS) equations. Since the NS solvers are continuum-based approaches, it is not easy to implement the non-slip boundary condition at the moving SL interface. Furthermore, the fluid flow calculation may be difficult to converge as the dendritic morphology becomes complicated with increasing solid fraction. In our previous work using a NS solver, it was found that for solid volume fractions above 0.3 the simulation could not proceed, because of the divergence of fluid flow calculation.

Recently, the lattice Boltzmann method (LBM) has rapidly emerged as a new powerful tool for the numerical simulation of fluid flow in complex geometries. Different from the conventional NS solvers, which are based on the macroscopic continuum equations, LBM is a mesoscopic kinetic-based approach that considers flows to be composed of a collection of pseudo-particles represented by a distribution function. The motion, collision and redistribution of these quasi-particles, constrained to move over a lattice, automatically represent the flow dynamics in the system. Compared to the conventional NS solvers, LBM has some attractive merits, such as simplicity of programming, high computational efficiency and good numerical stability for simulating complex fluid systems under complicated geometrical conditions. LBM can also be easily extended to numerically solve the heat and solute transport governed by convection and diffusion. Mathematically, the LBM can be regarded as a cellular automaton where the state at each node has vector character (fluid droplets with momentum vector). Thus, it can be incorporated naturally into the related simulation techniques such as the CA approach for the modeling of dendritic growth in a fluid flow.

In our recent work, we proposed a coupled model for the simulation of solutal dendrite growth with melt convection in the low Péclet number and low Reynolds number regime. In the model, the momentum and species transfer is numerically solved using the LBM, rather than via a continuum-based NS solver. Based on the LBM calculated solutal field that is governed by both convection and diffusion, the kinetics for dendritic growth is determined by the ZS model. The quantitative capabilities of the model were...
demonstrated by the comparison of simulated results with the relevant theories. The simulated growth Péclet number of the upstream tip as function of the flow Péclet number is close to the analytical Oseen–Ivantsov solution. The ratio of the selection parameters without flow and with flow is in good agreement with the prediction of the linearized solvability theory. In addition, the computational performance associated with numerical stability and time-efficiency was evaluated by the comparison with the ZS-NS model, in which the fluid flow and solute transport are calculated using a conventional NS solver based on the SIMPLE (Semi-Implicit Method for Pressure-Linked Equations) algorithm. It was found that the ZS-LBM model exhibits better numerical stability and higher computational efficiency than the ZS-NS model.

The simulations for the growth of single dendrite and multi-dendrites of Al–Cu alloys in the presence of forced melt convection were performed using the ZS-LBM model. The physical properties used were taken from literature. Figure 6 presents the simulated single dendrite morphologies, solute profiles, and flow fields for an Al–3.0wt%Cu alloy growing in an undercooled flowing melt with ΔT=4.0 K and various inlet flow velocities of (a) 0 (the case of pure diffusion), (b) 1.0×10^{-3} m/s, (c) 3.0×10^{-3} m/s, and (d) 5.0×10^{-3} m/s. The calculation was carried out on a domain of a 300×300 mesh with a mesh size Δx=0.4 μm. The solid volume fraction shown in Fig. 6 is maintained constant (F_s=0.07). The velocity vector plots represent the relative strength and the direction of flow. It is noted that in a purely diffusive environment the symmetrical solute field and dendrite shape are produced as shown in Fig. 6(a). On the other hand, when a forced melt flow is introduced, solute profile and dendrite shape are distorted by fluid flow significantly. The growth of the dendrite arms are promoted on the upstream side and inhibited on the downstream side, producing the asymmetrical dendrite features. With the increase of the inlet flow velocity, the influence of fluid flow on dendritic growth becomes stronger as shown in Figs. 6(b)–6(d).

It is quite evident that fluid flow washes the solute released at the SL interface away from the upstream region to the downstream region, resulting in an asymmetrical solutal field. Figure 7 illustrates that the liquid concentrations ahead of dendrite tips, which are measured when total solid volume fraction is F_s=0.07, vary with the inlet flow velocity. As shown, fluid flow causes a decrease and an increase in the concentrations around the dendrite tips of the upstream and downstream arms, respectively. With an increase of the inlet velocity, the effect of flow on the tip concentrations is enhanced. Regarding the situation of the perpendicular tip, the concentration is not influenced much by fluid flow in comparison with the case of pure diffusion.

As described previously, in the model the kinetics of dendritic growth is determined using a local composition equilibrium approach (the ZS model). According to this approach, during one time step interval, Δt, the increased solid fraction, Δf_s, of an interface cell is evaluated by Δf_s=(C_{liq}^{eq}-C_l)/[C_{liq}^{eq}(1-k)], where C_{liq}^{eq} is the local interface equilibrium concentration, C_l is the local actual liquid concentration, and k is the solute partition coefficient. During isothermal dendritic growth, the interface equilibrium composition, C_{liq}^{eq}, is influenced mainly by the interface curvature. It can be seen from Fig. 6 that the radii of different tips are approximately identical. It results in approximately

![Fig. 6. Simulated single dendrite morphologies of an Al–3.0 wt%Cu alloy growing in a flowing melt with ΔT=4.0 K and various inlet flow velocities: (a) U_o=0; (b) U_o=1.0×10^{-3} m/s; (c) U_o=3.0×10^{-3} m/s; (d) U_o=5.0×10^{-3} m/s (domain: 300×300, Δx=0.4 μm).](image)

![Fig. 7. Tip concentration as a function of inlet flow velocity for an Al–3.0 wt%Cu alloy growing in an undercooled melt with ΔT=4.0 K. Solid lines are the linear fits to the simulated data.](image)

![Fig. 8. Tip velocity as a function of inlet flow velocity for an Al–3.0 wt%Cu alloy growing in an undercooled melt with ΔT=4.0 K. Solid lines are the linear fits to the simulated data.](image)
identical tip equilibrium composition. The tip velocity is, therefore, mainly related to the tip actual liquid composition. Having a reduced actual liquid composition \( C_l \) at the upstream tip, the difference, \( \Delta C = C_l^{eq} - C_l \), in the upstream tip will be larger than that in the downstream tip. Accordingly, the enhanced velocity in the upstream tip and reduced growth of the downstream tip compared to the case without convection can certainly be expected. Figure 8 indicates that growth velocities of different tips vary with inlet flow velocity. Note that the growth velocities of the upstream and downstream tips are higher and lower than that without flow, respectively. As the inlet flow velocity increases, the velocity of the upstream tip continuously increases, while the one of the downstream tip experiences a monotone reduction. The perpendicular tip, however, holds a nearly unchanged velocity that is close to the one of pure diffusion. These trends are apparently corresponding to the concentration profiles shown in Fig. 7.

Figure 9 presents the evolution of dendritic morphology, solute and flow velocity profiles of multi-dendrites of an Al–4.5wt%Cu alloy growing in a corner flow \((U_m = V_m = 1.414 \times 10^{-3} \text{ m/s})\) with a cooling rate of 10 K/s. The simulation was performed in a domain consisting of \( 400 \times 400 \) mesh with a mesh size of \( \Delta x = 1 \mu \text{m} \). It can be seen that fluid flow also has a notable influence on the growth of multi dendrites, particularly at the early stage of solidification. Melt flows smoothly, from the top-left corner to the bottom-right corner, along the small dendrites, during which solute is transported from the upstream side to the downstream side of each dendrite. The dendritic growth is enhanced towards the direction of incoming flow and largely suppressed on the downstream side. As the dendrites grow close to each other, the flow gradually fades away in the inter-dendrite region. The liquid composition increases as solidification proceeds. The outside shell of the dendrites, where the final solidification of the solute-enriched liquid occurs, exhibits a higher composition as shown in Fig. 9(c). Note well that the model is able to perform the simulation of convective multi-dendritic growth at a high value of \( F_s \) equal to 0.93.

3.3. Divorced Eutectic Microstructures of Spheroidal Graphite Cast Iron

The multiphase model described in Chap. 2 was applied to simulate the divorced hypoeutectic solidification of SG cast iron. The physical properties used were taken from references.\(^{39,40}\) The degree of surface energy anisotropy, \( \varepsilon \), and the degree of kinetic anisotropy, \( \delta_a \), for the simulation of primary austenite dendrite growth were taken as 0.04 and 0.6, respectively. Figure 10 presents the evolution of the microstructure and solute field for a hypoeutectic SG cast iron with an initial composition \( C_0 = 3.993 \text{ wt\% C} \). The calculation was performed in a domain consisting of \( 400 \times 400 \) meshes with a mesh size of 2 \( \mu \text{m} \). The imposed cooling rate (heat extraction) was taken as \( T = -3.44 \exp(-0.0031t) \), where \( t \) is the time. It is seen that the solidification of hypoeutectic iron starts with the growth of primary austenite dendrites (Fig. 10(a)). As the temperature decreases to the eutectic range, some graphite nuclei precipitate from the liquid (Fig. 10(b)). When graphite spheroids touch austenite dendrites, they are engulfed fast by austenite to form the austenite shells. Then, the growth of austenite from the liquid becomes isotropic, because of the isotropic carbon diffusion field around graphite nodules (Fig. 10(c)). On the other hand, graphite spheroids continue to grow from the austenite through solute diffusion in austenite. The final microstructure exhibits austenite grains with several graphite nodules. The carbon concentration near graphite spheroids is very low as shown in Fig. 10(d). The simulated microstructure features are quite similar to the experimentally observed ones.\(^{41}\)

A comparison between the simulated cooling curve and
the experimental one for a hypo-eutectic SG iron with an initial composition of $C_0 = 4.13$ wt% ($3.47$ wt% C, $1.98$ wt% Si) is presented in Fig. 11. The extraction rate used in the calculation was $\dot{T} = 2.6299 \ln{t} - 12.179$ at $1554 \text{K} > T > 1452 \text{K}$ and $T = 0.6576 \ln{t} - 4.9732$ at $1452 \text{K} \geq T \geq 1273 \text{K}$. It can be seen that when the temperature is down to about $1430 \text{K}$, the slope of cooling curve is decreased, indicating the formation of primary austenite dendrites. When the temperature reaches around the eutectic temperature, the released latent heat due to eutectic solidification yields recalescence phenomenon. It is noted that the simulated curve exhibits less primary austenite arrest and eutectic recalescence, but is in general agreement with the experimental profile.

4. Conclusions

The two and three dimensional CA based models and derived coupling models were developed for the simulation of microstructure formation during alloy solidification. The quantitative capabilities of the proposed models are demonstrated by validating the simulations with relevant theories and experimental data. The models reproduce realistic dendritic and eutectic morphologies with acceptable computational efficiency. It is found that LBM, a new numerical tool for fluid flow calculation, is more numerically stable and computationally efficient than NS solvers for convective dendrite simulation. Efforts will be dedicated continuously to further improve the present models, develop new coupling models for simulating microstructure formation of multi-phases in multi-scales, and extend the applications of microstructure simulation into various practical materials processes.

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