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Quantitative phase-field model for dendritic growth with two-sided diffusion

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Abstract. A quantitative phase-field (PF) model with an anti-trapping current (ATC) is developed to simulate the dendritic growth with two-sided diffusion. The asymptotic analysis is performed at the second-order for the PF equations coupled with nonlinear thermodynamic properties and an ATC term under the equal chemical potential condition. The PF mobility and ATC are derived based on the asymptotic analysis in the thin interface limit, and the solute drag model. Then the model is reduced to the dilute solution limit for dendrite solidification in binary alloys. The test of convergence with respect to the interface width exhibits an excellent convergent behavior of the proposed model. The performance of the model is then validated by the comparison of PF simulations to the predictions of the Gibbs-Thomson relation, and of the linearized solvability theory, for the isothermal dendritic growth of an Fe-1.5mol.%C alloy. The results demonstrate quantitative capabilities of the model that effectively suppresses the abnormal solute trapping effect when the interface is taken artificially wide. It is also found that the present model can quantitatively describe dendrite growth with various solid diffusivities, ranging from the case with one-sided diffusion to the symmetrical model.

1. Introduction
Phase-field (PF) method has emerged as a powerful tool to simulate microstructure evolution during solidification process [1]. Yet, the PF model in the sharp interface limit has encountered the efficiency difficulty to describe realistic microstructures on experimentally relevant length and time scales. Based on the thin interface limit, Karma and Rappel [2] developed a quantitative PF model to simulate dendritic growth of pure materials in a much larger system even at low undercooling.

For the case of alloy solidification, however, it is demonstrated that the PF model in the thin interface limit, with different diffusivities in the two phases, suffers from the three spurious effects of efficient chemical potential jump across the interface, interface stretching, and surface diffusion [3].
Karma et al. [4, 5] proposed a PF model with an anti-trapping current (ATC) to eliminate the abnormal effects in the case of one-sided dilute alloy solidification with zero solute diffusivity in the solid. The extension of the ATC scheme to the two-sided model, involving diffusion in the solid, was initially attempted by Gopinath et al. [6]. The ATC, however, has a singularity problem when the model is reduced to the one-sided case. Another attempt was made by Steinbach [1], and an extrapolated form of ATC was proposed. Based on the matched asymptotic analysis in the thin interface limit, Ohno and Matsuura [7] proposed a quantitative two-sided PF model with ATC for dilute alloy solidification.

This paper presents a quantitative PF model with an ATC scheme to simulate dendrite growth in binary alloys, involving asymmetrical two-sided solute diffusion. The PF mobility and ATC are derived based on the second-order asymptotic analysis in the thin interface limit, and the solute drag model [8, 9]. The asymptotic analysis is performed for the PF equations coupled with nonlinear thermodynamic properties and an ATC under the equal chemical potential condition. To validate the model against the classic theories of dendritic growth, the model is reduced to the dilute solution limit. After demonstrating the convergent behavior, the performance of the model is validated through extensive comparisons of the PF simulations to the predictions of the Gibbs-Thomson relation and of the linearized solvability theory.

2. Isotropic phase-field model with nonlinear thermodynamic properties

Based on the approach proposed by Kim [10], the PF equations coupled with nonlinear thermodynamic properties for isothermal solidification can be written as

\[ M_0 \partial_t \phi = K \nabla^2 \phi - \frac{(8/\pi^2) \sigma f' (\phi)}{\phi} - g_\phi \Delta G_m / V_m \]  

(1)

\[ \partial_t u = \nabla \cdot (M_l \phi \nabla \mu / V_m + \xi a_\phi (u_l - u_s) \nabla \phi (\nabla \phi / |\nabla \phi|)) \]  

(2)

where \( \phi \) is the PF variable, \( M_0 \) is the PF mobility, \( \nabla = \{ \partial_x, \partial_y \} \) is the gradient operator for two-dimensions (2D), and \( \partial_t \) is the time derivative. \( \Delta G_m = \{ g_m^\phi (u_l) - g_m^\phi (u_s) - \mu_m (u_l - u_s) \} \) is the chemical driving force for isothermal solidification, \( g_m^\phi (u_l) \) and \( g_m^\phi (u_s) \) are the mole free energies of the solid and liquid phases, \( V_m \) is the mole volume, \( K \) is the gradient energy coefficient, \( \sigma \) is the potential height, \( f(\phi) = (\pi^2/8) |\phi| \) is a parabolic potential with double obstacles, \( u = u_s (1 + h_\phi (\phi))/2 + u_l (1 - h_\phi (\phi))/2 \) is the concentration, \( M_l \phi = M_l q_\phi (\phi) = M_l / M_s (1 + m_\phi (\phi))/2 + (1 - m_\phi (\phi))/2 \) is the diffusion mobility at the interface, \( M_l \) and \( M_s \) are the diffusion mobility in the liquid and solid phases, and \( \mu_m \) is the chemical potential, restricted by the equal chemical potential condition at the interface: \( \mu_m = \mu_1 (\partial g_m^\phi / \partial u_l) = \mu_2 (\partial g_m^\phi / \partial u_s) \). The model yields \( \tilde{\xi} = \pi \sqrt{3/2} \sigma \) and \( \sigma = \pi \sqrt{8 \cdot K \sqrt{3}} \sigma \), where \( \tilde{\xi} \) is the PF interface width and \( \sigma \) is the chemical potential. The second term on the right-hand side of equation (2) is the solute ATC term.

To perform asymptotic analysis, the dimensionless length and time scales are chosen as \( d = \sigma g_0 \) and \( t_0 = d^2 / D \), where \( D = M_0 g_0 \) for the case \( M_l = M_s \). Thus, the dimensionless transformation can be taken as follows: \( \tilde{r} = r / d_0 \), \( \tilde{t} = t (d / d_0) \), \( \tilde{\nabla} = \nabla / d \), \( \tilde{\nabla} = \tilde{\nabla} / (d / d_0) \), \( \tilde{\nu}_n = \nu_n (d / d_0) \), \( \tilde{\kappa} = d \kappa \), where \( \nu_n \) is the interface normal velocity, and \( \kappa \) is the interface curvature. The dimensionless energy scale, \( g_0 \), is determined by \( g_0 = \max \{ \Delta G_m / V_m \} \). Thus, the dimensionless phase-field model is expressed as

\[ \tau_\phi \nabla^2 \partial_t \phi = \nabla^2 \nabla \nabla \phi / \sigma - 8 / \pi^2 \cdot f' (\phi) - a_s \cdot \nabla \cdot g_\phi (\phi) \cdot \Delta G \]  

(3)

\[ \partial_t u = \nabla \cdot (q_s (\phi) \nabla \mu + \varepsilon \cdot a_\phi (\phi) (u_l - u_s) \nabla \phi (\nabla \phi / |\nabla \phi|)) \]  

(4)
where $\Delta \tilde{G} = (\Delta G_m/V_m)/g_0$, $\tilde{\mu} = (\mu_m/V_m)/g_0$, and $a_1 = \pi^2/16$.

The second-order matched asymptotic analysis for the PF equations shown in equations (3) and (4) is carried out in order to obtain the PF mobility and ATC. According to the asymptotic analysis, the spurious interface effects caused by the problem of asymmetrical two-sided diffusion with an artificial interfacial width can be suppressed by solving the following three constraints:

$$
\int_{-\infty}^{\infty} \left[ \Lambda_{\delta}(\phi_0) - \Lambda_{\delta}(\phi(+\infty)) \right] d\eta - \int_{-\infty}^{\infty} \left[ \Lambda_{\delta}(\phi_0) - \Lambda_{\delta}(\phi(-\infty)) \right] d\eta = 0
$$

where $\Lambda_{\delta}(\phi_0) = p_{\delta}(\phi_0)$, $h_{\delta}(\phi_0)$, and $m_{\delta}(\phi_0)$, respectively, and $p_{\delta}(\phi_0) = [h_{\delta}(\phi_0) - 2a_{\delta}(\phi_0)\partial_{\eta}\phi_0 - q_{\delta}(\phi_0(-\infty))\chi_0/\chi_0]/q_{\delta}(\phi_0)$. $g_{\delta}(\phi)$, $h_{\delta}(\phi)$, and $m_{\delta}(\phi)$ are the interpolation functions of the chemical energy, concentration, and diffusion mobility, respectively.

They are constructed as a function of the parameter, $\delta$, by

$$
g_{\delta}(\phi) = \frac{1 + h_{\delta}(\phi)}{2} = \frac{1 + m_{\delta}(\phi)}{2} = \begin{cases} 0 & \text{for } 0 \leq \phi \leq \delta \text{ (1-}\lambda \leq \eta \leq +\infty) \\ (\phi - \delta)/(1-2\delta) & \text{for } \delta < \phi < 1-\delta \text{ (1+}\lambda < \eta < 1-\lambda) \\ 1 & \text{for } 1-\delta \leq \phi \leq 1 \text{ (}-\infty \leq \eta \leq 1+\lambda) \end{cases} \tag{5}
$$

The function $a_{\delta}(\phi)$ in equation (4) required to determine the ATC, can be calculated by

$$a_{\delta}(\phi) = k_{\eta} (\phi, \delta) ((2/\pi) \sqrt{\phi(1-\phi)} (M_1 - M) / M_0(\Omega), \ (\delta < \phi < 1-\delta) \tag{6}$$

where $M_0(\Omega) = [(1-\Omega(M)^2 + \Omega(M_0)^2)]^{1/3}$, $\pi_0$ is the initial concentration, and $k_{\eta}(\phi, \delta) = [1-h_{\eta}(\phi)]/[4\psi(1-\phi)]$, $(\delta < \phi < 1-\delta)$.

By applying the solvability condition of the inner expansion of the $\phi$ equation at the second order, the PF mobility, $M_{\phi}$, can be expressed as

$$\pi^2 / (16\xi M_{\phi}) = 1/M_{\text{fric}} + \xi(u_s - u_i)^2 / (4\tilde{M}_{\phi}(\Omega)) \tag{7}$$

where, $k_{\mu\nu}(\delta) = [4(1-2\delta)\sqrt{(1+\delta+\pi(1+8\delta+8\delta^2)-32\delta \arccos(\sqrt{\delta}) - 4(1+8\delta^2) \arcsin(\sqrt{\delta})}) / [\pi(1-2\delta)^2]]$, $M_{\phi}(\Omega)^{-1} = k_{\mu\nu}(\delta)\tilde{M}(\Omega)^{-1}$ and $M_{\text{fric}}$ is the interface mobility caused by the solvent atoms rearranging themselves from one lattice into another lattice [8].

According to the solute drag model [8], the rate of the total Gibbs energy dissipation during the motion of the interface, $\dot{v}_a/M_{\text{eff}}$, controlled by the coupled processes of the friction of the interface (solvent atoms rearrange) and the trans-interface diffusion (solute drag), can be written as

$$\dot{v}_a^2 / M_{\text{eff}} = \dot{v}_a^2 / M_{\text{fric}} + Q_{\text{sd}} \tag{8}$$

where $\dot{v}_a/M_{\text{fric}}$ is for overcoming the friction of the interface [9], and $Q_{\text{sd}}$ is for overcoming the solute drag. Through the matched asymptotic analysis, we have $Q_{\text{sd}} = \dot{v}_a^2 \xi(u_s - u_i)^2 / (4\tilde{M}_{\phi}(\Omega))$.

According to equation (8), the effective interface mobility, $M_{\text{eff}}$, can be expressed as

$$1/M_{\text{eff}} = 1/M_{\text{fric}} + Q_{\text{sd}} / \dot{v}_a^2 \tag{9}$$

Substituting equation (9) into equation (7), the PF mobility can also be expressed as

$$M_{\phi} = \pi^2 M_{\text{eff}} / (16\xi) \tag{10}$$

Substituting equations (9) and (10) into the solvability condition of the inner expansion of the $\phi$ equation at the first order, $-\Delta G_m/V_m = \pi^2 v_a / (16\xi M_{\phi}) + \sigma\lambda$, we obtain
\[-\Delta G_a / V_a = v_a / M_{ric} + Q_{ad} / \tilde{v}_a + \sigma \kappa = v_a / M_{ric} + v_a \tilde{z}(u_s - u_l)^2 / (4 \tilde{\mu}_l(\Omega)) + \sigma \kappa = v_a / M_{eff} + \sigma \kappa \quad (11)\]

Assuming \( M_{ric} = \infty \) or \( \beta_{ric} = 0 \) for the case of solidification, where \( \beta_{ric} \) is the interface kinetic coefficient calculated by \( \beta_{ric} = T_{ad}(LM_{ric}) \), and \( L \) is the latent heat of pure metal, we obtain \( \tilde{z}_a = 4 \tilde{\mu}_l(\Omega)(u_s - u_l)^2 / (L / T_0) \beta_{ad} \) from equation (9), where \( \beta_{eff} = T_{ad}(LM_{eff}) \) is the effective interface kinetic coefficient. Using this \( \tilde{z}_a \), the effect of solute drag, \( Q_{ad} \), could be maintained as a constant for different interface widths. Accordingly, the PF mobility in the thin interface limit can be expressed as
\[ M_{\phi}^{-1} = (4 / \pi^2) \tilde{z}_a (u_s - u_l)^2 / \tilde{\mu}_l(\Omega) \quad (12) \]

3. Anisotropic phase-field model in the dilute binary alloy system

Taking the crystalline anisotropy of fourfold symmetry into account, the orientation dependent interface width can be expressed as \( \tilde{z}_a = \xi(\theta) + \Delta z(\theta) \), where \( \theta = \arctan(\partial / \partial \phi) \), \( A_1(\theta) = 1 + e_4 \cos(4\theta) \), and \( e_4 \) is the energy anisotropy strength. Thus, the PF equation for the isothermal dendritic growth in dilute binary alloys can be written as
\[ M_\phi' = \nabla \cdot (\tilde{\kappa}_l(\theta) \nabla \phi) - \tilde{z}_a(\theta) \partial / \partial \phi \tilde{\mu}_l(\Omega) (k_s - 1)(u_s - u_l) / V_a \quad (13) \]
where \( k_s = u_s / u_l \) is the equilibrium partition coefficient, \( u_s \) and \( u_l \) are the equilibrium concentration in the solid and liquid, respectively. \( R \) is the gas constant.

The orientation dependences are also introduced to the PF mobility given in equation (12) to obtain \( M_{\phi}^{-1}(\theta) = (4 / \pi^2) \tilde{z}_a(\theta) \tilde{\mu}_l(\Omega)(u_s - u_l)^2 / \tilde{\mu}_l(\Omega) M_{\phi}^{-1}(\theta) \). For dilute binary alloys, \( M_s / M_r = D_s / (k_s D_s) \). Thus, the PF mobility of dilute alloys with crystalline anisotropy can be expressed as
\[ M_\phi' = (4 / \pi^2) \tilde{z}_a(\theta) \tilde{\mu}_l(\Omega) \tilde{D}_l(\Omega) (k_s - 1)(u_s - u_l) / V_a \quad (14) \]
where \( \tilde{D}_l(\Omega) = \tilde{k}_{s, s}(\delta) \tilde{\Omega}^4 \), \( \tilde{\Omega}^4 = (1 - \Omega^2(k_s^2)(\Omega D_s))^{-1} \), and \( \tilde{z}_a(\theta) = \tilde{z}_a A_1(\theta) \).

With the assumption of dilute alloys, the concentration field satisfies \( u_s = k_s u_l \) and \( u_l = u / p_\phi(\theta) \), where \( p_\phi(\theta) = k_s(1 + h_s(\theta)) / 2 + (1 - h_s(\theta)) / 2 \). The diffusion equation can thus be described as
\[ \partial / \partial \phi = \nabla \cdot (q_s(\phi) \nabla u / p_\phi(\theta) + \tilde{z}_a(\phi)(u_s - u_l) \partial / \partial \phi \nabla \phi / \tilde{\mu}_l(\Omega)) \quad (15) \]
where \( q_\phi(\theta) = k_s(\theta) / 2 + \delta / 2 + (1 - h_s(\theta)) / 2 \), and \( a_\phi(\theta) = k_s(\theta) \). \( \Omega \) is evaluated by \( \exp(-D_s / (k_s D_s)) \) to satisfy the condition of \( \lim \exp(-D_s / (k_s D_s)) / D_s = 1 \).

4. Results and discussion

4.1. Dendrite morphology

The PF model described in Section 3 was applied to simulate dendritic growth of an Fe-C alloy. The physical parameters of Fe-C alloys were taken from reference [11]. Other simulation parameters were given as follows: \( d_s = \Gamma(u_s - u_l)^4 / m_s^4 = 0.04566 \) \( \mu m \), \( \beta_{eff} = 50 \) \( sK / m \), \( \tilde{z}_a = 20 d_s \), \( \epsilon = 0.04 \), \( \delta = 0.08 \), and the interface width was taken as 5 grid points. All the parameters used in the present work were the same as stated here, unless specified otherwise.

Figure 1 shows the concentration fields and ATC of the steady-state dendrite growth for an Fe-0.15 mol.\% C alloy with \( \Omega_0 = (u_s - u_l) / (u_l - u_s) = 0.55 \) at the temperature of \( T_0 = T_M - 5K \). The domain is
1600×800 grid with $\xi=3.75\ d_0$. Different scales are used in the left and right boxes to better visualize the concentration variations in the solid and liquid, respectively. The vectors at the interface illustrate the magnitude and direction of the ATC. Note that the ATC has a maximum value at the tip. Apparently, the interface velocity reaches the highest at the tip, and the effect of abnormal solute trapping should increase with the interface velocity. Thus, the largest ATC is needed to eliminate the abnormal solute trapping at the tip.

Figure 1. Simulated concentration fields of dendrite growth for an Fe-0.15mol.%C alloy at $\Omega_0=0.55$. The left and right boxes show concentration maps in the solid and liquid, respectively. The vectors indicate the magnitude and direction of the anti-trapping current.

4.2. Computational convergent performance

The computational convergent performance of the present model was tested with respect to various interface thicknesses. In order to represent the same physical length of 1200$d_0$, the grid sizes used were 1600×1600, 1200×1200, 800×800, 600×600, 500×500, 400×400, 300×300, 240×240, and 200×200 for $\xi=1.875d_0, 2.5d_0, 3.75d_0, 5d_0, 6d_0, 7.5d_0, 10d_0, 12.5d_0, and 15d_0$, respectively. Other conditions were identical with those used for figure 1. After dendritic growth reached the steady-state, the tip velocity, $v^*_n$, tip radius, $\rho^*$, and tip composition in the liquid, $u^*_l$, were measured, and the average values were calculated from the measured values of several time step intervals. The partition coefficient, $k_e$, was computed from the tip compositions in the liquid and solid at the interface. Figure 2 shows the steady-state tip parameters, including growth velocity, radius, composition in the liquid, and the partition coefficient, as a function of interface thickness, $\xi/d_0$. The converged solution of tip parameters are obtained when the interface thickness, $\xi/d_0$, is less than about 10. It has been demonstrated that in the thin interface limit, convergence needs to satisfy the condition that the interface width must be much smaller than the radius of local curvature. Ramirez et al. [12] suggested that the ratio of tip radius to interface width, $\rho^*/\xi$, should be larger than about 10 to obtain converged results. Note that for the case of figure 2, the interface thickness $\xi/d_0 = 10$ is corresponding to the ratio $\rho^*/\xi = 2.7376$. It can be expected that for a larger tip radius, $\rho^*$, the converged solution could be obtained with a larger interface thickness, $\xi/d_0$. Consequently, the present model exhibits an excellent convergent behavior.

In the thin interface limit, the convergence is limited by two independent conditions of $\xi << \rho^*$, and $\xi << D/v_n$ [5, 10]. For the case of figure 2, $D/v_n$ is about 95$d_0$. Apparently, the convergent range of the interface width in figure 2 satisfies the two limiting conditions.
4.3. Comparison with the Gibbs-Thomson relation

To validate the accuracy of the present model, the evolution of tip composition in the liquid simulated by the present PF model was compared with those calculated from the Gibbs-Thomson (GT) relation. Taking the dynamic effect and crystallographic anisotropy into account, the GT relation at the dendrite tip can be expressed as

$$u_t = u_v - \frac{V_n}{RT_m (1-k_v)} \left[ (1+\varepsilon_1) \frac{v^*}{M_{eff}} + (1-15\varepsilon_1) \frac{\sigma}{\rho^*} \right] = u_v - \frac{(1+\varepsilon_1) \beta_{eff} v^* + (1-15\varepsilon_1) \Gamma / \rho^*}{m_v} \tag{16}$$

where $V_n = T_d R (1-k_v)/(LV_m)$ is the liquidus slope, and $\Gamma = T_d \alpha L$ is the GT coefficient. In the absence of dynamic effect, i.e., $\beta_{eff} = 0$, the GT relation at the dendrite tip is expressed as

$$u_t = u_v - \left[ (1-15\varepsilon_1) \Gamma / (\rho^* \cdot m_v) \right] \tag{17}$$

Figure 3 shows the profiles of tip composition in the liquid, $u_t$, varying with time, obtained from the PF simulations, the GT relation with dynamic effect by equation (16), and the GT relation without dynamic effect by equation (17), for the two interface widths $\xi = 3.75d_0$ and $\xi = 12.5d_0$. The equilibrium composition is also given in the figure for comparison. The tip velocity, $v^*$, and tip radius, $\rho^*$, used for calculating equations (16) and (17) were obtained from the PF simulations. As shown, the profiles of PF simulation agree well with those calculated from the GT relation with dynamic effect for both interface widths, indicating that the abnormal solute trapping is indeed nearly eliminated. In addition, the data of PF simulations and the GT relation by equation (16) are lower than that obtained from the GT relation without the dynamic effect by equation (17). This difference is apparently caused by the effect of the dynamic undercooling.

The computational efficiency of the present model is acceptable. For example, the calculation times for figures 3 (a) and 3 (b) are 21050 s and 295 s, respectively, on a PC Dual-Core, CPU-i3 530.
4.4. Comparison with the linearized solvability theory

The second validation was performed by comparing the PF simulations with the linearized solvability theory for the effect of solid diffusivity, $D_s$, on the selection parameter, $\sigma^*$. According to the linearized solvability theory, the following relation is held during the steady-state dendrite growth at low undercooling [13]

$$\sigma^* = 2\sigma_0^*/(1+k_sD_s/D_l)$$

where $\sigma^*=2D_s\rho_0/(v_s(\rho^*)^2)$, and $\sigma_0^*=2D_s\rho_0/(v_s(\rho_0^*)^2)$ is the selection parameter for 2D non-symmetry case ($k_sD_s\neq D_l$), and for 2D symmetrical case ($k_sD_s$=D_l), respectively. For this validation, the simulations were carried out with different values of $D_s$ by setting the realistic values of $k_s$ and $D_l$ as constant. The values of $v_s^*$ and $\rho_0^*$ used for calculating $\sigma_0^*$ in equation (18) were obtained from the PF simulations with $\xi=3.75d_0$. Figure 4 (a) presents the profiles of the selection parameter, $\sigma^*$, as a function of $k_sD_s/D_l$. The PF simulation plots were calculated by $\sigma^*=2D_s\rho_0/(v_s(\rho)^2)$ with the two interface widths $\xi=3.75d_0$ and $\xi=12.5d_0$. The good agreement between the PF simulation and the linearized solvability theory prediction illustrates that the present PF model can reasonably describe dendrite growth ranging from the case of $k_sD_l/D_l=0$ (one-sided model) to the symmetrical case of $k_sD_s/D_l=1$.

In the view of the linearized solvability theory [13], the selection parameter for symmetrical case, $\sigma_0^*$, is a function of interface energy anisotropy, $\varepsilon$, and the Péclet number, $P_c$. For two dimensions, the deduced solvability condition can be expressed by the following integral equation:

$$\int_{-\infty}^{\infty} \frac{A(x)^{1/2} A(x)^{1/4} (1-ix)^{1/4}}{(1+x^2)^{3/4}} \exp\left\{ \frac{S_0(x)}{\sigma_0^*} - \frac{P_c}{2} (ix + x^3/2) \right\} dx = 0$$

where $A(x)=1-15\varepsilon x + 120\varepsilon x^2 (1+x^2)^2$, $S_0(x)=\int_0^x (1-ix)^{1/4} (1+ix)^{3/4} A(s)^{1/2} ds$, and $i$ is the imaginary unit.\n
The solution of equation (19) determines $\sigma_0^*$ as a function of $\varepsilon$ and $P_c$. The selection parameter, $\sigma_0^*$, as a function of anisotropy, $\varepsilon$, simulated by the PF model with $\xi=3.75d_0$ and $\xi=12.5d_0$ was compared with those calculated from the linearized solvability theory by equation (19) with $P_c=0$. For this comparison, $\sigma_0^*$ of PF simulations was calculated based on equation (18) ($\sigma_0^*=\sigma(1+k_sD_s/D_l)/2$). The comparison is shown in figure 4 (b), and indicates that when anisotropy, $\varepsilon$, is smaller than around 0.05, the profiles obtained from the PF simulations with two interface widths agree well with the one predicted by the linearized solvability theory.
Conclusions
A quantitative PF model with an anti-trapping current (ATC) is developed to simulate dendritic growth involving two-sided solute diffusion. The PF mobility and ATC are derived based on the second-order asymptotic analysis and the solute drag model. Model tests are performed in terms of the convergent behavior with respect to the interface width, and the comparison of the PF simulations to the GT relation and the linearized solvability theory, for the isothermal dendritic growth of an Fe-1.5mol.%C alloy. The convergent solution is obtained when the ratio of tip radius to interface width, \( \rho \xi \), is less than 3, exhibiting an excellent convergent behavior of the proposed model. The simulated tip composition agrees well with the prediction of the GT relation involving the dynamic effect, when the interface is extended to \( \xi = 12.5d_0 \). Good agreements are also found for the comparisons of the PF simulations to the predictions of the linearized solvability theory regarding the selection parameter as functions of solid diffusivity, and of interface energy anisotropy.

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References