Phase-field modeling of liquid droplet migration in a temperature gradient

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Abstract. The migration of liquid droplets in a solid phase caused by temperature gradient zone melting (TGZM) is simulated by employing a quantitative phase-field (PF) model proposed by Echebarria et al. The PF simulation results are compared with the predictions of an analytical model that describes the droplet migration for both static and dynamic conditions, allowing the direct solution of the time dependent migration velocity of a liquid droplet that is initially located at an arbitrary position in the mushy zone. For dynamic conditions as e.g. during directional solidification, criteria for the critical pulling velocity and critical droplet position are suggested and validated by the PF simulations. When the pulling velocity is lower than the critical pulling velocity, the droplet will migrate through the moving liquidus into the bulk liquid. The droplet velocity gradually increases as it is approaching liquidus. On the other hand, when a pulling velocity higher than the critical pulling velocity is imposed, the droplet will travel through the moving solidus into the fully solid region while the droplet velocity decreases with time. The droplets initially located above the critical position migrate toward liquidus, while the others sink into the bulk solid. The effect of the temperature gradient on the droplet migration kinetics is investigated by both PF simulations and analytical predictions. The results confirm that the upward droplet migration velocity increases, while the time needed for a liquid droplet to move through the entire mushy zone decreases with increasing temperature gradient. The PF simulation results compare well with the analytical predictions.

1. Introduction

During directional solidification in steep temperature gradients, coupled local solidification and remelting in the mushy zone can occur, which is known as temperature gradient zone melting (TGZM). Typical phenomena of TGZM involve liquid droplets, films, or interdendritic pools migrating in the solid phase, or secondary dendrite arms moving in the liquid phase, in both cases toward higher temperatures [1-4]. TGZM influences the solidifying microstructure and microsegregation drastically. Motivated by the scientific and practical importance, numerous experimental and theoretical investigations have been performed to study the kinetics of TGZM and its inference on the solidified microstructures and microsegregation [4-12].
Over the recent decades, in parallel to the advances of rigorous analytical models and more refined experimental techniques, numerical simulation has developed rapidly and has become a powerful approach for studying microstructure evolution [13]. The phase-field (PF) method is an elegant and integrated simulation technique for quantitatively describing arbitrary complex topological changes in phase transformations without the need of explicitly tracking the moving interface. Various investigations on dendritic growth during directional solidification have been performed using the PF method [14-20]. Nevertheless, most PF studies focus on microstructure evolution during solidification, but neglect the effect of melting. Numerical modeling of TGZM phenomena involving both solidification and melting has so far remained scarce.

Recently, an analytical model describing liquid droplet migration caused by TGZM for both static and dynamic conditions was proposed by the present authors [21]. In this paper, the migration of liquid inclusions in a solid phase due to TGZM is studied by PF simulations. The effects of pulling velocity, initial droplet position, and temperature gradient on droplet migration kinetics are investigated. The simulation results are compared with the analytical predictions.

2. Governing equations of the phase-field model

In the present work, a two-dimensional (2D) quantitative PF model with an anti-trapping current for directional solidification of dilute binary alloys, as first proposed by Echebarria et al. [14], is adopted to simulate the migration of droplets in a temperature gradient. The model is based on the assumptions of zero diffusivity in the solid (one-sided diffusion) and a low phase transformation velocity. The temperature field is expressed as \( T(y) = T_0 + G(y-V_p t) \), where \( T_0 \) is the temperature at the cold end, \( G \) is the temperature gradient, and \( V_p \) is the pulling velocity during directional solidification. Based on the assumption of a dilute binary alloy, \( T_0 \) is determined as a function of the initial solute composition, \( c_s^0 \), where

\[
T_0 = T_m - |m| c_s^0 = T_m - |m| c_s^0 / k,
\]

and \( T_m \) is the melting temperature of the pure solvent, \( m \) is the liquidus slope, and \( c_s^0 = (T_m - T_0) / |m| \) is the equilibrium liquid concentration at \( T_0 \). In the 2D Cartesian coordinate system \((x, y)\), the governing equations of the PF variable and dimensionless solute supersaturation are expressed as

\[
\tau_0 \left[ 1 - (1-k) \left( \frac{y-V_p t}{l_f} \right)^2 \right] \partial^2 \phi = \nabla \cdot \left( D q_f \nabla \phi + a_f W_0 \left[ 1 + (1-k) U \right] \nabla \phi \right) + \nabla \cdot \left( \lambda g_f \phi \right),
\]

(1)

\[
\left( \frac{1+k}{2} - \frac{1-k}{2} \cdot h(\phi) \right) \partial_t U = \nabla \cdot \left( c_f \phi \nabla U \right) + a \phi W_0 \left[ 1 + (1-k) U \right] \nabla \phi | \nabla \phi | + \left[ 1 + (1-k) U \right] \frac{1}{2} \partial_t \phi
\]

(2)

where \( \phi \) is the PF variable with \( \phi = 1 \) for the solid and liquid phase, respectively, \( W_0 \) is the interface thickness, \( U = (c_s - c_f^0) / (c_s^0 (1-k)) \) is the dimensionless solute supersaturation, \( k \) is the partition coefficient, \( c_f \) is the local composition of the liquid droplet, \( D \) is the diffusion coefficient in the liquid. \( \lambda = a W_0 / d_0 \) is the coupling constant, where \( a_1 = 0.8839 \), \( d_0 = \Gamma / \Delta T_0 \) is the solute capillary length, \( \Gamma \) is the Gibbs-Thomson coefficient, and \( \Delta T_0 = |m| (1-k) c_s^0 \) is the freezing range. \( \tau_0 = \frac{a_2 W_0^2}{D} \) is the relaxation time, where \( a_2 = 0.6267 \). \( l_f = \Delta T_0 / G \) is the mushy zone length. The interpolation functions, \( g(\phi) \), \( q(\phi) \), and \( h(\phi) \), are expressed as

\[
g(\phi) = \phi - (2/3) \phi^3 - (1/5) \phi^5,
\]

\[
q(\phi) = (1/2) (1+k-(1-k) \cdot h(\phi)),
\]

and \( h(\phi) = \phi \), respectively. \( \nabla = \{ \partial_x, \partial_y \} \) is the 2D gradient operator, and \( \partial_t \) is the time derivative.

The simulation system is initialized by setting the domain length, grid size, and the selected parameters. Equations (1) and (2) are solved using an explicit finite difference scheme with the time step determined by \( \Delta t = \Delta x^2 / (4.5D) \), where \( \Delta x \) is the grid size. The zero-flux boundary condition is applied to numerically calculate both the phase field and concentration field. The physical parameters of succinonitrile-acetone (SCN-ACE) alloys used in the present work are taken from reference [22].
3. Solutions of the analytical model

Allen and Hunt [4] proposed an analytical model that describes liquid droplets migrating in a stationary temperature gradient. The migration velocity of a droplet, \( V_d \), is given by

\[
V_d = \frac{d\xi_v(t)}{dt} = -\frac{D}{c_i'(1-k)}\frac{\xi_c'(\xi_d)}{\xi_d}, \text{ with } \frac{\xi_c'(\xi_d)}{\xi_d} = -\frac{G}{|m|},
\]

where \( \xi_v(t) \) is the position of the droplet as a function of time \( t \), \( c_i'(\xi_d) \) is the droplet composition. Since \( c_i'(\xi_d) \) varies with time, the migration velocity of a droplet, \( V_d \), is given by equation (3) cannot be explicitly solved. Thus, an explicit solution for the time dependent \( V_d \) is proposed through solving a first-order ordinary differential equation of the variable \( \xi_d(t) \) derived from equation (3). Then, the time dependent position of a liquid droplet, initially located at an arbitrary position in the mushy zone, can be obtained by solving the nonlinear ordinary differential equation [21]. When a non-zero pulling velocity is imposed, the dimensionless position of the droplet, \( \tilde{\xi}_d(\tilde{t}) \), is calculated as

\[
\tilde{\xi}_d(\tilde{t}) = \frac{\varepsilon}{1-\frac{1}{f}} - \frac{1-f^{-1}[\varepsilon-1(1+\tilde{\xi}_0)(k-1)e\exp(\varepsilon-1+\tilde{\xi}_0)(k-1)e-(k-1)^2\cdot t)]}{(k-1)e},
\]

where \( \tilde{\xi}_0 = y_0/l_r \), \( \tilde{t} = tD/l_r^2 \) and \( \varepsilon = V_p[V_p/l_r/D] \) are the dimensionless initial droplet position, time, and pulling velocity, respectively. The droplet is located at an arbitrary position in the mushy zone, and satisfies \( 0 \leq \tilde{\xi}_0 = \tilde{\xi}_d(0) \leq 1 \), where \( \tilde{\xi}_0 = 0 \) and \( \tilde{\xi}_0 = 1 \) represent the dimensionless initial droplet location at the initial positions of the moving solidus and the moving liquidus, respectively. \( f^{-1} \) is the inverse function of \( f(w) = w\exp(w) \). The dimensional position of the droplet \( y_d(t) \) can be obtained by the dimensional transformation of equation (4) by \( \tilde{\xi}_d = y_d/l_r \), \( \tilde{\xi}_0 = y_0/l_r \), \( \tilde{t} = tD/l_r^2 \) and \( \varepsilon = V_p[l_r/D] \).

Evaluating the derivative of \( y_d(t) \), the solution of the time dependent migration velocity of a liquid droplet, \( V_d \), is obtained by

\[
V_d = \frac{dy_d}{dt} = \frac{DG}{(1-k)[|m|c_i^0 - G(y_d - V_p)|]}.
\]

Equation (5) indicates that the droplet migration kinetics due to TGZM is directly influenced by the pulling velocity. There is a critical pulling velocity \( V_{p,cr} \) corresponding to the initial droplet location, \( y_0 \). On the one hand, when the pulling velocity, \( V_p \), is lower than \( V_{p,cr} (V_p < V_{p,cr}) \), the droplet migration velocity, \( V_d \), will be higher than \( V_p (V_p > V_p) \), and the droplet will migrate through the moving liquidus into the bulk liquid. On the other hand, when a pulling velocity higher than \( V_{p,cr} \) is imposed \( (V_p > V_{p,cr}) \), the droplet migration velocity is lower than the pulling velocity \( (V_d < V_p) \), and the droplet will travel through the moving solidus into the fully solid region. The critical pulling velocity is calculated by

\[
V_{p,cr} = \frac{DG}{(1-k)[|m|c_i^0 - Gy_0]}.
\]

According to equation (6), the critical liquid droplet position is defined as

\[
y_{0,cr} = \frac{(1-k)[|m|c_i^0 - DG]}{(1-k)GV_p}, \text{ and } y_{0,cr} = \frac{y_{0,cr}}{l_r}.
\]

For a given constant \( V_p \), the migrating droplet with \( y_0 > y_{0,cr} \) will migrate toward liquidus and get integrated in the bulk liquid. Inversely, the migrating droplet with \( y_0 < y_{0,cr} \) will gradually approach solidus and finally sink into the bulk solid. Accordingly, equations (6) and (7) are the criteria for the critical pulling velocity and critical droplet position, both yielding constant relative positions of the migrating droplet with respect to the moving liquidus and solidus.
4. Results and discussion

4.1. Effect of pulling velocity

PF simulations and analytical predictions with different pulling velocities are performed for SCN-ACE alloys. Figure 1 presents the time evolution of droplet migration velocity, \( V_d \), and droplet location, \( y_d \), obtained by the PF simulation, and the analytical prediction of a SCN-0.6 wt.% ACE alloy with \( V_p=2 \mu m/s \) and \( G=12000^\circ C/m \). At the beginning of the simulation, the domain with a 150×2400 grid and \( \Delta x=0.2 \mu m \) is initialized with a solid matrix. The solidus is initially located at 16\( \mu m \) above the bottom wall. The solid composition below solidus is uniform with a value of 0.6 wt.% ACE, while a solid composition gradient, corresponding to the local temperature between solidus and liquidus, is initialized according to the equilibrium phase diagram. This initialization of the composition field in solid corresponds to the experimental situation after a few minutes of equilibration time [7,8]. A liquid droplet with a radius of 8\( \mu m \) is allocated at 179.5 \( \mu m \) above the bottom of the domain, corresponding to \( \tilde{y}_0=0.5 \), and the initial liquid composition determined from the phase diagram at the respective local temperature. The critical pulling velocity, \( V_{p,c,r} \), calculated by equation (6) is 4.71 \( \mu m/s \). Thus, the pulling velocity used in the simulation of figure 1 is lower than \( V_{p,c,r} \). It leads to a droplet velocity increasing with time as shown in figure 1 (a). As discussed in section 3, in this case the droplet will approach (and pass through) liquidus. The locations of the droplet, the moving liquidus, \( T_s \), and solidus, \( T_s \), as a function of time, determined for the pre-set \( V_p=2 \mu m/s \), are plotted in figure 1 (b). As shown, within a simultaneously migrating mushy zone, the droplet migrates from the initial position toward the moving liquidus, due to the fact that \( V_p \) is lower than \( V_{p,c,r}=4.71 \mu m/s \).

![Figure 1](https://example.com/figure1.png)

**Figure 1.** Comparison of PF and analytical model results regarding the time evolution of (a) droplet velocity and (b) droplet location for a SCN-0.6 wt.% ACE alloy at \( V_p=2 \mu m/s \) and \( G=12000^\circ C/m \), corresponding to \( \tilde{y}_0=0.5 \) and \( V_{p,c,r}=4.71 \mu m/s \).

PF simulation and analytical calculation have also been performed to study the case of \( V_p>V_{p,c,r} \). The pulling velocity is set to \( V_p=6 \mu m/s \). Other conditions are identical with those of figure 1. The time evolution of the droplet velocity and location with \( V_p=6 \mu m/s \), respectively, as obtained by the PF simulation and analytical model are compared in figure 2 (a) and (b). The profiles of the moving liquidus and solidus vs. time, determined by the pre-set \( V_p=6 \mu m/s \), are also plotted in figure 2 (b). As shown in figure 2 (a), the droplet velocity gradually decreases with time. Figure 2 (b) indicates that the droplet location goes upwards with time, confirming that a droplet always migrates toward the high temperature in a temperature gradient. Yet, the migrating velocity of the droplet is lower than the pulling velocity under the condition of \( V_p>V_{p,c,r} \), implying that the droplet migrates slower than the mushy zone. Therefore, the droplet gradually approaches the solidus position as shown in figure 2 (b).

It is noted from figures (1) and (2) that the simulated profiles are slightly lower than the analytical predictions. This might be caused by the following reasons. First, the analytical model neglects, while
the PF simulation includes, the effect of curvature that exerts a small but perceptible influence on the droplet velocity. Second, the diffuse interface in the PF model inevitably leads to some deviations from the precise thermodynamic equilibrium concentrations, which leads to a minor error that however can accumulate for long migration distances. Despite the mentioned differences between the two models, the agreement is still satisfying.

4.2. Effect of initial droplet position
In order to examine the effect of initial droplet position on the migration behaviour of droplets, the PF simulation is performed for five droplets migrating in a solid matrix of a SCN-0.9 wt.% ACE alloy at \( G = 10000^\circ C/m \), corresponding to \( \tilde{y}_0 = 0.5 \) and \( V_{p,cr} = 4.71 \mu m/s \).

![Figure 2](image1.png)

**Figure 2.** Comparison of PF and analytical model results regarding the time evolution of (a) droplet velocity and (b) droplet location for a SCN-0.6 wt.% ACE alloy at \( V_p = 6 \mu m/s \) and \( G = 12000^\circ C/m \), corresponding to \( \tilde{y}_0 = 0.5 \) and \( V_{p,cr} = 4.71 \mu m/s \).

| Time, \( t \) (s) | Droplet velocity, \( V_d \) (\( \mu m/s \)) |
|------------------|------------------------------------------|
| 0                | PF model                                 |
| 0                | Analytical model                         |

![Figure 3](image2.png)

**Figure 3.** Simulated sequence of liquid droplet positions for a SCN-0.9 wt.% ACE alloy at \( G = 10000^\circ C/m \) and \( V_p = 2.62 \mu m/s \), corresponding to \( \tilde{y}_{0,cr} = 0.5 \): (a) 3.2 s, (b) 48 s, (c) 96 s. The initial positions of the five droplets are \( \tilde{y}_0 = 0.14, 0.25, 0.5, 0.63, \) and 0.74, respectively.
temperature. It is clear that the lower the local temperature, the higher are the equilibrium compositions of both the solid and liquid phases. All droplets with various \( y_0 \) migrate upwards with time in a fixed coordinate system. The droplet marked as “3” is initially located at the critical droplet position \( y_0 = 0.5 \). During the process, the relative position of droplet “3” with respect to liquidos and solidus remains essentially unchanged, while the relative position of other droplets evidently changes. The droplets marked as “4” and “5” initially located at \( y_0 = 0.63 \) and 0.74, respectively, gradually approach liquidus. When the migration time is around 96 s, droplet “5” is migrating through the moving liquidus into the bulk liquid. On the other hand, the droplets marked as “1” and “2” with \( y_0 = 0.14 \) and 0.25, respectively, gradually approach solidus. When the time is around 96 s, the location of droplet “1” is partly below the solidus.

4.3. Effect of temperature gradient

Figure 4 presents the droplet migration velocity varying with time, obtained from the PF simulations and the analytical predictions for a SCN-0.3 wt.% ACE alloy with different temperature gradients. The PF simulations are performed in a domain of a 150×2000 grid with \( \Delta x = 0.2 \mu m \) at \( V_p = 2 \mu m/s \). At the beginning of the simulations, the domain is initialized with a solid matrix. One liquid droplet with a radius of \( 8 \mu m \) is assigned at the initial solidus position, i.e., \( y_0 = 0 \). Corresponding to the temperature gradients of 8000~12000°C/m, the critical pulling velocities calculated by equation (6) are \( V_{p,cr} = 4.08~6.12 \mu m/s \), which are higher than \( V_p \). Thus, the droplets will migrate to approach liquidus. Simulations are stopped when the liquid droplet reaches the liquidus position. As shown in figure 4, the droplet migration velocity increases with time for the three temperature gradients. As expected a higher temperature gradient leads to a higher droplet migration velocity, and a shorter time needed for the droplet to reach the liquidus position and a certain velocity. For example, when the temperature gradients are 8000, 10000, and 12000°C/m, the times to reach the velocity of 10\( \mu m/s \) are around 60 s, 30 s, and 17 s, respectively.

It is noted that the profiles obtained from PF simulations and analytical solutions for \( G = 12000°C/m \) show the best possible agreement. With decreasing temperature gradient, the deviation between the profiles obtained from the two models gradually becomes evident. It is understandable that the accumulated deviation between the two models increases with the time needed for a droplet to reach liquidus, which becomes lower for a lower temperature gradient.

Another phenomenon to be noted from figure 4 is that the initial droplet velocity, \( V_{dl,0} \), is non-zero and it varies with temperature gradient. By substituting \( t = 0 \) into equation (5), \( V_{dl,0} \) can be calculated by

\[
V_{dl} \big|_{t=0} = \left. \frac{dy_p}{dt} \right|_{t=0} = \frac{DG}{(1-k)[|m| c_I^0 - G|y_0|]}.
\] (8)

It is found that \( V_{dl,0} \) calculated by equation (8) is identical with \( V_{p,cr} \) by equation (6). Equation (8) indicates that \( V_{dl,0} \) is proportional to the temperature gradient. As shown in figure 4, the values of \( V_{dl,0} \) obtained from PF simulations and the analytical model are close to 4.08\( \mu m/s \), 5.10\( \mu m/s \) and 6.12\( \mu m/s \), for \( G = 8000, 10000 \) and 12000°C/m, respectively.

The case of \( V_p > V_{p,cr} \) for various temperature gradients is also investigated by both PF and analytical models. The PF simulations are performed in a domain of a 200×2500 grid with \( \Delta x = 0.2 \mu m \), and \( G = 5000, 6000, 7000°C/m \), respectively. As discussed in section 4.1, in the case of \( V_p > V_{p,cr} \), the droplet migrates slower than the moving mushy zone, and it will approach solidus. Thus, at the beginning of simulation, one liquid droplet with a radius of 16\( \mu m \) is assigned at the initial liquidus position, i.e., \( y_0 = l_T \). According to equation (6), the conditions of \( y_0 = l_T \) and \( G = 5000~7000°C/m \) yield critical pulling velocities of \( V_{p,cr} = 8.5~11.9 \mu m/s \). Thus, a pulling velocity of \( V_p = 15 \mu m/s \) that is higher than the critical pulling velocity is imposed. Simulations are stopped when the liquid droplet reaches
the solidus position. Figure 5 shows the time evolution of the droplet migration velocity obtained from the two models for a SCN-0.3 wt.% ACE alloy at the conditions of $V_p=15 \mu m/s$ and $G=5000\text{°C}/m$. As expected, similar to the case of $V_p<V_p,cr$ in figure 4, the droplet migration velocity increases with increasing temperature gradient. For example, when the migration time is 5 s, the droplet migration velocities are around 6.8, 8.3, and 10.1$\mu m/s$, for $G=5000, 6000, \text{and} 7000\text{°C}/m$, respectively. As opposed to figure 4, however, during the droplet migration toward solidus, the droplet migration velocity decreases with time for each temperature gradient. In addition, it is noted that for a higher temperature gradient, a shorter time is needed for the droplet to migrate from liquidus to the solidus position. This is because a higher temperature gradient generates a shorter mushy zone length. The mushy zone lengths determined by $l_m=|m|(1-k)c_s^0/G$ are 392$\mu m$, 327$\mu m$, and 280$\mu m$, for $G=5000, 6000, \text{and} 7000\text{°C}/m$, respectively. Accordingly, the time required for a liquid droplet to go through the entire mushy zone decreases with increasing temperature gradient, although the upward velocity of the droplet migration increases with increasing temperature gradient as shown in figure 5.

![Figure 4](image1.png)  
Figure 4. Comparison of PF and analytical model results regarding the time evolution of droplet velocity for a SCN-0.3 wt.% ACE alloy at $V_p=2 \mu m/s$ ($V_0=0$) and various temperature gradients. (Symbols: PF model, lines: analytical model)

![Figure 5](image2.png)  
Figure 5. Comparison of PF and analytical model results regarding the time evolution of droplet velocity for a SCN-0.3 wt.% ACE alloy at $V_p=15 \mu m/s$ ($V_0=l_r$) and various temperature gradients. (Symbols: PF model, lines: analytical model)

5. Conclusions

Liquid droplet migration in a solid phase of SCN-ACE alloys caused by TGZM is simulated by employing a quantitative phase-field model for directional solidification. The simulation results are compared with an analytical model that describes the liquid droplet migration during TGZM for both static and dynamic conditions. In the analytical model, criteria are proposed for critical pulling velocity and critical droplet position, both yielding constant relative positions of the migrating droplet with respect to the moving liquidus and solidus.

The effect of the pulling velocity on the droplet migration kinetics is investigated. It is found that when the pulling velocity is lower than the critical pulling velocity, the droplet migrates from the initial location toward the moving liquidus, exhibiting an increasing velocity with time. However, when a pulling velocity higher than the critical pulling velocity is imposed, the droplet velocity gradually decreases with time. While the droplet always moves toward the high temperature direction, for a migration velocity of the droplet that is lower than the pulling velocity, the mushy zone migrates faster than the droplet. As a result, the droplet gradually approaches the moving solidus.
The migration behaviour of droplets with different initial locations has been studied. All droplets with various initial positions migrate upwards with time in a fixed coordinate system. The higher the position where the droplet is initially located, the faster it migrates. For a droplet that is initially located at the critical droplet position, its relative position with respect to the moving liquidus and solidus remains essentially unchanged. The droplets initially located above and below the critical position gradually approach liquidus and solidus, respectively.

The PF simulated evolution of droplet velocity as a function of time is also compared with the results of the analytical model for different temperature gradients. The results show that for the pulling velocity either higher or lower than the critical pulling velocity, the upward droplet migration velocity increases, while the time needed for a liquid droplet to go through the entire mushy zone decreases with increasing temperature gradient. It is found that the initial droplet velocity is non-zero and equals the critical pulling velocity, and it is also proportional to the temperature gradient.

It is found that the simulation data are slightly lower than the analytical predictions. This is considered to be caused by the two main reasons. First, the analytical model neglects, while the PF simulation includes the effect of curvature. Second, the diffuse interface in the PF model leads to some deviations from the precise thermodynamic equilibrium concentrations. Nevertheless, the PF simulation results are found to compare well with the analytical predictions, demonstrating the validity of the analytical model.

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