Simulating dendritic growth with convection

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Abstract

Starting with the effect of forced flows on the morphologies of growing dendrites, previous work on simulating dendritic growth with convection is summarized. In our work a fixed mesh for the temperature and a conformable mesh for velocity and concentration in a binary alloy are used; this method captures the morphology and motion of the complex solid-liquid interface. Convection is driven by thermo-solutal buoyancy and solidification contraction. Examples include: the natural convection near a dendrite of a pure substance growing in its under-cooled liquid; the dendritic growths of a pure substance and an alloy in their undercooled liquids, in which the convection is driven by buoyancy and solidification contraction; and the effects of convection driven by thermosolutal buoyancy and solidification contraction during the directional solidification of an alloy. Solidification contraction dominates the convection pattern, when the concentration of the alloy-element is dilute.

Keywords: Dendritic solidification; Binary alloys; Interface tracking

1. Introduction

Numerical modeling of dendritic growth without convection has been studied for two decades, using the phase-field method, the level-set method and explicit interface-tracking methods. The extension of these methods to include convection, however, is more recent. For pure substances, Tönhardt et al. [1] used a phase-field to simulate dendritic growth with forced flow and saw that growth of the side-branches was promoted on the upstream side. Tong et al. [2] also simulated the effects of forced flow on dendrite-growth using phase-field methods. Al-Rawahi et al. [3] and Udaykumar et al. [4] did simulations involving forced flow using front-tracking. Three-dimensional simulations of equiaxed dendrites of pure substances in forced convection were reported by Jeong et al. [5] and Boettinger et al. [6].

Simulations of dendritic growth with natural convection are few. Bänsch et al. [7] used a sharp interface for thermal convection around equiaxed dendrites. Tönhardt et al. [8] used a phase-field method. For small under-coolings, convection has a profound effect on dendrites; for larger under-coolings, the influence of thermal convection is small.

Simulation of non-dilute alloys is challenging even with no convection because of widely different length and time scales in the energy and mass transport and the partitioning of solute between phases with a strong dependence of the liquidus temperature on concentration [9]. Convection further confounds the problem. To deal with flow and moving boundaries various meshes have been used: fixed Cartesian-meshes and adaptive ones. The former include diffuse-interface methods, where the moving interface has a finite thickness of a few grid spacings [2,3,10], and the sharp interface methods, where interface conditions (thermodynamic and kinetic constraints) are applied directly [11]. Adaptive meshes may or may not conform to the moving interface. These comprise: (1) conformal mapping for simple geometries [12]; (2) node/mesh-moving methods that preserve the mesh structure [13]; and (3) re-meshing as the interface moves [14]. Others have used adaptive meshes that are locally refined and regenerated [5,8] or a coarse mesh, which is refined in the regions of steep gradients [15].

With finite-differences, a Cartesian-mesh has drawbacks: it is difficult to locally refine the grid, unless a fine grid is used throughout; and applying interface-conditions is difficult. In the generalized immersed boundary

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method [10], the forcing term is iteratively calculated and interpolated to the nodes until the velocity agrees with the interface velocity. Finite volumes with sharp interface were used by Udaykumar et al. [11], but the method can produce inaccuracies [16]. An adaptive-conformal mesh can be refined near the interface, and interface-conditions can be applied precisely. The trade-off is the need to regenerate the mesh every time-step and to interpolate to the new mesh.

2. Meshing for the finite-element method

We use a sharp-interface, finite-element model to simulate dendritic solidification of binary alloys with convection. The model was applied to dendritic growth of alloys without convection in Zhao et al. [14]. An adaptive mesh (very fine at the interface) is used to solve the concentration and momentum equations. The solid-liquid interface is explicitly tracked, and the interfacial conditions are applied directly [17]. The energy equation is solved on a fixed mesh of bilinear/triangular elements. The method requires very efficient re-meshing and interpolation between two different meshes [14,18,19]. Convection, including that driven by contraction and both thermal and solutal buoyancy, has been modeled.

We validated simulations for classical scenarios: for flow past a stationary cylinder for Reynolds numbers up to 100 we achieved excellent agreement with Fornberg [20]; for flow induced by an oscillating circular cylinder we produced results that compared almost exactly with the experimental data of Dütsch et al. [21]; and for the Benard instability we reproduced, almost exactly, the critical Rayleigh number and obtained excellent agreement with experiments [22]. Dendritic-growth with thermal convection was validated using the work of Tönhardt et al. [8].

Details regarding the tracking scheme and interaction between the moving interface, without convection, and the fixed mesh are in [9,14,17]. For dendritic growth into an undercooled pure melt, the model was tested against solvability theory in predicting the tip growth velocity. The model also predicts the outcomes of the linear stability theory of plane-front solidifcation. Buoyed by all these calculations, the present model is deemed appropriate for simulating dendritic solidification with convection.

3. Simulations of dendritic growth with convection

Figure 1 is an example of thermal convection near a dendrite that is growing in an under-cooled liquid. Thermal buoyancy, caused by latent heat release, forms two vortices above the crystal, which leads to the corresponding isotherms. Figures 2(a) and 2(b) compare the equiaxial dendrites of a pure substance and counterpart alloy when there is no convection. With convection caused by solidification contraction, growth of the side branches is more pronounced (Figs. 2(c) and 2(d)). Figure 3 shows directional solidification of a dilute alloy with thermo-solutal convection. The solidification contraction drastically changes the convection from recirculating cells (Fig. 3(a)) to flow downwards (Fig. 3(b)).

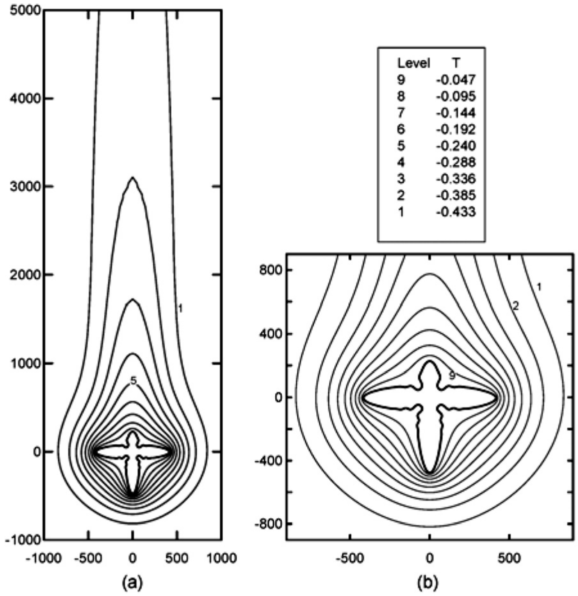

Fig. 1. Isotherms around a growing dendrite of succinonitrile showing the effects of natural convection: (a) full computational domain; (b) same as (a) but enlarged and near the dendrite.

4. Conclusions

To capture the morphology of growing dendrites using finite element methods, a conformable mesh for velocity and concentration and a fixed mesh for temperature have been used. The technique is robust enough to reproduce convection and solidification in many different cases of known results and to study coupling of natural convection and dendritic growths of pure substances or alloys growing in their under-cooled liquids or under directional solidification conditions. The convection can be driven by thermosolutal-buoyancy and solidification contraction. The contraction dominates the convection pattern when the concentration of the alloy element is dilute.

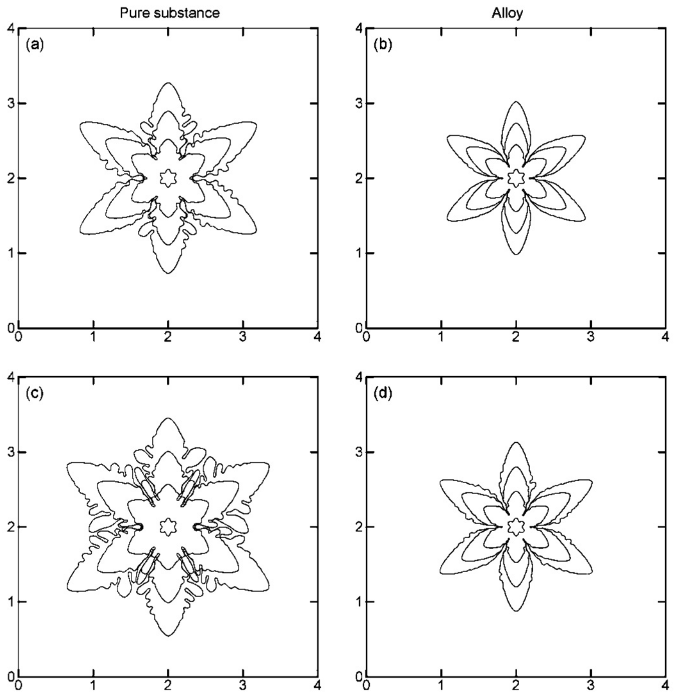

Fig. 2. Comparison of interface morphology in equi-axial solidification of a pure substance and an alloy with and without contraction-induced convection: (a) pure substance without convection; (b) alloy without convection; (c) pure substance with convection; (d) alloy with convection.

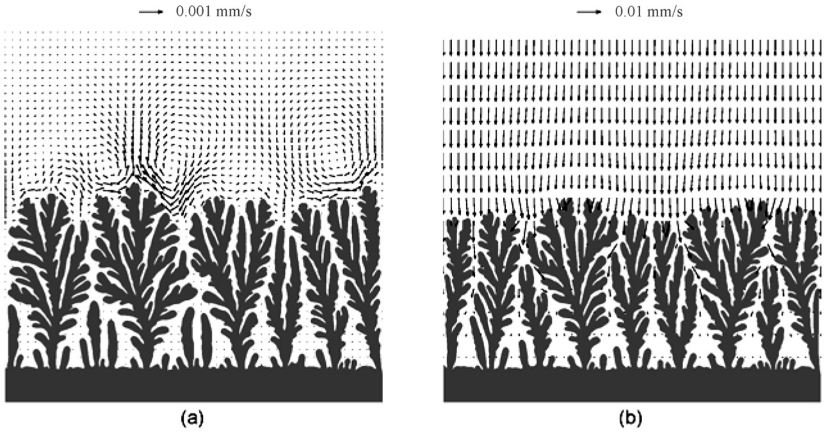

Fig. 3. Dendrites and velocity vectors in directional solidification of Pb-0.2wt%Sb alloy with thermosolutal convection: (a) at 3.4 s without contraction; and (b) at 3.4 s with contraction.

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