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Numerical investigations of drop solidification on a cold plate in the presence of volume change

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ABSTRACT

We present a front-tracking/finite difference method for simulation of drop solidification on a cold plate. The problem includes temporal evolution of three interfaces, i.e. solid–liquid, solid–gas, and liquid–gas, that are explicitly tracked under the assumption of axisymmetry. Method validation is carried out by comparing computational results with exact solutions for a two-dimensional Stefan problem, and with related experiments. We then use the method to investigate a drop solidifying on a cold plate in which there exists volume change due to density difference between the solid and liquid phases. Numerical results show that the shape of the solidified drop is profoundly different from the initial liquid one due to the effects of volume change and the tri-junction in terms of growth angles ϕ_{gr} on the solidification process. A decrease in the density ratio of solid to liquid ρ_{sl} or an increase in the growth angle results in an increase in the height of the solidified drop. The solidification process is also affected by the Stefan number *St*, the Bond number *Bo*, the Prandtl number *Pr*, the Weber number *We*, the ratios of the thermal properties of the solid to liquid phases k_{sl} and C_{psl}. Increasing *St*, *Bo*, *Pr*, *We*, or k_{sl} decreases the solidified drop height and the time to complete solidification. Moreover, the solidification growth rate is strongly affected by *St*, k_{sl} and C_{psl}. An increase in any of these parameters hastens the growth rate of the solidification interface. Contrarily, increasing ρ_{sl} decreases the growth rate. However, other parameters such as ϕ_{gr}, *Bo*, *Pr* and *We* have minor effects on the solidification growth rate.

Introduction

Solidification processes that involve solid, liquid and gas appear in many methods of growing crystals from melts such as Czochralski crystal growth (Porrini, 2001), float-zone processing (Markvart, 2000), laser welding (Booth, 2004), and spraying (Minemoto and Takakura, 2007). The three phases meet at a tri-junction, and the solid phase comes directly from the melt. The evolution of the solidification interface, i.e. the interface separating solid and liquid, and the tri-junction conditions determine the form of the solidified product. In addition, density difference between solid and liquid in conjunction with the tri-junction effect can produce a curious shape (Ajaev and Davis, 2004). Volume change caused by this density variation also leads to formation of porosity, stresses or microcracks (Lee and Hwang, 1996; Raessi and Mostaghimi, 2005).

A drop solidifying on a cold plate, which includes the above-mentioned aspects, has received much attention. Anderson et al. (1996) did an experiment using water, which experiences volume expansion upon solidification, to check the dynamical conditions at the tri-junction. Hu and Jin (2010) used a molecular tagging thermometry technique to reveal heat transfer and the phase change process of water. Some other experimental studies using water can be found in Enríquez et al. (2012), and Snoeijer and Brunet (2012). In these works, freezing started at the cold plate, and the solidification interface moved upward continuously. Afterward, the frozen drop had a conical tip near the axis of symmetry, very different from the initial water drop, due to volume expansion and the tri-junction effect. Similar revelations with silicon (Si), germanium and indium antimonide have been found (Itoh et al., 2014; Satunkin, 2003). In industrial applications, formation of solid from the melt on a cold plate has been widely used to produce single crystal particles for high efficiency solar cells (Conklin and Stevens, 1995; Padovani and Stevens, 1997) and for use in semiconductors (Nakata, 1998). To understand the process, a

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simplified model (Snoeijer and Brunet, 2012) has been used. Another simple model with the dynamical tri-junction conditions has been used in Anderson et al. (1996). However, these models do not clarify heat transfer and the flow field during solidification.

Even though there have been many experimental studies, fully resolved direct numerical simulations of this problem are still lacking. Schultz et al. (2001) used a boundary integral method to investigate a drop solidifying on a cold plate, but neglecting the gravity effect. A similar method with fixed contact angles has been used by Ajaev and Davis (2004) to consider the effect of the density difference and contact angles on the solidification process of a spherical drop in space. Gravity has been neglected. Virozub et al. (2008) included the gravity and surface tension effects in the problem of a drop solidifying on a cold plate. The Young–Laplace equation in conjunction with a constant growth angle was numerically solved to find the position of the liquid–gas front. In another work (Pasandideh-Fard et al., 2002), the volume of fluid method combined with the enthalpy method has been used to investigate the solidification process of a metal drop spreading and solidifying on a cold plate. However, volume change upon solidification was not accounted for. We recently have included all above-mentioned aspects in the simulation of the drop solidification, but detailed investigations have not been reported (Vu et al., 2013).

It appears that detailed numerical calculations on the solidification process of a liquid drop on a cold plate, which includes volume change upon solidification, are still lacking in the literature. Our literature search, summarized above, has not turned up systematic information on how volume change, tri-junction, gravity, surface tension and so on affect the process. In addition, no simulations have considered the detailed flow fields within and around the drop during solidification. These gaps motivate our present study on this problem, which is extremely important both academically and in its industrial applications (Conklin and Stevens, 1995; Nakata, 1998; Padovani and Stevens, 1997). Here, we apply the front-tracking/finite difference method for dendritic solidification (Al-Rawahi and Tryggvason, 2002) and impose simple tri-junction conditions to simulate a drop solidifying on a cold plate. We examine on the effects of various parameters such as the solid-to-liquid density ratio (volume change), the growth angle (tri-junction condition), the Stefan number, the Weber number (interfacial tension acting on the gas–liquid interface), the Bond number (gravity) as well as the thermal property ratios of the solid to the liquid on the solidification process.

Mathematical formulation and numerical parameters

Fig. 1 shows the investigated problem. An axisymmetric drop on a cold plate held at cold temperature T_c, surrounded by ambient gas at temperature T_g, solidifies from the bottom. Initially, the liquid's temperature is set to a value T_h that is greater than or equal to its melting temperature T_m. We assume that the fluids are incompressible, and Newtonian. Volume change is assumed to occur only at the phase change front. For computation purposes, we treat all phases as one continuum with variable properties such as density ρ, viscosity μ, thermal conductivity k and heat capacity C_p. In terms of this single-field representation, the momentum and thermal energy equation are

$$\frac{\partial}{\partial t}\rho\mathbf{u} + \nabla\cdot\rho\mathbf{u}\mathbf{u} = -\nabla p + \nabla\cdot\mu(\nabla\mathbf{u} + \nabla\mathbf{u}^T) + \rho\mathbf{g} + \int_f \sigma\kappa\mathbf{n}_f\delta(\mathbf{x}-\mathbf{x}_f)dS \tag{1}$$

$$\frac{\partial}{\partial t}(\rho C_p T) + \nabla\cdot(\rho C_p T\mathbf{u}) = \nabla\cdot(k\nabla T) + \int_f \dot{q}\delta(\mathbf{x}-\mathbf{x}_f)dS \tag{2}$$

Here, $\mathbf{u}$ is the velocity vector, p is the pressure, and $\mathbf{g}$ is the gravitational acceleration. At the interfaces, denoted by f, σ is the interfacial tension acting on the gas–liquid front. κ is twice the mean curvature, and $\mathbf{n}_f$ is the normal vector to the interface. The Dirac delta function $\delta(\mathbf{x}-\mathbf{x}_f)$ is zero everywhere except for a unit impulse at the interface $\mathbf{x}_f$. T and the superscript T denote respectively the temperature and the transpose. S indicates the drop and solidification surfaces. D/Dt is the material derivative. $\dot{q}$ is the heat flux at the solidification interface, given as

$$\dot{q}_f = k_s\frac{\partial T}{\partial n}\Big)_s - k_l\frac{\partial T}{\partial n}\Big)_l \tag{3}$$

where the subscript s and l represent solid and liquid, respectively. The velocity field can be written as

$$\mathbf{u} = \mathbf{u}_l I_s + \mathbf{u}_s(1-I_s) \tag{4}$$

where I_s is an indicator function which is one in the fluids (i.e. liquid and gas) and zero in the solid. I_s is determined from front properties

$$\nabla I_s = \int_f \delta(\mathbf{x}-\mathbf{x}_f)\mathbf{n}_f dS \tag{5}$$

Since the solid phase is stationary, $\mathbf{u}_s = \mathbf{0}$, the assumption that volume change occurs only at the solidification front yields the following mass conservation equation

$$\nabla\cdot\mathbf{u} = \frac{1}{L_h}\left(\frac{1}{\rho_s}-\frac{1}{\rho_l}\right)\int_f \delta(\mathbf{x}-\mathbf{x}_f)\dot{q}_f dS \tag{6}$$

where L_h is the latent heat of fusion. Detailed derivations of the above equations can be found elsewhere, e.g. Esmaeeli and Tryggvason (2004a), noting that we have here a stationary solid. The effect of the temperature on the surface tension force acting on the gas–liquid interface (Nas and Tryggvason, 2003) is given by

$$\sigma = \sigma_0 - \beta_\sigma(T - T_m) \tag{7}$$

where σ_0 and β_σ are the surface tension coefficient at a reference temperature (i.e. T_m) and the Marangoni tension coefficient.

We choose the wetting radius R (see Fig. 1) as a scaling length, and $\tau_c = \rho_l C_{pl} R^2/k_l$ as the characteristic time scale. The characteristic velocity scale is thus taken to be $U_c = R/\tau_c$. With the above choices, it is possible to show that the dynamics of the problem is governed by the Prandtl number Pr, the Stefan number St, the Bond number Bo, the Weber number We, the Marangoni number Ma, the density ratios ρ_{sl} and ρ_{gl}, the viscosity ratios μ_{sl} and μ_{gl}, the thermal conductivity ratios k_{sl} and k_{gl}, and the heat capacity ratios C_{psl} and C_{pgl}

$$Pr = \frac{C_{pl}\mu_l}{k_l},\quad St = \frac{C_{pl}(T_m - T_c)}{L_h},\quad Bo = \frac{\rho_l g R^2}{\sigma_0},$$
$$We = \frac{\rho_l U_c^2 R}{\sigma_0},\quad Ma = \frac{\beta_\sigma R(T_m - T_c)}{\mu_l\alpha_l} \tag{8}$$

$$\rho_{sl} = \frac{\rho_s}{\rho_l},\quad \rho_{gl} = \frac{\rho_g}{\rho_l},\quad \mu_{sl} = \frac{\mu_s}{\mu_l},\quad \mu_{gl} = \frac{\mu_g}{\mu_l}, k_{sl} = \frac{k_s}{k_l},$$
$$k_{gl} = \frac{k_g}{k_l},\quad C_{psl} = \frac{C_{ps}}{C_{pl}},\quad C_{pgl} = \frac{C_{pg}}{C_{pl}} \tag{9}$$

The temperature is non-dimensionalized as $\Theta = (T - T_c)/(T_h - T_c)$. The non-dimensional time is $\tau = t/\tau_c$.

Numerical method and validation

The numerical technique used in the present study is the front-tracking/finite difference method (Al-Rawahi and Tryggvason, 2002; Esmaeeli and Tryggvason, 2004a, 2004b) with modification to account for the presence of three phases, phase