Fluid Flow, Heat Transfer, and Solidification Near Tri-junctions

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Abstract

Steady, two-dimensional fluid flow and heat transfer are considered near tri-junctions at which solidification is occurring. Meniscus-defined configurations as well as closed configurations such as directional solidification are examined. The local wedge geometry admits separable solutions in plane polar coordinates. Over the class of functions which have bounded temperatures and velocities at the corner, LOCAL SOLUTIONS, those which satisfy all local boundary conditions, and PARTIAL LOCAL SOLUTIONS, those which satisfy all but the normal-stress boundary condition, are considered. The aim in this work is to describe local fluid flow and heat transfer in problems where solidification is occurring by identifying singularities in the heat flux and stress which are present at the tri-junction, determining the dependence of these singularities on the wedge angles, and determining when specific wedge geometries are selected. It is found that the locally dominant flow is that due to the expansion or contraction of the material upon solidification.

1. Introduction

Corner flows always are present at the "edges" of fronts that define phase transformation. For example, if a droplet of volatile liquid spreads on a heated surface, the evaporative mass loss near the contact line modifies the local dynamics[1]. Contact lines joining multiple-phase/multiple-field regions occur frequently in crystal growth systems. Meniscus-defined processes such as float-zone, and Czochralski systems, as well as other solidification processes are in this category (e.g. see Brown[2]).

Two-dimensional isothermal viscous flow in a corner region has been studied by several authors. Dean and Montagnon[3] considered a wedge bounded by two rigid planes and determined properties of the flow as functions of the wedge angle. Michael[4] considered the same geometry but with one solid boundary and one free surface and found that in order for the free surface to be stress-free the wedge angle must be π. Moffatt[5] considered these cases as well as the case of a wedge bounded by two free surfaces and described in detail situations in which sequences of eddies, now known as Moffatt vortices, can be present in the flow. Proudman and Asadullah[6] considered a two-fluid system where the two fluids meet along a flat surface. They found that the presence of a second phase with small viscosity resulted in a new mode of flow not obtained by a single-phase analysis. Anderson and Davis[7] considered two-fluid isothermal flow in a wedge bounded by two rigid planes of arbitrary angle. They identified singularities in the flow, Moffatt vortices, as well as geometries consistent with separable local solutions. They showed that the two modes identified by Proudman and Asadullah[6] are present for all wedge angles.

Anderson and Davis[8] analyzed non-isothermal corner flow in single- and double-wedge geometries. They identified heat transfer modes which are the analogs to the flow modes found by Proudman and Asadullah[6]. They also found that in order for the free surface to be stress-free, a non-isothermal planar free surface must leave a planar rigid boundary at an angle of π, the same angle as that found by Michael[4] for a isothermal rigid/free wedge.

The goal of the present work is to extend the isothermal and non-isothermal corner flow results to cases of systems in which phase transformation is occurring. In Section 2 solidification is considered. The aim is to determine those wedge angles for which solutions exist, and identify the strengths of singularities in the stresses and heat fluxes as functions of the wedge angles.

The class of solutions to be considered have bounded temperatures and velocities at the wedge vertex. Furthermore, both LOCAL SOLUTIONS, those which satisfy *all* local boundary conditions, and PARTIAL LOCAL SOLUTIONS, those which, when free surfaces are present, satisfy all local boundary conditions with the exception of the normal-stress boundary condition, are sought. PARTIAL LOCAL SOLUTIONS are important in the description of the local flow valid for infinite surface tension (or zero capillary number). When perturbation methods for small capillary number are used, conditions on the flow imposed by the normal-stress boundary condition do not appear in the leading-order problem and therefore PARTIAL LOCAL SOLUTIONS can be viewed as leading-order solutions for these cases[7,8]. PARTIAL LOCAL SOLUTIONS also describe cases in which there exists an appropriate spatially-varying pressure distribution outside the free surface such that the normal-stress boundary condition is satisfied without further restriction on the flow[5]. Under such an assumption, the restriction of small capillary number is not necessary. When such provisions are made for the pressure, these solutions satisfy all local boundary conditions and can be thought of as specialized LOCAL SOLUTIONS.

2. Non-isothermal Flow with Solidification

Consider local fluid flow and heat transfer near contact lines at which solidification is occurring. The first problem of study is meniscus-defined solidification systems. The analysis is generic in that the local wedge geometry is present in many problems in this category, e.g. Czochralski systems, float-zone systems, and surface welding systems[2]. Later, a directional solidification system is considered.

Table 1: Types of boundary conditions for flow with solidification.

	Hydrodynamic		Thermal		
	$\theta = 0$	$\theta = \alpha_2$	$\theta = -\alpha_1$	$\theta = 0$	$\theta = \alpha_2$
Meniscus-Defined Growth	rigid, nonmaterial	free	nf	melting temp heat balance	nf
Directional Solidification	rigid, nonmaterial	rigid	nf	melting temp heat balance	nf

In each case, there is heat transfer in two phases but flow in just one. For simplicity thermocapillary effects are neglected. The boundary conditions for these two systems are outlined in Table 1. Here "rigid, nonmaterial" indicates that there is a net mass flux through the surface due to solidification resulting in nonzero normal and tangential velocities, "rigid" and "free" indicate planar rigid and planar free surfaces, respectively, "nf" indicates a no-flux thermal boundary condition, "melting temp" indicates that the solidification front at $\theta = 0$ is at the melting temperature, T_M, and "heat balance" indicates that the jump in heat flux across the interface is balanced by the release of latent heat. Note that the flow has a locally-driven component due to the phase transformation at the solidification front.

Meniscus-Defined Systems: The geometry is shown in figure 1. The solid phase is represented by the wedge between $\theta = 0$ and $\theta = -\alpha_1$ and the liquid phase is represented by the wedge between $\theta = 0$ and $\theta = \alpha_2$. The boundary between the two phases, $\theta = 0$, is the solidification front. Each boundary is assumed to be planar. The radial distance from the corner is r. In a typical meniscus-defined crystal growth system the third region (or wedge) would represent a gas phase, which here is taken to be passive. A reference frame is defined in which the solidification front is stationary and the solid/gas interface is parallel to the pulling velocity, $\boldsymbol{V}$, (i.e. the steady-state case).

The energy equations for both the solid and the liquid contain translational terms due to the moving reference frame. However, these equations simplify near the corner region. The governing equations for this system are

$$\nabla^2 T_S = 0 \quad \text{in the solid} \tag{2.1a}$$

$$\nabla^2 T_L = 0 \quad \text{in the liquid} \tag{2.1b}$$

and

$$\nabla^4 \psi = 0 \quad \text{in the liquid} \tag{2.1c}$$

when $r \ll \min(\mathcal{K}_L^{(th)}/|\boldsymbol{V}|, \mathcal{K}_S^{(th)}/|\boldsymbol{V}|, \nu/|\boldsymbol{V}|, \mathcal{K}_L^{(th)}/U, \mathcal{K}_S^{(th)}/U, \nu/U)$ where $\mathcal{K}_L^{(th)}$ and $\mathcal{K}_S^{(th)}$ are the thermal diffusivities of the liquid and solid, respectively, ν is the kinematic viscosity, and U is a velocity scale. The thermal boundary conditions are

$$\frac{\partial T_S}{\partial \theta} = 0 \quad \text{on } \theta = -\alpha_1 \tag{2.2a}$$

$$T_S = T_L = T_M \qquad \text{on } \theta = 0 \tag{2.2b}$$

$$\frac{\rho_S L_v v_n r}{k_L} = k\frac{\partial T_S}{\partial \theta} - \frac{\partial T_L}{\partial \theta} \qquad \text{on } \theta = 0 \tag{2.2c}$$

$$\frac{\partial T_L}{\partial \theta} = 0 \qquad \text{on } \theta = \alpha_2 \tag{2.2d}$$

where T_M is the melting temperature, ρ_S is the solid density, L_v is the latent heat, and $k \equiv k_S/k_L$ is the ratio of thermal conductivities (solid to liquid). Note that $v_n = -|\boldsymbol{V}|\sin\alpha_1$ and $v_t = |\boldsymbol{V}|\cos\alpha_1$ are the normal and tangential components of the velocity of the solidification front. The hydrodynamic boundary conditions are

$$\frac{\partial \psi}{\partial r} = -\rho v_n \quad \text{on } \theta = 0 \tag{2.3a}$$

$$\frac{1}{r}\frac{\partial \psi}{\partial \theta} = v_t \quad \text{on } \theta = 0 \tag{2.3b}$$

$$\psi = 0 \quad \text{on } \theta = \alpha_2 \tag{2.3c}$$

$$\frac{\partial^2 \psi}{\partial \theta^2} = 0 \quad \text{on } \theta = \alpha_2 \tag{2.3d}$$

$$-p + \frac{2\mu}{r}\left(\frac{1}{r}\frac{\partial \psi}{\partial \theta} - \frac{\partial^2 \psi}{\partial r \partial \theta}\right) = 0 \quad \text{on } \theta = \alpha_2 \tag{2.3e}$$

where $\rho \equiv \rho_S/\rho_L$ is the density ratio (solid to liquid), p is the pressure, and μ is the viscosity. When $|\boldsymbol{V}| = 0$, there is no solidification, $v_n = v_t = 0$, and the system is locally unforced;

this corresponds to a single-phase rigid/free wedge problem (see Moffatt[5] or Anderson and Davis[7]). The forcing terms in equation (2.3) drive a flow with $\psi \sim r$. When $\rho = 1$ there is no locally generated flow at the solidification front. When $\rho > 1$ fluid is pulled toward the solidification front from infinity in order to conserve mass. When $\rho < 1$ the flow is oppositely directed.

The heat balance boundary condition (2.2c) suggests that the particular solution for the temperature is linear in r. However, the homogeneous solution, satisfying

$$k\frac{\partial T_S}{\partial \theta} = \frac{\partial T_L}{\partial \theta} \tag{2.4}$$

is also possible. The homogeneous solution will be dominant if it approaches zero slower than r, the radial dependence of the particular solution, as $r \to 0$.

Locally, there is no direct coupling between the thermal and flow problems, so we can determine the thermal and flow solutions separately. They are linked through the restrictions they each place on the wedge angles. The *particular* solution to thermal problem, which is linear in r and balances terms on the left-hand-side of equation (2.2c), is given by

$$T_S^{(p)} = T_M + A_S^{th} r \sin\theta \tag{2.5a}$$

$$T_L^{(p)} = T_M + \left(kA_S^{th} - \frac{\rho_S L_v v_n}{k_L}\right) r \sin\theta. \tag{2.5b}$$

This solution requires that $\alpha_1 = \alpha_2 = \pi/2$. The *homogeneous* contributions to the thermal fields are given by

$$T_S^{(h)} = T_M + A^{th} r^{\tau} \sin\tau\theta \tag{2.6a}$$

$$T_L^{(h)} = T_M + A^{th} k r^{\tau} \sin\tau\theta \tag{2.6b}$$

with the constraints

$$\alpha_1 = (p/q)\alpha_2 \tag{2.7}$$

$$\tau = (q\pi)/(2\alpha_2) \tag{2.8}$$

where p and q are any positive, odd integers. It is important to note here that either the particular *or* or homogeneous thermal field may be dominant near the corner. Specifically, when $\tau < 1$, the homogeneous thermal field is dominant. It follows from equation (2.8) that only the case $q = 1$ gives $\tau < 1$. This requires $\alpha_2 > \pi/2$. To see that no larger values of q give $\tau < 1$ note that for $q \geq 5$, $\tau < 1$ requires that $\alpha_2 > 5\pi/2$; such angles are not physically possible. For $q = 3$, $\tau < 1$ requires that $\alpha_2 > 3\pi/2$. However, (2.7) requires that $\alpha_1 = (p/3)\alpha_2$. So $\alpha_1 > p\pi/2 \geq \pi/2$ and $\alpha_1 + \alpha_2 > 2\pi$, which is not physically possible. By a similar argument we can deduce that $\tau < 1$ only when $\alpha_1 = \alpha_2$ (i.e. $p = 1$ and $q = 1$). Therefore, the homogeneous thermal field is dominant only when $\alpha_1 = \alpha_2 > \pi/2$.

Next, we consider the flow problem. We assume a streamfunction given by

$$\begin{aligned}\psi = \; & r^{\sigma+1}[A_\sigma \cos(\sigma+1)\theta + B_\sigma \sin(\sigma+1)\theta + C_\sigma \cos(\sigma-1)\theta + D_\sigma \sin(\sigma-1)\theta] \\ & + r^2(A_1 \cos 2\theta + B_1 \sin 2\theta + C_1\theta + D_1) \\ & + r(A_0 \cos\theta + B_0 \sin\theta + C_0\theta\cos\theta + D_0\theta\sin\theta)\end{aligned} \tag{2.9}$$

where A_i, B_i, C_i, D_i for $i = 0, 1, \sigma$ ($\sigma \neq 0, 1$) are unknown constants to be determined by the boundary conditions. In general, one or more of these coefficients will be left undetermined by the local analysis; these are in principle determined by matching to an outer flow. The exponent σ, which arises as a separation constant, may be complex and is taken to have positive real part. Values of σ with $\mathrm{Re}(\sigma) < 0$ are not considered since they lead to unbounded velocities at the wedge vertex, $r = 0$. The dominant contribution to the flow corresponds to the exponent of r with the smallest real part.

Both LOCAL SOLUTIONS and PARTIAL LOCAL SOLUTIONS are sought. The LOCAL SOLUTION satisfying the boundary conditions (2.3) is given by

$$\psi = r|\boldsymbol{V}|(\rho \sin\alpha_1 \cos\theta + \cos\alpha_1 \sin\theta) \tag{2.10}$$

provided that the condition

$$\rho \sin\alpha_1 \cos\alpha_2 + \cos\alpha_1 \sin\alpha_2 = 0 \tag{2.11}$$

is satisfied. Notice that this is simply a uniform flow feeding the solidification and corresponds to zero normal and zero tangential stress on the free surface $\theta = \alpha_2$. When $\rho = 1$, this flow corresponds to a uniform translation at the pulling speed $|\boldsymbol{V}|$. Note that when $\alpha_2 = \pi$ there are no physically allowable values of α_1 satisfying condition (2.11). Therefore, one cannot superpose onto this flow an unforced flow, corresponding to $|\boldsymbol{V}| = 0$, which requires $\alpha_2 = \pi$ in order to satisfy all local boundary conditions[4].

It is of interest to determine the wedge angles which satisfy the restrictions placed by the thermal fields as well as by the flow field. First note that when $\alpha_1 = \alpha_2$, equation (2.11) gives $\sin 2\alpha_1 = 0$ for all values of ρ. This suggests that $\alpha_1 = \alpha_2 = \pi/2$. As a result, the only thermal field of interest is the particular solution (2.5). In this case, both the temperature and streamfunction are linear in r.

These local results show that the growth angle ϕ (see figure 1), which is defined by

$$\phi = -\pi + \alpha_1 + \alpha_2, \tag{2.12}$$

must be zero. This can be compared with the results of Surek and Chalmers[9] who used a float-zone technique to measure ϕ. They studied silicon ($\rho = 0.909$) and germanium ($\rho = 0.9546$) and found values of ϕ to be 11° and 8°, respectively. The fact that our predicted value is $\phi = 0$ may suggest that the local angle found here is present on a smaller scale than the angle observed.

Next, PARTIAL LOCAL SOLUTIONS are sought. The same thermal-field results apply as given by equations (2.5)-(2.8). Now, however, the normal-stress condition (2.3e) on $\theta = \alpha_2$ is relaxed. The streamfunction is given by

$$\tilde{\psi} = \tilde{\psi}_I + r|\boldsymbol{V}|\left\{\rho \sin\alpha_1 \cos\theta + \cos\alpha_1 \sin\theta \right. \tag{2.13}$$
$$\left. - \frac{\rho \sin\alpha_1 \cos\alpha_2 + \cos\alpha_1 \sin\alpha_2}{\alpha_2 - \cos\alpha_2 \sin\alpha_2}\left[\theta\cos(\theta - \alpha_2) - \cos\alpha_2 \sin\theta\right]\right\}$$

where $\tilde{\psi}_I$ represents the homogeneous contribution to the flow corresponding to isothermal flow in a rigid/free wedge and is given by Anderson and Davis[7] by their equations (2.22), (2.28), (2.29), (2.30), or (2.32), depending on α_2, where the exponent σ in the most general case is given by

$$\sigma \sin 2\alpha_2 - \sin 2\sigma\alpha_2 = 0. \tag{2.14}$$

This restriction on σ is that found by Moffatt[5] for a rigid/free wedge. Regardless of the value of α_2 and regardless of the isothermal contribution to the flow, the *local* flow is always dominated by the locally-driven flow due to phase change. There is an r^{-1} singularity in the stress at the corner due to the term in the streamfunction proportional to $r\theta\cos(\theta - \alpha_2)$. Note that this singularity is not present in the LOCAL SOLUTIONS.

One must interpret the restrictions placed on the wedge angles, α_2 and α_1, and exponents, τ and σ. The thermal problem requires that $\alpha_1 = \alpha_2 \geq \pi/2$. The particular thermal field (2. 5) is dominant when the equality holds and the homogeneous thermal field (2.6) is dominant otherwise. The value of τ is given by $\tau = \frac{1}{2}\pi/\alpha_2$. Note that when $\alpha_1 = \alpha_2 > \pi/2$ the heat flux is singular. Also note that neither α_1 nor α_2 can exceed π. Equation (2.14) determines the value of σ for the flow field and does not involve the solid angle, α_1. While the value of σ is given by equation (2.14), the stress field now has an r^{-1} singularity due to the terms in the streamfunction proportional to $r\theta\cos\theta$ and $r\theta\sin\theta$. This is the dominant singularity.

DIRECTIONAL SOLIDIFICATION SYSTEM: The geometry for this system is shown in figure 2. The boundaries $\theta = \alpha_2$ and $\theta = \alpha_2 - \pi$ are rigid surfaces and $\theta = 0$ represents the solid/liquid interface. The container, or ampoule, is pulled upwards with velocity $\boldsymbol{V}$. A reference frame is used in which the solid/liquid interface is stationary.

The problem formulation remains the same as for the meniscus-defined systems with the exception of the hydrodynamic boundary conditions. For the directional solidification system these are

$$\frac{\partial\psi}{\partial r} = -\rho v_n \quad \text{on } \theta = 0 \tag{2.15a}$$

$$\frac{1}{r}\frac{\partial\psi}{\partial\theta} = v_t \quad \text{on } \theta = 0 \tag{2.15b}$$

$$\psi = 0 \quad \text{on } \theta = \alpha_2 \tag{2.15c}$$

$$\frac{1}{r}\frac{\partial\psi}{\partial\theta} = -|\boldsymbol{V}| \quad \text{on } \theta = \alpha_2. \tag{2.15d}$$

Here $v_n = -|\boldsymbol{V}|\sin\alpha_2$ and $v_t = -|\boldsymbol{V}|\cos\alpha_2$. Notice that there is no free surface upon which thermocapillarity can act.

The thermal problem is the same as in the meniscus-defined systems. However, since the present geometry has a total wedge angle, $\alpha_1 + \alpha_2$, of π, the results are limited to the case $\alpha_1 = \alpha_2 = \pi/2$. Therefore, the thermal fields are given by equation (2.5) and are nonsingular. The streamfunction given by equation (2.9). As in the meniscus-defined case, the inhomogeneous boundary terms must be balanced by the terms linear in r. In this case the streamfunction is given by

$$\psi = \frac{2D_\sigma r^{\sigma+1}}{(\sigma+1)\sin\sigma\frac{\pi}{2}}g(\theta,\sigma) + r|\boldsymbol{V}|\left\{\rho\cos\theta + \frac{(1-\rho)}{(\frac{\pi}{2})^2 - 1}\left[\theta\sin\theta + \frac{\pi}{2}(\theta\cos\theta - \sin\theta)\right]\right\} \tag{2.16}$$

where $g(\theta,\sigma)$ is given by

$$\frac{g(\theta,\sigma)}{\sin\sigma\frac{\pi}{2}} \equiv \cos\theta\sin\sigma\theta - \frac{\sin\sigma(\frac{\pi}{2}-\theta)}{\sin\sigma\frac{\pi}{2}}\sigma\sin\theta \tag{2.17}$$

and σ by

$$\sigma \pm \sin\sigma\frac{\pi}{2} = 0. \tag{2.18}$$

This restriction on σ is that found by Dean and Montagnon[3] for a rigid/rigid wedge of angle $\pi/2$. Note that the largest contribution locally is due to the term linear in r. The contribution from the far field only becomes important away from the corner. Typical flows showing the contribution from the first *two* dominant terms in the streamfunction are sketched in figure 3. The two sketched flows shown in this figure correspond to $|\boldsymbol{V}| = 1$, $\rho = 1$, $\alpha_2 = \pi/2$, and $D_\sigma = 1$ (upper figure) and -1 (lower figure). While the far field flow has a significant effect on the flow a finite distance from the corner, the flow sufficiently near the corner is always dominated by that associated directly with the solidification process (see inset). Recall that there is a r^{-1} singularity in the stress due to the presence of the terms $\theta\sin\theta$ and $\theta\cos\theta$, which vanish only when $\rho = 1$.

3. Summary

We have presented a local picture of fluid flow and heat transfer near tri-junctions at which solidification is occurring. The class of solutions sought are those with bounded temperatures and velocities at the wedge vertex. Locally, the governing equations simplify to Laplace's equation and the biharmonic equation for the temperature and streamfunction, respectively. Separable solutions for the temperature and streamfunction are written as $T \sim r^{\tau} f_{\tau}(\theta)$ and $\psi \sim r^{\sigma+1} f_{\sigma}(\theta)$, respectively. For the streamfunction, one distinguishes between LOCAL SOLUTIONS, those which satisfy all local boundary conditions, and PARTIAL LOCAL SOLUTIONS, those which satisfy all local boundary conditions except for the normal-stress boundary condition. The analysis provides locally valid solutions that identify the types of singularities present at the corner and shows how these singularities vary with the wedge angles.

Two different systems are considered; meniscus-defined solidification systems and directional solidification systems. The analysis is generic in that many different solidification configurations have the same type of local tri-junction region.

In the meniscus-defined solidification system it is found that for LOCAL SOLUTIONS the resulting flow is just a uniform flow towards the solidification front and has both the solid and liquid wedge angles, α_1 and α_2, respectively, equal to $\pi/2$. This gives a growth angle, ϕ, of zero. This flow is nonsingular. Since the unforced version of the flow problem is the rigid/free wedge problem studied by Michael[4] and since a liquid wedge angle of π is not allowed in this system, no unforced flow solution can be superposed. For LOCAL SOLUTIONS, the dominant temperature exponent is $\tau = 1$; therefore the heat flux is never singular. For PARTIAL LOCAL SOLUTIONS the streamfunction has a locally-driven component due to the solidification but now, due to the relaxation of the normal-stress boundary condition, an unforced flow solution can be superposed. However, the locally dominant flow is that driven by the solidification. The temperature and velocity exponents, τ and σ, are functions of the wedge angles; there is no dependence on the density ratio. The stress field always has an r^{-1} singularity. The heat flux is singular only when both solid and liquid wedge angles are equal and greater than $\pi/2$.

In the directional solidification system the dominant flow is again the component driven by the phase transformation. The solidification front is found to be locally perpendicular to the sidewalls. The heat flux is always nonsingular.

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Figure 1: Meniscus-defined solidification: a typical tri-junction in a Czochralski crystal growth system. We use a reference frame in which the solid/liquid interface is stationary and the solid/gas interface is parallel to the pulling velocity, $\boldsymbol{V}$. The growth angle, ϕ, is shown.

Figure 2: Directional solidification: the tri-junction in a typical directional solidification system. The container walls are represented by the solid boundaries $\theta = \alpha_2$ and $\theta = \alpha_2 - \pi$ and the solid/liquid interface is represented by the boundary $\theta = 0$. We use a reference frame in which the solid/liquid interface is stationary.

Figure 3: Directional solidification: sketches of two possible flow fields for the directional solidification system. The parameters used here are $\boldsymbol{V} = 1$, $\rho = 1$, $\alpha_1 = \alpha_2 = \pi/2$, and $D_\sigma = 1$ (upper figure), -1 (lower figure). Here the first two dominant terms in the streamfunction have been considered. We see that the flow away from the corner depends on the far-field flow but that sufficiently near the corner the flow is completely driven by the phase-change process as shown in the inset.