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THERMOCAPILLARY FLOW NEAR A "COLD CORNER"

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The velocity field in a neighborhood of the point of contact between the free and solid boundaries is studied numerically for the problem of noncrucible zone melting in a two-dimensional model formulation. A distinct Prandtl boundary layer on the solid boundary and a Marangoni boundary layer on the free boundary and high gradients of the longitudinal velocity along the free boundary in the immediate vicinity of the "cold corner" are observed. It is found for the first time that with distance from the solid boundary, the velocity curve has a maximum, which is not typical of the ordinary flow near the solid boundary.

Introduction. In recent years, problems related to noncrucible zone melting are of great scientific and applied interest. The melting can be described as follows: a liquid zone is formed in a crystal (usually of cylindrical shape) which is placed inside a heater. Investigations of these problems can be divided into three groups: studies aimed at qualitative analysis of hydrodynamic phenomena [1] and experimental [2] and numerical studies. The goal of these investigations is to find the velocity and temperatures fields over the entire flow region [3]. The stability of the liquid zone has been examined in many papers (see, for example, [4, 5]). Asymptotic methods of solution have not been developed as yet. In numerical methods of solutions, which reflect adequately the situation in the central flow region, difficulties arise in work with corner regions. This is due to the fact that the liquid acceleration along the free boundary due to the Marangoni effect and the subsequent deceleration on the solid boundary cause fluctuations of the surface velocity near the "cold" walls. One method of overcoming these difficulties is proposed in [3], and another is considered in the present paper. The problem is investigated in a two-dimensional formulation: the Moffatt asymptotic relation [6] is used in the immediate vicinity of the contact point, the Prandtl–Batchelor scheme [7] in the flow core, and numerical calculation in the intermediate region.

1. Formulation of the Problem. Let the liquid phase occupy a rectangular region bounded by two solid rectilinear parallel boundaries between the solid and liquid phases and two rectilinear free boundaries between the liquid and the gas that are orthogonal to the former. The liquid is assumed to be viscous and incompressible and the flow is steady. A constant temperature gradient A, treated as a parameter, is specified on the free boundaries.

The characteristic liquid-flow velocity can be evaluated [8] by the formula

$$U = (h\nu)^{1/3}\Big(\frac{A|\sigma_T|}{\rho\nu}\Big)^{2/3},$$

where h is the characteristic length of the melting zone (the height of the rectangle), ν is the kinematic viscosity coefficient, σ_T is the coefficient in the linear dependence of the surface-tension coefficient on the temperature, and ρ is the density.

If the temperature gradient A is rather high and the above-mentioned physical parameters correspond to a melted semiconductor, the velocity reaches several centimeters per second. This is liquid flow at large Reynolds numbers, because, by definition, $\mathrm{Re} = Uh/\nu$.

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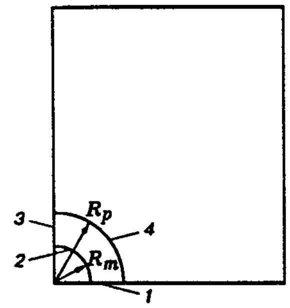

Fig. 1. Flow region: 1) solid boundary; 2) boundary of radius R_m (the Moffatt solution is applicable on it); 3) free boundary; 4) boundary of radius R_p (the Prandtl–Batchelor solution is applicable on it).

Thus, assuming that all streamlines in the rectangular region are closed, it is reasonable to use the Prandtl–Batchelor scheme [7]. However, immediately in the "cold" corner this scheme is inappropriate. Assuming that interesting effects occur in close proximity to the corner, we distinguish a sector in the corner and use its radius as a new characteristic dimension. Assuming that the attachment condition on the solid boundary (see Sec. 2) and the velocity-continuity condition are satisfied, for the liquid flow in this sector (the radius is small) we can use the Stokes approximation [9]:

$$\nabla p - \Delta \mathbf{v} = 0, \qquad \nabla \cdot \mathbf{v} = 0.$$

Here p is the pressure and $\mathbf{v}$ is the velocity vector. In this case, it is reasonable to use the Moffatt solution [6].

The region of investigation is chosen so that the Moffatt solution is valid on one boundary of the circular sector, the Prandtl–Batchelor solution is valid on the other boundary, the third boundary is free, and the fourth boundary is solid (Fig. 1).

In the region obtained, we solve complete Navier–Stokes equations written in polar coordinates (r, φ), in terms of the vorticity ω and stream function ψ:

$$\nu\Big(\frac{\partial^2\omega}{\partial r^2} + \frac{1}{r}\frac{\partial\omega}{\partial r} + \frac{1}{r^2}\frac{\partial^2\omega}{\partial\varphi^2}\Big) + \frac{1}{r}\Big(-\frac{\partial\omega}{\partial r}\frac{\partial\psi}{\partial\varphi} + \frac{\partial\omega}{\partial\varphi}\frac{\partial\psi}{\partial r}\Big) = 0,$$

$$\frac{\partial^2\psi}{\partial r^2} + \frac{1}{r}\frac{\partial\psi}{\partial r} + \frac{1}{r^2}\frac{\partial^2\psi}{\partial\varphi^2} = -\omega.$$

2. Derivation of Boundary Conditions. On the solid immovable boundary 1, the attachment condition [8]

$$u = 0, \quad v = 0, \tag{2.1}$$

where u and v are the velocity components along the x and y axes, respectively, is written in terms of the stream function as

$$\psi = 0, \quad \frac{\partial\psi}{\partial\varphi} = 0. \tag{2.2}$$

On the free boundary 3, the kinematic condition [8]

$$u = 0 \tag{2.3}$$

in terms of the stream function has the form

$$\psi = 0. \tag{2.4}$$

The dynamic condition is equivalent to two scalar conditions [8]. One of these (the equality of the difference between the normal pressure and atmospheric pressure to the capillary pressure) is assumed to be satisfied on the plane free boundary in a first approximation owing to the smallness of the capillary number $\text{Ca} = \sigma_T A/\sigma_0$, and the second condition should be satisfied:

$$2\rho\nu \mathbf{s} \cdot D \cdot \mathbf{n} = p - p_0 + \frac{\partial \sigma}{\partial s} \Longrightarrow P_{xy} = \rho\nu\left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}\right) = A|\sigma_T|. \tag{2.5}$$

Here $\mathbf{s}$ is a tangent vector, D is the strain tensor, $\mathbf{n}$ is the external normal vector to the free surface, $p_0 = \text{const}$ is the average pressure, P_{xy} is the strain-tensor component, $\sigma = \sigma_0 + \sigma_T(T - T_0)$ is the surface tension, $\sigma_0 = \text{const}$ is the average surface tension, T is the temperature, and $T_0 = \text{const}$ is the average temperature.

Equation (2.5) in terms of the vorticity has the form

$$\omega = \frac{A|\sigma_T|}{\rho\nu}. \tag{2.6}$$

The boundary 2 is chosen from considerations of applicability of the Moffatt solution, i.e., from the condition of smallness of the Reynolds number. For this, in the rectangular region we consider the equations

$$u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y} = -\frac{1}{\rho}p_x + \nu\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right), \qquad u\frac{\partial v}{\partial x} + v\frac{\partial v}{\partial y} = -\frac{1}{\rho}p_y + \nu\left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2}\right)$$

subject to the following boundary conditions: (2.1) on the solid boundary and (2.3), (2.5), and $T = Ay$ on the free boundary. Here p_x and p_y are the pressure-gradient components.

Let V be the velocity increment in the boundary layer and δ the thickness of the boundary layer. Then, from the equations and the boundary conditions we obtain

$$\frac{\rho\nu V}{\delta} = A|\sigma_T|, \qquad \frac{V^2}{h} = \frac{\nu V}{\delta^2},$$

whence we can estimate the thickness of the Marangoni boundary layer:

$$\delta = \left(\frac{\rho\nu^2 h}{A|\sigma_T|}\right)^{1/3}.$$

From the estimate of the Reynolds number through the estimate of the velocity increment V,

$$\text{Re} = \left(\frac{A|\sigma_T|h^2}{\rho\nu^2}\right)^{2/3}, \qquad V = (h\nu)^{1/3}\left(\frac{A|\sigma_T|}{\rho\nu}\right)^{2/3},$$

we can determine the radius of the boundary 2 $[\text{Re} = (VR_m/\nu) \ll 1]$:

$$R_m \ll \frac{1}{h^{1/3}}\left(\frac{\nu^2\rho}{2A|\sigma_T|}\right)^{2/3}$$

(R_m is of the order of $3 \cdot 10^{-5}$ cm).

We turn to constructing a Moffatt-type solution. In the plane case, the solution of the equation $\Delta\Delta\psi = 0$, which is equivalent to the Stokes system, is sought in form of the series

$$\psi = \sum_{k=1}^{\infty} r^k g_k(\varphi). \tag{2.7}$$

Substituting solution (2.7) into known formulas [9] for the strain-tensor components, we obtain

$$\begin{aligned} P_{rr} &= -p + 2\rho\nu\left(-\frac{\partial\psi}{\partial\varphi}\frac{1}{r^2} + \frac{1}{r}\frac{\partial^2\psi}{\partial\varphi\partial r}\right) = -p + 2\rho\nu(-r^{k-2}g_k'(\varphi) + kr^{k-2}g_k'(\varphi)), \\ P_{r\varphi} &= \rho\nu\left(\frac{1}{r^2}\frac{\partial^2\psi}{\partial\varphi^2} - \frac{\partial^2\psi}{\partial r^2} + \frac{1}{r}\frac{\partial\psi}{\partial r}\right) = \rho\nu(r^{k-2}g_k''(\varphi) - r^{k-2}g_k(\varphi)k(k-1) + kr^{k-2}g_k(\varphi)), \\ P_{\varphi\varphi} &= -p + 2\rho\nu\left(-\frac{1}{r}\frac{\partial^2\psi}{\partial r\partial\varphi} + \frac{1}{r^2}\frac{\partial\psi}{\partial\varphi}\right) = -p + 2\rho\nu(-kr^{k-2}g_k'(\varphi) + r^{k-2}g_k'(\varphi)), \end{aligned} \tag{2.8}$$

where P_{rr}, $P_{r\varphi}$, and $P_{\varphi\varphi}$ are the strain-tensor components. From (2.8) it is evident that terms with $k < 2$ give infinite stresses as $r \to 0$. This is impossible in the present problem, and, hence, only terms with $k \geqslant 2$

are retained. The solution is sought in the form $g_k(\varphi) = B\sin k\varphi + C\cos k\varphi + D\sin(k-2)\varphi + E\cos(k-2)\varphi$. The stream function and vorticity should satisfy boundary conditions (2.2), (2.4), and (2.6), which give the following conditions for $g_k(\varphi)$:

$$g_k(0) = 0, \qquad g_k'(0) = 0, \qquad g_k\Big(\frac{\pi}{2}\Big) = 0,$$
$$g_k''\Big(\frac{\pi}{2}\Big) = -\frac{A|\sigma_T|}{\rho\nu} \quad \text{for} \quad k = 2, \quad g_k''\Big(\frac{\pi}{2}\Big) = 0 \quad \text{for} \quad k \neq 2.$$

As a result, we obtain a system of four equations for four unknown coefficients B, C, D, and E. These equations are compatible for integer values of k, as shown by solution of the equation

$$k^2(k-2)\sin\frac{k\pi}{2}\cos(k-2)\frac{\pi}{2} + k(k-2)^2\cos\frac{k\pi}{2}\sin(k-2)\frac{\pi}{2}$$
$$= k^3\sin(k-2)\frac{\pi}{2}\cos\frac{k\pi}{2} + (k-2)^3\cos(k-2)\frac{\pi}{2}\sin\frac{k\pi}{2},$$

obtained by setting to zero the determinant of the corresponding matrix. The presence of real solutions ensures the absence of a periodic solution structure of the type of a chain of eddies. This follows immediately from [6] because, in the problem considered, the angle of contact of the solid and free boundaries is 90°, which exceeds the critical angle of 78°.

In view of the smallness of r, it is reasonable to ignore all terms with $k > 2$, and the solution have the form

$$\psi = r^2\frac{A|\sigma_T|}{\rho\nu}\Big(\frac{1}{2\pi}\sin 2\varphi - \frac{1}{4}\cos 2\varphi - \frac{1}{\pi}\varphi + \frac{1}{4}\Big).$$

Next, taking into account that $\omega = -\Delta\psi$, we write the condition for the vorticity as

$$\omega = \frac{A|\sigma_T|}{\rho\nu}\Big(\frac{4}{\pi}\varphi - 1\Big).$$

On boundary 4, the Prandtl–Batchelor [7] solution is assumed to be correct. To construct it in the rectangular region specified above, we solve the equation

$$\Delta\psi = -\Omega \tag{2.9}$$

subject to the boundary condition $\psi = 0$. Here Ω is the constant vorticity treated as the second parameter of the problem (the first parameter is the temperature gradient A). The solution of the inhomogenous equation (2.9) is sought as the sum of two solutions $\psi = \hat{\psi} + \Phi$: the partial solution $\hat{\psi} = (\Omega/2)x(l-x)$ for the inhomogenous equation (2.9) subject to the boundary conditions $\hat{\psi} = 0$ for $x = 0$ and $x = l$ and the general solution for the homogeneous equation $\Delta\Phi = 0$ subject to the boundary conditions $\Phi = 0$ for $x = 0$ and $x = l$, and $\Phi = -(\Omega/2)x(l-x)$ for $y = 0$ and $y = h$ $(0 \leqslant x \leqslant l)$. In turn, the homogeneous equation is solved by the method of separation of variables with subsequent expansion into a Fourier series in sinuses, extending the function $f(x) = -(\Omega/2)x(l-x)$ in an uneven manner (to the region $-l \leqslant x \leqslant 0$, where l is the length of the rectangle). This solution is not given herein. Thus, the conditions on boundary 4 have the form

$$\omega = \Omega, \qquad \psi = \frac{\Omega}{2}R_p\cos\varphi(l - R_p\cos\varphi) + \sum_{k=1}^{\infty} a_k \sin\frac{k\pi R_p\cos\varphi}{l},$$

where $a_k = 0$ for even k, and

$$a_k = -4\frac{\Omega l^2}{\pi^3 k^3}\Big(\cosh\frac{k\pi R_p\sin\varphi}{l} + \frac{1-\cosh(k\pi h/l)}{\sinh(k\pi h/l)}\sinh\frac{k\pi R_p\sin\varphi}{l}\Big) \tag{2.10}$$

for uneven k (R_p denotes the radius of the external boundary of the region for which the Prandtl–Batchelor solution is valid).

Hence, it is obvious that on boundaries 2–4 conditions exist for both ψ and ω, and on boundary 1 there is no condition for ω. The latter can be obtained using the approximate condition of [10], which is based on numerical representation of the condition for ω in terms of the condition for ψ using a Taylor series expansion. It is easy to see that in the "upper" corner, i.e., at the point of contact of the 3rd and 4th boundary, the conditions for ω do not join. It is known, however, that for thermocapillary-liquid flow at Re $\gg 1$, a Marangoni boundary layer is formed on the free boundary. This layer helps to smooth the condition for the "upper" corner [8]. A similar situation arises in the "lower" corner, i.e., at the point of contact of the 1st and 4th boundaries, where smoothing is performed using a Prandtl boundary layer. Thus, the problem is completely formulated.

3. Method of Numerical Solution. Introduction of polar coordinates made it possible to use a rectangular grid to find a numerical solution, which was obtained by a time-like iteration method, i.e., by introduction of fictitious time. We used the Peaceman–Rachford scheme (the equations were split by directions) with a "cross" stamp. For the equations in ψ, the difference analog is

$$\frac{\psi_{k,j}^{n+1/2} - \psi_{k,j}^{n}}{\tau/2} r_j^2 = r_j^2 \frac{\psi_{k,j+1}^{n+1/2} - 2\psi_{k,j}^{n+1/2} + \psi_{k,j-1}^{n+1/2}}{h_r^2} + r_j^2 \omega_{k,j}^{n}$$

$$+ r_j \frac{\psi_{k,j+1}^{n+1/2} - \psi_{k,j-1}^{n+1/2}}{2h_r} + \frac{\psi_{k+1,j}^{n} - 2\psi_{k,j}^{n} + \psi_{k-1,j}^{n}}{h_\varphi^2},$$

$$\frac{\psi_{k,j}^{n+1} - \psi_{k,j}^{n+1/2}}{\tau/2} r_j^2 = r_j^2 \frac{\psi_{k,j+1}^{n+1/2} - 2\psi_{k,j}^{n+1/2} + \psi_{k,j-1}^{n+1/2}}{h_r^2}$$

$$+ r_j \frac{\psi_{k,j+1}^{n+1/2} - \psi_{k,j-1}^{n+1/2}}{2h_r} + \frac{\psi_{k+1,j}^{n+1} - 2\psi_{k,j}^{n+1} + \psi_{k-1,j}^{n+1}}{h_\varphi^2}.$$

For ψ, the scheme is absolutely stable [11].

In the same manner, we write the difference analog of equations for ω, in which a counterflow difference scheme is used for convective terms [11]. The scheme is considered conditionally stable. All four equations are easily reduced to

$$a_j f_{k,j}^{n+1/2} + b_j f_{k,j+1}^{n+1/2} + c_j f_{k,j-1}^{n+1/2} + A_j = 0, \quad a_k f_{k,j}^{n+1} + b_k f_{k+1,j}^{n+1} + c_k f_{k-1,j}^{n+1} + A_k = 0.$$

The solution is performed by a diagonal-sweep method. Care should be taken that the condition of diagonal predominance $|a_j| \geqslant |b_j| + |c_j|$ is satisfied. Note that for $\psi_{k,j}^n$ it always holds.

To perform this estimate, in the program we adjust the step in the fictitious time τ in each time layer to the solution. The following numerical parameters of a germanium alloy were used: $\rho = 5.571$ g/cm^3; $\nu = 1.35 \cdot 10^{-3}$ cm^2/sec; $|\sigma_T| = 0.2$ g/(sec$^2\cdot$deg); $R_m = 10^{-7}$ cm; $R_p = 0.4$ cm; $l = 3$ cm; $h = 4$ cm; $5 \leqslant A \leqslant 10$ deg/cm; $A|\sigma_T|/(20\rho\nu) \leqslant \Omega \leqslant A|\sigma_T|/(4\rho\nu)$ sec^{-1}. By virtue of the smallness of the kinematic viscosity ν, it is convenient to perform scaling using R_p as the unit.

4. Calculation Results. For the problem of steady thermocapillary flow of a viscous incompressible liquid near the "cold" corner, we solved complete Navier–Stokes equations in the above-mentioned region bounded by the free, solid, and two specially chosen boundaries on which boundary conditions were formulated. Analysis of the resulting velocity fields yields a distinct Prandtl boundary layer on the solid boundary and a distinct Marangoni boundary layer on the free boundary. In addition, we obtained high gradients of the longitudinal velocity along the free boundary in the immediate vicinity of the "cold" angle. This was noted in [3] as the main difficulty in work with a "cold" corner.

Figure 2 shows curves of both velocity components at the solid boundary for four small values of x in the interval 10^{-3}–10^{-2} cm., i.e., at four close distances from the "cold" corner.

It is evident from Fig. 2a that with distance from the solid boundary, there is a maximum, which is untypical of ordinary flow at a solid boundary. This fact has not been described in the literature. From the viewpoint of physics, this phenomenon is similar to the processes occurring in a wall jet [12], for which the velocity curves have a similar shape.

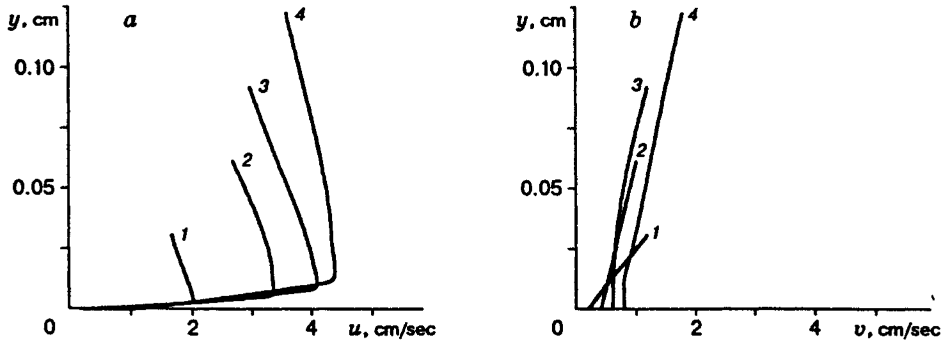

Fig. 2. Curves of the velocity components u (a) and v (b) for close distances from the "cold" corner (curves 1–4) at the solid boundary ($A = 5$ deg/cm and $\Omega = 6.649\ \text{sec}^{-1}$).

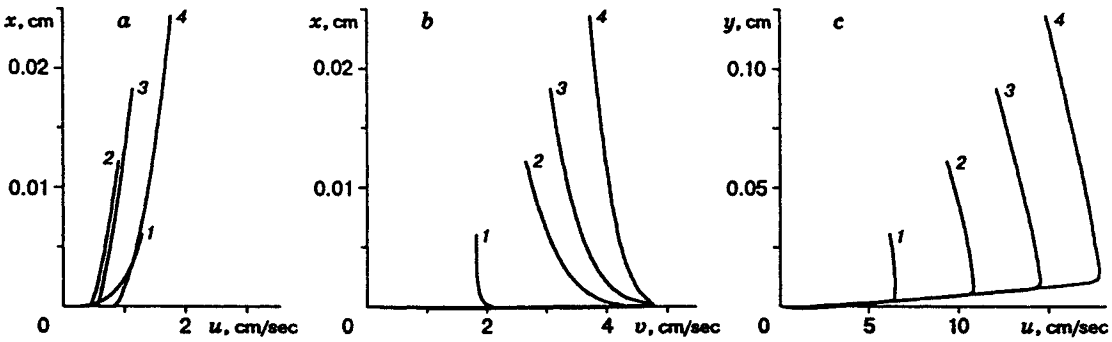

Fig. 3. Curves of the velocity components ($A = 5$ deg/cm) at the free boundary, $\Omega = 6.649\ \text{sec}^{-1}$ (a and b) and near the solid boundary, $\Omega = 33.245\ \text{sec}^{-1}$ (c); the notation is the same as in Fig. 2.

The velocity curves at the free boundary for four small values of y (in the interval 10^{-3}–10^{-2} cm) are shown in Fig. 3. Here of interest is the behavior of the velocity component directed parallel to the free boundary and having a maximum on the free boundary (Fig. 3b).

We note that with increase in both the temperature gradient A and the vorticity Ω, the modulus of the maximum velocity on the free boundary in the indicated region increases. In this case, the qualitative flow pattern does not change, as can be seen from Figs. 2a and 3c which give results for one value of the parameter A and two extreme values of the parameter Ω.

Conclusion. The problem considered can be called "too model" because of the assumption of a free surface "plane." However, the algorithm of solution applied to this problem is also suitable for the problem of a cylindrical free surface under the assumption of axisymmetric flow without swirling. The Moffatt solution can be used in studies of the region located in the immediate vicinity of the line of the three-phase contact, the Prandtl–Batchelor solution is applicable for the entire flow region, and numerical solution is performed for a similarly distinguished region. We note that the Prandtl–Batchelor scheme now implies consideration of the equation $w_t = kr$, where $k = \text{const}$ (k is a new parameter and w is a single nonzero vortex component). In this case, only representations of a_k change in the Prandtl–Batchelor solution (2.10), where Bessel functions are used instead of the hyperbolic functions, i.e., in the boundary condition for ψ on the boundary 4: $r = R_p$.

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