DETERMINATION OF THE INTERFACIAL BOUNDARIES DURING THE FORCED FLOW OF A LIQUID IN A SUPERCOOLED TUBE OF FINITE LENGTH

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The paper proposes an approximate method for determining the interfacial boundaries under conditions in which there are competing interactions of dissipative heat liberation and phase change.

# INTRODUCTION

In practically important processes involving the forced flow of liquids in supercooled pipelines, when frontal freezing of the liquid occurs from the wall, the important problem arises of determining the interfacial boundaries over the length of the pipe.

An approximate consideration of this problem is carried out in the present paper on the basis of an analytical solution obtained earlier [1] of the problem of the forced flow of a liquid in an infinitely long tube under conditions of phase change and the dissipative liberation of heat. The possibility of utilizing this solution is connected with the assumption that the picture of the flow changes slowly over the length of the tube, when considerable changes occur only over lengths which considerably exceed the tube diameter. In this case the time of passage of the phase front inwards can be determined, as in [1, 2], by using steady-state heat fluxes which do not depend explicitly on the coordinate z, and it is assumed that the temperature T and the velocity  $v_z$  depend only on the radius r. This is equivalent to the well-known lubrication approximation [3] in the hydrodynamic theory of lubrication, where it is assumed that by describing the complete developing flow in a circular tube with a cross section equal to the local gap it is possible to describe the actual flow in a tube whose radius varies over its length.

The steady-state profile of the interfacial boundaries over the tube length and the headflow characteristics are derived in the present paper.

By changing in the limit to the model of the infinite tube [1], the zone of applicability of this model is indicated. An analysis is also made of the effect of the entry zone on the flow characteristics.

# Statement of the Problem

We will consider the flow of a Newtonian liquid in a tube of circular cross section having radius  $r_0$  and length l, at the walls of which a constant temperature  $T_0$  is maintained which is smaller than the temperature of the phase change  $T_{\pm}$ . The liquid undergoes a phase change of the first type as a result of the cooling, and an internal interfacial surface is formed at  $r_{\pm}$ . The temperature dependence of the viscosity is assumed in the form  $n = n_0 \exp$ (E/RT). The equations for heat conduction and flow are written with the following assumptions: 1) the times of thermal and hydrodynamic relaxation are much smaller than the characteristic time of phase change, i.e., the following conditions are satisfied:

$$\frac{c_1}{Q_*} \quad \frac{RT_*^2}{E} \ll 1; \quad \frac{\lambda_1}{\eta(T_*)Q_*} \quad \frac{RT_*^2}{E} \ll 1;$$

2) the effects of the inertia terms in the equations of motion and of the convective terms in the equation of heat conduction are small, and the profile of the phase surface varies little over the tube length; 3) the flow velocity at any point is directed practically along the tube axis ( $v_z > v_r$ ); 4) the changes in the axial components of the velocity and temperature along the tube axis are much smaller than their changes over the tube radius:  $\partial v_z/\partial z << \partial v_z/\partial r$ ,  $\partial T/\partial z << \partial T/\partial r$ .

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845

When these assumptions are taken into account, the equations of continuity, heat conduction, and motion in the liquid phase ( $r < r_{x}$ ) can be written as:

$$\frac{1}{r} \frac{\partial}{\partial r} (rv_r) + \frac{\partial v_z}{\partial z} = 0;$$
(1)

$$\frac{1}{r} \frac{\partial}{\partial r} (r\tau_{rz}) = \frac{\partial P}{\partial z}, \quad \tau_{rz} = \eta \frac{\partial v_z}{\partial r}; \quad (2)$$

$$\frac{\partial^2 T}{\partial r^2} + \frac{1}{r} \frac{\partial T}{\partial r} + \frac{1}{\lambda_1} \frac{\partial v_z}{\partial r} \tau_{rz} = 0.$$
 (3)

In the solid phase (for  $r_0 > r > r_*$ ) the equation of heat conduction in the absence of a heat source applies:

$$\frac{\partial^2 T}{\partial r^2} + \frac{1}{r} \frac{\partial T}{\partial r} = 0.$$
 (4)

The last term in Eq. (3) expresses the rate of dissipative heat liberation.

The boundary conditions can be written as follows:

$$r = r_0; T = T_0;$$
 (5)

$$r = 0; \quad \frac{\partial T}{\partial r} = 0, \quad \frac{\partial v_z}{\partial r} = 0, \quad \frac{\partial v_r}{\partial r} = 0;$$
 (6)

 $r=r_*: \quad T=T_*, \quad v_z=v_r=0,$ 

$$Q_* \rho_1 \frac{\partial r_*}{\partial t} = \lambda_2 \frac{\partial T}{\partial r} \bigg|_{r=r_*+0} - \lambda_1 \frac{\partial T}{\partial r} \bigg|_{r=r_*-0}.$$
(7)

The second of the relationships in Eq. (7) expresses the Stefan condition.

# Determination of the Interfacial Boundaries

The interfacial boundary is determined from the following considerations: a) since the profile of the phase surface varies only slowly over the tube length, considerable changes in the axial component of the velocity  $v_{z}$  can only occur over distances which are much larger than the tube radius, so that  $v_{z}$  can be determined from the solution of the "infinite" model [1]; b) since the effects of the inertia terms in the equations of motion and of the convective terms in the heat conduction equation are small, the heat fluxes to the right and left of the phase interface can also be determined from the solution of the "infinite" problem, and, as a result, the process of propagation of the phase front does not depend explicitly on the condinate z; c) the profile of the interfacial boundary is determined essentially from the condition that the time of passage of the phase front is equal to the time after which the axial velocity component decreases to zero.

By using the solution of the steady-state system of equations (2)-(6) given in [1], the steady-state heat fluxes to the right and left of the phase boundary can be written as:

$$\lambda_{2} \frac{\partial T}{\partial r}\Big|_{r=r_{*}+0} = -\frac{2\lambda_{1}}{r_{*}} \frac{(T_{0}-T_{*})}{\ln(r_{*}/r_{0})^{2}},$$

$$\lambda_{1} \frac{\partial T}{\partial r}\Big|_{r=r_{*}-0} = \frac{-2\lambda_{1}RT_{*}^{2}}{Er_{*}} \left[2 - \sqrt{4 - \frac{Er_{*}^{4}}{8RT_{*}^{2}\lambda_{1}\eta(T_{*})} \left(\frac{\partial P}{\partial z}\right)^{2}}\right].$$
(8)

By substituting (8) into (7), it is found that

$$\frac{dr_{*}}{dt} = \frac{2}{Q_{*}\rho_{1}r_{*}} \left[ \frac{-\lambda_{2}(T_{0}-T_{*})}{\ln(r_{*}/r_{0})^{2}} + \frac{2\lambda_{1}RT_{*}^{2}}{E} - \frac{\lambda_{1}RT_{*}^{2}}{E} \sqrt{4 - \frac{Er_{*}^{4}}{8RT_{*}^{2}\lambda_{1}\eta(T_{*})} \left(\frac{\partial P}{\partial z}\right)^{2}} \right]$$
(9)

By substituting the temperature dependence of the viscosity into Eq. (2), the steadystate distribution of the axial velocity component is found as [1]:

$$v_{z} = \frac{dz}{dt} = \left(\frac{\partial P}{\partial z}\right)^{-1} \frac{16RT_{*}^{2}\lambda_{1}}{Er_{*}^{2}} \left\{\frac{q}{4} - \frac{qr^{2}r_{*}^{2}}{q(r^{4} - r_{*}^{4}) + 4r_{*}^{4}} + \sqrt{\frac{q}{4-q}} \left[\operatorname{arctg} \sqrt{\frac{q}{4-q}} - \operatorname{arctg} \left(\frac{r^{2}}{r_{*}^{2}}\sqrt{\frac{q}{4-q}}\right)\right]\right\}.$$
(10)

The pressure gradient  $\partial P/\partial z$  is determined from the condition that the flow rate must be constant,  $Q = 2\pi \int_{0}^{r_{*}} v_{z} r dr = \text{const}$ :

$$\frac{\partial P}{\partial z} = \frac{4\pi}{Q} \frac{RT_*^2 \lambda_1}{E} q.$$
 (11)

The parameter  $q = q(r_*)$  is determined from the relationship

$$\kappa \left(\frac{r_*}{r_0}\right)^4 = q \left(4 - q\right)/2; \quad \kappa = \frac{Er_0^4}{16RT_*^2 \lambda_1 \eta \left(T_*\right)} \left(\frac{\partial P}{\partial z}\right)^2. \tag{12}$$

The axial coordinate of the interfacial boundary  $z_{\star}(r)$  is determined by integrating with respect to time the longitudinal velocity component  $v_z = v_z(r, r_{\star}(t))$ , which depends explicitly on the radial coordinate  $r_{\star}$  (see Eq. (10)):

$$z_* = \int_0^{t_*} v_z(r, r_*(t)) dt,$$
(13)

where  $t_{\dot{x}} = t_{\dot{x}}(r)$  is determined from the condition  $v_z = 0$  when  $t = t_{\dot{x}}$ .

It is obvious that  $r_{*}(t_{*}) = r$ . By converting in Eq. (13) to integration with respect to  $r_{*}$ , it is found that

$$z_*(r) = \int_0^r v_z(r, r_*) \frac{dt}{dr_*} dr_*.$$
 (14)

By using Eqs. (9)-(12) the determination of the position of the interfacial boundary can be reduced to satisfying the quadrature of Eq. (14).

# Results of the Calculations

The calculations were carried out for the following combinations of parameters:

$$\sqrt{\frac{RT_*\lambda_1}{E\eta(T_*)}} = 0.25 \,\mathrm{m/sec}; \ \sqrt{\frac{E}{RT_*^2\lambda_1\eta(T_*)}} r_0^2 = 4 \ (\mathrm{m}^2 \cdot \mathrm{sec})/\mathrm{kg}$$

Since the solution of the problem does not require a condition at the exit of the tube, the quantity z can be treated not only as the longitudinal coordinate but also as the length of the tube. It is apparent that with the boundary condition  $r_{\star} = r_0$  at z = 0, the profile of the interfacial boundary can only decrease monotonically.

It is clear from Fig. 1 that an inlet zone can be distinguished on the profiles of the interfacial boundaries, beyond which the position of the interfacial boundary almost ceases to vary over the length of the tube and coincides with that calculated from the model of flow in a tube of infinite length under conditions of dissipative heat liberation and phase change [1] (dashed lines in Fig. 1). Thus, the boundary beyond which this model is applicable is determined by the dependence of the length of the inlet zone on the parameters of the problem.

Figures 2a and b show the dependence of the parameter z<sub>in</sub> on the dimensionless groups

$$\gamma = \frac{Q}{4\pi r_0^2} \sqrt{\frac{E\eta(T_*)}{RT_*^2 \lambda_1}}; \quad S = \frac{\lambda_2 E(T_* - T_0)}{2\lambda_1 RT_*^2}, \tag{15}$$

which characterize the flow rate and degree of supercooling of the tube wall, respectively.

The zone of applicability of the model of flow in a tube of infinite length is given by the condition  $l >> z_{in}$ , where l is the tube length.



Fig. 1. Monotonically decreasing profiles of the interfacial boundaries at various degrees of supercooling of the tube wall: 1) S = 0.04; 2) S = 0.01; 3) S = 0.005;  $\gamma = 0.049$ .

Fig. 2. Dependence of the length of the inlet zone  $z_{in}$ , m, on the flow rate, S = 0.02 (a) and on the degree of supercooling of the wall,  $\gamma = 0.049$  (b).



Fig. 3. Comparison of the flow-head characteristic curves for the infinite and finite tube models; S = 0.02. G is given in N/m<sup>3</sup>.

Fig. 4. Monotonically increasing profiles of the interfacial boundaries at various degrees of supercooling of the tube walls: 1) S = 0.01; 2 S = 0.02; 3) S = 0.1.

Comparison of the results of calculating the flow-head characteristic curve from the model proposed in [1] and from the model proposed in the present paper shows that they are qualitatively in agreement. At small degrees of supercooling of the wall they appear to be nonmonotonic (see [1]). The calculations were carried out for tubes of lengths greater than  $z_{in}$ . Figure 3 shows the difference G in the values of the pressure drop obtained from the models for flow in tubes of infinite and finite lengths as a function of the flow rate Q.

The decrease of G as the flow rate increases is explained by the fact that the value of G is determined by the length of the inlet zone, which decreases as the flow rate increases (see Fig. 2a).

From Eqs. (11) and (12) it follows that over the length of the tube the following relationship is valid between the dimensionless pressure gradient  $\kappa$  and the dimensionless flow rate  $\gamma$  (see (12), (15)):

 $\varkappa = \frac{16\gamma^2}{\left[\frac{1}{2}\left(\frac{r_*}{r_0}\right)^4 + 4\gamma^2\right]^2}$  (16)

At the entry to the tube, when  $r_{1} = r_{0}$ , relationship (16) assumes the form:

$$\varkappa = \frac{16\gamma^2}{(1/2 + 4\gamma^2)^2}$$

It can be shown that the relationship  $\alpha(\gamma)$  has a maximum value of  $\alpha = 2$  at  $r_* = r_0$ , i.e., that within the framework of the present model and under the conditions of a specified flow rate the pressure gradient cannot be greater than the value corresponding to  $\alpha = 2$ .

When a layer of solid material is formed at the inlet of the tube for any reason (for instance, when liquid is fed into a supercooled tube) it is possible to form a monotonically decreasing solid layer. In this case, the profile of the interfacial surface is calculated

within the scope of the present model with the condition  $r_* \neq r_0$  at the tube inlet. The results of such a calculation are shown in Fig. 4.

#### NOTATION

t, time; r, local value of radius; r<sub>0</sub>, tube radius; r<sub>\*</sub>, radial coordinate of interfacial surface; z, longitudinal coordinate; z<sub>\*</sub>, longitudinal coordinate of interfacial surface; z<sub>in</sub>, length of inlet zone; l, tube length; T, temperature; T<sub>\*</sub>, temperature of phase change; T<sub>0</sub>, tube wall temperature; R, universal gas constant; E, energy of activation of viscous flow; Q<sub>\*</sub>, specific heat of the phase change; P, pressure; Q, liquid flow rate;  $\varkappa$ ,  $\gamma$ , S, q, dimensionless parameters; G, difference in pressure drops calculated by various models;  $\lambda_1$ ,  $\lambda_2$ , thermal conductivities of the liquid and solid phases, respectively;  $\rho_1$ ,  $c_1$ , density and heat capacity of liquid phase;  $\nu_z$ ,  $\nu_r$ , axial and radial components of the liquid velocity;  $\tau_{rz}$ , shear stress;  $\eta$ , viscosity;  $\eta_0$ , preexponential multiplier.

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NUMERICAL ANALYSIS OF THE TRANSPORT PHENOMENON IN SEMICONDUCTOR DEVICES

AND STRUCTURES.

5. THREE-DIMENSIONAL MODELING OF VLIS ELEMENTS

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The high efficiency of a multidimensional numerical analysis of semiconductor devices is confirmed in an example of three-dimensional modeling of bipolar integral circuit structures.

A change in the configuration of the components in the plane of the crystal, i.e., their topology, is the approach approved in practice for improving the characteristics of LIC and VLIC elements. In this case, despite the possible significant machine time expenditures, the three-dimensional modeling of transport processes occurring in the elements [1, 2] is necessary in principle. Such an analysis in the preliminary stage of VLIC design permits complete investigation, without involving significant material expenditures, of the influence of different topological factors on the structure properties, which is extremely important for the engineer-developer in the creation of new optimized structures of elements and investigation of the influence of the changes made on the whole integrated circuit. As is known, this latter is realized by involving the programs of the circuit engineering design stage [2].

Traditionally it is considered that execution of a rigorous three-dimensional numerical analysis (coordinate solution of the problem mentioned) of just several stationary states of the element by solving the fundamental system of equations [3] is impossible in a reasonable time even on an ES-1060 type computer.

The inconsistency of such an assertion is shown in this paper. Results are cited for this that have been obtained for two fundamental kinds of bipolar structures of integrated circuits and that confirm the high efficiency of the universal program developed for threedimensional numerical modeling of VLIC elements later designated "TREADE." Underlying it is the generalized and perfected method of previous papers [3-6].

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