DYNAMIC RELATIONS FOR A MOVING PHASE INTERFACE

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In the theory of two-phase media motion two limiting cases are usually examined: the Stefan problem [1], in which the motion of the media is neglected, and the Rayleigh problem on bubble growth [2], in which the phase change is not taken into account.

However, there are problems of flow stratification, behavior of vapor bubbles subject to strong superheating or pressure discontinuities, shock wave propagation in a two-phase medium, and others in which increased requirements are presented on the accuracy of the account for the phase interaction conditions at their interface, and therefore in the solution of these problems we cannot neglect either the motion or the phase transformations.

In the following we attempt to obtain such conditions, which become the corresponding limiting cases in the Rayleigh and Stefan problems.

1. For a correct phenomenological account for the interaction conditions at the phase interface we can use the results of strong discontinuity theory in gasdynamics with additional account for surface tension [3, 4]. In so doing we use the mass, momentum, and energy conservation laws.

From the mass conservation law

$$\frac{d}{dt}\int_{\Omega} \rho\, d\Omega = 0 \tag{1.1}$$

and the continuity equation for continuous media, with the aid of the expression [5]

$$\frac{d}{dt}\int_{\Omega} \varphi\, d\Omega = \int_{\Omega} \left(\frac{d\varphi}{dt} + \varphi \operatorname{div} \mathbf{W}\right) d\Omega + \int_{\sigma} [\varphi U]\, d\sigma \quad (U = W_n - N) \tag{1.2}$$

follows the first compatibility equation condition

$$[\rho U] = 0 \tag{1.3}$$

Here ρ is the density; W is the velocity of the particles of the medium; U is the normal velocity of the medium relative to the front; N is the phase-interface velocity in the normal direction; Ω is the isolated volume of moving liquid; σ is the portion of phase interface bounded by the surface Σ of volume Ω; brackets denote the difference of the values (jump) of the quantity φ on the two sides of the interface; and the subscripts 1 and 2 relate to the liquid and vapor, respectively.

The second compatibility condition follows from the momentum conservation law:

$$\frac{d}{dt}\int_{\Omega} \rho \mathbf{W}\, d\Omega = \int_{\Omega} \mathbf{f}\, d\Omega + \int_{\Sigma} \chi\, d\sigma + \oint_{\Gamma} \alpha (\mathbf{n} \times \boldsymbol{\tau})\, d\Gamma \quad (\chi = -p\mathbf{n}) \tag{1.4}$$

where **f** is the volume force density; χ is the surface force density (we neglect viscosity in the case in question); p is pressure; **n** is the vector of the outward normal to the interface; α is the (constant) surface tension coefficient; τ is the vector tangent to the contour Γ – the boundary of the surface σ.

With account for (1.2) and the continuity equation, (1.4) takes the form

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$$\int\limits_{\Omega}\rho\,\frac{d\mathbf{W}}{dt}\,d\Omega+\int\limits_{\sigma}[\rho U\mathbf{W}]\,d\sigma=\int\limits_{\Omega}\mathbf{f}\,d\Omega-\oint\limits_{\Sigma}p\mathbf{n}\,d\sigma+\oint\limits_{\Gamma}\alpha\,(\mathbf{n}\times\boldsymbol{\tau})\,d\Gamma \tag{1.5}$$

After transformations of the surface and contour integrals with account for the equation of motion, we obtain the second condition on the interface:

$$[\rho\,U\mathbf{W}+p\mathbf{n}]=-2\alpha H\mathbf{n} \tag{1.6}$$

where H is the average curvature of the surface.

The third condition on the interface follows from the energy conservation law

$$\frac{d}{dt}\left\{\int\limits_{\Omega}\rho\left(\frac{W^2}{2}+E\right)d\Omega+\int\limits_{\sigma}\alpha\,d\sigma\right\}\int\limits_{\Omega}\mathbf{W}\mathbf{f}\,d\Omega+\oint\limits_{\Sigma}(\chi\mathbf{W}-\mathbf{q}\mathbf{n})\,d\sigma+\oint\limits_{\Gamma}\{\mathbf{W}\alpha\,(\mathbf{n}\times\boldsymbol{\tau})\}\,d\Gamma \tag{1.7}$$

Here, **q** is the heat flux through unit area of the interface; E is the internal energy density.

We use (1.2) and the Gauss-Ostrogradskii formula to transform (1.7):

$$\int\limits_{\Omega}\left\{\rho\,\frac{d}{dt}\left(\frac{W^2}{2}+E\right)-\mathbf{W}\mathbf{f}+\operatorname{div}(p\mathbf{W}+\mathbf{q})\right\}d\Omega+\alpha\,\frac{d}{dt}\int\limits_{\sigma}d\sigma$$

$$=-\int\limits_{\sigma}\left[(p\mathbf{W}+\mathbf{q})\,\mathbf{n}+\rho U\left(\frac{W^2}{2}+E\right)\right]d\sigma+\alpha\oint\limits_{\Gamma}\{\mathbf{W}\,(\mathbf{n}\times\boldsymbol{\tau})\}\,d\Gamma$$

The volume integral on the left equals zero by virtue of the energy equation. After several transformations we obtain

$$[(p\mathbf{W}+\mathbf{q})\mathbf{n}+\rho\,U\,({}^1\!/_2W^2+E)]=-2\alpha HN \tag{1.8}$$

As a result we have the compatibility equations on the phase interface

$$[\rho\,U]=0,\qquad [W_\tau]=0,\qquad [\rho\,U^2+p]=-2\alpha H \tag{1.9}$$

$$[\rho U\,({}^1\!/_2U^2+i)+q_n]=0 \tag{1.10}$$

$$(i=E+p\,/\,\rho)$$

Here i is the enthalpy.

The last condition of (1.10) shows that examination of problems with phase change without account for the thermal fluxes is meaningful only for fast processes. In fact, in the latter case $[U^2]=-2[i]$, and since $-[i]=L$ (L is the heat of vaporization) U must have values close to $2\cdot10^3$ m/sec for water.

If heat conduction is not neglected, the hydrodynamic conditions (1.9) and (1.10) alone are not sufficient for a unique solution. This can be seen from the example of the Stefan [1] and Rayleigh [2] problems, where the following conditions are used in addition to the hydrodynamic conditions:

$$i_2-i_1=L,\qquad T_1=T\,(p),\qquad T_2=T\,(p) \tag{1.11}$$

where T and T(p) are the temperatures at the interface and at the line of phase equilibrium, respectively.

Conditions (1.11) assume equilibrium of the system. The application of (1.11) to processes in highly superheated liquid in the case of shock thermal fluxes or when shock waves pass through two-phase media is not justified. For such fast processes the missing conditions have been obtained [6] in the kinetic examination of the phase-change problem. These conditions are the expressions for the mass, energy Q, and momentum G fluxes in terms of the thermodynamic parameters of the phases at the boundary:

$$\rho U=\left(\frac{k}{2\pi m}\right)^{1/2}\left[T^{1/2}\,\frac{\rho''^2}{\rho'}\right],\quad Q=\left\{\frac{1}{2\pi}\left(\frac{k}{m}\right)^3\right\}^{1/2}\left[T^{3/2}\left(2+\ln\frac{\rho'}{\rho''}\right)\frac{\rho''^2}{\rho'}\right] \tag{1.12}$$

$$G=\frac{k}{2m}\left[T\,\frac{\rho''^2}{\rho'}\right]$$

Here m is the molecular mass; K is Boltzmann's constant; the single and double primes relate to the liquid and vapor, respectively; and the bracketed expressions are to be taken first for the liquid parameters and then for the vapor parameters at the interface, as before.

2. To compare the resulting compatibility conditions with the analogous conditions of [1, 7, 8], we examine the dynamics of the change of a spherical vapor bubble in a large liquid volume.

For a bubble of radius R the system of equations (1.9), (1.10) takes the form

$$[\rho U] = 0, \qquad [W_\tau] = 0, \qquad [\rho U^2 + p] = -2\alpha / R \tag{2.1}$$

$$\rho U[{}^1\!/_2 U^2 + i] + [q_n] = 0 \tag{2.2}$$

$$(U = W_R - R^\cdot)$$

We assume that at infinity the liquid is at rest and locate the coordinate origin at the center of the bubble.

We neglect the influence of the gravity force; then the liquid motion will depend only on the radius vector of the liquid element. From the equations of hydrodynamics of a viscous incompressible liquid follows

$$W_r = \frac{a(t)}{r^2}, \qquad p = \rho\left(\frac{a^\cdot}{r} - \frac{a^2}{2r^4}\right) + p_\infty(t) \tag{2.3}$$

If we neglect the effect of phase change on bubble growth dynamics, i.e., if we take $W_{1R} = R^\cdot$, and if we also neglect the quantity $[\rho U^2]$ in comparison with $2\alpha/R$, then from (2.3) and the compatibility conditions (2.1) we obtain one of the limiting cases – the Rayleigh equation [2]

$$RR^{\cdot\cdot} + {}^3\!/_2 R^{\cdot 2} = (p_2 - p_\infty - 2\alpha / R) / \rho' \tag{2.4}$$

The authors of [7] and [8], assuming that p_2 is the saturated vapor pressure at the liquid temperature at the interface, used (2.4) to describe vapor bubble growth dynamics in superheated liquid. They used the boundary condition for the heat conduction equation in the liquid at the moving vaporization surface

$$\left.\frac{\partial T}{\partial r}\right|_{r=R} = \left|\frac{L\rho''}{\lambda'} R^\cdot\right. \tag{2.5}$$

Here λ' is the thermal conductivity. Equation (2.5) is the heat-balance equation for the phase interface and accounts partially for the effect of phase change on bubble growth.

Condition (2.5) is obtained from (2.2) if we neglect: 1) heat flow in the vapor; 2) the quantity $[{}^1\!/_2 U^2]$ in comparison with [i], and if we take $-[i] = L$.

For moderate liquid superheats (1–10°K) and low pressures this neglect of the dynamic terms is justified by the good agreement between the theoretical and experimental [9] results.

However, as noted previously, in taking the Rayleigh equation as the basis the authors of [7, 8] neglect the role of the phase change in Eq. (2.1) for the mass and momentum flux, which is not justified in many cases.

For the other limiting case, the Stefan problem, the compatibility conditions with account for surface tension are obtained from (2.1) in the form

$$W_1 = W_2 \text{ and } p_1 = p_2 - 2\alpha / R \quad \text{for} \quad \rho' \approx \rho''$$

and from (2.2)

$$\left[\lambda' \frac{\partial T}{\partial r}\right] = L\rho R^\cdot \quad \text{for} \quad -[i] = L$$

and the interface motion is determined entirely by heat transfer.

Let us make clear what changes occur when we account for phase change in the dynamics of the vapor bubble growth. From the first equalities of (2.1) and (2.3) follows

$$R^\cdot = a(t) / R^2 (1 - \rho'' / \rho') \tag{2.6}$$

Excluding a(t) from this expression by means of relation (2.3) and using (2.1), we obtain

$$RR^{\cdot\cdot} + \frac{1}{2}\left(3 - \frac{\rho''}{\rho'}\right) R^{\cdot 2} - \frac{(\rho'')^\cdot}{\rho' - \rho''} RR^\cdot = \frac{1}{\rho' - \rho''}\left(p_2(T) - p_\infty - \frac{2\alpha}{R}\right) \tag{2.7}$$

where $p_2(T)$ is the saturated vapor pressure in the bubble for the temperature T at the interface, and p_∞ is the pressure at infinity.

It follows from (2.7) that significant deviations from the case studied in [7, 8] can be expected, first, for $\rho'' \approx \rho'$ for example, with bubble growth near the critical point T^*; second, when $(\rho'')^{\cdot}$ is large, specifically with a pressure jump at infinity or for high superheats.

3. To illustrate the role of the additional terms obtained in (2.7), let us analyze its solution for

$$\rho'' \approx \rho', \quad (\rho'')^{\cdot} \ll 1, \quad p_2 - p_\infty = \Delta p = \mathrm{const} \tag{3.1}$$

Under these assumptions (2.7) admits the single quadrature

$$\zeta^{\cdot} = e^{-{}^1\!/_2(2+\vartheta)(\zeta-1)}\left(\frac{2\Delta p\,\{e^{(2+\vartheta)(\zeta-1)} - 1\}}{\rho' R_0^2\vartheta\,(2+\vartheta)} - \frac{4\alpha}{\rho' R_0^3\vartheta}\int\limits_1^{\zeta}\frac{e^{(2+\vartheta)(\zeta-1)}}{\zeta}\,d\zeta\right)^{1/2} \tag{3.2}$$

$$\left(\vartheta = 1 - \frac{\rho''}{\rho'}, \; \zeta = \frac{R}{R_0}\right)$$

Here R_0 is the initial radius of the nucleus; we set $R^{\cdot} = 0$ for $t = 0$. For the initial bubble growth stage the resulting solution (3.2) simplifies considerably if we take into account the smallness of $\zeta - 1$

$$\zeta^{\cdot} = \sqrt{\frac{2(\Delta p R_0 - 2\alpha)}{\rho' R_0^3\vartheta}}\left\{1 - \left(1 + \frac{1}{2}\vartheta\right)(\zeta - 1)\right\}\sqrt{\zeta - 1} \tag{3.3}$$

The solution of the Rayleigh equation (2.4) with condition (3.1) can be obtained from (3.3) for $\rho'' = 0$. We see from comparison of this solution with (3.3) that phase change leads to change of the initial bubble growth by a factor of $f = 1/\sqrt{\theta}$.

Thus, for low pressures, when $\rho'' \ll \rho'$, the phase change is retarded by the influence of the dynamic terms to the degree that vapor bubble growth takes place nearly the same as for a gas bubble. For $T \approx T^*$ the deviations from the solutions of [7, 8] become significant even for low superheats.

4. To determine the influence of the additional terms in (2.7) on vapor bubble growth dynamics near T^* under the same assumptions used in [7, 8], calculations were made using the Minsk-2 digital computer. The maximum liquid superheat at temperatures near T^* was determined using the method of [10, 11].

The system of equations defining bubble growth dynamics used for the calculation has the form

$$RR^{\cdot\cdot} + \frac{3 - \rho''/\rho'}{2}R^{\cdot 2} - RR^{\cdot}\frac{(\rho'')^{\cdot}}{\rho' - \rho''} = \frac{1}{\rho' - \rho''}\left(p_2(T) - p_\infty - \frac{2\alpha}{R}\right) \tag{4.1}$$

$$\frac{dp}{dT} = \frac{L\rho'\rho''}{(\rho' - \rho'')T} \tag{4.2}$$

$$T = T_0 - \frac{2L\rho''}{c'\rho'\sqrt{\pi a'}}\int\limits_0^t R^{\cdot\cdot}(t')(t - t')^{1/2}dt' \qquad \left(a' = \frac{\lambda'}{c'\rho'}\right) \tag{4.3}$$

Here c' is the heat capacity, a' is the thermal diffusivity, and T_0 is the initial system temperature. Equation (4.3) yields the temperature at the bubble wall in the initial period of its growth (for $R \approx R_0$) [8] and is the solution of the heat conduction problem through a moving vaporization surface.

If we take as the initial conditions for the system (4.1)–(4.3) the radius of the nucleus corresponding to the given superheat

$$R_0' = 2\alpha/(p_0 - p_\infty) \tag{4.4}$$

(where p_0 is the saturated vapor pressure at the temperature T_0) and $R_0^{\cdot} = 0$, then the system will be in equilibrium. The external conditions must be altered to bring the bubble out of equilibrium. The initial bubble radius will be taken equal to $R_0 = R_0' + \Delta$, $\Delta \ll R_0$.

The solutions of (4.1)–(4.3) together with the initial conditions were obtained by the Runge-Kutta method refined by subdivision of the step. For comparison and check of the computation technique, calculations were made with superheats $\Delta T = T_0 - T_\infty = 3$ and 5°K for water at $T_\infty = 373$°K and $p_\infty = 10^5$ N/m², i.e., for the same conditions as in [7, 8].

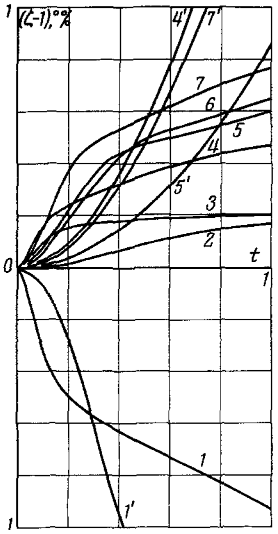

Fig. 1

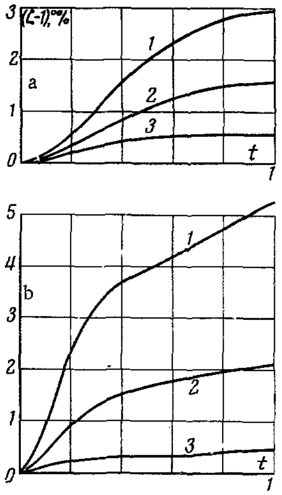

Fig. 2

Fig. 1. Relative radius change $\zeta - 1$ versus time t, in nsec, for $T_0 = 641°K$ and $\Delta\tau = 0.03°K$: 1) $R_0 = 2 \cdot 10^{-8}$ m, 2) $R_0 = 5 \cdot 10^{-7}$ m, 3) $R_0 = 2.8 \cdot 10^{-8}$ m, 4) $R_0 = 3 \cdot 10^{-8}$ m, 5) $R_0 = 1 \cdot 10^{-7}$ m, 6) $R_0 = 5 \cdot 10^{-8}$ m, 7) $R_0 = 6 \cdot 10^{-8}$ m. Primes indicate calculations using (2.4).

Fig. 2. Relative radius change $\zeta - 1$ versus time t, in nsec, combinations of values of T_0 and $\Delta\tau$ shown in parentheses in °K: 1 (641, 0.5), 2 (643, 0.2), 3 (647, 0.03). a) $R_0 = 1 \cdot 10^{-7}$ m, b) $R_0 = 3 \cdot 10^{-8}$ m.

Since in this case $\rho'' \ll \rho'$, the system of equations (4.1)–(4.3) coincides in first approximation with the system used for calculation in [7, 8]. In fact, calculations made of the system of equations (4.1)–(4.3) agreed well with the solutions obtained in [7, 8]. This gives some confidence in the correctness of this computational technique for other initial conditions as well.

However, near the critical point the calculations of water vapor bubble growth and collapse dynamics using the system of equations (4.1)–(4.3) led to a significant difference from the solutions obtained from Eq. (2.4), (4.2), and (4.3), used in [7, 8], which is seen from Fig. 1.

It was found from the numerical calculation, that, first of all, for $T \approx T^*$ the term $RR^{\bullet}\ \rho''/(\rho'-\rho'')$ in (4.1) is of the same order as the remaining terms of the equation; second, the bubble growth time $t \sim R/R^{\bullet}$ for $R \approx R_0$ is of the same order as the characteristic time R^2/a of the heat-conduction process (i.e., heat conduction cannot be neglected).

We see from the curves (Fig. 1) that at the initial time the growth (or collapse) rate is greater by f times than that given by (2.4). Then the nature of the bubble growth in accordance with (2.4) and (2.7) is different. Solution (2.7) has an inflection point and then grows in proportion to t to a power whose exponent is less than 1. This would be expected, since for $T \approx T^*$ and $\rho' \approx \rho''$ the asymptotic behavior of the bubble near the critical point should be described by the well-known Stefan solution [1]. The initial slowing in the bubble growth (collapse) is associated with the manifestation of surface tension.

It appears that in this case the physical process of bubble growth is analogous to the process of specimen crystallization from a melt; bubble growth takes place together with movement motion of the isotherm $T = T(p_2)$, where $T(p_2)$ is the phase change temperature, i.e., the bubble behavior actually differs from the solution in [7, 8], where "repulsion" (dynamic terms) is significant, since $\rho'' \ll \rho'$.

In contrast with solution (2.4), solution (2.7) depends nonmonotonically on R_0: for each T_0 there is an R_0 for which the bubble growth rate is maximal (Fig. 1).

The variation of vapor bubble growth as a function of T_0 is shown in Fig. 2. We see from the curves that with approach to T^* the bubble growth and condensation process slows considerably. This corresponds to the general tendency for slowing of processes near the phase change point of the second kind (specifically, near the critical point of the substance), which is associated with the singularities at this point of the isothermal compressibility, heat capacity, and other thermodynamic quantities.

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