NUMERICAL CALCULATION OF GROWTH OF A GAS BUBBLE FROM A SOLUTION

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The problem of growth of a solitary gas bubble from a solution is considered, and a method is presented for numerical solution.

We will formulate the basic mathematical relationships describing the process of growth of a single gas bubble of spherical form from a solution with an initial content of dissolved gas C_0. The equation of convective gas diffusion in the liquid in a spherical coordinate system centered at the bubble nucleus has the form

$$\frac{\partial C}{\partial t} = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial C}{\partial r}\right) - v\frac{\partial C}{\partial r}, \tag{1}$$

where D is the diffusion coefficient; $C = C(r, t)$, gas concentration in solvent; $\xi(t)$, current bubble radius; $v(r, t)$, velocity of liquid flow produced by bubble growth. From the continuity equation we can easily obtain the law of change in velocity as a function of coordinate r and time t

$$v(r, t) = \frac{\xi^2}{r^2}\frac{d\xi}{dt}. \tag{2}$$

Since bubble growth occurs due to transport of gas within the liquid to the liquid–vapor phase boundary, from the mass balance equation the following conditions follow, relating the change in gas mass content in the bubble to mass flow in the liquid phase at the boundary $r = \xi(t)$:

$$\frac{1}{3\xi^2}\frac{d}{dt}(\rho\xi^3) = D\frac{\partial C}{\partial r}\bigg|_{r=\xi(t)}. \tag{3}$$

In the future we will assume the gas ideal; then in correspondence with the equation of state the relationship between density ρ and gas pressure P in the bubble will have the form

$$\rho = \frac{MP}{RT}, \tag{4}$$

where M is the molecular weight of the gas; R, universal gas constant; and T, absolute temperature.

The second condition at the interphase boundary follows from the balance of forces acting on the bubble from the direction of the liquid (the liquid pressure P' at the point of bubble formation, including hydrostatic pressure of the liquid column and the pressure above the solution, the surface tension force, viscosity force, and inertial force of the liquid mass) and the forces directed from the bubble toward the liquid, i.e., the gas pressure P in the bubble. At moderate bubble growth rates the inertial force of the liquid mass may be neglected [2]. Then the force balance equation may be written in the form

$$P = P' + 4\mu\frac{1}{\xi}\frac{d\xi}{dt} + \frac{2\sigma}{\xi}, \tag{5}$$

where μ is the coefficient of dynamic viscosity and σ is the surface tension coefficient. Moreover, the gas pressure within the bubble and the dissolved gas concentration at the boundary with the vapor phase will be assumed to be related by the Siberts law

$$C(\xi, t) = \varkappa\sqrt{P}, \tag{6}$$

where $\varkappa$ is the solubility constant.

It follows from Eq. (5) that the critical bubble radius ξ_0 satisfies the relationship

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$$\xi_0 = \frac{2\sigma}{P_0} \frac{1}{1 - \frac{P'}{P_0}}, \tag{7}$$

where P_0 is the pressure of the gas in equilibrium with a liquid of composition C_0 (defined by Eq. (6)). The necessary condition for nucleus formation, as follows from Eq. (7), is

$$P_0 > P'.$$

In particular, at P' = 0 the critical bubble radius ξ_0 will be

$$\xi_b = \frac{2\sigma}{P_0}. \tag{7'}$$

We will now formulate initial conditions. At the initial moment of time we will assume the liquid phase composition constant

$$C(r, 0) = C_0, \tag{8}$$

and the bubble radius equal to the critical value*

$$\xi(0) = \xi_0. \tag{9}$$

Moreover, in the liquid at a sufficiently large distance L from the bubble we will assume the condition

$$C(L, t) = C_0 \tag{10}$$

to be fulfilled.

The unknowns in the problem of Eqs. (1)-(9) are the functions C(r, t), v(r, t), P(t), together with the bubble growth law, i.e., the function $\xi = \xi(t)$. In contrast to the classical Stefan problem, the value of the desired function C(r, t) on the interphase boundary is unknown and subject to definition.

We introduce the dimensionless parameters

$$\bar{r} = r/\xi_b, \ \bar{C} = C/C_0, \ \bar{P} = P/P_0, \ \bar{\xi} = \xi/\xi_b. \tag{11}$$

Replacing the dimensioned characteristics of Eqs. (1)-(10) by dimensionless ones, it can be shown that the solution depends on the following dimensionless characteristics:

$$\bar{r}, \ \mathrm{Fo} = Dt/\xi_b^2, \ P_T = \rho_0/C_0, \ P_s = P_0/P', \ \mathrm{Ta} = \mu DP'/\sigma^2. \tag{12}$$

The parameter P_S characterizes the degree of solution supersaturation relative to the external pressure; the parameter P_T (also expressable as $P_T = RT\varkappa^2/MC_0$) is a characteristic of the conditions of thermodynamic equilibrium between vapor phase and solution.

The parameter Ta is a measure of the ratio of the force characteristics (viscosity and surface tension) to diffusion, and characterizes the similarity of bubble growth conditions on the vapor–liquid boundary.

We will omit the rewriting of Eqs. (1)-(10) using the dimensionless parameters of Eqs. (11), (12), but use the defining parameters of Eq. (12) to process the results of numerical experiment.

As is well known, numerical integration of the equations of heat and mass transfer with convective terms is plagued by difficulties connected with replacement of the first derivative by difference relationships, so that approximation by one-sided differences (depending on the sign, right- or left-handed) is unsatisfactory with respect to accuracy of the solution obtained, while use of the central difference leads to a nonmonotonic difference scheme. Samarskii [1] has proposed a monotonic scheme for solution of a parabolic equation, based on perturbation of the divergent term in the equation, and ensuring second-order accuracy.

In the present study, for the difference approximation of Eq. (1) a movable Lagrangian network was used, upon which the approximation of the left side of Eq. (1) can be accomplished in an especially simple manner.

Let $\omega^{(k)}\{r_i^{(k)}, i = 1, 2, \ldots, N\}$ be the set of network node points at the time $t = t_k$, with $r_i^{(k)} = \xi(t_k)$.

*Condition (9) is a condition of unstable equilibrium, so that in numerical calculations the initial bubble radius is taken larger than critical by a sufficiently small value.

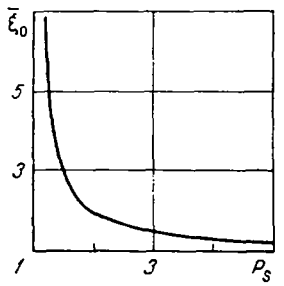

Fig. 1

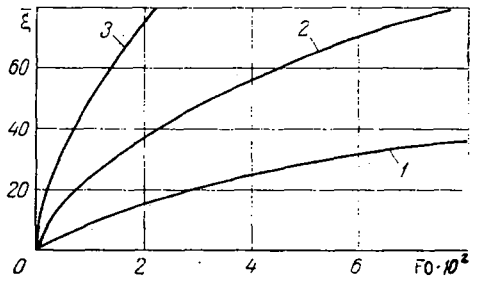

Fig. 2

Fig. 1. Relative nucleus radius vs P_S.

Fig. 2. Relative bubble radius vs. Fo for various P_S at $P_T = 10$: 1) $P_S = 1.5$; 2) 2; 3) 3.

Then the coordinates of the network nodes at time $t = t_{k+1} = t_k + \tau_k$ can be calculated in the following manner:

$$r_i^{(k+1)} = r_i^{(k)} + \tau_k v_i^{(k+1)}, \tag{13}$$

where τ_k is the step in time; $v_i^{(k+1)} = v(r_i^{(k+1)}, t_{k+1})$ is the velocity of liquid motion at a point with radius $r_i^{(k+1)}$ at the time $t = t_{k+1}$.

We write Eq. (1) in the form

$$\frac{dC}{dt} = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 D \frac{\partial C}{\partial r}\right),$$

where d/dt indicates the substantial derivative, then approximate this equation on the network $\omega^{(k+1)}$

$$\frac{C_i - \check{C}_i}{\tau_k} = \frac{1}{r_i^2}\frac{1}{\hbar_i}\left[d_{i+\frac{1}{2}}\frac{(r_i + 0.5h_{i+1})^2}{h_{i+1}}(C_{i+1} - C_i) - d_{i-\frac{1}{2}}\frac{(r_i - 0.5h_i)^2}{h_i}(C_i - C_{i-1})\right]. \tag{14}$$

Here $C_i = C_i(r_i^{(k+1)}, t_{k+1})$, $\check{C} = C(r_i^{(k)}, t_k)$, $h_i = r_i^{(k+1)} - r_{i-1}^{(k+1)}$, $h_{i+1} = r_{i+1}^{(k+1)} - r_i^{(k+1)}$, $\hbar_i = 0.5(h_{i+1} + h_i)$. The coefficients of the difference equation $d_{i+1/2}$, $d_{i-1/2}$ are calculated by the method proposed in [1].

We introduce a certain standard step h and require that the positions of the liquid–vapor phase boundary at the times $t = t_{k+1}$ and $t = t_k$ differ by the standard step, i.e., we assume that

$$\xi(t_{k+1}) - \xi(t_k) = h.$$

Let τ_k be the time step at which the boundary is displaced by the standard step. Then in accordance with Eq. (2) the velocity of liquid motion at node points of the network $w^{(k+1)}$ $\{r_i^{(k+1)}, i = 1, 2, \ldots, N\}$ can be calculated in the following manner:

$$v_i^{(k+1)} = \left(\frac{\xi(t_{k+1})}{r_i^{(k+1)}}\right)^2 \frac{h}{\tau_k}. \tag{15}$$

We write the difference analog of conditions (3), (5), and (6)

$$\frac{1}{3}\cdot\frac{\rho^{(k+1)}\xi_{k+1}^3 - \rho^{(k)}\xi_k^3}{\tau_k} = d_{\frac{3}{2}}\frac{C_2^{(k+1)} - C_1^{(k+1)}}{h_2^{(k+1)}}\xi_{k+1}^2, \tag{16}$$

$$P_{k+1} = P' + 4\mu\frac{1}{\xi_{k+1}}\frac{h}{\tau_k} + \frac{2\sigma}{\xi_{k+1}}, \tag{17}$$

$$C_1^{(k+1)} = \varkappa\sqrt{P_{k+1}}, \tag{18}$$

where $\xi_{k+1} = \xi(t_{k+1})$; $P_{k+1} = P(t_{k+1})$; $\rho^{(k+1)} = MP_{k+1}/RT$.

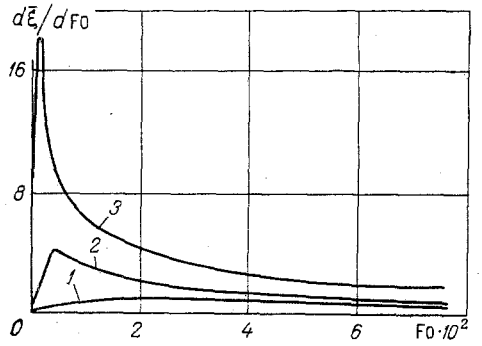

Fig. 3

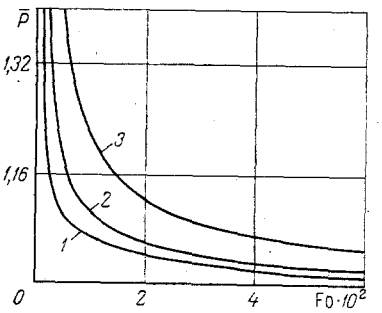

Fig. 4

Fig. 3. Dimensionless bubble growth rate vs. Fo for various P_S at P_T = 10: 1) P_S = 1.5; 2) 2; 3) 3.

Fig. 4. Relative gas pressure in bubble vs. Fo for various P_S at P_T = 10: 1) P_S = 3; 2) 2; 3) 1.5.

Combining with Eqs. (13)-(18) difference relationships for initial conditions (8), (9) and boundary condition (10), at each time step we obtain a system of nonlinear difference equations for determination of concentration at network nodes, gas pressure in the bubble, liquid motion velocity, and the displacement rate of the interphase boundary. For solution of this nonlinear algebraic problem we construct an iteration process in the following manner. We choose as the initial approximation for the time step $\tau_k^{(1)}$ its value in the preceding time layer, then calculate with Eqs. (13), (15), (17) the first approximations for the network $\omega^{(k+1)}$, velocites $v_i^{(k+1)}$, and pressure P_{k+1}. Then using Eq. (18) and the difference analog of condition (10), we solve the system of nonlinear algebraic equations (14) by the drive method. The following approximation for the time step is defined by Eq. (16)

$$\tau_k^{(s+1)} = \frac{[\rho_s^{(k+1)}(\xi_k + h)^3 - \rho^{(k)}\xi_k^3]\, h_{1,s}^{(k+1)}}{3d_3^{(k+1)}[C_{2,s}^{(k+1)} - C_{1,s}^{(k+1)}]\,\xi_{k+1}^2},$$

where the index s in the notation for concentrations, density, and spatial network step $h_i^{(k+1)}$ indicates that these values are taken from the s-th iteration.

The sequence of calculations described above is repeated until

$$\left| 1 - \frac{\tau_k^{(s+1)}}{\tau_k^{(s)}} \right| < \varepsilon.$$

Thus, at each step of the iteration process there occurs a readjustment of the spatial network $\omega^{(k+1)}$. When the iteration process converges, then the network will be structured in accordance with the calculated instantaneous velocity of bubble motion and the liquid velocity field.

It follows from Eqs. (7), (7'), (11) that the relative radius of the nucleus depends only on the dimensionless quantity P_S. Figure 1 shows the dependence of $\bar{\xi}_0$ on P_S.

Analysis of the range of variation of the defining parameters of Eq. (12) for hydrogen and nitrogen dissolved in metals reveals that the parameter Ta changes within the limits 10^{-4}-10^{-6}, i.e., is insignificant, so that it may be neglected in further analysis.

Of the two parameters P_S and P_T, P_S proves to have the greater effect on the dimensionless characteristics (in dimensioned units this is the degree of solution supersaturation).

Figures 2-4 present the dependence of relative bubble radius $\bar{\xi}$, relative bubble growth rate $d\bar{\xi}/dF_o$, and relative pressure $\bar{P}$ upon Fourier number for various values of the parameters P_S and P_T.

One should note the nonmonotonic character of the dimensionless bubble growth rate as a function of Fo, where with increase in P_S and P_T the maximum in dimensionless growth rate increases and shifts toward lower Fo.

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BUBBLE DEFORMATION IN AN ELECTRIC FIELD

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The problem of expansion of bubbles in a compressible liquid upon application of an electric field is solved. The effect of the electric field on phase transition is evaluated.

It has been experimentally established [1, 2] that under the influence of an electric field bubbles and droplets suspended in a dielectric field expand in the direction along the field independent of the ratio between dielectric permittivities of the medium ε_2 and the inclusions ε_1. A theoretical description of this effect is of interest in refining the peculiarities of heat exchange in an electric field [3].

The existing calculations of bubble deformation [1, 2] do not agree with experimental results without the assumption that the electrostriction pressure in the liquid is "fictitious" [1] or that the coefficient of liquid surface tension is strongly dependent on the electric field vector [2].

We will demonstrate that consideration of the compressibility of the liquid in solution of the equation of equilibrium of the interphase boundary leads to results which agree qualitatively with experimental data

$$\frac{1}{R_1}+\frac{1}{R_2}=\frac{P_1(\rho_1)-P_2(\rho_2)}{\delta}-\frac{\varepsilon_0(\varepsilon_2-\varepsilon_1)}{2\delta}\left(\frac{\varepsilon_1}{\varepsilon_2}E_{n1}^2+E_{t1}^2\right)+\rho_2\frac{\partial\varepsilon_2}{\partial\rho_2}\frac{\varepsilon_0E_2^2}{2\delta}-\rho_1\frac{\partial\varepsilon_1}{\partial\rho_1}\frac{\varepsilon_0E_1^2}{2\delta}, \quad (1)$$

where ρ_1, ρ_2 are densities; P_1, P_2, pressures; E_{t_1}, E_{n_1}, tangential and normal components of the field within the inclusion on the boundary with the medium; E_1, E_2, field intensities; δ, surface tension; R_1, R_2, major radii of curvature of the surface.

In contrast to the case of an incompressible liquid Eq. (1) is insufficient for determination of the bubble deformation, since the liquid density becomes variable in an inhomogeneous electric field as produced by the bubble. Electrostriction causes flow of some of the liquid from a region of weak field to a region of strong field, with the density and hydrostatic pressure increasing at the equator and decreasing at the poles of the bubble in comparison to the analogous parameters far from the bubble. After establishment of a stationary state the pressure distribution is described by the equation [4]

$$P_2(\rho_2)-\rho_2\frac{\partial\varepsilon_2}{\partial\rho_2}\frac{\varepsilon_0E_2^2}{2}=P_0, \quad (2)$$

where P_0 is a quantity dependent on the geometry of the electrode system creating the field, and the conditions at the boundary of the liquid volume. In experiments, apparently, case (a) is often realized, wherein the field occupies a small portion of the liquid volume and liquid flow is not inhibited at all. Then P_0 is equal to the hydrostatic pressure P_{ex}, existing in the liquid before field application. In case (b), where the influx of liquid is impossible or has not occurred

$$P_0=P_{ex}-\rho_2\frac{\partial\varepsilon_2}{\partial\rho_2}\frac{\varepsilon_0E_0^2}{2}. \quad (3)$$

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