MOVEMENT OF GAS BUBBLES IN A LIQUID LAYER IN THE PRESENCE OF DIFFUSION AND CHEMICAL REACTIONS

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The problem of a bubbling reactor, in which gas and liquid are mixed by the passage of bubbles of gas through a liquid layer, is discussed. We give the results of a numerical solution of the system of equations describing the processes occurring in the reactor in the case where there are no chemical reactions, and also in the case where chemical reactions take place at constant temperature.

The bubbles are formed by gas jets which issue from special nozzles mounted in the bottom of the reactor. The gas jet issuing from the nozzle breaks up into separate bubbles, which rise under the action of buoyancy forces. The bubbling process was investigated experimentally in [1-3].

For the total diffusion flux from a bubble the formula [4]

$$I = Ac_0\left(\frac{Du_1}{l}\right)^{1/2}$$

is usually used. Here I is the total diffusion flux, A is a constant which is experimentally determined, D is the diffusion coefficient, u_1 is the speed of ascent of the bubble, l is the characteristic dimension of the bubble, and c_0 is the saturation concentration.

The values usually used for small (undeformed) bubbles are $A = \sqrt{\pi/3}$, $l = 2a$, where a is the bubble radius. It has been established that the speed of ascent of a bubble depends significantly on the Reynolds number u_1a/ν, where ν is the kinematic viscosity of the liquid.

1. We consider the problem of solution of gas bubbles in a liquid. Let h be the depth of the layer of liquid in the reactor and u_1 the speed of ascent of the bubble; the x axis is directed upward along the reactor axis.

We assume that c_1 – the concentration of dissolved substance in the bubble – is small, the bubbles are all of the same size and do not break up into smaller bubbles nor unite to form larger ones. The speed of ascent of the bubbles will then be constant [4]. We assume that the Dalton and Henry laws hold for a bubble. Then the concentration of dissolved substance at the gas-liquid interface and c_1 will be connected by the relationship $c_2^\circ = \psi c_1$, where ψ is a constant, and c_2° is the saturation concentration.

Let t be the time, μ be the specific mass transfer coefficient for unit volume of the mixture (which depends on the number of bubbles per unit volume of the mixture, their size, etc.), and c_2 be the concentration of dissolved substance in the liquid. The process occurring in the reactor can be described by the following system of equations:

$$\frac{\partial c_1}{\partial t} + u_1\frac{\partial c_1}{\partial x} = -\mu(\psi c_1 - c_2), \quad \frac{\partial c_2}{\partial t} - D_2\frac{\partial^2 c_2}{\partial x^2} = \mu(\psi c_1 - c_2) \tag{1.1}$$

with initial and boundary conditions

Moscow. Translated from Zhurnal Prikladnoi Mekhaniki i Tekhnicheskoi Fiziki, No. 1, pp. 131-135, January-February, 1971. Original article submitted July 13, 1970.

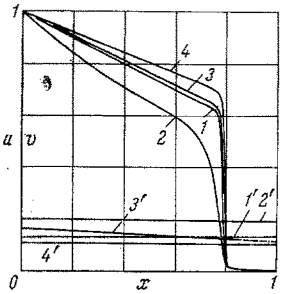

Fig. 1

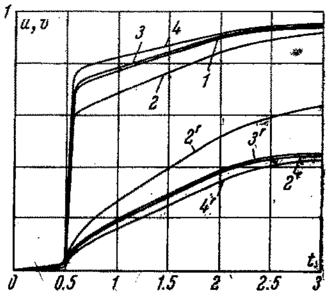

Fig. 2

$$
\begin{gathered}
c_1(x,0)=0, \qquad c_2(x,0)=0, \qquad c_1(0,t)=c_1^{\circ} \\
[\partial c_2/\partial x]_{x=0}=0, \qquad [\partial c_2/\partial x]_{x=l}=0
\end{gathered} \tag{1.2}
$$

Here D_2 is the turbulent diffusion coefficient, and c_1° is the initial concentration of dissolved substance in the bubble [5-8].

We assume that the medium consists of a liquid and discrete bubbles. No diffusion takes place between the bubbles. The first equation of system (1.1), which describes the change in concentration c_1, contains only a convective term (u_1 is the speed of the bubble relative to the liquid). The second equation of system (1.1) corresponds to the diffusion process (there is no convective term, the liquid is stationary, $D_2 \partial^2 c_2/\partial x^2$ is the diffusion term).

The terms on the right side of the equations of systems (1.1) are the source intensities, which are proportional to the difference in saturation concentration at the bubble boundary and the concentration of dissolved substance in the liquid.

We introduce new functions and dimensionless variables

$$
\bar{t}=\frac{u_1 t}{h}, \qquad \bar{x}=\frac{x}{h}, \qquad u=\frac{c_1}{c_1^{\circ}}, \qquad v=\frac{c_2}{c_1^{\circ}}
$$

System (1.1) and conditions (1.2) in dimensionless variables take the form

$$
\frac{\partial u}{\partial t}+\frac{\partial u}{\partial x}=-\gamma(\lambda u-v) \qquad \frac{\partial v}{\partial t}-D\frac{\partial^2 v}{\partial x^2}=\gamma(\lambda u-v) \tag{1.3}
$$

$$
\begin{gathered}
u(x,0)=0, \; v(x,0)=0, \; u(0,t)=1 \\
\left[\frac{\partial v}{\partial x}\right]_{x=0}=0, \qquad \left[\frac{\partial v}{\partial x}\right]_{x=1}=0
\end{gathered} \tag{1.4}
$$

The strokes above the variables t, x, and D_2, as in all that follows, are omitted.

Here D_2, γ, λ are dimensionless coefficients, corresponding to the diffusion coefficient, mass transfer coefficient, and Henry constant.

System (1.3) with conditions (1.4) was solved numerically on an electronic digital computer.

The system of equations (1.3) was replaced by difference equations.

In the semistrip $x \in [0, 1]$, $t \geq 0$, a rectangular net $x = j\Delta x$, $t = i\Delta t$ ($j = 0, 1, 2, \ldots, n$; $i = 0, 1, \ldots$) was constructed.

Since at the initial instant the boundary and initial conditions are inconsistent, there will be a solution in the form of a jump of concentration u.

The position of the jump is given by the characteristic of the first equation of system (1.3). The equation of the characteristic is $x - t = 0$. Hence, for the solution of the first equation of system (1.3) we chose an explicit three-point scheme (corner), stable at $r = \Delta t/\Delta x \leq 1$ and having first order of accuracy. Here we used the "through" count method. On the right of the difference equation u is taken on the upper layer to avoid a "surge," which is physically unreal.

The second equation of system (1.3) was approximated by a "weighted" six-point scheme. Initially, owing to the inconsistency of the boundary conditions, we regarded the weight θ as unity and used two-point approximations of the boundary conditions, but subsequently, after calculation of the first q layers in time, we assumed θ equal to a half and took more accurate three-point approximations of the boundary conditions.

When the concentration (u) front reached x = 1, we used an absolutely stable four-point scheme, with second order of accuracy [9-11], to calculate the first equation of the system.

The calculations were performed for four combinations of values of the parameters D_2, γ, and λ, viz.,

1 (10, 1.5, 0.5), *2* (10, 1.5, 0.75), *3* (1, 1.5, 0.5), *4* (10, 1.0, 0.5) .

The steps for the variables were taken as $\Delta x = \Delta t = 0.02$. A further reduction of the steps had practically no effect on the results.

We give the values of u and v in relation to x for t = 0.8 and in relation to t for x = 0.5 for the first variant

$t = 0.8$

$x = 0$	0.40	0.78	0.80	1.0
$u = 1.000\,000$	0.788 520	0.609 078	0.049 353	0.047 911
$v = 0.139\,946$	0.138 143	0.134 628	0.134 443	0.133 651

$x = 0.5$

$t = 0$	0.40	1.0	2.0	3.0
$u = 0.000\,000$	0.007 077	0.769 043	0.903 137	0.938 426
$v = 0.000\,000$	0.040 614	0.193 069	0.377 327	0.446 037

The distributions of the dimensionless concentrations u and v over the length of the reactor are shown in Fig. 1 for four variants at time t = 0.8. Curves 1, 2, 3, 4 show the distribution of u; the curves with the dashed numbers give the distribution of v.

The distributions of u and v for four variants in the reactor cross section x = 0.5 in relation to time are illustrated in Fig. 2. Curves 1, 2, 3, 4 show the distribution of u; the curves with the dashed numbers give the distribution of v.

2. We consider the case where a substance dissolved from the gas bubble reacts with a substance present in the liquid. We assume, as before, that the Dalton and Henry laws hold. We regard the process as isothermic. We denote the concentration of substance in the liquid which reacts with the substance dissolved from the bubbles by c_3, the rate constant of the chemical reaction by k, the stoichiometric coefficient by ν, the exponents characterizing the order of the reaction by a_1 and a_2, and the coefficient of turbulent diffusion of the substance reacting with the substance dissolved from the gas bubble by D_3 [12, 13].

Thus, in the case of bubbling with a chemical reaction an equation for c_3 has to be added to the system (1.1), and a term $kc_1^{a_1}c_2^{a_2}$, obtained from the laws of chemical kinetics, has to be added to the right side of the second equation of system (1.1).

We have to write the corresponding boundary and initial conditions for c_3.

The system of equations in this case in dimensionless variables will have the form

$$\begin{gathered}\frac{\partial u}{\partial t} + \frac{\partial u}{\partial x} = -\gamma(\lambda u - v)\\ \frac{\partial v}{\partial t} - D_2\frac{\partial^2 v}{\partial x^2} = \gamma(\lambda u - v) - kv^{a_1}w^{a_2}\\ \frac{\partial w}{\partial t} - D_3\frac{\partial^2 w}{\partial x^2} = -\nu k v^{a_1}w^{a_2}\end{gathered} \tag{2.1}$$

The initial conditions are

$$u(x, 0) = 0 \qquad v(x, 0) = 0, \qquad w(x, 0) = w_0 \tag{2.2}$$

and the boundary conditions

$$\begin{gathered}u(0, t) = 1, \qquad [\partial v/\partial x]_{x=0} = 0, \qquad [\partial v/\partial x]_{x=1} = 0\\ [\partial w/\partial x]_{x=0} = 0, \qquad [\partial w/\partial x]_{x=1} = 0\end{gathered} \tag{2.3}$$

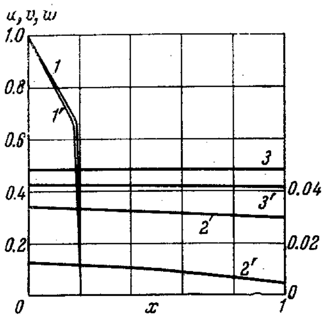

Fig. 3

Here D_2 and D_3 are dimensionless diffusion coefficients; k, γ, and λ are dimensionless coefficients corresponding to the rate constant of the chemical reaction, the mass transfer coefficient, and the Henry constant; $\omega = c_3/c_1°$.

A difference scheme [14] was used to solve system (2.1) with conditions (2.2) and (2.3).

In the semistrip $x \in [0, 1]$, $t \geq 0$, a main rectangular net $x = j\Delta x$, $t = i\Delta t$, and an auxiliary net $x = j\Delta x$, $t = \frac{1}{2}i\Delta t$ ($j = 0, 1, 2, \ldots, n$; $i = 0, 1, \ldots$) were constructed.

The first equation of system (2.1) was solved in exactly the same way as (1.3).

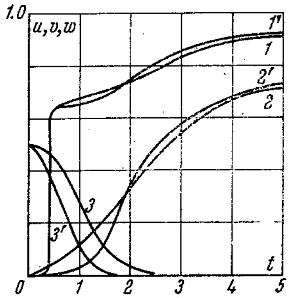

Fig. 4

Since the boundary conditions are inconsistent, we used a two-point approximation of the boundary conditions for the first q layers and then a more accurate three-point approximation for subsequent layers.

We took equal steps for the time and space variables to avoid "smearing" of the concentration front (u). The calculations were performed for Δt and Δx equal to 0.02. To check the accuracy we calculated some variants with steps $\Delta t = \Delta x = 0.01$, and a_1 and a_2 taken as unity which corresponds to a second-order reaction.

Some variants were calculated by iteration schemes [11]. These calculations gave results which were practically the same as the calculations by the scheme of [14], but the iteration schemes required more machine time.

The calculations were performed for two combinations of values of the parameters k, γ, λ, D_2, and D_3, viz.,

1 (10, 1.5, 0.8, 10, 10), *2* (100, 1.5, 0.8, 10, 10)

We give the values of u, v, and w in relation to x for t = 0.2 and in relation to t for x = 0.4 for the first variant:

$t = 0.2$

$x = 0$	0.18	0.20	1.0
$u = 1.000\,000$	0.661 378	0.001 397	0.000 739
$v = 0.018\,382$	0.017 198	0.016 816	0.011 214
$w = 0.494\,980$	0.494 996	0.495 015	0.495 282

$x = 0.4$

$t = 0$	0.4	1.0	2.0
$u = 0.000\,000$	0.008 216	0.670 496	0.756 894
$v = 0.000\,000$	0.041 978	0.133 630	0.343 744
$w = 0.500\,000$	0.468 916	0.282 363	0.028 475

The distributions of the dimensionless concentrations u, v, and w in relation to x for t = 0.2 are shown for two variants in Fig. 3. Curves 1, 2, and 3 show the distributions of u, v, and w, respectively, for the first variant; the curves for the second variant are denoted by dashed numbers. Figure 4 shows the distribution curves of u, v, and w in relation to time for x = 0.4.

Curves 1, 2, and 3 show the distributions of u, v, and w, respectively, for the first variant; the curves for the second variant are denoted by dashed numbers.

The authors thank L. A. Chudov for advice and interest in the work.

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