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NUMERICAL SOLUTION OF A NONSTEADY EXTRACTION PROBLEM IN THE CASE OF NONLINEARITY OF THE MASS-TRANSFER-COEFFICIENT RELATION

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A numerical solution is presented to an extraction problem with a variable mass-transfer coefficient and variable concentration of the external medium and a nonlinear condition of equilibrium on the surface of the body.

Well-known analytical solutions [1, 2] to the problem of nonsteady mass transfer during extraction were obtained for relatively simple cases, when the mass-transfer coefficient was assumed constant over the duration of the process. These solutions often differ significantly from the empirical data. In these cases, there is no regular regime [3], which can be attributed to several factors. Among these factors are a variable mass-transfer coefficient, polydispersity [4], the simultaneous extraction of several substances, and kinetic nonequivalence of the pores [5].

The study [2] examined special cases of mass transfer. The study [1] found the region of a regular regime with $\beta = 0$. The report [6] approximately solved the problem with allowance for the linear dependence of the mass transfer coefficient on concentration. The investigation [7, 8] obtained a solution in the case of a mass-transfer coefficient dependent on concentration without approximations limiting the form of the function but with $Bi = \infty$. These studies investigated exponential and rational dependences of the mass-transfer coefficient on concentration. Other particular solutions were obtained for a constant mass transfer coefficient and $\beta \neq 0$ [9-14].

This article presents a numerical solution of the above problem for three classic forms (plate, T = 0; cylinder, T = 1; sphere, T = 2) with a variable mass-transfer coefficient, variable concentration of the external medium, and nonlinear condition of equilibrium on the surface of the body.

Formulated in this way, the problem is described by the equation

$$\frac{\partial C_2}{\partial \tau} = \frac{1}{x^T}\frac{\partial}{\partial x}\left[x^T D_e(C_2)\frac{\partial C_2}{\partial x}\right]. \quad (1)$$

Equation (1) is supplemented by the following boundary and initial conditions:

$$\frac{\partial C_2}{\partial x} = 0;\ x = 0;\ \tau \geqslant 0, \quad (2)$$

$$W\frac{\partial C_1}{\partial \tau} = -N\varepsilon_1 D_2(C_2)\,S\frac{\partial C_2}{\partial x};\ x = R, \quad (3)$$

$$C_1 = \varkappa(C_2);\ x = R, \quad (4)$$

$$C_2 = C_{20};\ C_1 = C_{10};\ \tau = 0. \quad (5)$$

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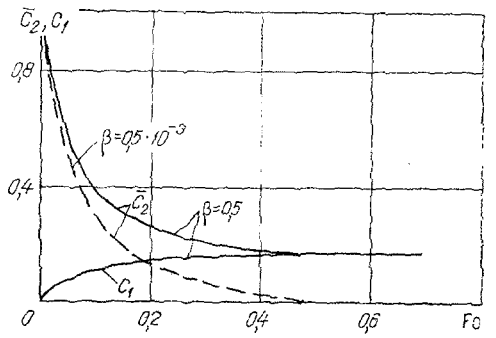

Fig. 1. Dependence of $\bar{C}_2$ and C_1 on Fo with $\beta = 0$ and $\beta \neq 0$.

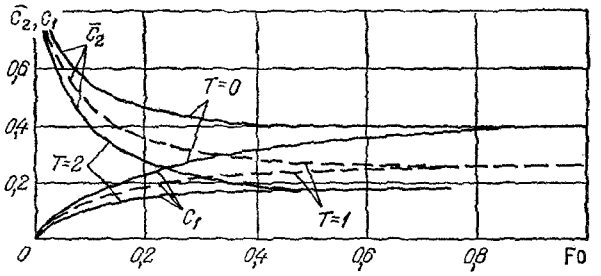

Fig. 2. Dependence of $\bar{C}_2$ and C_1 on Fo for T = 0, 1, and 2 with $\beta = 0.5$.

We use the following relations to write Eq. (1) and the boundary and initial conditions in dimensionless form:

$$\frac{C_2-\bar{C}_{20}}{C_{20}-\bar{C}_{20}}=\vartheta_2;\quad \bar{C}_{20}=\frac{C_{10}}{\varkappa}, \tag{6}$$

$$\frac{x}{R}=\varphi, \tag{7}$$

$$\frac{D_e}{D_{e0}}=D_e^*, \tag{8}$$

$$\mathrm{Fo}=\frac{D_{e0}\tau}{R^2}, \tag{9}$$

$$\frac{C_2-\bar{C}_{20}}{C_1-\bar{C}_{20}}=\vartheta_1, \tag{10}$$

$$\lambda(\vartheta_2)=\frac{N\varepsilon_1 S D^*(\vartheta_2)R^3}{W}. \tag{11}$$

After making a substitution of variables, we obtain Eq. (1) and conditions (2)-(5) in the following form

$$\frac{\partial\vartheta_2}{\partial(\mathrm{Fo})}=\frac{1}{\varphi^T}\frac{\partial}{\partial\varphi}\left[\varphi^T D^*(\vartheta_2)\frac{\partial\vartheta_2}{\partial\varphi}\right], \tag{12}$$

$$\left.\frac{\partial\vartheta_2}{\partial\varphi}\right|_{\varphi=0}=0, \tag{13}$$

$$\frac{\partial\vartheta_1}{\partial(\mathrm{Fo})}=\lambda(\vartheta_2)\left.\frac{\partial\vartheta_2}{\partial\varphi}\right|_{\varphi=1}. \tag{14}$$

We solve system (12)-(14) numerically by the finite differences method, using an implicit second-order approximation scheme both for the equation and for the boundary conditions. Due to the nonlinearity, we obtain the solution by means of iterations [15, 16].

We use the solution obtained to study the effect of the form of the mass-transfer-coefficient relation $D_e = D_e(C_2)$ on concentration C_2. Following [7, 8], we use two methods of expressing this relation:

$$D_e = \frac{D_{eo}}{1 + a_1 C_2}, \tag{15}$$

$$D_e = D_{eo} \exp(a_2 C_2). \tag{16}$$

We checked the solution by comparing the results obtained with Eqs. (15) and (16) with the results in [17] obtained for the case $\beta = 0$, i.e. without allowance for the effect of a change in concentration in the surrounding medium. The comparison was done with a value of the parameter h = 0.167 and 0.833 ($a_1 > 0$) and h = 1.25 ($a_1 < 0$), where $h = (1 + a_1 C_{1p})/(1 + a_1 C_{1o})$. The results agreed well in both cases.

During the numerical experiments we studied the effect of the hydraulic modulus and the form of the body on the course of the extraction process with a mass-transfer coefficient varying according to Eq. (15) and a variable concentration of the external medium. During occurrence of the nonsteady process, the hydraulic modulus — the ratio of the quantity of liquid phase to the quantity of solid phase — has a substantial effect on the degree of extraction. There should be an increase in the degree of extraction with an increase in the hydraulic modulus. This relationship is confirmed by Fig. 1, which shows the functions $\overline{C}_2 = f(Fo)$ and $C_1 = f(Fo)$ for $\beta \approx 0$ ($\beta = 0.5 \cdot 10^{-3}$) and $\beta \neq 0$ ($\beta = 0.5$).

In the first case, when the hydraulic modulus approaches infinity, the extraction process proceeds considerably more rapidly than when the modulus has a finite value.

The effect of the form of the particles on the extraction rate can be seen from Fig. 2, which shows the change in concentration in both cases for three classic forms — plate, cylinder, and sphere — under identical conditions for the process. It follows from the figure that extraction takes place most rapidly when the particles are spherical and least rapidly when they are in plate form.

NOTATION

β, ratio of quantity of extracted substance in the solid phase to quantity of same in the liquid phase, kg/m³; C_1, concentration of substance in the liquid phase, kg/m³; Bi, Biot criterion; τ, time; sec; x, direction of mass transfer, m; T, parameter considering the form of the body; D_e, mass-transfer coefficient, m²/sec; W, quantity of the liquid phase, m³; C_2, concentration of the substance in the solid phase, kg/m³; N, number of particles; S, surface of the particles normal to the direction x, m²; R, characteristic dimension of the particles, m; , equilibrium function on the surface of the particles; C_{2o}, C_{1o}, initial concentrations, kg/m³; ε_1, internal porosity of the solid, m³/m³; Fo, Fourier criterion; φ, relative length; D_{eo}, mass-transfer coefficient at $C_2 \to 0$, kg/m³; $\overline{C}_{2o}$, initial mean concentration; D_e^*, relative mass-transfer coefficient; ϑ_1, ϑ_2, dimensionless concentrations; $D^*(\vartheta_2)$, dimensionless diffusion coefficient; a_1, a_2, constants; λ, dimensionless mass-transfer complex; h, parameter; $\overline{C}_2$, mean concentration in the solid phase, kg/m³; C_{1p}, equilibrium concentration in the liquid phase, kg/m³.

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LIMITS OF APPLICABILITY OF THE BOHM FORMULA

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A comparison is made between the densities of ion current on spherical and cylindrical probes calculated by Bohm's approximate formula and on the basis of a rigorous numerical solution of Vlasov's system of equations.

Probe methods of diagnosing plasmas have now found wide application. If the plasma is of sufficiently low density, the concentration of charged particles can be calculated from the Bohm formula [1]

$$n_i = \frac{I_i}{ae\,(2\,kT_e/m_i)^{1/2}S}. \tag{1}$$

The coefficient $a = 0.8$ for a spherical probe and 0.4 for a cylindrical probe. As was noted in [2], Eq. (1) is valid if the mean free path of the particles of the plasma λ is much greater than the probe dimension r_0 and if r_0 is much greater than the thickness of the space-charge layer Δ. Also, the value of T_i of the ions must be much less than the electron temperature. The potential of the probe φ_0 must be negative and of sufficient magnitude. These conditions reduce to the following system of inequalities:

$$\lambda \gg r_0 \gg \Delta, \tag{2}$$

$$T_e \gg T_i, \tag{3}$$

$$e\varphi_0/kT_i \ll 0. \tag{4}$$

Conditions (2)-(4) are encountered in practice in measurements in a glow-discharge plasma and in low-pressure arcs if the concentration of charged particles $n_i \gtrsim 10^{10}$ cm^{-3}. The validity of Eq. (1) was checked repeatedly by comparing probe measurements with measurements obtained by other independent methods. We performed one such comparison using results for a molecular plasma flow coming out of a plasmatron. We used a cylindrical probe with its axis parallel to the flow axis. The concentration of charged particles in the flow was about 10^{12} cm^{-3}. Under these conditions, the thickness of the space-charge layer proves to be much less than the probe radius. Thus, the end effect can be ignored [3]. By selecting a probe with a length much greater than its radius, we also succeeded in establishing conditions such that the directed velocity had no effect on the ion saturation current. The con-

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