UNSTEADY CONVECTION MASS TRANSFER INSIDE A DROP IN THE PRESENCE OF VOLUME CHEMICAL REACTION*

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Unsteady diffusion inside a moving drop of material dissolved in a stream of viscous liquid is investigated at high Péclet numbers. The diffusing material in the drop volume may take part in a first-order chemical reaction. The case is considered, when the concentration of the dissolved substance in the liquid surrounding the drop is uniform, and its transport inside the drop depends on the velocity field distribution and the concentration only in that region (the internal problem). The flow in the drop is assumed to be steady and to correspond to a spherical Hill vortex (at low Reynolds number).

Previously the internal problem was investigated assuming constant concentration along the streamline /1,2/, which is obviously unsuitable /3/ in the region of a diffusion boundary layer which occurs when there is no chemical reaction for times less than a^2/D , where a is the drop radius and D the diffusion coefficient. To define the diffusion inside the drop the equation /4/ for the concentration averaged over the drop surface was considered. When the difference between the concentration and its averaged value is negligibly small (a quantity of the order of $1/P_{e}$, where Pe is the Peclet number), the investigation of the concentration distribution in the drop is analogous to that considered earlier in /1/. Calculations of the concentration distribution for times of the order of the order of (a/U) ln Pe requires taking into account the solute transport along the drop axis of symmetry.

Below, using the method of joined asymptotic expansions inside the drop, several regions are established, the concentration distribution is determined in each of them, and the stream of material diffusing through the drop surface in the neighbourhood of the front and rear stagnation point are established. The non-monotonic properties of the decrease of the modified stream with time is explained.

1. Let a steady stream of viscous incompressible fluid, moving at velocity U away from the drop, flow over the drop of radius a. In a spherical system of coordinates with origin at the drop centre (the angle θ is measured from the direction of the oncoming stream) the unsteady concentration distribution $c(r, \theta, t)$ of the diffusing substance inside the drop when there is a first-order volume chemical reaction is defined by the following equation in dimensionless variables:

$$\frac{\partial c}{\partial t} + v_r \frac{\partial c}{\partial r} + \frac{v_{\theta}}{r} \frac{\partial c}{\partial \theta} = \frac{1}{Pe} \left(\frac{1}{r^2} \frac{\partial}{\partial r} r^2 \frac{\partial c}{\partial r} + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \sin \theta \frac{\partial c}{\partial \theta} \right) - kc$$
(1.1)

$$v_r = -\frac{1}{r^2 \sin \theta} \frac{\partial \Psi}{\partial \theta}, \quad v_{\theta} = \frac{1}{r \sin \theta} \frac{\partial \Psi}{\partial r}$$

$$\Psi = \frac{r^2}{2} \left(1 - r^2 \right) \sin^2 \theta, \quad Pe = \frac{1}{e^2} = \frac{v_{\theta} a}{D}, \quad v_{\theta} = \frac{\mu U}{2(\mu + \mu')}$$

(in which the radial coordinate is related to the drop radius and the concentration to the concentration of the solute on the drop surface). Here D is the diffusion coefficient, μ and μ' are the dynamic viscosities of the fluids outside and inside the drop, and k is the dimensionless rate of chemical reaction.

At the initial instant of time the diffusing substance is not inside the drop, while at the surface the concentration is independent of time, i.e.

$$c(r, \theta, 0) = 0, r \neq 1$$
 (1.2)

$$c(1, \theta, t) = 1, t \neq 0$$
 (1.3)

At fairly high rate of chemical reaction at all times and for any value of k at short times the solute diffusing into the drop is concentrated in a thin layer close to the drop surface and its axis. Together with the large Péclet number this enables us to use the method of joined asymptotic expansions to solve the problem. We separate several regions inside the drop in

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each of which Eq.(1.1) is simplified, and shall seek solutions of these simplified equations that satisfy the initial condition (1.2) and the boundary condition (1.3) and are merged at the boundary of the separate regions (time is a parameter). The separation into regions is achieved by an asymptotic analysis of the solution in the region of the boundary layer and of the following separated regions (see, e.g. /5/).

2. In the region of the diffusion boundary layer (region 1 in Fig.1), Eq.(1.1) in the variables $y = (1 - r)/\epsilon$ and $v = \cos \theta$ allowing only for zero-order terms in ϵ can be written in the form

$$\frac{\partial^2 c_1}{\partial y^2} - 2y v \frac{\partial c_1}{\partial y} - (1 - v^2) \frac{\partial c_1}{\partial v} = kc_1 + \frac{\partial c_1}{\partial t}$$
(2.1)

Here and henceforth, the subscript denotes the number of the region in Fig.1.

Replacing the independent variables $\psi_1,\,\omega_1,\,\tau_1$ by $y,\,v,\,t$, where



and replacing c_1 (ψ_1 , τ_1 , ω_1) by

$$C_{1}(\psi_{1},\tau_{1},\omega_{1}) = \left(\frac{1+v}{1-v}\right)^{k/2} c_{1}(\psi_{1},\tau_{1},\omega_{1})$$
(2.2)

we transform Eq.(2.1) into the form of the heat-conduction equation

$$\frac{\partial C_1}{\partial \tau_1} = \frac{\partial^2 C_1}{\partial \psi_1^2} \tag{2.3}$$

A similar change of variables for the equation of unsteady convective diffusion was proposed in /6-8/, and substitution (2.3) was considered in /3/.

The boundary conditions for Eq.(2.3) with the indicated transformations and the boundary condition (1.3) have the form

$$C_1(0, \tau_1, \omega_1) = \left(\frac{1 + v(\tau_1, \omega_1)}{1 - v(\tau_1, \omega_1)}\right)^{k/2}, \quad \tau_1 \neq 0$$

$$C_1(\infty, \tau_1, \omega_1) = 0$$

The analog of the initial condition for Eq.(2.3) is

 $C_1(\mathbf{\psi}_1, 0, \omega_1) = f(\mathbf{\psi}_1, \omega_1), \ \mathbf{\psi}_1 \neq 0$

This function will be determined after constructing the solution in all regions from the joining condition. Note that the above transformations of independent variables and the relatio $f(\psi_1, \omega_1) = 0$ when t = 0 ensures that the initial condition (1.2) is satisfied.

Thus the concentration distribution in the boundary layer close to the drop surface is given by the expression

$$c_{1}(\psi_{1},\tau_{1},\omega_{1}) = \frac{1}{2\sqrt{\pi}} \left(\frac{1-\nu(\tau_{1},\omega_{1})}{1+\nu(\tau_{1},\omega_{1})}\right)^{k/2} \times \left[\frac{1}{\sqrt{\tau_{1}}} \int_{0}^{\infty} f(\xi,\omega_{1}) E(\xi,\psi_{1},\tau_{1}) d\xi + \right.$$

$$\psi_{1} \int_{0}^{\tau_{1}} \left(\frac{1+\nu(\eta,\omega_{1})}{1-\nu(\eta,\omega_{1})}\right)^{k/2} \exp\left(-\frac{\psi_{1}^{2}}{4(\tau_{1}-\eta)}\right) \frac{d\eta}{(\tau_{1}-\eta)^{s/s}} \left]$$

$$E(\xi,\psi_{1},\tau_{1}) = \exp\left(-\frac{(\psi_{1}-\xi)^{2}}{4\tau_{1}}\right) - \exp\left(-\frac{(\psi_{1}+\xi)^{4}}{4\tau_{1}}\right)$$
(2.4)

In the second integral of solution (2.4) we change the variable of integration $x = \frac{1}{2}\psi_1$ $(\tau_1 - \eta)^{-1/2}$. As a result we obtain the following expression for the concentration

$$c_{1} = \frac{1}{2\sqrt{\pi}} \left(\frac{1-\nu}{1+\nu}\right)^{k/2} \frac{1}{\sqrt{\tau_{1}}} \int_{0}^{\infty} f(\xi, \omega_{1}) E(\xi, \psi_{1}, \tau_{1}) d\xi +$$

$$\frac{2}{\sqrt{\pi}} \int_{u}^{\infty} \left(\frac{1-\nu}{1+\nu} \frac{1+\zeta(x)}{1-\zeta(x)}\right)^{k/2} \exp(-x^{2}) dx, \quad u = \frac{1}{2} \psi_{1} / \sqrt{\tau_{1}}$$
(2.5)

where the function $\zeta(x)$ is given by

$$\tau_1 - \frac{\psi_1^*}{4x^4} = \frac{2 - \zeta(x)}{3} (1 + \zeta(x))^2 - \frac{|2 - \varkappa(\omega_1)|}{3} (1 + \varkappa(\omega_1))^2$$



To determine the concentration in the neighbourhood of the rear stagnation point (region 2) it is necessary to obtain the asymptotic form of solution (2.5) as $v \rightarrow 1$ and for a fixed value of y. The first term of formula (2.5) is a small quantity when $v \rightarrow 1$, and the main contribution to the limit value is made by the second term. In the neighbourhood of v = 1 the following approximation hold:

$$\tau_1 = (1 - \nu)^2 (e^{4t} - 1), \ 1 - \zeta (x) = (1 - \nu) \sqrt{1 + (y / x)^2}$$

Consequently

$$\lim_{v \to 1} c_1 = \frac{2}{\sqrt{\pi}} \int_p^{\infty} \left(1 + \frac{y^2}{x^2} \right)^{-k/4} \exp\left(-x^2\right) dx, \quad p = y \left(e^{4t} - 1\right)^{-1/4}$$
(2.6)

In the rear stagnation point the variables y and $\varphi = \theta/\epsilon$ are of the order of unity. Let us assume that the concentration derivatives with respect to y and φ are also of the order of unity. Then Eq.(1.1), after linearization of coefficients, simplifies to

$$\frac{\partial^2 c_2}{\partial y^2} + \frac{\partial^2 c_2}{\partial \varphi^2} - 2y \frac{\partial c_2}{\partial y} + \left(\varphi + \frac{1}{\varphi}\right) \frac{\partial c_1}{\partial \varphi} = kc_2 + \frac{\partial c_2}{\partial t}$$
(2.7)

For this equation we have the initial condition $c_1 = 0$ when t = 0 and the boundary condition $c_2 = 1$ when y = 0. It is also necessary that the solution of this equation is joined as $\varphi \to \infty$ with the asymptotic form (2.6). If we limit the search for the solution of Eq. (2.7), which is independent of φ , it can be shown that Eq.(2.6) is the solution of the present problem, i.e.

$$c_2(y, \varphi, t) = \lim_{y \to 1} c_1$$
 (2.8)

In a cylindrical system of coordinates z, $\eta = e^{-t/r} \sin \theta$ with z axis oriented along the polar axis, the equation of Convective diffusion for the concentration distribution in the region of convective transport (region 3) has the form

$$(1-z^{\mathbf{s}})\frac{\partial c_{\mathbf{s}}}{\partial z}+\eta z\frac{\partial c_{\mathbf{s}}}{\partial \eta}=kc_{\mathbf{s}}+\frac{\partial c_{\mathbf{s}}}{\partial t}$$

For this equation we have the initial condition $c_3 = 0$ when t = 0. The general solution of this equation is

$$c_{3} = \left(\frac{1+z}{1-z}\right)^{k/2} F(\psi_{3}, \omega_{3})$$

$$\psi_{3} = \frac{\eta^{3}}{2} (1-z^{2}), \quad \omega_{3} = t - \frac{1}{2} \ln \frac{1-z}{1+z}$$
(2.9)

The condition for joining at the boundary of regions 1 and 3 enables us to determine the function $F(\psi_3, \omega_3)$. For limited values of k, solution (2.5), when $v \rightarrow 1$ and $\psi_1 \neq 0$ has the asymptotic form

$$\lim_{\gamma \to 1} c_1 = \left(\frac{\varepsilon \psi_1}{4 (1-r)}\right)^{k/2} \left[\frac{1}{2 \sqrt{\pi \tau_1^0}} \int_0^\infty f\left(\xi, \omega_1\right) E\left(\xi, \psi_1, \tau_1^0\right) d\xi + \frac{2}{\sqrt{\pi}} \int_{u^*}^\infty \left(\frac{1+\zeta(x)}{1-\zeta(x)}\right)^{k/2} \exp\left(-x^2\right) dx \right]$$
$$u^0 = \frac{\psi_1}{2 \sqrt{\tau_1^0}}, \quad \tau_1^0 = \frac{4}{3} - \frac{2-\chi(\omega_1)}{3} \left(1+\chi(\omega_1)\right)^2$$
$$\frac{4}{3} - \frac{\psi_1^3}{4x^2} = -\frac{2-\zeta(x)}{3} \left(1+\zeta(x)\right)^2$$

Taking into account that in the joining region $\psi_3 = \psi_1$ and $\omega_3 = \omega_1 - \frac{1}{3} \ln (\varepsilon \psi_3/8)$, we obtain for the function $F(\psi_3, \omega_3)$ the expression

$$F(\psi_{3}, \omega_{3}) = \left(\frac{e\psi_{3}}{8}\right)^{k/2} \left[\frac{1}{2\sqrt{\pi\tau_{s}(\omega_{2}^{0})}} \int_{0}^{\infty} f(\xi, \omega_{3}^{0}) E(\xi, \psi_{3}, \omega_{3}^{0}) d\xi + \cdots \right]$$

$$\frac{2}{\sqrt{\pi}} \int_{u_{s}}^{\infty} \left(\frac{1+\zeta(x)}{1-\zeta(x)}\right)^{k/2} \exp(-x^{2}) dx = \frac{\psi_{3}}{2\sqrt{\tau_{s}(\omega_{3}^{0})}}$$

$$\omega_{3}^{0} = \omega_{3} + \frac{1}{2} \ln(e\psi_{3}/8), \quad \tau_{3}(\omega_{3}^{0}) = \frac{4}{3} - \frac{1}{3} (2 - \frac{1}{3} ($$

Near the drop axis of symmetry (region 4) we introduce new variables z and $\rho = e^{-1}r \sin \theta = e^{-1}r\eta$. Assuming that in that region the concentration derivatives with respect to the new variables are of the order of unity and taking the leading terms into account, we obtain the following condition:

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we obtain

$$(1-z^2)\frac{\partial c_4}{\partial z} + \rho z \frac{\partial c_4}{\partial \rho} + \frac{\partial^2 c_4}{\partial \rho^3} + \frac{1}{\rho} \frac{\partial c_4}{\partial \rho} = kc_4 + \frac{\partial c_4}{\partial t}$$
(2.11)

The solution of this equation must satisfy two joining conditions

$$\lim_{z \to 1} c_4 = \lim_{y \to \infty} c_2, \quad \lim_{\rho \to \infty} c_4 = \lim_{\phi \to 0} c_3 \tag{2.12}$$

and the initial condition $c_4 = 0$ when t = 0. The asymptotic form of solution (2.8) has the form

$$\lim_{y\to\infty}c_2=\frac{2}{\sqrt[y]{\pi}}y^{-k/2}\int\limits_p^\infty\xi^{k/2}\exp\left(-\xi^2\right)d\xi$$

For the concentration in region 3 as $\psi_3 \rightarrow 0$, taking into account that

$$\tau_{s}(\omega_{s}^{0}) = \frac{\varepsilon^{2}\psi_{s}^{2}}{16} \left(\frac{1+z}{1-z}\right)^{s} e^{4t}, \quad 1-\zeta(x) = \frac{\psi_{s}}{2x}$$

$$\lim_{\psi_{s} \to 0} c_{s} = \frac{2}{\sqrt{\pi}} \left(\frac{\varepsilon}{2}\right)^{k/2} \left(\frac{1+z}{1-z}\right)^{k/2} \int_{p_{s}}^{\infty} x^{k/3} \exp\left(-x^{2}\right) dx, \quad (2.13)$$

$$p_{3} = \frac{2}{\varepsilon} \frac{1-z}{1+z} e^{-3t}$$

It can be shown that the expression for the concentration (2.13)

$$c_4(z,t) = \lim_{\psi_1 \to 0} c_3(z,\psi_2,\omega_3)$$

is the solution of Eq.(2.11) and satisfies the joining conditions (2.12) and the initial condition, if in conformity with the stated accurracy of the asymptotic expansion, the terms with exponentially small order are neglected.

The concentration distribution in the region of convective transport must be joined with the boundary-layer solution

$$\lim_{t \to -1} c_1 = \lim_{z \to -1} c_3 \tag{2.14}$$

If we take into account that the relation $\omega_3 \Rightarrow \omega_1 + \frac{1}{3} \ln (\epsilon \psi_1/8)$ holds as $\nu \rightarrow -1$ and $z \rightarrow -1$, then we obtain the following limit values of the concentration in regions 1 and 3:

$$\begin{split} \lim_{\mathbf{v} \to \mathbf{1}} c_{1} &= \left(\frac{4\left(1-r\right)}{\varepsilon \psi_{1}}\right)^{k/2} f\left(\psi_{1}, \omega_{1}\right), \quad \psi_{1} \neq 0\\ \lim_{x \to \mathbf{1}} c_{2} &= \left(\frac{\varepsilon \psi_{2}\left(1-r\right)}{16}\right)^{k/2} \left[\frac{1}{2\sqrt{\pi \tau_{2}\left(\omega_{1}^{0}\right)}} \int_{0}^{\infty} f\left(\xi, \omega_{1}^{0}\right) E\left(\xi, \psi_{2}, \tau_{3}\left(\omega_{1}^{0}\right)\right) d\xi + \frac{2}{\sqrt{\pi}} \int_{\omega_{1}^{0}}^{\infty} \left(\frac{1+\zeta\left(x\right)}{1-\zeta\left(x\right)}\right)^{k/2} \exp\left(-x^{2}\right) dx \right]\\ u_{3}^{0} &= \frac{1}{2} \frac{\psi_{3}}{\sqrt{\tau_{3}\left(\omega_{1}^{0}\right)}} , \quad \omega_{1}^{0} = \omega_{1} + \ln \frac{\varepsilon \psi_{1}}{8} \end{split}$$

From the joining condition (2.14) we obtain the integral equation for determining the function $f(\psi_1, \omega_1)$

$$f(\psi_{1}, |\omega_{1}) = \left(\frac{\varepsilon\psi_{1}}{8}\right)^{k} \left[\frac{1}{2\sqrt{\pi\tau_{s}}(\omega_{1}^{0})} \int_{0}^{\infty} f(\xi, \omega_{1}^{0}) E(\xi, \psi_{1}, \tau_{3}(\omega_{1}^{0})) d\xi + \frac{2}{\sqrt{\pi}} \int_{\omega_{1}}^{\infty} \left(\frac{1+\zeta(x)}{1-\zeta(x)}\right)^{k/2} \exp(-x^{2}) dx \right], \quad u_{1}^{0} = \frac{\psi_{1}}{2\sqrt{\tau_{s}}(\omega_{1}^{0})}$$
(2.15)

For limited values of k > 1/2 or for any k with $t \ll \ln (8/\epsilon)$ to within terms of the order of ϵ the solution of Eq.(2.15) is the first iteration

$$f(\psi_1, \omega_1) = \frac{2}{\sqrt{\pi}} \left(\frac{e\psi_1}{8}\right)^k \int_{\omega_1}^{\infty} \left(\frac{1+\zeta(x)}{1-\zeta(x)}\right)^{k/2} \exp\left(-x^2\right) dx$$
(2.16)

Equation (2.15) enables the asymptotic form of the function $f(\psi_1, \omega_1)$ as $\psi_1 \rightarrow 0$ and limited values of k to be obtained. In this case the solution is determined by the second term on the right-hand side of Eq.(2.15) in which

$$\tau_3 = \frac{1}{4} \left(\frac{e\psi_1}{4} \right)^4 \left(\frac{1-v}{1+v} \right)^2 e^{4t}, \quad 1-\zeta(x) = \frac{\psi_1}{2x}$$

The final form of the asymptotic form of the function $f(\psi_1, \omega_1)$ as $\psi_1 \rightarrow 0$ is

$$f(\psi_1, \omega_1) = \frac{2}{\sqrt{\pi}} \left(\frac{\varepsilon}{4}\right)^k \psi_1^{k/2} \int_{u_4}^{\infty} x^{k/2} \exp(-x^2) dx, \ u_1^0 = \frac{1}{4} \psi_1 \exp(-2\omega_1^0)$$

and enables us to find the limit of solution (2.5), necessary for determining the concentration at the forward stagnation point, as $v \rightarrow -1$ and for a fixed value of y. Note that in this case

$$\begin{aligned} x &= -1 + (1 + v) e^{-xt}, \ \tau_1 = (1 + v)^2 (1 - e^{-\varepsilon t}) \\ 1 &+ \zeta (x) = (1 + v) \sqrt{1 - (y/x)^2} \end{aligned}$$

After some transformations, we obtain

$$\lim_{V \to -1} c_1 = \frac{4}{\pi} \left(\frac{\varepsilon}{2}\right)^k (1 - e^{-4t})^{-1/2} \exp\left(-\frac{y^2}{1 - e^{-4t}}\right) \int_0^\infty d\lambda \times$$

$$\exp\left(-\frac{\lambda^2}{1 - e^{-4t}}\right) \lambda^{k/2} \operatorname{sh} \frac{2y\lambda}{1 - e^{-4t}} \int_{u_1}^\infty dx x^{k/3} \exp\left(-x^2\right) +$$

$$\frac{2}{\sqrt{\pi}} \int_{p_1}^\infty \left(1 - \frac{y^2}{x^2}\right)^{k/4} \exp\left(-x^2\right) dx, \quad u_1 = \frac{4e^{-2t}}{e^{4\lambda}}, \quad p_1 = \frac{y}{\sqrt{1 - e^{-4t}}}$$
(2.17)

Let us assume that at the front stagnation point (region 5) the concentration derivatives with respect to the variables y and $\alpha = e^{-1} (\pi - \theta)$ are of the order of unity. Retaining the leading terms in Eq.(1.1), we obtain

$$\frac{\partial^2 c_b}{\partial y^2} + \frac{\partial^2 c_b}{\partial \alpha^2} + 2y \frac{\partial c_b}{\partial y} + \left(\frac{1}{\alpha} - \alpha\right) \frac{\partial c_b}{\partial \alpha} = kc_b + \frac{\partial c_b}{\partial t}$$
(2.18)

The solution of this equation must satisfy the initial $c_s = 0$ condition when t = 0 and the boundary condition $c_s = 1$ when y = 0, and, also, the two joining conditions

$$\lim_{\alpha \to \infty} c_5 = \lim_{\nu \to -1} c_1, \quad \lim_{\nu \to \infty} c_5 = \lim_{\tau \to -1} c_4$$

It can be shown by direct substitution that expression (2.17) is the solution of Eq.(2.18), that satisfies the conditions derived above.

This result can be arrived at by the following reasoning. In Eq.(2.18) we make the change of variables

$$c_b = e^{-kt}C_b, \ \xi = ye^{2t}, \ \tau = \frac{1}{4} (e^{4t} - 1)$$

This reduces it to the form

$$\frac{\partial C_5}{\partial \tau} = \frac{\partial^2 C_5}{\partial \xi^2}$$

Reverting to the old variables, we have

 $c_{5} = \lim_{n \to \infty} c_{1}$

If we note that the main contribution to the limit of the first term of expression (2.17) as $y \to \infty$, is made by the neighbourhood of the point $y = \lambda$, while the second term is of higher order of smallness, it is possible to ascertain that the joining of the solutions in regions 5 and 4 is assured. In the same way it can be established that formula (2.19) is the solution of Eq.(2.18) that satisfies all of the stated conditions.

Thus five regions have been separated in the drop, in each of which the concentration distribution has been obtained The limits of these expressions as $t \rightarrow \infty$ correspond to the steady concentration distribution presented in /9/.

3. Let us calculate the dimensionless density of the diffusion stream through the drop surface using the concentration distribution in the region of the diffusive boundary layer. After integration by parts and replacing in the second term of formula (2.4) the variable of integration, we obtain the following expression for the flow density:

$$j = -\frac{1}{e} \left(\frac{\partial v_1}{\partial y}\right)_{y=0} = \frac{1-v^2}{e\sqrt{\pi}} \left[\frac{e^{-k\xi}}{\sqrt{\tau_1}} + k \int_0^t \frac{e^{-k\xi}}{\sqrt{\tau_1}(v, x(\xi, v))} d\xi - \frac{1}{2\tau_1\sqrt{\tau_1}} \left(\frac{1-v}{1+v}\right)^{k/2} \int_0^\infty \xi f(\xi, \omega_1) \exp\left(-\frac{\xi^2}{4\tau_1}\right) d\xi \right]$$

$$\tau_1 (v, x(\xi, v)) = \frac{1}{s} (2-v) (1+v)^2 - \frac{1}{s} (2-x) (1+x)^2$$

$$x(\xi, v) = (1+v - (1-v) e^{2\xi})/(1+v + (1-v) e^{2\xi})$$

(2.19)

where the function $f(\xi, \omega_1)$ is determined from the integral equation (2.15).

To determine the diffusion stream density in the neighbourhood of the rear and front stagnation points we use formulas (2.8) and (2.19) respectively. We obtain

$$j_{2} = -\frac{1}{e} \left(\frac{\partial c_{3}}{\partial y}\right)_{y=0} = \frac{2}{e \sqrt{\pi}} \left[\frac{e^{(2-k)t}}{\sqrt{1-e^{-4t}}} - (2-k) \int_{0}^{t} \frac{e^{(2-k)\tau}}{\sqrt{1-e^{-4\tau}}} d\tau\right]$$

$$j_{5} = -\frac{1}{e} \left(\frac{\partial c_{5}}{\partial y}\right)_{y=0} = \frac{2}{e \sqrt{\pi}} \left[\frac{e^{-kt}}{\sqrt{1-e^{-4t}}} + k \int_{0}^{t} \frac{e^{-k\tau} d\tau}{\sqrt{1-e^{-4\tau}}} - \frac{4}{\sqrt{\pi}} \frac{(e/2)^{k}}{(1-e^{-4t})^{1/2}} \int_{0}^{\infty} d\lambda \exp\left(-\frac{\lambda^{2}}{1-e^{-4t}}\right) \lambda^{1+k/2} \int_{u_{1}}^{\infty} x^{k/2} \exp\left(-x^{2}\right) dx\right]$$

When calculating the total dimensionless stream of solute through the drop surface

$$I = \int_{-1}^{1} j \, dv$$

it is necessary, first, to solve numerically, for instance by the method of iterations, integral equation (2.15). However, as previously noted, when k > 1/2 or for any other values of k, but $t \ll \ln (8/s)$, it is possible to restrict the calculation to the first iteration, which yields an accuracy of order ε . Below, for calculating streams formula (2.16) was used for the function $f(\psi_1, \omega_1)$.

The time-dependence of the local flow for various points of the drop surface are shown in Fig.2. The calculations were made for the values of parameters Pe = 100 and k = 0.5.



Curve *l* corresponds to the stream at the front stagnation point, 2 to $\theta = \frac{2}{3}\pi$, $3 - \theta = \frac{1}{2}\pi$, and 4 at the rear stagnation point. It can be seen that during times $t \approx 1$ the local stream is constant, and only later, when $t \approx 3$, is it reduced due to the effect of transport along the drop axis of the solute, subsequently reaching a constant. This effect is fairly strong at the forward stagnation point, it rapidly decreases as θ increases, becomes insignificant when $\theta = \pi/2$, and is entirely absent at the rear stagnation point.

The time-dependence of the total stream is shown in Fig.3 for $Pe = 10^4$ and k = 0.75 by curve 1, for $Pe = 10^4$ and k = 0.5 by curve 2, for $Pe = 10^3$ and k = 0.5 by curve 3, and for $Pe = 10^3$ and k = 0.5 by curve 4. It is seen that as Pe and k increase the effect of the material transported along the drop on the stream is reduced.

In the unsteady problem without chemical reaction the results obtained, shown in Fig.4 define only the beginning of the effect of the substance transported along the drop axis. Calculations were carried out for the following values: Pe = 80 by curve 1, Pe = 250 by curve 2, for $Pe = 3 \cdot 10^3$ by curve 3 and for $Pe = 10^4$ by curve 4. As Pe increases the "shelf" of the stream curve which corresponds to the stage when the stream becomes steady lengthens in time, and the effect of the substance diffusing along the drop axis on the stream is negligibly small.

It follows from the results obtained that at the beginning of the process of solute transport through the drop surface, molecular diffusion takes place in a direction normal to the streamlines, and convective transport occurs along the streamline in the region of the boundary layer. During the time $t \approx 1$ the process of mass transfer becomes steady and remains such up to a time $t \approx T = \ln (8\sqrt{Pe})$, when the substance transported along the drop axis of symmetry begins to effect the diffusion stream. The process of unsteady diffusion was investigated in /3/ using the diffusion boundary layer method without taking into account the transport of material along the axis. Hence the results of that investigation are only applicable for defining the initial stage of the process up to a time $t \approx T$. The internal unsteady problem was also investigated in /1/, where it was assumed that the concentration along a streamline was constant. The results of that calculation are represented in Fig.4 /2/ for Pe=80 by curve 5, and for Pe = 250 by curve 6. The Kronig-Brink equation is unsuitable for defining convective diffusion at small times $t \leq 1$. In the absence of chemical reaction with Pe ≥ 1 during times $t \geq T$ that equation approximately describes the mass transfer process. However, the question of the correct selection of the initial distribution for this equation remains open. For Pe ≈ 100 during times of order T the mean concentration of the diffusing material reaches $t \approx 0.5$ which shows the unsuitability of the Kronig-Brink method for defining a considerable part of the mass transfer process.





Fig.5

In /10-12/, where the unsteady problem was investigated using finite difference methods, results that agree satisfactorily were obtained only when $Pe \leq 20$. For Pe > 100, the results of calculations are noticeably different. The results of a numerical solution in /10/ of the internal unsteady problem are compared in Fig.5 with those of the present paper with Pe = 80 and k = 0. Curve 1 shows the dependence of the modified stream $I_1 = \frac{1}{3}Ped \ln \frac{1}{2}dt$ on time. Curve 3 corresponds to the modified stream obtained in /10/. The difference reaches 30% of the flow magnitude, which is obviously connected with the need to take into account higher order terms in the method of joining asymptotic expansions and, also, with the accuracy of the numerical methods used in /10/. The question of using finite difference methods for equations with a large parameter was investigated on the model equation of convective diffusion in /13/, where it was shown that to achieve satisfactory accuracy, stiff limits must be imposed on the step of three-dimensional variables.

The internal unsteady problem with a chemical reaction of the first order was considered in /2/, using the method developed in /1/. The numerical solution of this problem in /14/ yielded results that differed considerably from those in /2/, when the chemical reaction rate was high. As is clear from the present paper, this discrepancy is due to the inadmissibility of the assumption that the concentration is constant along a streamline.

The non-monotonic form of the decrease of the modified stream with time was also considered. Thus in /2/ this peculiarity was explained by the error in the numerical calculations, and the authors overlooked the non-monotonicity in their calculations. The results of this paper indicate that the modified stream non-monotonicity (see Fig.5) is related to the presence of a shelf of the total stream, and is explained by the fact that during a certain time interval the concentration distribution in the boundary layer region is quasisteady.

If the chemical reaction rate constant satisfies the condition $k\sqrt{Pe} \gg 1$, then, as follows from the earlier estimates /9/ in solving the steady problem, the results of our investigation are suitable for defining the mass transfer process inside the drop at all times.

REFERENCES

- KRONIG R. and BRINK J., On the theory of extraction from falling droplets. Appl. Sci. Res., A, Vol.2, No.2, 1951.
- DANKWERTS P.V., Absorption by simultaneous diffusion and chemical reaction into particles of various shapes and into falling drops. Trans. Faraday Soc., Vol.47, No.9, 1951.
- LEVICH V.G., KRYLOV V.S. and VOROTILIN V.P., On the theory of unsteady diffusion from a moving drop. Dokl. Akad. Nauk SSSR, Vol.161, No.3, 1956.

- BRIGNELL A.S., Solute extraction from an internally circulating spherical liquid drop. Int. J. Heat Mass Transfer, Vol.18, No.1, 1975.
- SIH PING HUEI and NEWMAN J., Mass transfer to the rear of a sphere in Stokes flow., Int. J. Heat Mass Transfer, Vol.10, No.12, 1967.
- CHAO B.T., Transient heat and mass transfer to translating droplet. Trans. ASME, Ser. C. J. Heat Transfer, Vol.91, No.2, 1969.
- RUCKENSTEIN E., Unsteady mass transfer near fluid-liquid interfaces. Chem. Engng. Sci. Vol.25, No.11, 1970.
- POLIANIN A.D. and PRIADKIN P.A., On unsteady convection heat and mass exchange in fluid at high Péclet numbers. PMTF, No.6, 1981.
- 9. GOLOVIN A.M. and ZHIVOTIAGIN A.F., The effect of volume chemical reaction on mass transfer inside a drop at high Péclet numbers. Vestn. MGU, Ser. 1, Matem. Mekhan., No.4, 1979.
- 10. JOHNS L.E. and BECKMANN R.B., Mechanism of dispersed-phase mass transfer in a viscous single-drop extraction system. AIChE Journal, Vol.12 No.1, 1966.
- 11. BRAUER H., Unsteady state mass transfer through the interface of spherical particles, II. Int. J. Heat Mass Transfer, Vol.21, No.4, 1978.
- 12. BROUNSTEIN B.I. and RIVKIND V. Ia, The internal problem of mass and heat exchange with closed streamlines at high Péclet numbers. Dokl. Akad. Nauk SSSR, Vol.260, No.6, 1981.
- 13. PRICE H.S., VARGA R.S. and WARREN J.E., Application of oscillation matrices to diffusionconvection equations. J. Math. and Phys. Vol.45, No.3, 1966.
- 14. WATADA H., HAMIELEC, A.E. and JOHNSON A.I., A theoretical study of mass transfer with chemical reaction in drops. Canad. J. Chem. Eng., Vol.48, No.3, 1970.

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THE METHOD OF DISCRETE SINGULARITIES IN PLANE PROBLEMS OF THE THEORY OF ELASTICITY*

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Plane problems of the theory of elasticity are reduced to sets of singular integral equations for which a direct method of solution is developed, similar to the method of discrete vortices used in aerodynamics. Numerical solutions of a number of plane problems of the theory of elasticity are considered, stable numerical solutions are obtained, and their convergence is proved.

When solving problems of the theory of elasticity by reducing them to integral equations, the tendency usually was to get away from the singular integral equations (SIE), and to reduce them to regular integral equations of the first or second kind /1,2/. A similar situation occurs when solving other problems, for example, in electrodynamics /3/. It appeared, however, that numerical solutions of regular integral equations of the first kind on a computer were unstable. Regular integral equations of the second kind, obtained in the theory of elasticity, possess eigenfunctions /2/, and therefore their numerical solution on a computer by direct methods is also unstable. In view of these inconveniences in reducing the problems to regular integral equations, they are reduced to SIE, for which a stable method (the method of "discrete vortices" /4/) for their numerical solution has been developed.

Below, a similar approach is developed for solving plane problems of the theory of elasticity. These problems for bounded simply connected regions, whose boundary is a closed Liapunov curve, are reduced to SIE of the first kind with Hilbert kernels in complex conjugate functions. The conditions are obtained that ensure the uniqueness of the solution of these equations. The equations are solved numerically using the method of discrete singularities, which is a development of the method of discrete vortices. The idea of this method consists in exchanging the set of SIE for a set of linear algebraic equations in unknown functions with boundary points selected in some special way, and specially situated in relation to points at which the values of the required functions are found.

⁶³²