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DIFFUSION TO A PARTICLE IN A SHEAR GAS FLOW IN THE CASE OF ARBITRARY KINETICS OF THE SURFACE REACTION*

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Diffusion to a particle in a shear flow at small Peclet and Reynolds numbers is considered in the case when a chemical reaction, the rate of which depends on the concentration in an arbitrary manner, takes place at its surface. The heat and mass transfer in a particle in a translational flow of viscous incompressible fluid at small Peclet and Reynolds numbers were studied in /1—7/. The diffusion mode of the reaction at the particle surface was studied in /1—3/, and a heterogeneous reaction of the first, second and arbitrary order were considered in /4—6/, /4/ and /7/ respectively. The papers /8—10/ deal with the case of diffusion mode of reaction at the particle surface freely suspended in a shear flow.

Using a spherical r, θ, λ-coordinate system attached to the particle, we can describe the reagent transfer process in the fluid using the following convective diffusion equation and boundary conditions:

$$\Delta_r c = P u_i \frac{\partial c}{\partial x_i}, \quad c = \frac{c_\infty - c_*}{c_\infty}, \quad P = \frac{aU}{D} \tag{1}$$

$$r \to \infty,\ c \to 0;\ r = 1,\ \partial c/\partial r + f(1 - c) = 0, \quad f(x) = ak'(Dc_\infty)^{-1}F(c_\infty x),\ F(0) = 0 \tag{2}$$

Here c_* is the concentration, P is the Peclet number, a is the particle radius, D is the diffusion coefficient, U is the characteristic flow rate, Δ is the Laplace operator, k' is the reaction rate constant and $k'F$ is the rate of chemical reaction. Here and henceforth the repeated indices will denote summation.

In the case of an arbitrary shear flow of an incompressible fluid, the velocity distribution away from the particle has the form

$$r \to \infty,\ u_i \to G_{ij}x_j,\ G_{ii} = 0 \tag{3}$$

We shall assume for definiteness that the dimensionless coefficients in (3) and the characteristic flow rate in (1) can be expressed in terms of the elements of the shear coefficients matrix G_{ij}^* as follows:

$$G_{ij} = G_{ij}^* |G_{ij}^*|^{-1}, \quad U = a|G_{ij}^*|, \quad |G_{ij}^*| = \max_{i,j}|G_{ij}^*|$$

Let us investigate the boundary value problem (1), (2) using the method of merging asymptotic expansions in terms of the small Peclet numbers /1—10/. The flow region is divided into two subregions, the inner $\{1 \leqslant r \leqslant O(P^{-1/2})\}$ and the outer $\{O(P^{-1/2}) \leqslant r \leqslant \infty\}$ subregion /8—10/. As usual, a "compressed" coordinate $\rho = P^{1/2}r$ is introduced in the outer subregion and the solution is sought in each of the subregions separately, in the form of the inner and outer expansion. In the course of constructing an asymptotic solution we use the boundary condition (2) at the particle surface in the inner region, and boundary conditions at infinity in the outer region. The unknown constants appearing in the solution can be found using the merging procedure. Similarly /10/ we can show that in the case of a Stokes shear flow past a plane, and concentration distribution in the outer region $\{O(P^{-1/2}) \leqslant r \leqslant \infty\}$ is expressed in terms of the fundamental solution of the equation $\Delta_\rho\Psi = G_{ij}\rho_j \partial\Psi/\partial\rho_i$, in the form

$$c = P^{1/2}\Phi(P)[\Psi + O(P)^{1/2}], \quad \Psi = \ldots \quad \rho \to 0,\ \Psi \to \rho^{-1} \ldots \alpha \ldots \alpha(G_{ij}) \tag{4}$$

Here α is a numerical coefficient and Φ is an unknown function determined in the course of the problem. A general expression for the parameter α is given in /9/. In particular, in the

*Prikl.Matem.Mekhan.,45,No.4,763-766, 1981 case of simple shear (one nondiagonal element of the matrix G_{ij} is equal to unity and the rest are zero) $\alpha = 0.258$ /8/.

Using the results of /7,10/ we can show that for the inner expansion in the region $\{1 \leqslant r \leqslant O(P^{-1/2})\}$ the following representation holds:

$$c = \frac{q}{r} + \alpha q P^{1/2}\left(\frac{q_*}{r} - 1\right) + qPc_2 + \alpha q q_* P^{3/2} c_3 + o(P^{3/2}) \tag{5}$$
$$q_* = \omega_1(\omega_1 + 1)^{-1}, \quad \omega_n \equiv [\partial^n f / \partial x^n]_{x=1-q}$$

where q is the root of the equation

$$-q + f(1 - q) = 0 \tag{6}$$

Functions c_2 and c_3 satisfy the equation /10/

$$\Delta_r c_m = -r^{-3} u_i x_i \quad (m = 2,\ 3) \tag{7}$$

and boundary conditions

$$r = 1, \quad \frac{\partial c_2}{\partial r} - \omega_1 c_2 + \frac{1}{2}\alpha^2 q q_*^2 \omega_2 \omega_1^{-3} = 0 \tag{8}$$
$$r = 1, \quad \frac{\partial c_3}{\partial r} - \omega_1 c_3 - q\omega_2\omega_1^{-1} c_2 + \frac{1}{6}\alpha^2 q^2 q_*^2 \omega_3 \omega_1^{-3} = 0$$

which are obtained by substituting the expression (5) into the boundary conditions (2) at the particle surface, expanding into series and separating the terms accompanying the like powers of the small parameter $P^{1/2}$. Integrating (7) over the surface of the sphere S of radius $r > 1$ and taking into account the incompressibility of the fluid, we obtain, in accordance with /10/

$$\frac{1}{r^2}\frac{d}{dr} r^2 \frac{d}{dr}\langle c_m\rangle = -\frac{1}{4\pi r^2}\int\limits_S u_i n_i \, dS = 0 \tag{9}$$
$$\langle A\rangle \equiv \frac{1}{4\pi r^2}\int\limits_S A\, dS, \quad n_i = \frac{x_i}{r} \quad (m = 2, 3)$$

The general solution of (9) has the form

$$\langle c_m\rangle = a_m + b_m r^{-1} \tag{10}$$

Integration of the boundary conditions (8) over S at $r = 1$, yields two linear algebraic equations for determining the unknown coefficients a_m and b_m. Integration of (5) with (10) taken into account, and subsequent merging with the integral of the outer solution (4), yields deficient (linear) algebraic relations for determining the coefficients a_m and b_m in (10) and the unknown function Φ appearing in the expression (4). Let us write the final expression for the mean Sherwood number

$$\mathrm{Sh} = -\langle \partial c / \partial r\rangle|_{r=1} = \Phi(P) = q\{1 + \varepsilon + (1 + {}^1/_2 q q_* \omega_2 \omega_1^{-3})\varepsilon^2 + \tag{11}$$
$$(1 + {}^3/_2 q q_* \omega_2 \omega_1^{-3} - {}^1/_2 q^2 q_*^2 \omega_2^2 \omega_1^{-5} + {}^1/_6\, q^2 q_* \omega_3 \omega_1^{-4})\varepsilon^3 + O(\varepsilon^4)\},$$
$$\varepsilon = \alpha q_* P^{1/2}$$

The coefficients q, q_* and ω_n are defined in the formula (5) and (6).

In the case of the linear kinetics of the surface reaction $f(x) = kx$, the formula (11) simplifies and assumes the form

$$\mathrm{Sh} = q(1 - \alpha q P^{1/2})^{-1} + o(P^{1/2}), \quad q = k(k + 1)^{-1} \tag{12}$$

When $k \to \infty$ $(q \to 1)$, the expression (12) becomes identical with the result of /10/. Using direct substitution we can show that (11) can be obtained by solving the following algebraic (transcendental) equation

$$\mathrm{Sh} = f(1 - \mathrm{Sh}/\mathrm{Sh}_\infty) \tag{13}$$

where Sh_∞ is the Sherwood number in the case of a shear flow past a sphere for a diffusive reaction mode /10/, which corresponds to the value $q = 1$ $(k = \infty)$ in (12). It should be noted that the equation /13/ yields a correct result also in the case of a translational Stokes flow past a plane. We can show this by substituting into (13) the expression for Sh_∞ obtained in /1/, and solving the resulting equation for Sh. This procedure yields the result of /7/.

It can be shown that in the case of an arbitrary flow of an incompressible fluid past a spherical particle (a drop), equation (14) yields a correct result for at least first two terms of the asymptotic expansion of the mean Sherwood number Sh in terms of the small Peclet number (Sh_∞ corresponds to the diffusion reaction mode). The assertion can be proved as follows. At small Peclet numbers the zero term of the inner expansion is independent of the type of flow past the sphere and is determined by the expression (5) with $P=0$. This leads to the appearance of a supplementary (compared with the diffusion reaction mode) multiplier q in the principal term of the outer expansion. Moreover, the boundary condition at the sphere surface coincides, for the first term of the inner expansion c_1, with the first boundary condition of (8) when $\omega_2 = 0$, and the expression for c_1 is either given by the homogeneous Laplace equation, or it coincides with equation (7). In all cases the equation implies that the representation (10) holds for $\langle c_1 \rangle$. The boundary condition for $r=1$ yields a single linear equation for determining the coefficients a_1 and b_1, and the second necessary relation is obtained from the condition of merger with the principal term of the outer expansion. These equations together yield a_1 and b_1. Comparison of the two-term expansion obtained in this manner for the mean Sherwood number shows, that Sh coincides, with the required accuracy, with the root of the equation (13).

It can be shown that in the case of a particle of arbitrary form freely suspended in a shear flow, the following formula for the mean Sherwood number holds for the linear kinetics of the surface reaction:

$$Sh/Sh_0 = 1 + \alpha Sh_0 P^{1/2} + \alpha^2 Sh_0^2 P + O(P^{3/2}) \tag{14}$$

Here the mean Sherwood number Sh_0 corresponds to the mass transfer between the reacting particle with $j(x) = kx$, and the stationary medium (i.e. at $P=0$), and the coefficient α is found in accordance with /9/. The formula (14) is derived in the same manner, as that used in /10/ in investigating the case of a diffusion reaction mode ($k \to \infty$) just as the authors of /6/ generalized /2/ the results of /2/ to the case of a translational flow.

In the case of a solid sphere $Sh_0 = k(k+1)^{-1}$ and the formula (14) becomes, with the accuracy of up to $O(P^{3/2})$, (12).

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