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Translated by L.K.

UDC 532, 72

CONVECTIVE DIFFUSION TO A REACTING RIGID SPHERE IN STOKES FLOW

PMM Vol. 40, No. 5, 1976, pp. 892-897 Iu. A. SERGEEV (Moscow) (Received April 16, 1976)

The problem of convective diffusion to a reacting rigid sphere was solved earlier in [1] for small values of Péclet and Reynolds numbers and finite reaction velocities, using the method of matched asymptotic expansions. In the present paper the problem of diffusion to a rigid sphere in a Stokes flow at finite velocities of the first order chemical reaction at the sphere surface is solved for large values of the Péclet number. The method of solution is similar to that used in [2] in the problem of convective diffusion to a reacting flat plate in a longitudinal flow of a viscous fluid.

We consider a convective diffusion of material to a rigid sphere in a Stokes flow of a viscous incompressible fluid the speed of which, away from the sphere is U. We assume that the Péclet numbers P = aU/D (where a is the radius of the sphere and D is the diffusion coefficient of the material in the flow) are large. A first order chemical reaction with the velocity constant k takes place at the surface of the sphere. The process of convective diffusion at large Péclet numbers is described by the boundary layer diffusion equation which in the spherical (r, θ) -coordinate system with the origin at the center of the sphere and the polar axis pointing in the direction opposite to the direction of flow at infinity, has the form

$$v_r \frac{\partial c}{\partial r} + \frac{v_{\theta}}{r} \frac{\partial c}{\partial \theta} = D \frac{\partial^2 c}{\partial r^2}$$
(1)

Here v_r and v_{θ} are the radial and angular velocity components in the spherical

coordinate system. Equation (1) has the following boundary conditions :

$$r \to \infty, \quad c = c_0$$

$$r = a, \quad D \frac{\partial c}{\partial r} = kc$$

$$r = a, \quad \theta = 0, \quad c = c_0$$
(2)

where c_0 is the reagent concentration at a distance from the sphere. The last condition of (2) represents an additional condition that the flow is not depleted at the stagnation point.

The stream function in the diffusive boundary layer can be written for small y = r - a in the form

$$\begin{split} \psi \approx &-\frac{3}{4} U y^2 \sin \theta \\ \left(v_{\theta} = &-\frac{1}{r \sin \theta} \frac{\partial \psi}{\partial y} , \quad v_r = \frac{1}{r^2 \sin \theta} \frac{\partial \psi}{\partial \theta} \right) \end{split}$$

Let us introduce the variables

$$\varphi = \sqrt{-\psi}, \quad \xi = \int_{0}^{\theta} Da^{2} \frac{\sqrt{3}\overline{U}}{4} \sin^{2}\theta d\theta =$$

$$Da^{2} \frac{\sqrt{3}\overline{U}}{8} \left(\theta - \frac{\sin 2\theta}{2}\right)$$
(3)

In the (φ, ξ) variables the problem (1), (2) assumes the form

$$\frac{\partial c}{\partial \xi} = \frac{1}{\varphi} \frac{\partial^2 c}{\partial \varphi^2}, \quad \varphi \to \infty, \quad c = c_0$$

$$\varphi = 0, \quad D\zeta(\xi) \frac{\partial c}{\partial \varphi} = kc \quad \left(\zeta(\xi) \equiv \frac{\sqrt{3U}}{2} \sin\theta\right)$$

$$\varphi = 0, \quad \xi = 0, \quad c = c_0$$
(4)

where the function ζ (ξ) is obtained by inverting the transformation (3) for ξ . The solution of (4) is similar to the solution given in [2] of the problem of convective diffusion to a reacting flat plate in a longitudinal flow of a viscous fluid and is given in the appendix. From the second boundary condition in (4) and the appendix it follows that the diffusive flux to the surface of the sphere is given by the expression

$$j(\xi, 0) = j(\theta, 0) = \frac{kc_0}{\Gamma(^{3}/_{3})} \int_0^\infty \exp\left(-\gamma t^{s/_{3}}\right) e^{-t} t^{-1/_{3}} dt$$
(5)

where

$$\gamma = \frac{3^{s_{1}}\Gamma(1_{3})\xi^{1_{3}}}{2D\zeta(\xi)} = \varepsilon \frac{(\theta - 1_{2}\sin 2\theta)^{1_{3}}}{\sin \theta}$$
(6)
$$\varepsilon = \frac{3^{1_{3}}\Gamma(1_{3})ka^{s_{1}}}{2D^{s_{1}}U^{1_{3}}\Gamma(1_{3})}$$

The expression (5) for the differential flux can be written in the form of a series in

 γ which converges for any value of γ [2]

$$j(\theta, 0) = \frac{kc_0}{\Gamma(2/s)} \left\{ \sum_{n=0}^{N} \frac{(-1)^n}{n!} \Gamma\left(\frac{2+2n}{3}\right) \gamma^n + \right\}$$
(7)

$$\frac{1}{(N+1)!} \Gamma\left(\frac{4+2N}{3}\right) \gamma^{N+1} S_{N+1} \bigg\}, \quad S_{N+1} = O(1)$$

However, the above series converges extremely slowly even at $\gamma \ge 1$, therefore it is impractical to use (7) unless γ is small. For large γ we follow [2] and make the substitution $\gamma t^{2/3} = u$ to obtain the expression for the differential flux in the form

$$j(\theta, 0) = \frac{3}{2} \frac{kc_0}{\Upsilon} \frac{1}{\Gamma(2/3)} \int_0^\infty \exp\left[-\left(\frac{u}{\Upsilon}\right)^{4/2}\right] e^{-u} du$$
(8)

after which we expand the integrand into a series in powers of $\gamma^{-3/2}$. This yields the expression for the differential flux in the form

$$j(\theta, 0) = \frac{3^{s/s} c_0 D^{s/s} U^{1/s} \sin \theta}{\Gamma(1/s) a^{s/s} (\theta - 1/2) \sin 2\theta)^{1/s}} \left\{ \sum_{n=0}^{N} \frac{(-1)^n}{n!} \Gamma\left(\frac{2+3n}{2}\right) \gamma^{-s/s^n} + \frac{1}{(N+1)!} \Gamma\left(\frac{5+3N}{2}\right) \gamma^{-s/s(N+1)} R_{N+1} \right\}, \quad R_{N+1} = O(1)$$

The results obtained indicate that near the leading critical point the chemical reaction is the rate limiting step of the process of mass exchange irrespective of the value of the reaction velocity constant, while near the trailing critical point it is the convective diffusion of the material to the surface of the sphere that determines the rate of the process. In the intermediate region we have a mixed mode, and the expansions obtained above allow for this. The area of the surface of the sphere working in the diffusion mode increases with increasing reaction velocity constant. When $k \to \infty$ ($\gamma \to \infty$) the whole surface of the sphere enters the diffusion mode and the expression (9) becomes identical to that obtained in [2] for the limiting diffusive flux to a sphere. When

 $k \rightarrow 0$ the whole surface of the sphere is in the kinetic mode and $j(\theta, 0) = kc_0$.

Let us now determine the total flux I to the surface of the sphere. The mean Sherwood number $Sh = I / (4\pi a Dc_0)$ can be expressed, as follows from (5) and (8), by either of the following two integrals :

$$\mathrm{Sh} = \frac{1}{3^{1/s} \Gamma(1/s)} \varepsilon P^{1/s} \int_{0}^{\infty} \left\{ \int_{0}^{\pi} \exp\left[-\gamma(\theta) t^{s/s}\right] \sin\theta d\theta \right\} e^{-t} t^{-1/s} dt \qquad (10)$$

$$Sh = \frac{3^{a_{a}}}{2\Gamma(1/s)} P^{1/s} \int_{0}^{\infty} \left\{ \int_{0}^{\pi} \frac{\sin \theta}{(\theta - 1/2 \sin 2\theta)^{1/s}} \times \right.$$

$$exp\left[-\left(\frac{u}{\gamma(\theta)}\right)^{a_{s}} \right] \sin \theta d\theta \right\} e^{-u} du$$
(11)

Fig. 1 depicts the dependence of the Sherwood number on the parameter ε , obtained by numerical computation of the integrals (10) and (11). Here $\mathrm{Sh}_0 = [3^{*/_{\mathrm{orc}}*/_{\mathrm{o}}}/$

 $(8\Gamma(1/3))P^{1/3}$ is the Sherwood number for the limiting flux to the sphere which was calculated in [2].

At the high reaction velocities, i.e. at large values of the parameter ε , the total flux can be represented in the form of a series in powers of $e^{-3/s}$. To do this, we use the integral (11) expanding its exponent into a series in powers of $e^{-3/s}$.

The resulting series appearing in the inner integral of (11) converges uniformly in θ and can be integrated with respect to θ term by term Performing term by term integration in the outer integral of (11) as well, we obtain the series

$$\frac{3^{s/s}}{2\Gamma(1/s)} P^{s/s} \sum_{n=0}^{\infty} \varepsilon^{-s/sn} J_n$$

$$J_n = \frac{1}{n!} \Gamma\left(\frac{2+3n}{2}\right) \int_0^{\pi} \left[\frac{\sin\theta}{(\theta-1/2\sin2\theta)^{1/s}}\right]^{1+s/sn} \sin\theta d\theta$$
(12)

It can easily be shown that the series (12) converges to the integral (11). We can also obtain the following estimates for the residue term Q_{N+1} of the series $J_0 + I_0$ in the form

 $J_1 + \ldots$ in the form

$$|Q_{N+1}| < e^{-3/2(N+1)} \frac{\Gamma(5/2 + 3/2N)}{(N+1)!}$$

The problem thus reduces to calculating the integrals J_n . The results obtained can be conveniently represented in the form of an expansion of the mean Sherwood number in terms of the parameter $e^{-s|_2}$. Computing six integrals J_n yields the following expansion :

$$\begin{aligned} \mathrm{Sh} &= \mathrm{Sh}_{0} \left(1 - 1.135 \varepsilon^{-s_{2}} + 2.415 \varepsilon^{-3} - 1.167 \varepsilon^{-s_{2}} + 24.87 \varepsilon^{-6} - 205.4 \varepsilon^{-s_{2}} + \varepsilon^{-9} \pi^{1/2} \frac{4\Gamma(10)}{3.6!} T_{6} \right), \quad T_{6} < 1 \end{aligned}$$

Fig. 1 shows with a dashed line the dependence (13) of the Sherwood number on the parameter ε for large values of the latter. We note that a certain lack of agreement between the results obtained by computing the series (13) and those obtained using the integrals (10) and (11), is due to the slow convergence of (13). When ε is small, the integral (10) cannot be expanded in terms of ε . Mathematically, this is connected with the presence of a singularity near the point π in the integrand of the inner integral in (10). The singularity has the form $\exp\{-\varepsilon B / (\pi - \theta)\}(\pi - \theta)$ and it causes a nonuniform convergence of the series obtained by expanding the exponent. From the physical point of view this is connected with the fact that at small reaction velocities (small ε) a region in the neighborhood of the point $\theta = \pi$ still exists which is in the diffusion mode and in which $\gamma(\theta)$ can assume arbitrarily large values. It can easily be shown that in this case the region of small γ (an almost kinetic mode) and of large γ (an almost diffusion mode) make contributions of the same order $O(\varepsilon)$ towards the total flux, in contrast to the case of large ε when the contribution of the kinetic region to the total flux is vanishingly small.

We can estimate the region on the surface of the sphere corresponding to the transition from the kinetic to the diffusion mode using the relation $\gamma(\theta^*) = O(1)$. The shaded region of angles θ^* in Fig. 1 corresponds to the mixed kinetics, *I* denotes the kinetic region and *II* denotes the diffusion region.

The results obtained above enable us to estimate the effective thickness of the diffusive boundary layer $\delta = D (c_0 - c_{r=a}) / j_{r=a}$ for various values of ϵ . Using the expansions (7) and (9) and the second boundary condition of (2), we can show that

$$\delta = 1.08P^{-1/2} (\theta - 1/2 \sin 2\theta)^{1/2} / \sin \theta, \quad \varepsilon \to \infty$$

$$\delta = 0.78P^{-1/2} (\theta - 1/2 \sin 2\theta)^{1/2} / \sin \theta, \quad \varepsilon \to 0$$

The first of the above formulas coincides with one obtained in [2] for the thickness of the diffusive boundary layer in the case of a limiting flux. We can see that in the case of a kinetic mode the boundary layer is thinner than that in the diffusion mode. Numerical computations of the integrals (5) and (8) show that in the intermediate range of values of ε the boundary layer thickness increases with increasing ε .



It will be interesting to compare the above results with those obtained in [1] for small Péclet numbers. In Fig. 2 solid lines depict the dependence of the Sherwood number on the Péclet number for small (in accordance with [1], this is a particular case of a Stokes flow) and large values of the latter for various values of the dimensionless reaction velocity constant $k' = ka / D = [2\Gamma (2/3) / (3^{4/3}\Gamma (1/3))] P^{4/3}\varepsilon$. Curves 1 correspond to k' = 0.1, 2 - k' = 1, 3 - k' - 10, $4 - k' \to \infty$. Fig. 2 presents the possibility of interpolating for the intermediate values of the Péclet number and for any chemical reaction velocities. Examples of interpolation are shown in Fig. 2 by dashed lines.

A p p e n d i x. Below we give the solution of the problem (4). Substitution

$$z = \frac{2}{3} \phi_{z,\lambda}^{3/2}, \quad c(z, \xi) = z^{1/2} S(\xi, z)$$

reduces the Eq. (4) to the form which allows the application of the Setton's method which is analogous to the Goursat method of solving the problems in the theory of heat conduction (see e.g. [2]

$$\frac{\partial^2 S}{\partial z^2} + \frac{1}{z} \frac{\partial S}{\partial z} - \frac{1}{9z^2} S = \frac{\partial S}{\partial \xi}$$
(A1)

Equation (A1) admits the solutions [2]

$$\begin{aligned} \chi_{1,2}(\xi, z; \lambda, \rho) &= \frac{\lambda^{1/\mathfrak{s}} z^{1/\mathfrak{s}}}{2(\xi - \rho)} \exp\left[-\frac{z^2 + \lambda^2}{4(\xi - \rho)}\right] I_{\pm 1/\mathfrak{s}}\left[\frac{\lambda z}{2(\xi - \rho)}\right];\\ \xi &\leq \rho, z > 0, \ \chi_{1,2} \equiv 0 \end{aligned}$$

which are fundamental in the sense that any given boundary conditions can be satisfied by choosing a suitable contour L in the (λ, p) -plane and constructing the function

$$c(\xi, z) = \int_{L} [A_1(\lambda, p) \chi_1 + A_2(\lambda, p) \chi_2] [P(\lambda, p) d\lambda + Q(\lambda, p) dp]$$

Here the functions A_1 , A_2 , P, and Q must also be chosen in a prescribed manner with the boundary conditions taken into account. Following [2], we choose as the contour of integration the straight line $\rho = 0$ in the half-plane $\lambda \ge 0$ and set

$$A_i (\lambda, 0) P(\lambda, 0) = \lambda^{1/2} f_i (\lambda), \quad i = 1, 2.$$

The functions f_1 and f_2 are assumed continuous and bounded in the interval $(0, \infty)$. Then

$$c (\xi, z) = c_{1} (\xi, z) + c_{2} (\xi, z)$$

$$c_{i} = \int_{0}^{\infty} \frac{f_{i}(\lambda) \lambda^{2} z^{1/3}}{2\xi} \exp\left(-\frac{z^{2} + \lambda^{2}}{4\xi}\right) I_{j}\left(\frac{\lambda z}{2\xi}\right) d\lambda$$

$$i = 1, \quad j = \frac{1}{3}; \quad i = 2, \quad j = -\frac{1}{3}$$
(A2)

and the problem is reduced to choosing the functions f_1 and f_2 . The system of boundary conditions written in the variables ξ and z, has the form

$$\left(\frac{3}{2}\right)^{t_1} D\zeta(\xi) \lim_{z \to +0} \left(z^{t_1} \frac{\partial c(\xi, z)}{\partial z}\right) = k \lim_{z \to +0} c(\xi, z)$$

$$\lim_{z \to \infty} c(\xi, z) = c_0, \quad \lim_{z \to +0} c(\xi, z) = c_0$$
(A3)

Using the boundary conditions (A3) and the properties of the expansion (A2) obtained in [3] (and quoted in [2] for the problem of convective diffusion to a flat plate), we obtain

$$f_{2}(\lambda) = c_{0} - f_{1}(\lambda)$$
(A4)
$$\frac{3^{i_{1}s}}{\Gamma(i_{1}s)} D\zeta(\xi) \xi^{-i_{1}s} \int_{0}^{\infty} f_{1}(2\sqrt{\xi\rho}) e^{-\rho} d\rho = \frac{k}{\Gamma(i_{2}s)} \int_{0}^{\infty} [c_{0} - f_{1}(2\sqrt{\xi\rho})] e^{-\rho\rho^{-i_{1}s}} d\rho$$
(A5)

Changing the variables

 $\xi \rho = t$, $\xi = 1 / u$, $f_1 (2 \sqrt{t}) = \beta (t)$

we can reduce (A5) to the form

$$\eta(u) \int_{0}^{\infty} \beta'(t) e^{-ut} dt = \int_{0}^{\infty} [c_0 - \beta(t)] e^{-ut} t^{-1/s} dt \quad \eta(u) = \frac{3^{1/s} D\Gamma(2/s)}{k \Gamma(1/s)} \zeta\left(\frac{1}{u}\right) u^{-1/s}$$

Function $\beta(t)$ can now be found from the equation

...

$$\eta (u) \beta' (t) = [c_0 - \beta (t)] t^{-1/2}$$

the initial condition for which can be written in the form $\beta(0) = 0$. Solving this equation, we obtain the following expression for the function $f_1(t)$:

$$f_1(t) = \beta\left(\frac{t^2}{4}\right) = c_0 \left[1 - \exp\left(-\frac{3t^{4/s}}{8\eta}\right)\right]$$

n

and from this it follows that

$$\lim_{z \to +0} c(\xi, z) = \frac{c_0}{\Gamma(^2/_3)} \int_0^{\infty} \exp\left[-\frac{3}{2\eta} (\xi \rho)^{z/_3}\right] e^{-\rho} \rho^{-1/_3} d\rho$$
(A6)

The result (A6) obtained together with the first boundary condition of (A3), enables us to determine the diffusive flux on the surface of the sphere which is equal, with acc - ordance with the second boundary condition of (2), to $k \lim_{z \to +0} c(\xi, z)$, and this leads to formula (5).

The author thanks Iu. P. Gupalo and Iu. S. Riazantsev for unceasing interest and valuable discussions.

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Translated by L. K.

UDC 539, 3: 534, 1

DIFFRACTION OF A SPHERICAL ELASTIC WAVE BY A WEDGE

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(Received February 18, 1976)

A three-dimensional nonstationary problem of spherical elastic wave diffraction by a smooth solid wedge with arbitrary apex angle is considered. An exact solution in the form of a sum of two terms, the known acoustic solution and an additional part describing the influence of elasticity, and caused by the appearance of additional longitudinal and transverse diffraction waves, is obtained by the method of integral transforms with extraction of the sing ularities in the neighborhood of an edge. This latter term essentially distinguishes the elastic from the acoustic solution. The particular case of an incident wave with a jump in the stresses at the front is investigated in detail.

The corresponding acoustic problem has been examined in [1-4], where the solution in elementary functions was first obtained in [2]. Only the solution for the plane wave diffraction problem [5] is known for a wedge in the