CONVECTIVE DIFFUSION IN A PERIODIC ARRAY OF SPHERES FOR SMALL REYNOLDS NUMBERS

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It is shown that in flow past a system of spheres of radius a situated at the nodes of a cubic lattice with the period b in the direction of one of the principal translations of the lattice under the condition $(a/b)\cdot P^{1/3} \ll 1$ (P is the Péclet number, $P \gg 1$), the concentration of dissolved material absorbed by the sphere surfaces diminishes logarithmically at distances large compared with b, but small compared with $L = Pb^2/4\pi a$. At distances considerably larger than L, the decrease is described by an exponential law which coincides with the law of concentration decrease at distances much larger than b in the case of a spatially homogeneous distribution of the spheres. We consider the flow of an incompressible fluid with the velocity U past a system of spheres of radius a. We assume that the Reynolds number $R = Ua/\nu$ (where ν, the kinematic viscosity coefficient, is much larger than unity). Dissolved in the fluid is a material of concentration c which is absorbed by the sphere surfaces. The diffusion coefficient D is assumed to be sufficiently small for the Péclet number $P = Ua/D$ to be much larger than unity. The spheres are situated at the nodes of a cubic lattice with the period b. As will be shown below, it is necessary that $P(a/b)^3 \ll 1$. Under these assumptions the concentration varies in a thin (of the order $aP^{-1/3}$) diffusion layer near the surface of each sphere. A diffusion wake is formed behind each sphere. The transverse dimensions of this wake for a sufficiently widely spaced lattice ($aP^{1/3} \ll b$) exceed the effective thickness of the diffusion boundary layer, which enables us to reduce the problem of concentration absorption on the surface of the system of spheres to the problem considered by Levich [1] concerning the convective diffusion of a material of constant constant concentration flowing past a single sphere.

Hasimoto [2] considers the solution of the Stokes equation describing the motion of a viscous fluid past an array of spheres situated at the nodes of a cubic lattice. However, he does not give an expression for the velocity field applicable near the surface of some single sphere which is necessary to the solution of the diffusion problem.

In the method of Lamb [3] (§336) and Burgers [4], in dealing with the flow of a viscous stream past a single sphere, one considers the equation of motion in space, including the interior of the sphere, and not just the solution of the equation in the space outside the sphere with boundary conditions at the sphere surface. At the center of the sphere one places a concentrated force and a system of multipoles whose magnitude is chosen in such a way as to ensure fulfillment of the required boundary conditions.

This idea of introducing an effective potential is used in [2] to find the velocity field of a fluid flowing past an array of spheres. We propose a treatment of the effective potential method somewhat different from that of [2].

§1. We begin with the equation

$$\mu\Delta\mathbf{v} = \operatorname{grad} p + (\mathbf{F}_0 + a^2\mathbf{F}_1\Delta + \ldots)\sum_{\mathbf{n}}\delta(\mathbf{r} - \mathbf{r}_\mathbf{n}), \tag{1.1}$$

$$\operatorname{div}\mathbf{v} = 0 \qquad (\mathbf{r}_\mathbf{n} = n\mathbf{a} + m\mathbf{b} + l\mathbf{c})\,. \tag{1.2}$$

Here v is the velocity of the fluid at the point r; μ is the dynamic viscosity coefficient; p is the pressure; r_n is the radius-vector of the n-th node of the lattice (n, m, l = 0, 1, 2, ...). The density of the force exerted by the spheres on the fluid will be sought in the form of a series containing the δ-function and its derivatives with some constant coefficients F_0, F_1, etc. Introduction of these terms enables us to find a combination of particular periodic solutions which satisfies the condition of vanishing of the velocity at the sphere surfaces.

We shall then show that consideration of the first two terms of the series with the coefficients F_0 and F_1 enables us to pass to the Stokes solution for flow past a single sphere as $a/b \to 0$. The smallness of the rejected terms means that the highest-order derivatives of the correction of the velocity field produced by all the spheres are small as compared with the corresponding derivatives of the correction of the velocity field produced by the nearest sphere, except in the neighborhood of the sphere around which the flow is being considered. The method is therefore applicable only if $a/b \ll 1$.

Assuming summation over the recurring Greek-letter indices, we can write the required solution (as in [2]) in the form

$$v^\alpha = v_0^{\alpha} - \frac{F_0^{\beta} + a^2F_1^{\beta}\Delta}{4\pi\mu}\left(\delta_{\alpha\beta}S_1 - \frac{\partial^2 S_2}{\partial r^\alpha \partial r^\beta}\right) \tag{1.3}$$

where v^α are the components of the velocity of the fluid, and v_0^α are their limiting values for $a/b \to 0$,

$$S_1 = \frac{1}{\pi a^3}\sum_{\mathbf{k}\neq 0}{}' \frac{1}{k^2}e^{-2\pi i(\mathbf{k}\cdot\mathbf{r})},$$

$$S_2 = -\frac{1}{4\pi a^3}\sum_{\mathbf{k}\neq 0}{}' \frac{1}{k^4}e^{-2\pi i(\mathbf{k}\cdot\mathbf{r})}\,. \tag{1.4}$$

Here **k** is the vector of the reciprocal lattice, which is related to the vectors of the (original) lattice by the conditions $(\mathbf{k}\cdot\mathbf{a}) = n$, $(\mathbf{k}\cdot\mathbf{b}) = m$, $(\mathbf{k}\cdot\mathbf{c}) = l$.

We know (e.g., see [2]) the expansion of the lattice sums S_1 and S_2 in the neighborhood of small r to within terms of order $(r/b)^3$,

$$\delta_{\alpha\beta}S_1 - \frac{\partial^2 S_2}{\partial r^\alpha \partial r_\beta} = \frac{r^\alpha r^\beta}{2r^3} + \delta_{\alpha\beta}\left(\frac{1}{2r} + \frac{1.88}{b}\right). \tag{1.5}$$

Substituting expansion (1.5) into Eq. (1.3) and making use of the boundary condition $v^\alpha \equiv 0$ for $r = a$, we obtain

$$8\pi\mu a v_0^\alpha = F_0^\beta\,[n^\alpha n^\beta + \delta_{\alpha\beta}(1 - 3.76\,a/b)] - F_1^\beta(3n^\alpha n^\beta - \delta_{\alpha\beta}) \qquad (n^\alpha = r^\alpha/r)\,. \tag{1.6}$$

Equating the coefficients of the equal spherical harmonics, we obtain

$$F_0^\alpha = 6\pi\mu a U^\alpha, \qquad F_1^\alpha = \pi\mu a U^\alpha,$$

$$U^\alpha = \frac{v_0^\alpha}{1 - 2.84\,a/b}\,. \tag{1.7}$$

Thus, in the region $r^3 \ll b^3$, i.e., in the neighborhood of the isolated sphere, the velocity field of the fluid flowing past the system of spheres is given by

$$v^\alpha = U^\beta [\delta_{\alpha\beta} - 3(n^\alpha n^\beta + \delta_{\alpha\beta}) a / 4r + (3n^\alpha n^\beta - \delta_{\alpha\beta}) a^3 / 4r^3] . \tag{1.8}$$

As expected, the velocity field near the surface of the sphere is similar to the velocity field of a viscous stream flowing past a single sphere, except that the velocity **U** of the oncoming stream differs from v_0.

If $a^3 \ll b^3$, then there exists a region where $r \gg a$ and $r^3 \ll b^3$ and where expression (1.8) still holds. For this reason the velocity of the stream can be considered constant and equal to **U**.

§2. Before investigating convective diffusion in the stream flowing past an array of spheres, let us consider the problem of convective diffusion at the surface of a single sphere in the way of a stream of velocity **U**.

The equation of convective diffusion is

$$v \nabla c = D \Delta c . \tag{2.1}$$

In spherical coordinates the velocity components v_r, v_θ can be expressed in terms of the stream function ψ,

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

$$\psi = -{}^1/_2 U \sin^2\theta (r^2 - {}^3/_2 ar + {}^1/_2 a^3 / r) . \tag{2.2}$$

Following Levich [1], we retain only the most essential terms in the equation for the diffusion boundary layer,

$$v_r \frac{\partial c}{\partial r} + \frac{v_\theta}{r} \frac{\partial c}{\partial \theta} = D \frac{\partial^2 c}{\partial r^2} . \tag{2.3}$$

We make use of the von Mises transformations to convert from the variables r, θ to the variables ψ, θ, where

$$\psi = -{}^3/_4 U (r-a)^2 \sin^2\theta . \tag{2.4}$$

Repeating the analysis of [1], we obtain the equation

$$\frac{\partial^2 c}{\partial \xi^2} = \xi \frac{\partial c}{\partial t} \qquad (\xi = (-\psi)^{1/2},$$

$$t = \frac{Da^2 (3U)^{1/2}}{8} \left(\theta - \frac{\sin 2\theta}{2}\right)) \tag{2.5}$$

with the following boundary conditions:

at the surface of the sphere,

$$c(0, t) = 0, \qquad t \neq 0; \tag{2.6}$$

in the region outside the boundary layer,

$$\lim_{\xi \to \infty} c(\xi, t) = c_0; \tag{2.7}$$

for the concentration distribution in the stream entering the neighborhood of the run-on point,

$$c(\xi, 0) = c_0, \qquad \xi \neq 0 . \tag{2.8}$$

Equation (2.5) with boundary conditions (2.6)–(2.8) has the solution obtained by Levich [1],

$$c(\xi, t) = \frac{c_0}{\Gamma(^1/_3)} \gamma\left(\frac{1}{3}, \frac{\xi^3}{9t}\right)$$

$$\gamma\left(\frac{1}{3}, x\right) = \int_0^x e^{-u} u^{-2/3} du, \qquad \Gamma\left(\frac{1}{3}\right) = \gamma\left(\frac{1}{3}, \infty\right) . \tag{2.9}$$

The range of applicability of Eq. (2.2), and therefore of solution (2.9), is defined by the condition $\partial c / \partial r \gg c_0 / R$, which is fulfilled, as we see directly from Eqs. (2.9), if $\pi - \theta \gg P^{-1/3}$.

The principal terms of convective diffusion equation (2.1) in the domain $\pi - \theta \gg P^{1/3}$ satisfy the following equation (whose form is that of the heat conduction equation,

$$U \frac{\partial c}{\partial x} = D \left(\frac{\partial^2 c}{\partial y^2} + \frac{\partial^2 c}{\partial z^2}\right) \tag{2.10}$$

at large distances from the surface of the sphere ($r \gg a$) (in Cartesian coordinates with the x-axis directed along the oncoming stream).

The assumption of a constant velocity U can be justified by the fact that the characteristic distance along the x-axis along which the concentration varies is (as will be seen from our solution) on the order of $aP^{1/3}$, i.e., considerably larger than the radius of the sphere (the region in which the stream velocity differs markedly from U).

The second assumption made in deriving Eq. (2.11) has to do with the condition $|U \partial c / \partial x| \gg D |\partial^2 c / \partial x^2|$, whose fulfillment for a monotonically varying concentration follows from the condition $P \gg 1$.

If we had a boundary condition for Eq. (2.10), i.e., for c(0, y, z), we could write the solution of this equation as

$$c(x, y, z) = \int c(0, y', z') G(x, y-y', z-z') dy'dz',$$

$$G(x, y, z) = \frac{U}{4\pi D x} \exp\left[-\frac{U(y^2+z^2)}{4Dx}\right]. \tag{2.11}$$

The function c(0, y', z') can be determined as follows. Let us consider a conical surface with the fixed angle $\varepsilon = \varepsilon_0 \approx P^{-1/3}$. The concentration on this surface is given by Levich's formula (2.9) if we substitute in it the value $\theta = \pi - \varepsilon_0$ for t. To within terms of order 1/P we have $t = t_0 = {}^1/_8 \pi D a^2 (3U)^{1/2}$. Now, assuming that the concentration distribution on the conical surface is also defined by the angle ε_0, we let P go to infinity. Convective diffusion equation (2.1) throughout the domain, including the conical surface, then becomes the equation of convective transfer

$$v_r \frac{\partial c}{\partial r} + \frac{v_\theta}{r} \frac{\partial c}{\partial \theta} = 0 . \tag{2.12}$$

According to Eq. (2.12), the concentration distribution specified on the surface of the cone is carried inside along the streamlines. Thus, for $P \to \infty$ the concentration distribution inside the conical surface is given by expression (2.9) with t replaced by t_0,

$$c(\xi) = \frac{c_0}{\Gamma(^1/_3)} \gamma\left(\frac{1}{3}, \frac{\xi^3}{9t_0}\right). \tag{2.13}$$

Expression (2.11) for $P \to \infty$ must tend to the same expression sufficiently far away from the surface of the sphere ($x \gg a$). This implies that

$$c(0, y, z) = \frac{c_0}{\Gamma(1/3)} \Upsilon\left(\frac{1}{3}, \frac{\xi^3}{9t_0}\right)$$
$$\left(\xi^2 = \frac{U}{2}(y^2 + z^2)\right). \quad (2.14)$$

For sufficiently large x, expression (2.11) with boundary condition (2.14) can be written as

$$\frac{c(x, y, z)}{c_0} = 1 - \frac{G(x, x, z)}{\Gamma(1/3)} \iint \Gamma\left(\frac{1}{3}, \frac{\xi'^3}{9t_0}\right) \times$$
$$\times \left\{1 + \frac{U}{2Dx}(yy' + zz') - \right.$$
$$\left. - \frac{U}{4Dx}(y'^2 + z'^2) + \ldots \right\} dy'dz',$$
$$\Gamma\left(\frac{1}{3}, x\right) = \int_x^\infty e^{-u} u^{-2/3} du . \quad (2.15)$$

The second term in braces contributes nothing to the integral because of the oddness of the integrand. The contribution of the third term is small if $x \gg y_*^2 U/D$. But the quantity $y_* \approx (9t)^{1/3} U^{-1/2}$. It is therefore necessary that $x \gg (9t_0)^{2/3} / D \approx aP^{1/3}$ in order for the concentration distribution in the diffusion wake to coincide with the concentration distribution due to the point source

$$\frac{c(x, y, z)}{c_0} = 1 - \frac{(9t_0)^{2/3}}{2\Gamma(1/3) Dx} \exp\left[-\frac{U(y^2 + z^2)}{4Dx}\right]. \quad (2.16)$$

§3. Now let us consider convective diffusion in a stream flowing past an array of spheres situated at the nodes of a cubic lattice with the period $b \gg aP^{1/3}$. Outside the boundary diffusion layers the concentration distribution is determined by the diffusion wakes of all the spheres having (in accordance with §2) the form of diffusion wakes due to point sources. Due to the periodicity of the concentration distribution in the plane perpendicular to the stream (x = const), it is sufficient to consider the stream in the neighborhood of the sphere (kb, 0, 0),

$$\frac{c}{c_0} = 1 - \sum_{n=0}^{k-1} A_n \frac{a}{x_n'} \sum_{m, l} \exp\left[-\frac{U(y_m'^2 + z_e'^2)}{4Dx_n'}\right],$$
$$x_n' = x - nb, \qquad y_m' = y - mb, \qquad z_e' = z - lb . \quad (3.1)$$

The constant A_n can be determined from the condition that the difference between the fluxes of the dissolved material through the planes $x = x_1$ and $x = x_2$, of which one is taken in front of, and the other behind, the k-th sphere ($a \ll kb - x_1 \ll b$, $a \ll x_2 - kb \ll b$) is equal to the diffusion flux on the spheres lying inside the layer just defined. This implies that

$$I_k = c_0 U A_k \frac{a}{x} \int_0^\infty \exp\left(-\frac{U\rho^2}{4Dx}\right) 2\pi\rho d\rho = 4\pi D c_0 a A_k , \quad (3.2)$$

where I_k is the total diffusion flux on the surface of the k-th sphere.

We can compute I_k by considering the equation of convective diffusion in the boundary layer near the surface of the k-th sphere (2.3).

The appropriate boundary conditions can be obtained from Eq. (3.1).

The concentration distribution near the surface of the k-th sphere outside the diffusion boundary layer is produced by the diffusion wakes of all the spheres in the system situated to the left of the plane x = bk. The principal role in the sum is played by the term associated with the (k − 1)-th sphere. But since the lattice period b is much larger than $aP^{1/3}$, the diffusion wake of the (k − 1)-th sphere has a transverse width considerably larger than $aP^{-1/3}$, i.e., larger than the effective thickness of the diffusion boundary layer. The concentration changes markedly in the longitudinal direction in the diffusion wake at distance $aP^{1/3} \gg a$. In view of all these considerations, the concentration of the stream flowing past the k-th sphere in the region outside the diffusion boundary layer can be considered equal to the concentration which would be produced by all the diffusion wakes at the k-th node of the lattice. Hence,

$$\lim_{\xi \to \infty} c(\xi, t) = c_k, \qquad c(\xi, 0) = c_k, \qquad \xi \neq 0,$$
$$\frac{c_k}{c_0} = 1 - \sum_{n=0}^{k-1} \frac{A_n a}{(k-n)b} \sum_{m, l} \exp\left[-\frac{Ub(m^2 + l^2)}{4D(k-n)}\right]. \quad (3.3)$$

We have therefore reduced the problem to that of Levich [1]. The concentration distribution in the diffusion boundary layer is defined by formula (2.9) with c_0 replaced by c_k. The diffusion flux density on the surface of the k-th sphere is

$$j = D\left(\frac{\partial c}{\partial r}\right)_{r=R} = \frac{D(3U)^{1/3}}{2\Gamma(1/3)} \left(\frac{3}{t}\right)^{1/3} c_k \sin\theta . \quad (3.4)$$

The total diffusion flux on the surface of the k-th sphere is

$$I_k = 2\pi a^2 \int_0^\pi j \sin\theta \, d\theta = 4\pi D\lambda b c_k ,$$
$$\lambda = \frac{(3U)^{1/3}}{2Db\,\Gamma(1/3)} \left(\frac{9\pi}{8} Da^2\right)^{2/3} = 0.65 \frac{a}{b} P^{1/3} . \quad (3.5)$$

From relations (3.2) and (3.5) we infer that

$$A_k = \lambda b c_k / a c_0 . \quad (3.6)$$

We therefore have the following recurrence relation for the concentration in the neighborhood of the k-th lattice node:

$$\frac{c_k}{c_0} = 1 - \sum_{n=0}^{k-1} \frac{\lambda c_n}{(k-n) c_0} \sum_{m, l} \exp\left[-\frac{Ub(m^2 + l^2)}{4D(k-n)}\right]. \quad (3.7)$$

Making use of the theta function $\vartheta_3(z \mid \tau)$ defined in [5],

$$\vartheta_3(0 \mid \tau) = \sum_{m=-\infty}^{\infty} e^{i\pi\tau m^2} \quad (3.8)$$

we can rewrite expression (3.7) as

$$c_k = c_0 - \sum_{n=0}^{k-1} \frac{\lambda c_n}{k-n} \vartheta_3^2\left(0 \,\middle|\, \frac{iL}{b(k-n)}\right) \qquad \left(L = \frac{Ub^2}{4\pi D}\right). \quad (3.9)$$

For $k \gg 1$ Eq. (3.9) is equivalent to the integral equation

$$c(x) = c_0 - \int_0^{x-b} \frac{\lambda c(x')}{x - x'} \vartheta_3^2 \left(0 \,\Big|\, \frac{iL}{x - x'}\right) dx'. \qquad (3.10)$$

In the range $x \ll L$, neglecting terms of order $e^{-\pi L/x}$ and assuming that $\lambda \ll 1$, we obtain the following solution of Eq. (3.10):

$$c(x) = c_0 \Big/ \left(1 + \lambda \ln \frac{x}{b}\right). \qquad (3.11)$$

If $x \gg L$, then, using the imaginary Jacobi transform

$$\vartheta_3(0 \mid \tau) = (-i\tau)^{-1/2} \vartheta_3\left(0 \,\Big|\, -\frac{1}{\tau}\right) \qquad (3.12)$$

and neglecting terms of order $e^{-\pi}$, we can replace Eq. (3.10) by the simpler equation

$$c(x) = c_0 - \frac{\lambda}{L} \int_0^{x-L} c(x')\,dx' - \lambda \int_{x-L}^{x-b} \frac{c(x')}{x - x'}\,dx', \qquad (3.13)$$

whose solution is

$$\frac{c(x)}{c_0} = \left(1 + \lambda \ln \frac{L}{b}\right)^{-1} e^{-\lambda (x-L)/L}. \qquad (3.14)$$

Thus, the concentration of the oncoming stream in the neighborhood of the lattice nodes varies logarithmically for $x \ll L$ and decreases exponentially for $x \gg L$.

As we see from Eq. (3.1), at distances $x \sim L$ the effective width of the diffusion wake is comparable with the lattice period b. The concentration distribution in the range $x \ll L$ is therefore close to that which arises in flow past a single chain in an infinite medium. The effect of neighboring chains is not yet significant. For $x \gg L$ the solution of the problem obtained in the first approximation in the small parameter λ becomes the solution for spheres chaotically distributed in space. In fact, the equation for the average concentration in a region considerably larger than b^3 is described by the equation of convective transfer with absorption (for $P \gg 1$ the diffusion flux for the average concentration is negligibly small as compared with the convective flux),

$$L\,dc / dx = -\lambda c \qquad (3.15)$$

whose solution for $x \gg L$ clearly coincides with Eq. (3.14) to within a constant factor.

However, the range of applicability of this solution in the case of chaotically distributed spheres is $x \gg b$. If the spheres form chains, then it is only applicable for $x \gg L$. In the range $b \ll x \ll L$ the character of concentration variation in the neighborhood of spheres homogeneously distributed in space and of spheres arranged in chains differs qualitatively.

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REFERENCES

1. V. G. Levich, Physicochemical Hydrodynamics [in Russian], Fizmatgiz, 1959.

2. H. Hasimoto, "On the periodic fundamental solutions of the Stokes equations and their application to viscous flow past a cubic array of spheres," J. Fluid Mech., vol. 5, no. 2, 1959.

3. G. Lamb, Hydrodynamics [Russian translation], Gostekhizdat, 1947.

4. J. M. Burgers, Second Report on Viscosity and Plasticity, ch. III. Amsterdam, 1938.

5. E. T. Whittaker and J. N. Watson, A Course in Modern Analysis, part 2 [Russian translation], Fizmatgiz, 1963.

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