

Stokes flow through periodic arrays of spheres

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We treat the problem of slow flow through a periodic array of spheres. Our interest is in the drag force exerted on the array, and hence the permeability of such arrays. It is shown to be convenient to formulate the problem as a set of two-dimensional integral equations for the unknown surface stress vector, thus lowering the dimension of the problem. This set is solved numerically to obtain the drag as a function of particle concentration and packing characteristics. Results are given over the full concentration range for simple cubic, body-centred cubic and face-centred cubic arrays and these agree well with previous limited experimental, asymptotic and numerical results.

1. Introduction

The problem of slow flow through assemblages of fixed solid particles is important in many processes involving flow through porous media and packed bed reactors. In spite of its wide importance, solutions are generally limited to conditions of small particle concentration. The problem is thus one of both fundamental interest and of great practical utility.

We develop here a solution to the problem for the case in which the particles are spheres held fixed in regular periodic arrays. No restriction is made regarding the volume concentration of spheres in the lattice, but only certain types of isotropic packings may be treated practically from a computational point of view.

There are a number of methods by which this problem can be solved. Hasimoto (1959) obtained a perturbation solution that gave the drag on each sphere in terms of an expansion in fractional powers of the concentration of the packing. Hasimoto has given the first few terms and, while it is in principle possible to compute more terms of the expansion, the existing results are limited to dilute packings.

The problem can also be solved by finding numerical approximations to the pressure and velocity fields within the unit cell. The methods of finite differences and finite elements are two means of numerical solution. Both methods require the division of the fluid region into three-dimensional grids. Each different concentration of interest would require a different grid. The finite-difference method would experience difficulties at the curvilinear boundaries. The finite element method would require the integration of trial functions over each three-dimensional element. Both methods result in very large (with possibly hundreds or even thousands of unknowns) banded systems of equations. The bandwidths depend on how the gridpoints are numbered and are generally larger for the finite-element method.

A global Galerkin technique may also be used to obtain a numerical solution. In this method, trial functions defined over the entire domain are used to approximate the solution. The difference between the exact solution and the trial solution is made

to average zero over the domain with respect to a number of weight functions. This method requires a large number of three-dimensional integrations (usually done numerically) and the domain of integration changes for each concentration. The resulting system of equations is somewhat smaller than those resulting from the finite-difference or finite-element methods but the matrix is full rather than banded. Snyder & Stewart (1966) and Sorensen & Stewart (1974) have used the Galerkin method to determine the velocity and pressure profiles within cubic lattices. Because of the computational complexity, their results are generally limited to the concentration corresponding to closest packing.

The problem was solved in this study by a completely different technique. Since the quantity of primary interest is the relationship between the pressure drop, flow rate, packing characteristics, and particle concentration, we seek a method which gives these results in a direct way. As described below, the set of partial differential equations was reduced to a set of Fredholm integral equations of the first kind. The unknown is the surface stress vector and the parameters include the mean flow, packing characteristics, and particle concentration. The integral equations were then solved numerically by a Galerkin method to obtain the pressure drop through the porous medium.

The reduction of Stokes-flow problems to the equivalent integral equation is not new. It was first used as a basis of a computational technique by Youngren & Acrivos (1975), who solved problems involving a single particle of arbitrary shape; it has since been applied to free boundary problems; see Youngren & Acrivos (1976) and Rallison & Acrivos (1978). In extending this approach to multi-particle systems, it is convenient to develop the averaged equations describing the mean quantities. It is also necessary to proceed with some care because as we shall see, the fundamental singular solutions comprising the kernel of the integral equation are now infinite Fourier sums. Although this fact severely limits the class of multi-particle systems for which the integral representation is computationally feasible, it provides only a minor obstacle in the case of cubic arrays of spheres.

In §2, we define the problem and reduce it to an equivalent integral equation. Section 3 gives the details of the solution technique and the numerical results are given and discussed in §4.

2. Problem definition and derivation of integral equation

Consider the steady creeping flow of a Newtonian fluid through a periodic array of fixed spheres of radius a centred at positions

$$\mathbf{r}^{\alpha} = m_1 \mathbf{s}^{(1)} + m_2 \mathbf{s}^{(2)} + m_3 \mathbf{s}^{(3)} \quad (m_1, m_2, m_3 = 0, \pm 1, \pm 2, \dots). \quad (2.1)$$

The basis vectors $\mathbf{s}^{(i)}$ determine a unit cell of the array. The volume of this unit cell is given by

$$\tau_0 = \mathbf{s}^{(1)} \cdot (\mathbf{s}^{(2)} \times \mathbf{s}^{(3)}). \quad (2.2)$$

Let D be the region within the spheres comprising the array. Let E be the region exterior to D containing fluid. Let ∂D denote the interface between D and E , i.e. the surface of the spheres. The solution to the flow problem is governed by the usual Stokes equations for slow flow of a Newtonian fluid:

$$\frac{\partial v_i}{\partial x_i} = 0, \quad x_i \in E; \quad (2.3)$$

$$\sigma_{ij} = -p\delta_{ij} + \mu \left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i} \right), \quad x_i \in E; \quad (2.4)$$

$$\frac{\partial \sigma_{ij}}{\partial x_i} = 0, \quad x_i \in E; \quad (2.5)$$

$$v_i = 0, \quad x_i \in \partial D; \quad (2.6)$$

v_i is periodic, i.e. for all \mathbf{r}^α ;

$$v_i(\mathbf{x} + \mathbf{r}^\alpha) = v_i(\mathbf{x}), \quad \mathbf{x} \in E. \quad (2.7)$$

Our objective is to solve (2.3)–(2.7) to obtain the force exerted by the fluid on the solids in the lattice when the superficial velocity, \mathbf{V} , is specified.

The fundamental singular solution of this problem is comprised of the quantities $q_k(\mathbf{x}, \mathbf{y})$, $u_{ik}(\mathbf{x}, \mathbf{y})$, and $\tau_{ijk}(\mathbf{x}, \mathbf{y})$ which represent the pressure, the i th velocity component, and the ij component of the stress field at a point \mathbf{x} due to unit forces applied in the k direction at each position $\mathbf{y} + \mathbf{r}^\alpha$. These quantities satisfy

$$\frac{\partial u_{ik}(\mathbf{x}, \mathbf{y})}{\partial x_i} = 0, \quad (2.8)$$

$$\tau_{ijk}(\mathbf{x}, \mathbf{y}) = -q_k(\mathbf{x}, \mathbf{y})\delta_{ij} + \mu \left(\frac{\partial u_{ik}}{\partial x_j} + \frac{\partial u_{jk}}{\partial x_i} \right), \quad (2.9)$$

$$\frac{\partial \tau_{ijk}}{\partial x_j} = -\delta_{ik} \sum_{\alpha} \delta(\mathbf{x} - \mathbf{y} - \mathbf{r}^\alpha), \quad (2.10)$$

where \sum_{α} indicates a summation over all particles in the lattice. In addition we will require u_{ik} to have a zero mean within a unit cell. The fundamental singular solution is well known (Hasimoto 1959; Saffman 1973) to be

$$u_{jk} = \frac{1}{4\pi^2\mu\tau_0} \sum'_{\alpha} \left(\frac{\delta_{jk}}{|\mathbf{k}^\alpha|^2} - \frac{k_j^\alpha k_k^\alpha}{|\mathbf{k}^\alpha|^4} \right) \exp[2\pi i \mathbf{k}^\alpha \cdot (\mathbf{x} - \mathbf{y})], \quad (2.11)$$

$$q_k = \frac{(x_k - y_k)}{\tau_0} - \frac{i}{2\pi\tau_0} \sum'_{\alpha} \frac{k_k^\alpha}{|\mathbf{k}^\alpha|^2} \exp[2\pi i \mathbf{k}^\alpha \cdot (\mathbf{x} - \mathbf{y})], \quad (2.12)$$

where

$$\mathbf{k}^\alpha = m_1 \mathbf{b}^{(1)} + m_2 \mathbf{b}^{(2)} + m_3 \mathbf{b}^{(3)} \quad (m_1, m_2, m_3 = 0, \pm 1, \pm 2, \dots), \quad (2.13)$$

are vectors in the reciprocal lattice. The basis vectors $\mathbf{b}^{(i)}$ are given by

$$\mathbf{b}^{(1)} = \frac{1}{\tau_0} (\mathbf{s}^{(2)} \times \mathbf{s}^{(3)}), \quad \mathbf{b}^{(2)} = \frac{1}{\tau_0} (\mathbf{s}^{(3)} \times \mathbf{s}^{(1)}), \quad \mathbf{b}^{(3)} = \frac{1}{\tau_0} (\mathbf{s}^{(1)} \times \mathbf{s}^{(2)}) \quad (2.14)$$

and hence,

$$\mathbf{b}^{(i)} \cdot \mathbf{s}^{(j)} = \delta_{ij}. \quad (2.15)$$

Also, \sum'_{α} indicates a summation over all reciprocal lattice vectors \mathbf{k}^α except where $|\mathbf{k}^\alpha| = 0$.

Now restrict the points \mathbf{x} and \mathbf{y} to be within the region T , which we shall define as any unit cell which completely encloses the sphere centred at the origin. Let ∂T denote the surface of T . In addition, redefine E and D as the fluid and solid regions within T , and ∂D as the surface of the isolated sphere. The superficial velocity can now be defined as

$$V_i = \frac{1}{\tau_0} \iiint_E v_i(\mathbf{x}) d\mathbf{x}. \quad (2.16)$$

For \mathbf{x} and \mathbf{y} within T , equation (2.10) becomes

$$\frac{\partial \tau_{ijk}}{\partial x_j} = -\delta_{ik} \delta(\mathbf{x} - \mathbf{y}). \quad (2.17)$$

It then follows that

$$\iiint_E v_i(\mathbf{x}) \frac{\partial \tau_{ijk}(\mathbf{x}, \mathbf{y})}{\partial x_j} d\mathbf{x} = -v_k(\mathbf{y}). \quad (2.18)$$

From equations (2.3)–(2.5), (2.8)–(2.9) and (2.18), and the divergence theorem we obtain

$$-v_k(\mathbf{y}) = \iiint_E \left\{ v_i(\mathbf{x}) \frac{\partial \tau_{ijk}(\mathbf{x}, \mathbf{y})}{\partial x_j} - u_{ik}(\mathbf{x}, \mathbf{y}) \frac{\partial \sigma_{ij}(\mathbf{x})}{\partial x_j} \right\} d\mathbf{x} \quad (2.19)$$

$$= \iint_{\partial T} \left\{ v_i \tau_{ijk} - u_{ik} \sigma_{ij} \right\} n_j d\mathbf{x} - \iint_{\partial D} \left\{ v_i \tau_{ijk} - u_{ik} \sigma_{ij} \right\} n_j d\mathbf{x} \quad (2.20)$$

where n_j is the unit outward normal.

The quantity we seek to determine is the force, \mathbf{F} , exerted on each sphere by the fluid. This force is given by

$$F_i = \iint_{\partial D} f_i(\mathbf{x}) d\mathbf{x}, \quad (2.21)$$

where

$$f_i(\mathbf{x}) \equiv \sigma_{ij}(\mathbf{x}) n_j(\mathbf{x}). \quad (2.22)$$

Because of the force exerted on each sphere, there will be an overall or mean pressure gradient of $-\mathbf{F}/\tau_0$ through the array. In other words, the pressure can be decomposed into a periodic part and a linear part with gradient $-\mathbf{F}/\tau_0$, i.e.

$$p(\mathbf{x}) = -\frac{1}{\tau_0} F_j x_j + p'(\mathbf{x}), \quad (2.23)$$

where $p'(\mathbf{x})$ is periodic.

It should be observed that because $v_i(\mathbf{x})$ and $u_{ik}(\mathbf{x}, \mathbf{y})$ are periodic and because $p(\mathbf{x})$ and $g_k(\mathbf{x}, \mathbf{y})$ contain periodic parts, the quantity $v_i \tau_{ijk} - u_{ik} \sigma_{ij}$ can be decomposed into a periodic part and a non-periodic part:

$$\begin{aligned} v_i(\mathbf{x}) \tau_{ijk}(\mathbf{x}, \mathbf{y}) - u_{ik}(\mathbf{x}, \mathbf{y}) \sigma_{ij}(\mathbf{x}) &= -\frac{\delta_{ij}}{\tau_0} \{v_i(\mathbf{x}) (x_k - y_k) + u_{ik}(\mathbf{x}, \mathbf{y}) F_l x_l\} \\ &\quad + \text{a periodic part.} \end{aligned} \quad (2.24)$$

From equation (2.24) and the fact that

$$\iint_{\partial T} g(\mathbf{x}) n_i d\mathbf{x} = 0, \quad (2.25)$$

for any periodic function $g(\mathbf{x})$, equation (2.20) can be reduced to

$$\begin{aligned} -v_k(\mathbf{y}) &= -\frac{1}{\tau_0} \iint_{\partial T} \{v_i(\mathbf{x}) x_k + u_{ik}(\mathbf{x}, \mathbf{y}) F_l x_l\} n_i d\mathbf{x} \\ &\quad + \iint_{\partial D} u_{ik}(\mathbf{x}, \mathbf{y}) f_i(\mathbf{x}) d\mathbf{x}. \end{aligned} \quad (2.26)$$

With use of the divergence theorem, this can be reduced further to

$$-v_k(\mathbf{y}) = -\frac{1}{\tau_0} \iiint_E v_k(\mathbf{x}) d\mathbf{x} - \frac{F_i}{\tau_0} \iiint_T u_{ik}(\mathbf{x}, \mathbf{y}) d\mathbf{x} + \iint_{\partial D} u_{ik}(\mathbf{x}, \mathbf{y}) f_i(\mathbf{x}) d\mathbf{x}. \quad (2.27)$$

From the definition of \mathbf{V} and the fact that u_{ik} has zero mean it follows that

$$-v_k(\mathbf{y}) = -V_k + \iint_{\partial D} u_{ik}(\mathbf{x}, \mathbf{y}) f_i(\mathbf{x}) d\mathbf{x}, \quad \mathbf{y} \notin \partial D, \quad (2.28)$$

$$V_k = \iint_{\partial D} u_{ik}(\mathbf{x}, \mathbf{y}) f_i(\mathbf{x}) d\mathbf{x}, \quad \mathbf{y} \in \partial D. \quad (2.29)$$

Finally, equations (2.11) and (2.29) give the integral equation

$$V_k = \frac{1}{4\pi^2\mu\tau_0} \sum'_\alpha \left(\frac{\delta_{ik}}{|\mathbf{k}^\alpha|^2} - \frac{k_i^\alpha k_k^\alpha}{|\mathbf{k}^\alpha|^4} \right) \exp[-2\pi i \mathbf{k}^\alpha \cdot \mathbf{y}_1] \times \iint_{\partial D} \exp[2\pi i \mathbf{k}^\alpha \cdot \mathbf{x}] f_i(\mathbf{x}) d\mathbf{x}, \quad \mathbf{y} \in \partial D \quad (2.30)$$

which must be solved to obtain $f_i(\mathbf{x})$ and subsequently F_i .

3. Solution of the integral equation

It is obvious that equation (2.30) still requires a numerical solution. At first it may appear to be more difficult to solve than the original differential equations. One reason is that integral equations of the first kind tend to yield stiff algebraic equations upon discretization. Furthermore, the kernel is a three-dimensional Fourier series which is singular at $\mathbf{x} = \mathbf{y}$. The integral equation is not without its advantages, however.

The domain of the integral equation is the two-dimensional surface of a sphere whereas the domain of the differential equations is the three-dimensional fluid region. This gives the integral equation a great advantage over the differential equations with regard to the size of the numerical problem. In addition, a change in either the structure of the array or the concentration of the particles requires a change in the size and shape of the domain over which the differential equations must be solved. However, such a change in the packing affects only the kernel of the integral equation and not the domain. The integral equation involves only three unknowns, the three components of the surface stress vector. The differential equations involve four unknowns: the pressure and the three components of the velocity vector. This will also make a difference in the size of the numerical problem. Finally, it may be difficult to satisfy the boundary conditions exactly when the differential equations are solved. However, the conversion of the differential equations to the integral equation automatically satisfies all periodicity and boundary conditions.

The straightforward approach to solving equation (2.30) would be to use a collocation method. Integral equations are usually solved by collocation methods and in particular, Youngren & Acrivos (1975) have successfully used such a method to determine the drag on a single, arbitrarily shaped particle in Stokes flow. The basic idea behind any collocation method is to divide the domain of integration into N

discrete collocation points. The integral is approximated by a sum over all the collocation points and the integral equation is required to hold at each collocation point. For a vector integral equation such as equation (2.30), this results in a $3N \times 3N$ system of algebraic equations for the three unknowns at the N collocation points. Some difficulty is encountered because of the singularity in the kernel but as Youngren & Acrivos demonstrated, this difficulty can be overcome by analytic integration in the neighbourhood of the singularity.

However, in the present problem, collocation becomes unattractive because the kernel is a Fourier series. A collocation method for a vector equation, with N collocation points, would require up to $\frac{1}{2}(3N)(3N+1)$ evaluations of the kernel. Youngren & Acrivos encountered no difficulties even with $N = 144$ because the kernel in their problem was easily evaluated. In the present case, this would involve the evaluation of 93,528 three-dimensional Fourier series, which would be totally out of the question from a computational viewpoint. Therefore, a different method was used to solve equation (2.30). This involved the development of a Galerkin method.

Consider the equation we must solve for $\mathbf{f}(\mathbf{x})$:

$$V_k = \iint_{\partial D} u_{ik}(\mathbf{x}, \mathbf{y}) f_i(\mathbf{x}) d\mathbf{x}, \quad \mathbf{y} \in \partial D. \quad (3.1)$$

Suppose there exists a set of known basis functions, $\phi^j(\mathbf{x})$ which are complete over the domain ∂D . Then $\mathbf{f}(\mathbf{x})$ can be expressed as a linear combination of these basis functions:

$$f_i(\mathbf{x}) = \sum_{j=1}^{\infty} a_i^j \phi^j(\mathbf{x}). \quad (3.2)$$

Therefore, equation (3.1) can be rewritten

$$V_k = \sum_{j=1}^{\infty} a_i^j \iint_{\partial D} u_{ik}(\mathbf{x}, \mathbf{y}) \phi^j(\mathbf{x}) d\mathbf{x}, \quad \mathbf{y} \in \partial D. \quad (3.3)$$

In the usual way, it may be shown that

$$\iint_{\partial D} V_k \phi^l(\mathbf{y}) d\mathbf{y} = \sum_{j=1}^{\infty} a_i^j \iint_{\partial D} \left[\iint_{\partial D} u_{ik}(\mathbf{x}, \mathbf{y}) \phi^j(\mathbf{x}) d\mathbf{x} \right] \times \phi^l(\mathbf{y}) d\mathbf{y}, \quad l = 1, 2, 3, \dots \quad (3.4)$$

We now have a system of linear equations of infinite rank for the unknown coefficients a_i^j :

$$\sum_{j=1}^{\infty} A_{ik}^{jl} a_i^j = W_k^l, \quad l = 1, 2, 3, \dots, \quad (3.5)$$

where

$$A_{ik}^{jl} \equiv \iint_{\partial D} \left[\iint_{\partial D} u_{ik}(\mathbf{x}, \mathbf{y}) \phi^j(\mathbf{x}) d\mathbf{x} \right] \phi^l(\mathbf{y}) d\mathbf{y}, \quad (3.6)$$

and

$$W_k^l \equiv \iint_{\partial D} V_k \phi^l(\mathbf{y}) d\mathbf{y}. \quad (3.7)$$

If A_{ik}^{jl} were diagonal, equation (3.5) could be solved explicitly for every a_i^j and then equation (3.2) would provide an exact solution for $\mathbf{f}(\mathbf{x})$. Unfortunately, in this problem there is no known set of basis functions for which A_{ik}^{jl} is diagonal and so there is no

exact solution. However, the Galerkin technique may be used to find an approximate solution by truncating the expression for $\mathbf{f}(\mathbf{x})$ after N terms and solving the resulting finite problem, i.e.

$$f_i(\mathbf{x}) \simeq \sum_{j=1}^N a_i^j \phi^j(\mathbf{x}), \quad (3.8)$$

where

$$\sum_{j=1}^N A_{ik}^{jl} a_i^j = W_k^l, \quad l = 1, 2, 3, \dots, N. \quad (3.9)$$

One possible set of basis functions for this problem is given by

$$\left. \begin{aligned} \phi^1(\mathbf{x}) &= 1, & \text{0th order;} \\ \phi^2(\mathbf{x}) &= x_1, & \phi^3(\mathbf{x}) = x_2, & \phi^4(\mathbf{x}) = x_3, & \text{1st order;} \\ \phi^5(\mathbf{x}) &= x_1 x_1, & \phi^6(\mathbf{x}) = x_1 x_2, & \phi^7(\mathbf{x}) = x_1 x_3, & \text{2nd order;} \\ \phi^8(\mathbf{x}) &= x_2 x_2, & \phi^9(\mathbf{x}) = x_2 x_3, & \phi^{10}(\mathbf{x}) = x_3 x_3, & \\ \phi^{11}(\mathbf{x}) &= x_1 x_1 x_1, \text{ etc.}, & & & \text{3rd order.} \end{aligned} \right\} \quad (3.10)$$

These functions can be derived from spherical harmonic functions and thus they form a complete set over the surface of a sphere. As listed, not all of these functions are linearly independent (e.g. $\phi^5 + \phi^8 + \phi^{10} = a^2 \phi^1$) so some of them may be discarded. It can also be shown that if the array is isotropic (as are the three cubic arrays studied here) a considerable number of the coefficients a_i^j will be zero. First, none of the odd-ordered functions will contribute to \mathbf{f} . Secondly, we can take the flow to be in the 1-direction without loss of generality. Then it can be shown that for the function

$$\phi^j(\mathbf{x}) = x_1^p x_2^q x_3^t, \quad (3.11)$$

a_1^j is non-zero only if p, q and t are even; a_2^j is non-zero only if p is odd, q is odd, and t is even; and a_3^j is non-zero only if p is odd, q is even, and t is odd. We shall let the even integer M denote the order of the approximation if all the independent functions for which $p + q + t = M$ are included in the approximation. It can then be shown that the total number of non-zero coefficients to be determined is $\frac{1}{8}(M+2)(3M+4)$. One other consequence of the array being isotropic is that the matrix A_{ik}^{jl} takes the simplified form

$$A_{ik}^{jl} = \frac{1}{4\pi^2 \mu \tau_0} \sum_{\alpha} \left(\frac{\delta_{ik}}{|\mathbf{k}^{\alpha}|^2} - \frac{k_i^{\alpha} k_k^{\alpha}}{|\mathbf{k}^{\alpha}|^4} \right) \iint_{\partial D} \cos(2\pi \mathbf{k}^{\alpha} \cdot \mathbf{y}) \phi^l(\mathbf{y}) d\mathbf{y} \\ \times \iint_{\partial D} \cos(2\pi \mathbf{k}^{\alpha} \cdot \mathbf{x}) \phi^j(\mathbf{x}) d\mathbf{x}. \quad (3.12)$$

If the integrals appearing within A_{ik}^{jl} were to require evaluation for each specific value of \mathbf{k}^{α} , the computation of A_{ik}^{jl} would be hopelessly intractable (this would be similar to the downfall of the collocation method). Fortunately however, because of the simplicity of the basis functions and of the spherical surface, ∂D , the integrals can be evaluated analytically. It can be shown that, for any vector \mathbf{z} ,

$$\iint_{\partial D} \cos(\mathbf{z} \cdot \mathbf{n}) n_1^p n_2^q n_3^t d\mathbf{x} = 4\pi a^2 \sum_{i=0,1}^p \sum_{j=0,1}^q \sum_{k=0,1}^t \\ \times \frac{p!}{i!(\frac{1}{2}(p-i))!} \frac{q!}{j!(\frac{1}{2}(q-j))!} \frac{t!}{k!(\frac{1}{2}(t-k))!} \frac{z_1^i z_2^j z_3^k}{|\mathbf{z}|^{i+j+k}} F_{i+j+k}^{p+q+t}(|\mathbf{z}|), \quad (3.13)$$

where a is the sphere radius.

Here $\sum_{i=0,1}^p$ indicates a summation over the values

$$i = \begin{cases} 0, 2, 4, \dots, p, & \text{for } p \text{ even,} \\ 1, 3, 5, \dots, p, & \text{for } p \text{ odd,} \end{cases} \quad (3.14)$$

and

$$F_{2l}^{2m}(z) \equiv (-1)^l (2z)^{-(m-l)} j_{m+l}(z), \quad (3.15)$$

where $j_n(z)$ is the n th spherical Bessel function of the first kind.

All that remains is to define τ_0 and the reciprocal lattice vectors, \mathbf{k}^α , for a particular array before equation (2.30) can be solved. Given below are the lattice basis vectors, $\mathbf{s}^{(i)}$, the unit cell volume, τ_0 , and the reciprocal-lattice basis vectors, $\mathbf{b}^{(i)}$, for the three types of cubic packings with centre-to-centre distance d between nearest neighbouring particles.

(a) Simple-cubic packing (SC):

$$\left. \begin{aligned} \mathbf{s}^{(1)} &= d(1, 0, 0), & \mathbf{b}^{(1)} &= d^{-1}(1, 0, 0), \\ \mathbf{s}^{(2)} &= d(0, 1, 0), & \mathbf{b}^{(2)} &= d^{-1}(0, 1, 0), \\ \mathbf{s}^{(3)} &= d(0, 0, 1), & \mathbf{b}^{(3)} &= d^{-1}(0, 0, 1). \end{aligned} \right\} \quad \tau_0 = d^3, \quad (3.16)$$

(b) Body-centred cubic packing (BCC):

$$\left. \begin{aligned} \mathbf{s}^{(1)} &= 3^{-\frac{1}{2}}d(1, 1, -1), & \mathbf{b}^{(1)} &= \frac{1}{2}\sqrt{3}d^{-1}(1, 1, 0), \\ \mathbf{s}^{(2)} &= 3^{-\frac{1}{2}}d(-1, 1, 1), & \mathbf{b}^{(2)} &= \frac{1}{2}\sqrt{3}d^{-1}(0, 1, 1), \\ \mathbf{s}^{(3)} &= 3^{-\frac{1}{2}}d(1, -1, 1), & \mathbf{b}^{(3)} &= \frac{1}{2}\sqrt{3}d^{-1}(1, 0, 1). \end{aligned} \right\} \quad \tau_0 = (4/3\sqrt{3})d^3, \quad (3.17)$$

(c) Face-centred cubic packing (FCC):

$$\left. \begin{aligned} \mathbf{s}^{(1)} &= 2^{-\frac{1}{2}}d(1, 1, 0), & \mathbf{b}^{(1)} &= 2^{-\frac{1}{2}}d^{-1}(1, 1, -1), \\ \mathbf{s}^{(2)} &= 2^{-\frac{1}{2}}d(0, 1, 1), & \mathbf{b}^{(2)} &= 2^{-\frac{1}{2}}d^{-1}(-1, 1, 1), \\ \mathbf{s}^{(3)} &= 2^{-\frac{1}{2}}d(1, 0, 1), & \mathbf{b}^{(3)} &= 2^{-\frac{1}{2}}d^{-1}(1, -1, 1). \end{aligned} \right\} \quad \tau_0 = 2^{-\frac{1}{2}}d^3, \quad (3.18)$$

In all cases, the volume concentration of the array,

$$c = \frac{4}{3}\pi a^3/\tau_0, \quad (3.19)$$

is determined by the parameter a/d .

All the information required to obtain a numerical solution to equation (2.30) is now available. The only remaining matters of concern are (a) the number of Fourier series which must be evaluated, (b) the inversion of the system matrix, and (c) the convergence of the solution. As it turns out, after the integrations in equation (3.12) are performed, the series to be evaluated are no longer Fourier series. Instead, for an M th order approximation, they take the form

$$\sum_{\alpha} \frac{(k_1^\alpha)^p (k_2^\alpha)^q (k_3^\alpha)^t}{|\mathbf{k}^\alpha|^{p+q+t+2}} j_m(2\pi a|\mathbf{k}^\alpha|) j_n(2\pi a|\mathbf{k}^\alpha|), \quad (3.20)$$

where $p+q+t \leq 2M+2$ and $0 \leq l, m, n \leq M$. There is a limited number of such series, especially since the Bessel functions can be expressed in terms of trigonometric functions. For example, for $M = 12$, only 756 independent series evaluations are necessary to determine the matrix. Computationally, this did not prove to be unreasonable.

Packing	... SC	BCC	FCC	SC	BCC	FCC
Concentration	... 0.027	0.125	0.216	0.5236	0.6802	0.7405
Order						
0	2.004	4.366	7.095	9.53	9.6	8.4
2	2.008	4.441	7.702	28.04	86.1	135.8
4	2.008	4.447	7.757	40.91	131.8	214.4
6	—	4.447	7.758	41.82	157.6	370.8
8	—	—	—	42.03	161.8	418.1
10	—	—	—	42.07	162.3	425.4
12	—	—	—	42.10	162.6	429.8
Projected value	2.008 ± 0.001	4.447 ± 0.001	7.758 ± 0.001	42.14 ± 0.05	162.9 ± 0.3	435 ± 5

TABLE 1. Convergence of results for various concentrations and packings.

Integral equations of the first kind are often difficult to solve numerically because they tend to yield stiff system matrices. In this case, however, no problems of this sort were encountered. It was possible to vary the accuracy of the matrix elements slightly without significantly affecting the solution. Convergence of the solution was found to be quite rapid. Table 1 shows some typical results for the drag coefficient (defined by equation (4.1) below) computed at various orders of approximation. For dilute arrays, where the results reproduce those of Hasimoto, no approximations higher than 6th order were needed. For the close-packed arrays, 12th order approximations were sufficient to allow extrapolation of the results, with estimated errors of less than 2%. Tabulations of the coefficients a_i^j are available from the authors upon request.

4. Results and discussion

The results of the numerical computations are summarized and compared with other theoretical and experimental results in table 2. They are reported in terms of a drag coefficient, K , which is defined by the following equation for the drag on each sphere in the array:

$$F_i = 6\pi\mu a K V_i. \quad (4.1)$$

In addition, the pressure gradient in the array is related to K and the concentration, c , by

$$\frac{\Delta P}{L} = -\frac{9\mu}{2a^2} c K V. \quad (4.2)$$

It can easily be shown that the following expression gives K in terms of the numerically determined coefficients, a_i^j :

$$K = (6\pi\mu a |V|^2)^{-1} \lim_{N \rightarrow \infty} \sum_{j=1}^N a_i^j W_i^j. \quad (4.3)$$

This drag coefficient, K , is a function only of the geometry and concentration of the periodic array. When the array is infinitely dilute, $K = 1$ and the drag is simply the Stokes drag on a single sphere.

The comparison of our results with previous theoretical work deserves some discussion. It is important to point out that in contrast to other analytical or numerical

Concentration	SC packing		BCC packing		FCC packing	
	K	Previous results	K	Previous results	K	Previous results
0.000125	1.096	1.096†	1.098	1.098†	1.098	1.098†
0.001	1.212	1.212†	1.217	1.217†	1.217	1.217†
0.008	1.525	1.525†	1.539	1.539†	1.539	1.539†
0.027	2.008	2.009†	2.044	2.044†	2.044	2.044†
0.064	2.810	2.83†	2.889	2.889†	2.889	2.889†
0.125	4.292	4.5†	4.447	4.47†	4.446	4.47†
0.216	7.442	12†	7.739	8.0†	7.758	7.9†
0.343	15.4	—	16.3	20†	16.6	19†
0.45	28.1	—	31.7	—	33.5	—
0.5236	42.1	42.6†	51.7	48.4††	57.4	48.4††
—	—	40.4§	—	—	—	—
—	—	42.5	—	—	—	—
—	—	48.4††	—	—	—	—
0.6	—	—	88.9	93.8††	108	93.8††
0.6802	—	—	163	170¶	229	208††
—	—	—	—	208††	—	—
0.72	—	—	—	—	349	328††
0.7405	—	—	—	—	435	412§
—	—	—	—	—	—	398
—	—	—	—	—	—	424††

† Hasimoto (1959). ‡ Sorensen & Stewart (1974). § Snyder & Stewart (1966).
 || Martin *et al.* (1951). ¶ Susskind & Becker (1967). †† Equation (4.4).

TABLE 2. Drag coefficients for various concentrations and packings.

techniques the integral equation formulation conveniently provides a solution to this problem over the entire range of concentrations. Hasimoto's asymptotic expansion for small concentration is valid for dilute arrays but it fails for concentrated packings. On the other hand, standard numerical techniques of solving differential equations will not work well on dilute packings and thus these methods have only been applied to a few select densely packed arrays. Table 2 shows that our results compare very well with Hasimoto's results for concentrations up to about 0.2, above which Hasimoto's results begin to diverge. To our knowledge, this is the first time Hasimoto's results have been corroborated by an independent numerical technique. There have been relatively few numerical studies of this problem, and these have been for close packings. For simple cubic packing, Snyder & Stewart (1966) used a Galerkin method to obtain a drag coefficient of 40.4 ± 0.6 . Sorensen & Stewart (1974) later improved on that Galerkin solution and obtained 42.6 ± 0.2 . This last result agrees very well with our value of 42.1 ± 0.1 . Snyder & Stewart also obtained a coefficient of 412 for a dense face-centred cubic packing. This is within 6% of our value of 435.

There have also been some experimental studies of the pressure drop through periodic porous media. Drag coefficients of 42.5 and 398 were obtained from the data of Martin, McCabe & Monrad (1951) for simple cubic and face-centred cubic packings, respectively. The experiments of Susskind & Becker (1967) with body-centred cubic packings yielded a coefficient of 170. These values agree to within a few per cent with our results of 42.1, 435, and 163, respectively.

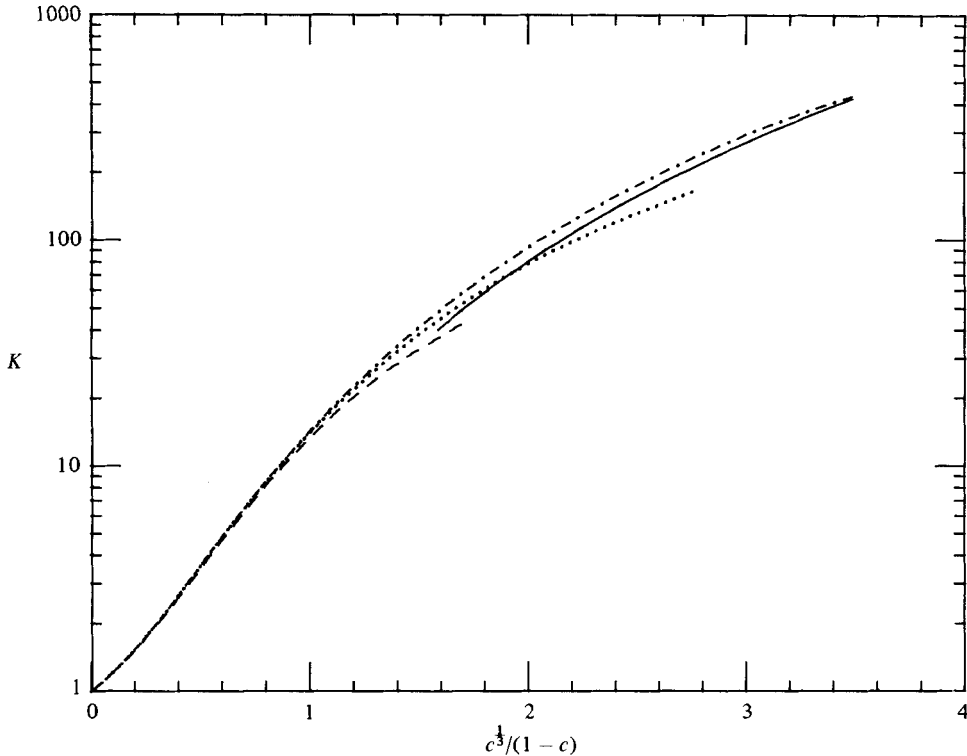


FIGURE 1. Drag coefficient as a function of concentration. The curves for various packings end at the concentration corresponding to closest packing. ---, simple cubic; ···, body-centred cubic; - · - ·, face-centred cubic; —, equation (4.4).

Our results may also be compared over a range of concentrations with the Carman empirical correlation which predicts that for random packings,

$$K \approx \frac{10c}{(1-c)^3}. \quad (4.4)$$

Figure 1 shows that for concentrations greater than 0.5, this correlation falls within 15% of our results for at least one of the three types of packings. This suggests that certain features of the flow through randomly packed beds may be modelled by periodic arrays of spheres. However, the choice of the packing geometry in such a model may require careful consideration since, as figure 1 also shows, at high concentrations, the geometry of the packing has a significant effect on the pressure drop.

In addition to the drag coefficient, we may examine the details of the surface stress variations for each of the packings considered. We restrict this discussion to solutions for closest packings, although results for other concentrations are available. From our Galerkin expansion, equation (3.8), and our numerically determined a_i^j , we may evaluate the three components of the surface stress vector. The component of \mathbf{f} in the direction of flow, f_1 , is shown in figures 2–4 for simple cubic, body-centred cubic and face-centred cubic packings respectively. (The drag is simply the mean of these functions.) In these figures, the co-ordinate system is chosen such that $\theta = 0$ corresponds to the forward stagnation point, the mean flow being in the x_1 direction, and $\phi = 0$ corresponds to the negative x_2 axis. ϕ, θ are the usual azimuthal and polar angles.

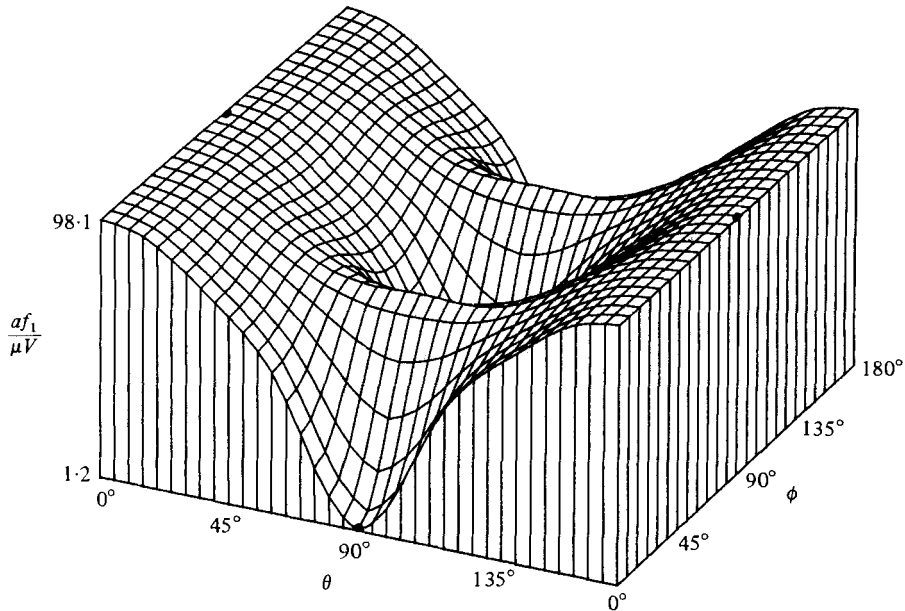


FIGURE 2. The surface stress component f_1 for simple cubic packing. In this and subsequent figures, contact points are marked by the dots.

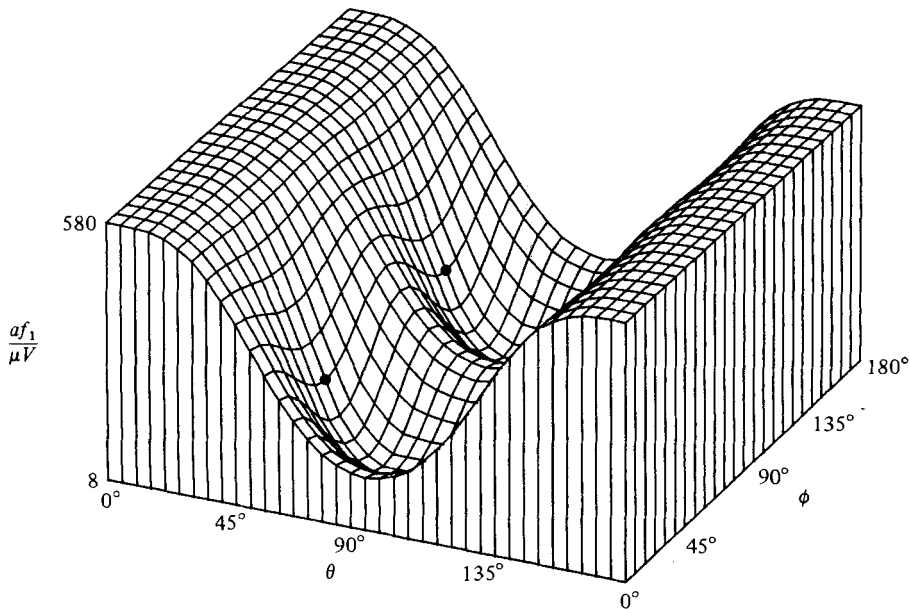
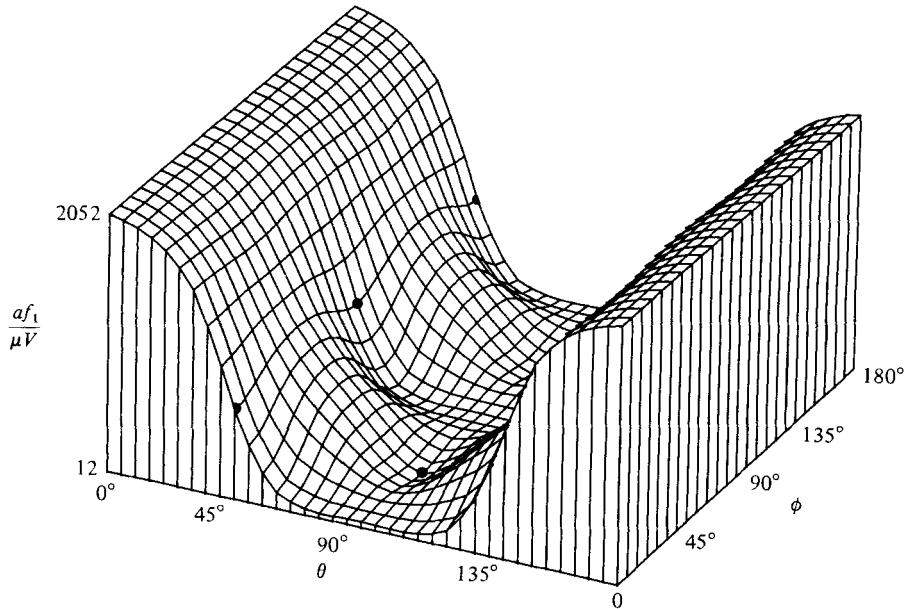
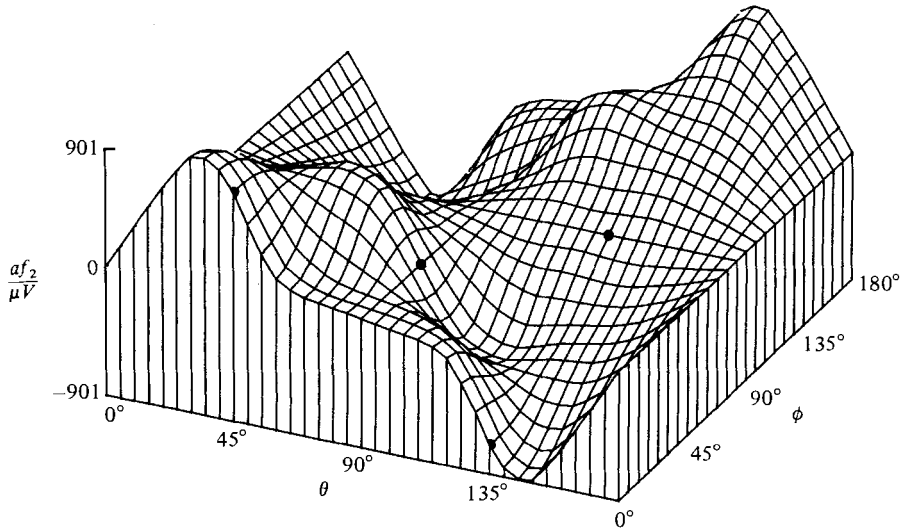


FIGURE 3. The surface stress component f_1 for body-centred cubic packing.

It is of interest to locate the points of contact on these figures (recall these results are for closest packing). In figure 2, for simple cubic packing, these are at $\theta = 0^\circ, 180^\circ$, and in the 'valleys' at $\theta = 90^\circ, \phi = 0^\circ, 90^\circ, 180^\circ$ (the latter two not visible). As might be expected, the normal stress contribution is large at the forward and rear stagnation points, and vanishes at $\theta = 90^\circ$. The shearing stress is minimal at points of contact,

FIGURE 4. The surface stress component f_1 for face-centred cubic packing.FIGURE 5. The surface stress component f_2 for face-centred cubic packing.

and large in the regions between contact points, a manifestation of the flow being constrained to channel through the open spaces in the lattice.

Figure 3 shows the stress component f_1 for the case of body-centred cubic packing. The same general features are evident. However, because there are now eight contact points, the tangential stress along the equator ($\theta = 90^\circ$) is more evenly distributed and larger than in the case of the simple cubic packing. The stress vector at the stagnation points is also larger, but this may be a misleading comparison as the void fraction (and hence the mean force) at closest packing is different for the three cases being discussed. What is clear however, is that the distribution of fluid flow in the lattice is more uniform the more complex the packing.

This is evident in figure 4, which gives f_1 for the face-centred cubic case, which has twelve points of contact at closest packing. The azimuthal variation is the weakest of the three cases and the stress at the equator the highest. It is also of interest to note that the results for this packing are closest to experimental results for random packings.

In figure 5 we show the stress component f_2 for the face-centred cubic packing, which of course has zero surface mean, but serves to demonstrate the complexity of the flow through the interstitial space.

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