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Brinkman screening and the covariance of the fluid velocity in fixed beds

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The phenomenon of Brinkman screening, whereby the fluid velocity disturbance produced by each particle in a fixed bed is attenuated by the forces that the fluid exerts on surrounding particles, plays a crucial role in limiting the range of velocity correlations in porous media and fixed beds. Koch and Brady [J. Fluid Mech. **154**, 399 (1985)] showed theoretically that Brinkman screening leads to a finite hydrodynamic diffusion coefficient for fluid phase tracers in dilute fixed beds. In this Letter, we present the results of two simulation techniques (lattice-Boltzmann method and a multipole method) confirming the screening of the fluid velocity covariance that underlies the Koch and Brady theory. © *1998 American Institute of Physics.* [S1070-6631(98)02612-9]

The slow decay of fluid velocity correlations with spatial position in a Stokes flow raises subtle issues concerning the existence of velocity covariances and hydrodynamic diffusion coefficients. The fluid velocity disturbance produced by flow past a single sphere decays like $1/r$, where r is the radial distance from the particle. Thus, an attempt to calculate the variance (or covariance) of the fluid velocity in an unbounded fixed bed or sedimenting suspension in the absence of inertia by adding the effects of the particles acting independently would lead to a volume integral that diverges at large r. The existence of system-size-independent velocity covariances and hydrodynamic diffusion coefficients remains a controversial issue for sedimenting suspensions.[1]

However, the understanding of hydrodynamic screening and dispersion in fixed beds of particles is more firmly established. Brinkman[2] suggested that the fluid velocity disturbance produced by a particle in a fixed bed should be described by equations

$$\nabla\cdot\langle\mathbf{u}\rangle_1=0, \tag{1}$$

$$\mu\nabla^2\langle\mathbf{u}\rangle_1-\nabla\langle p\rangle_1-(\mu/k)\langle\mathbf{u}\rangle_1=0, \tag{2}$$

that include the drag per unit volume exerted by the fluid on the surrounding particles, $\mu\langle\mathbf{u}\rangle_1/k$. Here, $\mathbf{u}$ and p are the fluid velocity and pressure, μ is the fluid viscosity, $\langle\cdot\rangle_1$ indicates a conditional ensemble average with the position of one particle fixed, $k=2a^2/(9\phi)$ is the permeability, ϕ is the particle volume fraction, and a is the particle radius. Hinch[3] derived this equation rigorously for a dilute fixed bed using the method of ensemble averaged equations. Previous numerical simulations have confirmed the predictions of Brinkman's equations for the conditionally averaged velocity[4] and the pressure drop in the bed.[5]

The conditionally averaged velocity obtained by solving Brinkman's equations (1) and (2) decays like $1/r$ at small radial distances from the fixed particle. However, it is screened and decays like $1/r^3$ at distances large compared with the Brinkman screening length, $k^{1/2}=a2^{1/2}/(3\phi^{1/2})$. Koch and Brady[6] showed that this screening leads to finite values of the fluid velocity variance, covariance and hydrodynamic fluid-tracer diffusivity in an unbounded fixed bed.

In a recent paper, however, Lowe and Frenkel[7] presented simulation evidence suggesting that finite hydrodynamic diffusion coefficients do not exist in unbounded random arrays of spheres. They used a lattice-Boltzmann method to compute the fluid velocity fields in arrays of 2400 spheres with a volume fraction of 0.45. The trajectories of fluid-phase tracers that experienced molecular diffusion and convection were also determined. The effective diffusivity of these tracers can be obtained as the time integral of the two-time covariance of the velocity of a fluid-phase tracer, i.e., $\langle\mathbf{u}'(t)\mathbf{u}'(0)\rangle$, where $\mathbf{u}'=\mathbf{u}-\langle\mathbf{u}\rangle$ is the fluctuation of the fluid velocity relative to the mean, and the angle brackets indicate an unconditional ensemble average. The simulations indicated that the 11-component of this temporal velocity covariance decayed like $1/t$ at long times t. Here the 1-axis is parallel to the mean velocity in the bed. This slow decay of the velocity covariance would lead to a logarithmic divergence of the effective diffusivity.

A slowly decaying temporal velocity covariance could arise from one of two physical effects: the spatial covariance of the velocity could be slowly decaying or some tracer particles could spend an infinite time trapped in some region of the porous medium. Koch and Brady[8] showed that a $1/t$ decay of the temporal velocity covariance could arise from tracer particles that come close to the no-slip surfaces of the fixed bed particles. After a time of order $(a/U)\mathrm{Pe}^{-1/3}$, however, molecular diffusion would allow the tracers to escape the boundary layer near the particles and lose their velocity correlation. Here, $\mathrm{Pe}=Ua/D$ is the Peclet number, U is the mean velocity in the medium, and D is the tracers' molecular diffusion coefficient. Thus, the theory for boundary-layer dispersion[8] predicts only a transient period of $1/t$ decay, whereas the simulations of Lowe and Frenkel[7] found this to be the long-time behavior of the temporal velocity covariance. Since the qualitative behavior observed by Lowe and Frenkel was not sensitive to the Peclet number and the grid resolution, it seems unlikely that it arose from tracers trapped in boundary layers near particle surfaces.

We may then conjecture that the slow temporal decay of $\langle \mathbf{u}'(t)\mathbf{u}'(0)\rangle$ observed in the Lowe and Frenkel simulations arose due to a slow decay of the two-position velocity correlation function $\langle \mathbf{u}'(\mathbf{x})\mathbf{u}'(\mathbf{0})\rangle$ with the magnitude x of the spatial separation of the two positions. Since the tracers are convected through the medium with an average velocity $U/(1-\phi)$, the $1/t$ decay of the temporal velocity covariance may be attributed to a slow $1/x$ decay of the spatial velocity covariance. In a dilute fixed bed the spatial velocity covariance can be computed from the conditionally averaged velocity using the relationship[6]

$$\langle \mathbf{u}'(\mathbf{x})\mathbf{u}'(\mathbf{0})\rangle \approx n\int d\mathbf{r}\langle \mathbf{u}'\rangle_1(\mathbf{x}|\mathbf{r})\langle \mathbf{u}'\rangle_1(\mathbf{0}|\mathbf{r}), \tag{3}$$

where n is the number of particles per unit volume. Evaluating the integral in (3) using the solution of Brinkman's equations (1), (2) leads to the result that the spatial covariance decays like $1/x^3$ at separations x that are much larger than the Brinkman screening length $k^{1/2}$. There are corrections to (3) (discussed in the appendix to Ref. 10) that involve the conditionally averaged velocity disturbance with two or more particles fixed. These corrections may be expressed in terms of multiple hydrodynamic reflections between the group of particles interacting through a Brinkman medium. Since each hydrodynamic reflection is subject to screening by the Brinkman medium, these higher order terms also decay like $1/x^3$. It may be noted that the contributions of higher order hydrodynamic reflections have been incorporated into calculations of the drag on a particle in a fixed bed.[3,9]

In view of the apparent contradiction between the Lowe and Frenkel simulations and the theoretical framework for understanding fluid velocity fluctuations and dispersion in fixed beds, it is desirable to perform further numerical simulations to determine the velocity covariance in a fixed bed. For simplicity, we will focus on the spatial velocity covariance. Since only the 11-component of the temporal velocity covariance was found to decay like $1/t$, we will consider the 11-component of the spatial covariance. The mean flow will tend to convect the tracer primarily in the 1-direction. Therefore, we will consider the dependence of $\langle u_1'(x_1,0,0)u_1'(0,0,0)\rangle$ on the separation x_1 of the two points in the direction parallel to the mean velocity. To assure that our conclusions do not result from artifacts of the simulation method, two simulation techniques will be applied: a multipole method and a lattice-Boltzmann method.

First, we consider the velocity covariance in a fixed bed of spheres determined by a fast multipole technique. Briefly,

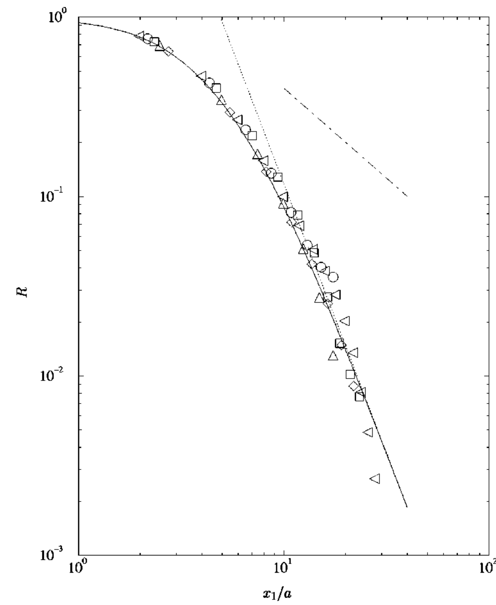

FIG. 1. The velocity correlation function in a random fixed bed of spheres with a volume fraction of 0.05 is plotted as a function of position x_1 in the direction parallel to the mean flow. The symbols are results of simulations using a fast multipole method with 500 (circles), 5000 (squares) and 8000 (diamonds) particles in cubic unit cells and 1500 (upward triangles) and 6000 (left triangles) particles in oblong cells whose lengths in the flow direction are twice as long as in the transverse directions. The solid line is the Brinkman theory, the dotted line is the asymptote $R=118(a/x_1)^3$ and the dash–dotted line is the slow decay required to give non-Fickian diffusion.

this method consists of representing the velocity field induced by particles in terms of force multipoles located at the center of the particles. The magnitude of these multipoles is determined by satisfying the no-slip boundary condition on the surface of each particle, as described in Mo and Sangani.[10] We are interested in arrays with a large number N of particles in each unit cell. In this case, it is advantageous to employ the rapid summation technique based on hierarchical grouping of particles described by Sangani and Mo.[11] For the relatively low volume fraction ($\phi=0.05$) considered in our study, the velocity disturbance caused by each sphere can be approximated as that resulting from the net force acting upon it. The $O(N)$ fast multipole algorithm[11] involves expanding the velocity induced by a group of particles in a series of force multipoles at a center of the group. We used force multipoles of $O(2^4)$ ($N_{sp}=5$ in the notation of Ref. 11) to represent the velocity induced by groups of particles. The velocity covariance was determined by averaging $u_1(\mathbf{r})u_1(\mathbf{r}+\mathbf{x})$ over position $\mathbf{r}$ (exploiting the translational invariance) and averaging over between 10 and 200 realizations of the random arrays. The velocity inside the particles was taken to be zero.

The variance of the velocity in all the simulations was found to be approximately 0.28. A calculation using the solution for Brinkman flow around a sphere in (3) yields a velocity variance of 0.20. The velocity correlation function $R(x_1)=\langle u_1(x_1,0,0)u_1(0,0,0)\rangle/\langle u_1^2\rangle$ is plotted as a function of position x_1/a in Fig. (1). The symbols correspond to simulations with N varying between 500 and 8000 in both cubic and oblong simulation cells. It may be seen that the velocity covariance decays rapidly at large separations

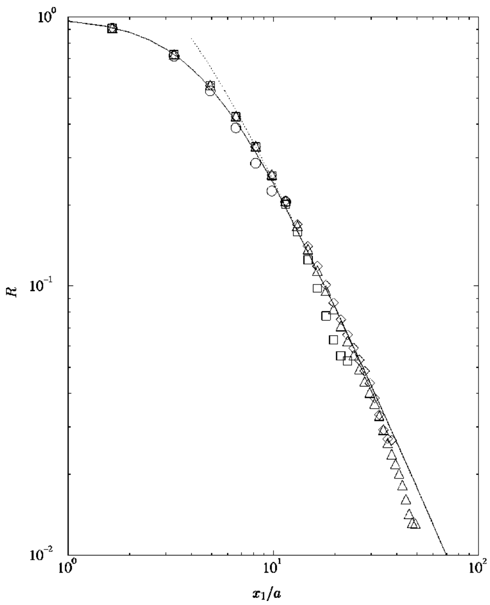

FIG. 2. The velocity correlation function in a random array of cylinders with a volume fraction of 0.0954 is plotted as a function of the position x_1 in the direction parallel to the mean flow. The symbols are results of lattice-Boltzmann simulations with 16 (circles), 64 (squares), 256 (diamonds) and 1024 (triangles) particles per unit cell. The solid line is the Brinkman theory, and the dotted line is the asymptote $R=[12.4\ln(x_1/a)-3.83](a/x_1)^2$.

$x_1/a>7$. The solid line is the theoretical prediction of (3) with a solution of Brinkman's equations for the conditionally averaged velocity. The dashed line is the long distance asymptote $R=118(a/x_1)^3$. For reference, the dash–dotted line indicates the slow decay of the velocity correlation function, $R\propto a/x_1$, that would be required to yield the non-Fickian dispersion observed in the Lowe and Frenkel simulations. It is clear that the velocity correlation function decays at a rate that is in good agreement with the Brinkman solution and the approximation (3) used in the Koch and Brady study of hydrodynamic diffusion in fixed beds.

The lattice-Boltzmann method will be applied to determine the fluid velocity covariance in the two-dimensional flow through a random array of aligned cylinders with $\phi=0.095$. The method we employ is described in detail by Ladd[12] and has been applied by Koch and Ladd[13] to determine the pressure drop/flow rate relationship in fixed arrays of cylinders. It is well known that two-dimensional Stokes flows have a longer range than three-dimensional flows and so this example provides a more rigorous test of Brinkman screening. A theoretical treatment of dispersion in random fibrous media has been developed by Koch and Brady.[14]

A calculation using the two-dimensional analog of (3) indicates that the spatial velocity covariance in a random array of cylinders should be proportional to $(a/x_1)^2\ln(x_1/a)$ for distances much larger than the Brinkman screening length, i.e., $x_1\gg k^{1/2}$. To test this prediction, we calculated the covariance for arrays of 16, 64, 256 and 1024 cylinders whose positions were chosen from a hard-disk distribution. The cylinders had an effective hydrodynamic diameter of 1.22 lattice spacings. With this small diameter, the flow on the length scale of the particle diameter is not well resolved. However, our primary interest here is in the long range behavior of the velocity. The Reynolds number was always less than 10^{-6} and the Mach number was sufficiently small so that compressibility effects were negligible. The covariance reported for each box size represents an ensemble average over 100 configurations of the random medium, except for the largest array where 50 configurations were used. The variance of the velocity obtained from the simulations was 0.65 whereas the variance obtained using the two-dimensional analog of (3) was 0.41. This deviation may result from the finite particle volume fraction. Nonetheless, the theory provides very accurate predictions for the spatial decay of the velocity correlation function as illustrated in Fig. 2. For sufficiently large values of x_1, the covariance decays like $\ln(x_1)/x_1^2$ as predicted on the basis of (3) and the Brinkman equations (1) and (2).

In summary, we have used lattice-Boltzmann and multipole simulation methods to determine the covariance of the fluid velocity in fixed beds of spheres and cylinders. The covariance of the fluid velocity in a fixed bed decays rapidly with spatial position. This decay is predicted well by theories based on a solution of Brinkman's approximation to the conditionally averaged equations of motion and the approximation (3) used in Koch and Brady's theory for hydrodynamic dispersion. No evidence was found of the long-range velocity correlations that would be required to yield non-Fickian dispersion.

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