Dispersion in an unconsolidated porous medium

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(Received 27 February 1991; accepted 3 June 1991)

The dispersion of passive scalar by Stokes flow through a dilute suspension of solid spheres fixed at random points in space is a basic model of mixing and transport in an unconsolidated porous medium. Earlier investigators have used a general theory of macroscopic transport to calculate the Lagrangian velocity autocorrelation function and the effective diffusivity of this system. If the tracer does not diffuse molecularly then the autocorrelation function has a "long tail," proportional to t^{-1}. Small molecular diffusivity provides a cutoff at long times and implies an effective diffusivity that increases as the logarithm of the Péclet number. In the present work the same results are obtained including the constants of proportionality, using an elementary Lagrangian argument that avoids the formalism of the macrotransport theory.

In a recent series of papers Koch and Brady[1–3] have developed a formalism for calculating the macroscopic transport properties of flow in a disordered medium.[4] They emphasize the utility and generality of a nonlocal theory which relates the flux at a point to the spatial–temporal average of the concentration about that point. The importance of a nonlocal description has long been recognized in theories of turbulent dispersion.[5] In this context it was realized from general considerations that the macroscopic formulation is nonlocal but, because of mathematical difficulties, approximations or phenomenological assumptions are required to calculate the form of the kernel in the transport equation.

By contrast Koch and Brady[3] solve a model of dispersion in a porous medium which does not require such approximations, and for which even dimensionless parameters in the kernel [e.g., $\pi^2/2$ in Eq. (1)] can be calculated exactly. The Koch and Brady model of a porous medium is a dilute bed of spherical solid particles fixed at random points in space through which a very viscous fluid, transporting passive scalar, is pumped.

In this Brief Communication we present an alternative and elementary derivation of some of the results obtained by Koch and Brady for this archetypical model of an unconsolidated porous medium. Our derivation is based on Lagrangian statistics and is simpler than the more general Eulerian formulation in Ref. 3. We show that the Lagrangian velocity autocorrelation function decays like

$$\mathscr{C}(t) \equiv \frac{1}{N} \sum_{i=1}^{i=N} u_i'(t) u_i'(0) \approx \frac{\pi^2}{2} \frac{\phi a U}{t} \tag{1}$$

when

$$\frac{a}{U} \ll t \ll P_e^{1/3} \frac{a}{U}.$$

Here a is the radius of a sphere, U is the mean fluid velocity, ϕ is the volume fraction of spheres,

$$P_e \equiv aU/D_{\rm mol}, \tag{2}$$

is the Péclet number, N is the number of tracer molecules in the ensemble and $u_i(t) = U + u_i'(t)$ is the velocity component in the direction of the mean flow of the ith molecule at time t.

Because of the slow algebraic decay of the correlation function in Eq. (1), Taylor's[6] expression for the effective diffusivity of the ensemble about the center of mass,

$$D_{\rm eff} = \int_0^\infty \mathscr{C}(t)\,dt, \tag{3}$$

diverges and the mean-square displacement about the center of mass of the tracer increases as $t \ln t$. A finite result is obtained only when $t \sim P_e^{1/3} a/U$ so that molecular diffusivity becomes important and results in an exponentially decaying correlation function

$$\mathscr{C}(t) \sim e^{-\mu t} \quad \text{when } t \gg P_e^{1/3}(a/U),$$

where

$$\mu^{-1} \sim P_e^{1/3}(a/U). \tag{4}$$

Fortunately it is not necessary to calculate μ in order to determine the leading-order asymptotic behavior of the effective diffusivity. Rather, from Eq. (3), the exponential cutoff of the correlation function gives the leading-order approximation

$$D_{\rm eff} \sim (\pi^2 \phi a U/6) \ln P_e. \tag{5}$$

This result (which is an example of the well-known logarithmic dependence of the effective diffusivity of a porous medium on the Péclet number[7]) first appeared in Ref. 1.

All of the conclusions summarized above are well known and most of them can be deduced by a combination of dimensional reasoning and simple statistical arguments such as those given by Baudet *et al.*[8] An apparent exception is the constant of proportionality, $\pi^2/2$, appearing in the asymptotic relation Eq. (1). To our knowledge this constant has been obtained only as a result of the Koch and Brady macrotransport formulation. The goal of this Brief Communication is to present an alternative simple calculation of this constant which does not require the formalism of the macrotransport theory in Refs. 1–3. Of course a systematic calculation of higher-order corrections certainly requires this apparatus, but for many purposes leading-order approximations such as Eqs. (1) and (5) suffice.

Suppose that at $t=0$ the volume occupied by a single sphere

$$\mathscr{V}=4\pi a^3/3\phi \tag{6}$$

contains $N\gg 1$ molecules of tracer. Consider those molecules that initially lie in a spherical shell, $a<r<a+\epsilon$ with $\epsilon\ll a$, which is concentric with the solid sphere. Persistent velocity correlations are due to those molecules which are still in the shell at $t\gg a/U$. Specifically, when $t\gg a/U$ the sum in Eq. (1) can be simplified because most of the terms are zero, and those that remain are mostly due to particles which have been detained at the sphere. Thus when $t\gg a/U$ the sum in (1) reduces to

$$\mathscr{C}(t)\approx\left(\frac{1}{N}\right)\left(\frac{4\pi a^2\epsilon N}{\mathscr{V}}\right)\left(\frac{V(t)}{4\pi a^2\epsilon}\right)(-U)^2=\frac{V(t)}{\mathscr{V}}U^2 . \tag{7}$$

Here $V(t)$ is volume of fluid initially in the shell that still remains in the shell at t. The first term in the middle expression of Eq. (7) is division by the number of particles in the ensemble. The second term is the number of particles initially in the shell. The third term is the fraction of these particles still in the shell at t. The product of the second and third terms is the number of nonzero terms in the sum Eq. (1). The fourth term is the value of each of these terms, since $u'(0)\approx u_i'(t)\approx -U$ for particles lingering in the shell.

To calculate $V(t)$ we use a local expansion of the Stokes streamfunction:

$$\psi=Ur^2\sin^2\theta\left(\frac{1}{2}-\frac{3}{4}\frac{a}{r}+\frac{1}{4}\frac{a^3}{r^3}\right). \tag{8}$$

Close to the sphere convenient local coordinates are

$$\begin{aligned} &s\equiv r-a, \quad 0\leqslant s\leqslant\infty,\\ &\alpha\equiv 2\pi a^2(1-\cos\theta), \quad 0\leqslant\alpha\leqslant 4\pi a^2, \end{aligned} \tag{9}$$

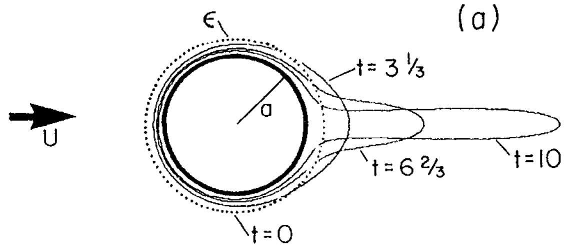
where α is the area of a spherical cap with semiangle θ. The approximate ($s\ll a$) equations of motion for a nondiffusing tracer particle are then

$$\begin{aligned} \dot{s}&=-\frac{\partial\hat{\psi}}{\partial\alpha}=-\frac{3U}{2}\left(\frac{s}{a}\right)^2\left(1-\frac{\alpha}{2\pi a^2}\right),\\ \dot{\alpha}&=\frac{\partial\hat{\psi}}{\partial s}=3U\left(\frac{s}{a^2}\right)\left(\alpha-\frac{\alpha^2}{4\pi a^2}\right), \end{aligned} \tag{10}$$

where

$$\hat{\psi}(s,\alpha)\equiv 2\pi\psi(r,\theta)\approx\frac{3}{2}U\left(\frac{s}{a}\right)^2\alpha\left(1-\frac{\alpha}{4\pi a^2}\right). \tag{11}$$

Because the flow is steady particles remain on streamlines and it is easy to calculate the time taken for a particle starting near one pole, $(s,\alpha)\approx(\epsilon,0)$, to enter the shell and leave at the antipodes, $(s,\alpha)\approx(\epsilon,4\pi a^2)$:



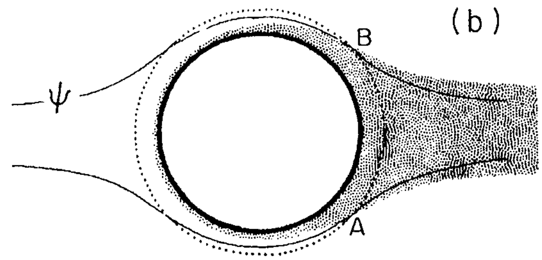


FIG. 1. (a) The shell has thickness ϵ and at $t=0$ it contains the red fluid. This figure shows the evacuation of this shell at three successive times in units of a/U. (b) This figure summarizes the geometry used to obtain (13). The stippled area is the red fluid which at this instant is leaving the dotted spherical shell through the cap AB. The cap is defined by the intersection of the stream surface ψ with the spherical shell.

$$T(\hat{\psi})=\sqrt{2\pi^3a^4/3U\hat{\psi}} . \tag{12}$$

Now we imagine that the fluid in the shell at $t=0$ is dyed red so that $V(t)$ is the volume of red fluid still in the shell at t. As $t\to\infty$ the red fluid leaves through a shrinking spherical cap centered on the pole $\alpha=4\pi a^2$. This process is illustrated in Fig. 1(a). In fact, solving $t=T(\hat{\psi})$ gives the stream surface whose intersection with the outer spherical shell instantaneously defines this cap through which the red fluid is exiting [see Fig. 1(b)]. Thus at $t\gg a/U$ all of the red fluid that remains in the shell is contained in the region between the stream surface $\hat{\psi}=2\pi^3a^4/3Ut^2$ and the solid sphere $r=a$. The area of the cap [the curve AB in Fig. 1(b)] is $4\pi^3a^6/9(U\epsilon t)^2$. The velocity perpendicular to the cap is approximately $3U\epsilon^2/2a^2$ so that the flux of red fluid out of the shell is

$$f(t)=-\frac{dV}{dt}=\frac{2\pi^3a^4}{3Ut^2} . \tag{13}$$

Integrating the relation above we find the amount of red fluid that remains in the shell as $t\to\infty$ is

$$V(t)\approx 2\pi^3a^4/3Ut . \tag{14}$$

With Eq. (14) we return to Eqs. (6) and (7) and obtain the asymptotic approximation in Eq. (1).

When the tracer is diffusive the expression for the correlation function in Eq. (7) is still valid but the calculation of $V(t)$ must be modified to allow for the diffusive escape of fluid from the shell. This requires the solution of the local approximation of the advection–diffusion equation for flow around a sphere:

$$C_t + \dot{s}C_s + \dot{\alpha}C_\alpha = D_{\rm mol}C_{ss}, \quad (15)$$

where $\dot{s}$ and $\dot{\alpha}$ are given in Eq. (10). This equation must be solved with the initial condition $C(\alpha,s,0) = 1$ in the shell $0 \leqslant s \leqslant \epsilon$, and an absorbing boundary condition $C(\alpha,\epsilon,t) = 0$. Then the function $V(t)$ in Eq. (7) is

$$V(t) = \int C\,dV, \quad (16)$$

where the integral is over the volume of the shell. Our earlier calculation of this quantity has avoided explicit solution of this partial differential equation by ignoring molecular diffusivity and evaluating the advective flux of tracer at the boundary of the shell. And, again ignoring molecular diffusivity, Koch and Brady[3] explicitly solve (15) using the method of characteristics. A solution of the diffusive case is difficult, but might be possible using the transformations discussed by Acrivos and Goddard.[9] Fortunately, if only the leading-order approximation in Eq. (5) is needed, then only well-known scalings for advection–diffusion near a solid wall[3,8,9] are required. These indicate that our earlier calculation, Eq. (14), based on purely advective evacuation of the shell, is accurate provided that the inequality in Eq. (1) is satisfied. When $t \sim P_e^{1/3}a/U$, diffusion across streamlines becomes important and accelerates the escape of tracer from the shell so that $V(t)$ decays exponentially. To leading order, Eq. (5), this is accounted for by stopping the integration in Eq. (3) when $t \sim P_e^{1/3}a/U$.

As an embellishment we turn to a simple model of heterogeneity by supposing that the solid spheres have different sizes. Denote the number of spheres per volume with radius in the interval $(a,a+da)$ by $\mathcal{N}(a)da$. Thus the volume fraction of solid is

$$\phi = \int_0^\infty \frac{4\pi a^3}{3}\mathcal{N}(a)da. \quad (17)$$

The preceding argument is easily generalized to include this complication. We consider a large volume $\mathcal{V}$ containing

$$S = \mathcal{V}\int_0^\infty \mathcal{N}(a)da \quad (18)$$

spheres and N molecules of tracer. If a_i is the radius of the ith sphere and this sphere is surrounded by a shell of thickness ϵ_i, then the generalization of Eq. (7) is

$$\mathscr{C}(t) = \frac{U^2}{\mathcal{V}}\sum_{i=1}^{i=S} V_i(t), \quad (19)$$

where V_i is the volume of fluid initially in the ith shell that remains in this shell at t. Now from Eq. (14) we have the generalization of (1),

$$\mathscr{C}(t) \approx \frac{2\pi^3 U}{3t\mathcal{V}}\sum_{i=1}^{i=S} a_i^4 = \frac{\pi^2\phi U}{2t}\frac{\int_0^\infty a^4\mathcal{N}(a)da}{\int_0^\infty a^3\mathcal{N}(a)da}. \quad (20)$$

This result is analogous to one found by Koch and Brady[10] using a different model of heterogeneity. They consider D'arcy flow through a porous medium with weak spherically symmetric fluctuations in permeability. As in Eq. (20), their final expression for an effective diffusivity is proportional to a fourth moment of number density. If this density decays slowly

$$\mathcal{N}(a) \sim a^{-4-\gamma} \quad \text{as } a\to\infty, \quad \text{where } 0<\gamma\leqslant 1, \quad (21)$$

then the integral in the numerator of Eq. (20) diverges and our calculation of the correlation function must be modified to circumvent this infinity. [Note that Eq. (21) gives only the large a behavior of $\mathcal{N}(a)$. In order to avoid a divergent expression for the inverse permeability we suppose that there is a cutoff at some small a.]

We conclude with a scaling argument along the lines of Bouchaud and Georges,[11] which shows that the expression in Eq. (20) is convergent and in fact $\mathscr{C}(t) \sim t^{-\gamma}$. The key observation is that in the volume occupied by the tracer there is a largest sphere with radius $a_{\max}$ so that there is an effective upper limit to the integral in the numerator of Eq. (20). This gives $\mathscr{C}(t) \sim t^{-1}a_{\max}^{1-\gamma}$; $a_{\max}$ is increasing as the tracer encounters even larger spheres and samples the tail of the distribution. Dimensional consistency gives $a_{\max} \sim Ut$ so that $\mathscr{C}(t) \sim t^{-\gamma}$.

ACKNOWLEDGMENTS

We thank Andrew Woods and Yves Pomeau for several useful suggestions.

This research was supported by the National Science Foundation.

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