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Heat and mass transport in random velocity fields with application to dispersion in porous media

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Abstract. The effective equations describing the transport of a Brownian passive tracer in a random velocity field are derived, assuming that the lengthscales and timescales on which the transport process takes place are much larger than the scales of variations in the velocity field. The effective equations are obtained by applying the method of homogenization, that is a multiple-scale perturbative analysis in terms of the small ratio ϵ between the characteristic micro- and macro-lengthscales. After expanding the dependent variable and both space and time gradients in terms of ϵ, equating coefficients of like powers of ϵ yields expressions to determine the dependent variable up to any order of approximation. Finally, a Fickian constitutive relation is determined, where the effective transport coefficients are expressed in terms of the ensemble properties of the velocity field. Our results are applied to the transport of passive tracers in the stationary flow field generated in dilute fixed beds of randomly distributed spheroids, finding the effective diffusivity as a function of the spheroid eccentricity. Our result generalizes the expression of Koch and Brady (1985), who considered spherical inclusions, and is readily applied to the cases of random beds of slender fibers and flat disks.

1. Introduction

In many natural and industrial settings it is often important to control the transport of passive scalar species, such as heat and mass, in random velocity fields. For example, when operating a packed bed reactor we want to maximize the overall mixing of the reacting species, while, on the other hand, when managing a landfill we want to minimize it. At first it would seem that, due to the complexity of the velocity field, the study of such processes is a hopeless endeavor. Our primary interest, however, is not the detailed knowledge of the microscale process, but rather its description on a coarse scale, that is on length- and time-scales that are much larger than the scales of variations of the velocity field. In fact, we expect that the macroscale transport process will be described through an effective-medium equation, with the effective parameters (such as the effective diffusivity or thermal conductivity) depending on the global characteristics of the microscale velocity field.

In this work, the effective equations will be determined by using the method of homogenization, that is a multiple-scale perturbative analysis in terms of the small ratio ϵ between the characteristic micro- and macro-lengthscales. The method of homogenization was first proposed in 1978 by Bensoussan, Lions and Papanicolaou [1], and was later extended in a series of books [2–4] and articles (see, for example, [5–11]). In this method, the dependent variable(s) of the problem is assumed to be expressible as a regular expansion in terms of a small parameter ϵ, equal to the ratio of the microscale to macroscale characteristic lengths. Finally the effective equation, which is satisfied by the leading-order term of that expansion, is expected to arise naturally from the ensuing regular perturbation analysis. Therefore the method of homogenization seems to be unsuitable to determine terms in the effective equation that are not of leading order, and which are often of the greatest interest.

Consider, for example, the transport of Brownian solute particles in a fluid flow field. Assuming that at the microscale the diffusive and convective timescales are of the same magnitude (see Section 2), at the macroscale convection will dominate diffusion. The method of homogenization, therefore, will determine only the convective term in the effective equation, while the more interesting $0(\epsilon)$ diffusion term is neglected and cannot be determined.

Sometimes the $O(\epsilon)$-term in the effective equation can be determined by using an artifice. For example, the effective diffusivity of a passive Brownian tracer convected in a flow field can be found using homogenization by simply 'knocking out' the convective term, that is formulating the problem in a reference frame that moves at the same speed as the average fluid velocity [1]. However, it is easy to realize [12, 13] that this stratagem cannot be applied when higher-order terms of the effective equation are sought after or when the dependent variables of the problem are tensors, such as velocity and deformation.

In the present article we propose a modification of the homogenization scheme that allows to remove these limitations and determine the effective equations of composite materials or suspensions up to *any* degree of approximation. This method is applied to the transport of Brownian solute particles convected by a random flow field. Eventually, a Fickian constitutive relation is derived, where the steady mass flux equals the product of the concentration gradient times an effective diffusivity tensor which, in its turn, is expressed in terms of the microscale characteristics of the velocity field. Finally, our results are applied to the transport of passive tracers in the stationary flow field generated by a random distribution of spheroids in dilute fixed beds, finding the effective diffusivity as a function of the spheroid eccentricity.

2. Formulation of the sample problem

Consider the convection of Brownian passive tracers in a random incompressible velocity field $\mathbf{v}$ which is statistically homogeneous and infinitely extended. Neglecting all interactions between the tracer particles, the conservation equation for the solute concentration $c(\mathbf{R}, \tau)$ at location $\mathbf{R}$ and time τ may be written as

$$\frac{\partial c}{\partial \tau} + \nabla \cdot (\mathbf{v}c) - D\nabla^2 c = 0 , \tag{1}$$

where D is the diffusion coefficient of the tracers, supplemented by the initial condition $c(\mathbf{R}, \tau) = c_0(\mathbf{R})$ at $\tau = 0$. Here the velocity field satisfies

$$\langle \mathbf{v}(\mathbf{R}, \tau) \rangle = \mathbf{V}; \qquad \nabla \cdot \mathbf{v} = 0 ,$$

where the bracket, $\langle A \rangle$, and, identically, the overbar $\bar{A}$ indicate the ensemble average of any quantity $A(\mathbf{R}, \tau)$ over an ensemble of velocity fields. Moreover, we shall assume that the correlation function

$$R_{ij}(\mathbf{R}, \tau) = \langle v_i(\mathbf{R}_1 + \mathbf{R}, \tau_1 + \tau) v_j(\mathbf{R}_1, \tau_1) \rangle$$

decays over a characteristic length l and time $\tau_d = l^2/D$.

The geometry of the problem is characterized by the two lengthscales l and L, indicating a typical correlation length of the velocity field and a characteristic linear dimension of the macroscale, respectively. Throughout this analysis we denote by $\epsilon = l/L \ll 1$ a small parameter, essential for the perturbation analysis that follows.

Now consider the local Peclet number $Pe = lV/D$, with V denoting a typical value of the fluid velocity; Pe is defined as the ratio between the timescales $\tau_c = l/V$ and $\tau_d = l^2/D$, characterizing convection and diffusion at the microscale, respectively. The analogous global Peclet number Pe_L is defined in terms of the macroscopic length L, so that $Pe_L = 0(\epsilon^{-1} Pe)$. As we will see, the most general case arises when convection and diffusion balance each other at the microscale, that is when $Pe = O(1)$, so that $Pe_L = O(\epsilon^{-1})$, i.e. convection dominates diffusion at the macroscale.

3. The method of homogenization

The homogenization procedure [1] can be summarized as a three-stage 'recipe'. In the first stage, each physical quantity is assumed to be representable by a locally random function, that is to depend separately on the macroscopic position vector $\mathbf{R}$, with $|\mathbf{R}| = O(L)$, and on the stretched coordinate $\mathbf{r} = \epsilon\mathbf{R}$, with $|\mathbf{r}| = O(l)$, in such a way that any function $f(\mathbf{r})$ is stationary random. In the second stage, all quantities, as well as their space derivatives, are expanded as regular perturbations of the small parameter ϵ. Finally, in the third stage, coefficients of like powers of ϵ are equated, producing a set of boundary value problems to determine the effective coefficients appearing in the final, effective equation. Throughout this procedure, the time variable does not play any role; in fact, it is scaled out of the problem.

In this work, we follow the guidelines that are sketched above, but with the difference that time, too, is homogenized. In fact, four timescales are easily identifiable, namely τ_c, $\tau_d = O(\tau_c)$, $\tau_C = L/V = \tau_c/\epsilon$ and $\tau_D = L^2/D = \tau_d/\epsilon^2$, characterizing convection and diffusion at the micro- and macro-scale, respectively. Therefore, we assume that each physical quantity depends separately on these time coordinates.

Now, in the first stage of homogenization, scaling the time and space variables according to

$$\mathbf{x} = \mathbf{R}/L, \ \mathbf{y} = \mathbf{r}/l, \qquad t = \tau/\tau_d, \ T_1 = \tau/\tau_C, \qquad T_2 = \tau/\tau_D , \tag{2}$$

we have:

$$c = c(\epsilon, \mathbf{x}, \mathbf{y}, t, T_1, T_2), \qquad \mathbf{v} = \mathbf{v}(\mathbf{y}, t), \qquad c_0 = c_0(\mathbf{x}, \mathbf{y}) . \tag{3}$$

Note that since $\mathbf{v}$ represents the stationary random velocity field, it depends on $\mathbf{y}$ and t only.

In the second stage of the method of homogenization we expand the space gradient, the time derivative, and the dependent variable c in terms of ϵ, i.e.

$$L\nabla = \nabla_x + \epsilon^{-1}\nabla_y; \qquad \frac{L^2}{D}\frac{\partial}{\partial\tau} = \frac{\partial}{\partial T_2} + \epsilon^{-1}\frac{\partial}{\partial T_1} + \epsilon^{-2}\frac{\partial}{\partial t}, \tag{4a, b}$$

and

$$c(\epsilon, \mathbf{x}, \mathbf{y}, T_2, T_1, t) = \sum_{n=0}^{\infty} \epsilon^n c^{(n)}(\mathbf{x}, \mathbf{y}, T_2, T_1, t) , \tag{5}$$

where each term $c^{(n)}$ in the uniformly valid expansion (5) is assumed to be locally ergodic [14, 15], that is expressible as the product of an ergodic, $\mathbf{y}, t$-dependent function by an $\mathbf{x}, T_1, T_2$-dependent part; in addition, the $c^{(n)}$ functions for $n \neq 0$ are defined only within a certain degree of arbitrariness that will be removed later.

Substituting (4) into (1) we obtain the governing equation,

$$\left(\frac{\partial}{\partial T_2} + \epsilon^{-1}\frac{\partial}{\partial T_1} + \epsilon^{-2}\frac{\partial}{\partial t}\right)c + \epsilon^{-1} Pe\,(\nabla_x + \epsilon^{-1}\nabla_y)\cdot(\mathbf{u}c) = (\nabla_x + \epsilon^{-1}\nabla_y)^2 c , \tag{6}$$

with $\mathbf{u} = \mathbf{v}/V$ an $O(1)$ quantity, to be solved with initial condition $c = c_0(\mathbf{x}, \mathbf{y})$ at $T_2 = T_1 = t = 0$.

4. Derivation of the effective equation

In this Section we carry out the third stage of the homogenization procedure, namely we substitute the expansion (5) for the concentration into the governing equation (6), and we collect equal powers of ϵ. At leading, $O(\epsilon^{-2})$ order we obtain:

$$\partial c^{(0)}/\partial t + Pe\,\nabla_y\cdot(\mathbf{u}c^{(0)}) - \nabla_y^2 c^{(0)} = 0 , \tag{7}$$

whose trivial solution is

$$c^{(0)} = c^{(0)}(\mathbf{x}, T_2, T_1) . \tag{8}$$

Now, considering that we want the macroscopic behavior of the system to be described by $c^{(0)}$, we can remove the arbitrariness in the definition (5) of the $c^{(n)}$-functions by imposing $c^{(0)} = \bar{c}$, which means

$$\langle c^{(n)}\rangle = \bar{c}\delta_{n,0} . \tag{9}$$

Although the condition (9) is not unique, it is the most logical and it simplifies our results, as will be shown later.

At the next, $O(\epsilon^{-1})$ order of equation (6) we obtain,

$$\frac{\partial c^{(1)}}{\partial t} + Pe\,\nabla_y\cdot(\mathbf{u}c^{(1)}) - \nabla_y^2 c^{(1)} = -\frac{\partial c^{(0)}}{\partial T_1} - Pe\,\mathbf{u}\cdot\nabla_x c^{(0)} + 2\nabla_x\cdot\nabla_y c^{(0)} , \tag{10}$$

in which the last term on the RHS is identically zero, in agreement with equation (8). Now we impose that equation (10) is solvable, that is the ensemble averages of its LHS and RHS are identically equal to each other. Considering that $c^{(1)}$ is locally random, we find:

$$\frac{\partial c^{(0)}}{\partial T_1} = -Pe\,\mathbf{u}^*\cdot\nabla_x c^{(0)} , \tag{11}$$

where

$$\mathbf{u}^* = \langle \mathbf{u} \rangle \tag{12}$$

is the effective solute velocity.

Now we look for solutions of equation (10) of the form,

$$c^{(1)}(\mathbf{x}, \mathbf{y}, T_2, T_1, t) = \mathbf{X}(\mathbf{y}, t) \cdot \nabla_{\mathbf{x}} c^{(0)}(\mathbf{x}, T_1, T_2) , \tag{13}$$

which is analogous to Taylor's asymptotic expansion [16]. Substituting (13) into (10), we see that equation (10) is identically satisfied, provided that the random vector function $\mathbf{X}(\mathbf{y}, t)$ is the solution of the following cell problem:

$$\partial \mathbf{X} / \partial t + \nabla_{\mathbf{y}} \cdot (Pe\, \mathbf{u}\mathbf{X} - \nabla_{\mathbf{y}} \mathbf{X}) = -Pe\, (\mathbf{u} - \bar{\mathbf{u}}) . \tag{14}$$

Since the vector function $\mathbf{X}(\mathbf{y}, t)$ in equation (14) is determined only within an arbitrary additive constant vector, we may assume the normalization condition

$$\langle \mathbf{X} \rangle = \mathbf{0} , \tag{15}$$

which is equivalent to (9) with $n = 1$.

At $O(1)$, we obtain:

$$\frac{\partial c^{(0)}}{\partial t} + Pe\, \nabla_{\mathbf{y}} \cdot (\mathbf{u} c^{(2)}) - \nabla_{\mathbf{y}}^2 c^{(2)} = -\frac{\partial c^{(0)}}{\partial T_2} - \frac{\partial c^{(1)}}{\partial T_1} - Pe\, \mathbf{u} \cdot \nabla_{\mathbf{x}} c^{(1)} + 2 \nabla_{\mathbf{x}} \cdot \nabla_{\mathbf{y}} c^{(1)} + \nabla_{\mathbf{x}}^2 c^{(0)} .$$

Now we apply the solvability condition to this equation and, considering that $c^{(2)}$ is locally random, substitution of (14) and (15) yields

$$\frac{\partial c^{(0)}}{\partial T_2} = \mathbf{q}^* : \nabla_{\mathbf{x}} \nabla_{\mathbf{x}} c^{(0)} , \tag{16}$$

where the non-dimensional effective diffusivity dyadic $\mathbf{q}^*$ is given by the following expression:

$$\mathbf{q}^* = \mathbf{I} - Pe \langle \mathbf{u}' \mathbf{X} \rangle , \tag{17}$$

with $\mathbf{u}' = \mathbf{u} - \bar{\mathbf{u}}$ denoting the fluctuation of the velocity field about its mean value.

Now we can characterize the transport of the solute particles by substituting the $O(\epsilon^{-1})$ convective term $\partial c^{(0)} / \partial T_1$ of equation (11) and the $O(1)$ diffusive term $\partial c^{(0)} / \partial T_2$ of equation (16) into (4b), finding the following effective equation in dimensional form

$$\frac{\partial \bar{c}}{\partial \tau} + \nabla_{\mathbf{R}} \cdot \bar{\mathbf{J}} = 0 , \tag{18a}$$

with

$$\bar{\mathbf{J}} = \bar{\mathbf{v}} \bar{c} - \mathbf{D}^* \cdot \nabla_{\mathbf{R}} \bar{c} , \tag{18b}$$

where $\mathbf{D}^* = D\mathbf{q}^*$. This equation is coupled with the effective initial condition $\bar{c}(\mathbf{R}, \tau = 0) = \langle c_0(\mathbf{x}, \mathbf{y}) \rangle$, which can be easily obtained from (9).

Here we should stress an intrinsic limitation of our method, namely that space and time in the effective equation (18) are spanned through the macroscopic lengthscale L and timescale L^2/D, respectively, which are assumed to be much larger than their microscopic counterparts. In fact, whenever the macroscopic lengthscale is not sufficiently large as when, for example, the correlation length l diverges, then anomalous diffusion takes place, that is the mean square displacement of a tracer particle grows faster (or slower) than linearly with time [17]. However in this case, since there is no separation of scales, the method of homogenization cannot be applied.

The expression (17) for the effective diffusivity is well known [7] for the case of a spatially periodic configuration, where the ensemble average is replaced by a volume average over the unit cell of the periodic array; it was first obtained by Brenner [18], who, considering that only the symmetric part of $\mathbf{q}$ enters the effective equation (18), rewrote (17) as

$$q^*_{ij} = \delta_{ij} - \langle (\nabla_k X_i)(\nabla_k X_j) \rangle .$$

Alternatively, the solution of equation (14) can be expressed in terms of the Green function $P(\mathbf{y}, t)$ as

$$\mathbf{X}(\mathbf{y}, t) = \int \mathrm{d}\mathbf{y}' \int \mathrm{d}t' \, P(\mathbf{y} - \mathbf{y}', t - t') \, \mathbf{u}'(\mathbf{y}', t') \, , \tag{19}$$

where $P(\mathbf{y}, t)$ satisfies the equation

$$\partial P / \partial t + \nabla_{\mathbf{y}} \cdot (Pe \, \mathbf{u} P - \nabla_{\mathbf{y}} P) = Pe \, \delta(\mathbf{y}) \delta(t) \, . \tag{20}$$

Therefore the effective diffusivity $\mathbf{q}^*$ in (17) can be rewritten as

$$\mathbf{q}^* = \mathbf{I} + Pe \int \mathrm{d}t \, \mathbf{R}(t) \, , \tag{21}$$

where

$$\mathbf{R}(t - t') = \int \mathrm{d}\mathbf{y}' \langle \mathbf{u}'(\mathbf{y}', t') P(\mathbf{y} - \mathbf{y}', t - t') \mathbf{u}'(\mathbf{y}, t) \rangle \tag{22}$$

is the average covariance of the fluid velocities at the points occupied by a Brownian tracer at the times $t > t'$ and t' [19]. Equation (21) coincides with Saffman's result [20]. When Pe is very large, the dispersion of the Brownian tracer coincides with that of the fluid particles. In fact, as $Pe \to \infty$, the solution of the advection equation (20) is

$$P(\mathbf{y} - \mathbf{y}', t - t') = \delta[\mathbf{y} - \mathbf{Y}(t \,|\, \mathbf{y}', t')] \, ,$$

where $\mathbf{Y}(t \,|\, \mathbf{y}', t')$ is the position at time t of a fluid particle that at time t' was located at $\mathbf{y}'$. Therefore the covariance $\mathbf{R}$ in (22) reduces to the Lagrangian velocity autocorrelation function,

$$\mathbf{R}(t - t') = \langle \mathbf{u}'(\mathbf{y}', t') \mathbf{u}'(\mathbf{Y}, t) \rangle \, , \tag{23}$$

and $\mathbf{q}^*$ now coincides with the effective eddy diffusivity [21–23].

An important feature of equation (21) is that it shows that for large Peclet numbers, as both P and $\mathbf{u}'$ are $O(1)$ quantities, the effective diffusivity is proportional to Pe. This result is consistent with the fact that the eddy diffusivity (i.e. $\mathbf{D}^*$ for $Pe \to \infty$) is proportional to Vl [19, 24].

5. Dispersion in fixed beds of randomly distributed spheroids

This is an extension of Koch and Brady's study [25] of the transport of a passive tracer in fixed beds composed of randomly distributed identical spheres. Here we assume that the bed is composed of a dilute suspension of identical spheroids fixed in space, randomly distributed and randomly oriented. Now, in the absence of convection, molecular diffusion is the only mechanism responsible for the transport of tracer particles, and the effective tracer diffusivity is a scalar which depends on the tracer molecular diffusivity and the distribution of the inclusions. However, when the fluid is convected through the fixed bed, the dispersion mechanism is mainly due to the convection of the tracer particles by the random velocity field generated at the microscale by the randomly-distributed inclusions. In this case, the effective tracer diffusivity can be determined by applying the results derived in the previous Section, namely equation (21) and (22), i.e.,

$$\mathbf{D}^* = D\mathbf{I} + \int d\mathbf{r}' \langle \mathbf{v}'(\mathbf{r}') P(\mathbf{r} - \mathbf{r}') \mathbf{v}'(\mathbf{r}) \rangle , \tag{24}$$

with P satisfying

$$\mathbf{v} \cdot \nabla P - D\nabla^2 P = \delta(\mathbf{r}) . \tag{25}$$

This expressions, which coincide with the results given by Koch and Brady [25], has been derived considering that the velocity field is stationary, as for any given configuration of the fixed bed the velocity field is time-independent. Since the transport process is ergodic, the ensemble average in (24) can be substituted by a volume average over a characteristic cell, obtaining

$$\mathbf{D}^* = D\mathbf{I} + \frac{1}{V_c} \int d\mathbf{r}_1 \int d\mathbf{r}_2 \, \mathbf{v}'(\mathbf{r}_1) P(r_1 - \mathbf{r}_2) \mathbf{v}'(\mathbf{r}_2) , \tag{26}$$

where V_c is the volume of the characteristic cell, $V_c = V_p/\phi$, with ϕ and V_p denoting the volume fraction and the volume of each spheroid, respectively.

The surface of a spheroid centered in the origin and with its symmetry axis pointing along the unit vector $\hat{\mathbf{n}}$ (see Fig. 1) is described by the equation,

$$[(\mathbf{r} \cdot \hat{\mathbf{n}})/a]^2 + [\mathbf{r} \cdot (\mathbf{I} - \hat{\mathbf{n}}\hat{\mathbf{n}})/b]^2 = 1 ,$$

where a and b are, respectively, the polar and equatorial radii, so that the spheroid volume is $V_p = \frac{4}{3}\pi a^2 b$. We will first consider the case where $a > b$, so that we deal with prolate spheroids; the case of oblate spheroids, with $a < b$, is analogous and we will only give the final result at the end of the paragraph. All geometric characteristics of the spheroids are described through their eccentricity e, defined as $e = [1 - (b/a)^2]^{1/2}$. In particular, the drag force exerted by the spheroid on a uniform fluid flow is [26, 27]

$$\mathbf{F} = -6\pi\mu a \mathbf{Z} \cdot \mathbf{V} , \tag{27}$$

where $\mathbf{V}$ is the unperturbed uniform velocity field, while $\mathbf{Z}$ is the drag dyadic,

$$\mathbf{Z} = Z_l \hat{\mathbf{n}}\hat{\mathbf{n}} + Z_t(\mathbf{I} - \hat{\mathbf{n}}\hat{\mathbf{n}}) , \tag{28}$$

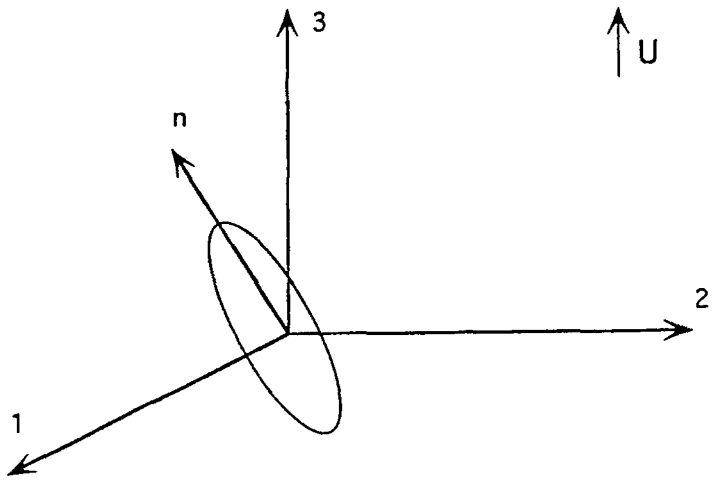

Fig. 1. Geometry of the problem.

where

$$Z_l = \frac{8}{3} e^3 \left[-2e + (e^2 + 1) \log \frac{1+e}{1-e} \right]^{-1}, \tag{29a}$$

$$Z_t = \frac{16}{3} e^3 \left[2e + (3e^2 - 1) \log \frac{1+e}{1-e} \right]^{-1}. \tag{29b}$$

Now, for small volume fractions ϕ of the bed particles, Hinch [28] showed that the velocity field $\mathbf{v}$ can be determined by holding one, randomly-oriented particle fixed at the origin $\mathbf{r} = \mathbf{0}$, while the effect of the other bed particles can be modelled in terms of a permeability coefficient in the Brinkman equations,

$$\nabla p + \frac{\mu}{\sigma} \mathbf{v} - \mu \nabla^2 \mathbf{v} = \mathbf{F} \delta(\mathbf{r}) + O(\phi), \tag{30a}$$

$$\nabla \cdot \mathbf{v} = 0. \tag{30b}$$

Here σ denotes the permeability of the bed which, in the dilute limit, equals the 'ratio' between the fluid velocity and the force per unit volume exerted on the fluid by the bed particles. In our case, considering that the spheroids are randomly oriented, $(\mu/\sigma) = 6\pi\mu a V_c^{-1} \zeta$, with $\zeta = \mathbf{Z}:\mathbf{I}/3$, that is

$$\sigma = \frac{2}{9} \frac{b^2}{\phi \zeta}. \tag{31}$$

In writing this expression we have implicitly considered that in the volume l^3, with $l = \sqrt{\sigma}$ denoting the Debye screening length, a large number of randomly oriented particles are included[1]. As noted by Koch and Brady [25, 29], although the term $(\mu/\sigma)\mathbf{v}$ is $O(\phi)$, it must be included in the momentum conservation equation (30a) even in the low-ϕ limit, since it has a large influence on the fluid velocity far from the fixed bed particle, allowing the convergence of the integral in equation (26). By modelling the porous particles in terms of

Stokeslets of strength $\mathbf{F}$ we introduce an $O(\phi)$ error in the subsequent analysis that can be neglected [25]. Since our unit cell is effectively infinitely extended, we can Fourier-transform the velocity field, defining

$$\hat{\mathbf{v}}(\tilde{\mathbf{k}}) = \int \mathbf{v}(\tilde{\mathbf{r}}) \exp(-i\tilde{\mathbf{k}} \cdot \tilde{\mathbf{r}})\, \mathrm{d}\tilde{\mathbf{r}}\,, \tag{32}$$

where $\tilde{\mathbf{r}} = \mathbf{r}/l$ and $\tilde{\mathbf{k}} = l\mathbf{k}$. Fourier-transforming Equations (30) we find:

$$\hat{\mathbf{v}}(\tilde{\mathbf{k}}) = -6\pi\lambda V[\mathbf{I} - \tilde{\mathbf{k}}\tilde{\mathbf{k}}/\tilde{k}^2] \cdot \mathbf{Z} \cdot \hat{\mathbf{1}}_3/(\tilde{k}^2 + 1)\,, \tag{33}$$

where $\lambda = a/\sqrt{\sigma}$, while $\hat{\mathbf{1}}_3$ is the unit vector along the direction of the unperturbed flow, i.e. $\mathbf{V} = V\hat{\mathbf{1}}_3$.

Now we evaluate $\hat{P}(\tilde{\mathbf{k}})$ from equation (25). Following Koch and Brady [25], we observe that at $0(l)$-distances, where the dominant contribution to the integral (26) occurs, the velocity disturbance is small, due to the Debye screening, so that $\mathbf{v} \approx \mathbf{V}$; consequently we find

$$\hat{P}(\tilde{\mathbf{k}}) = \frac{1}{V\sigma}\left(i\tilde{\mathbf{k}} \cdot \hat{\mathbf{1}}_3 + \frac{1}{Pe}\tilde{k}^2\right)^{-1}, \tag{34}$$

where $Pe = Vl/D$ is the Peclet number based on the screening length $l = \sqrt{\sigma}$. Equations (33) and (34) are now substituted into the expressions (26) for the effective diffusivity, which, after Fourier transforming, gives

$$\mathbf{D}^* = D\mathbf{I} + \frac{1}{V_c}\left[\frac{\sigma}{2\pi}\right]^3 \int \mathrm{d}^3\tilde{k} \langle \hat{\mathbf{v}}(-\tilde{\mathbf{k}})\hat{P}(\tilde{\mathbf{k}})\hat{\mathbf{v}}(\tilde{\mathbf{k}})\rangle_{\mathbf{n}}\,, \tag{35}$$

with $\langle \cdot \rangle_{\mathbf{n}}$ denoting the average over the (random) spheroid orientation. Finally, after some easy algebraic manipulations, (35) yields

$$\mathbf{D}^* = D\mathbf{I} + \frac{3Va}{\zeta}\frac{1}{(2\pi)^2}\int \mathrm{d}\tilde{\mathbf{k}} \left\langle \frac{[(\mathbf{I} - \tilde{\mathbf{k}}\tilde{\mathbf{k}}/k^2) \cdot \mathbf{Z} \cdot \hat{\mathbf{1}}_3]^2}{(\tilde{k}^2 + 1)^2(i\tilde{\mathbf{k}} \cdot \hat{\mathbf{1}}_3 + \tilde{k}^2/Pe)} \right\rangle_{\mathbf{n}}. \tag{36}$$

This integral can be solved when $Pe \gg 1$, giving, after a long but straightforward calculation,

$$\mathbf{D}^* = \frac{3Va}{4\zeta}\langle \tilde{Z}_1^2\hat{\mathbf{1}}_3\hat{\mathbf{1}}_3 + \tilde{Z}_2^2(\tfrac{19}{8}\hat{\mathbf{1}}_1\hat{\mathbf{1}}_1 + \tfrac{1}{8}\hat{\mathbf{1}}_2\hat{\mathbf{1}}_2) + 3\tilde{Z}_1\tilde{Z}_2\hat{\mathbf{1}}_1\hat{\mathbf{1}}_3\rangle_{\mathbf{n}}\,, \tag{37}$$

where $\hat{\mathbf{1}}_1$ is a unit vector perpendicular to $\hat{\mathbf{1}}_3$ and laying in the plane of $\hat{\mathbf{1}}_3$ and $\hat{\mathbf{n}}$, so that $\hat{\mathbf{1}}_3 \times \hat{\mathbf{1}}_1 \cdot \hat{\mathbf{n}} = 0$, $\hat{\mathbf{1}}_2$ is a unit vector forming an orthogonal triad with $\hat{\mathbf{1}}_1$ and $\hat{\mathbf{1}}_3$, while $\tilde{Z}_1$ and $\tilde{Z}_2$ denote the following scalars,

$$\tilde{Z}_1 = Z_t - (Z_t - Z_l)\cos^2\alpha; \qquad \tilde{Z}_2 = -(Z_t - Z_l)\sin\alpha\cos\alpha\,, \tag{38}$$

with $\cos\alpha = \hat{\mathbf{n}} \cdot \hat{\mathbf{1}}_3$. Now, since the spheroid has a random orientation, averaging over all orientations gives:

$$\mathbf{D}^*/Va = D_l\hat{\mathbf{1}}_3\hat{\mathbf{1}}_3 + D_t(\mathbf{I} - \hat{\mathbf{1}}_3\hat{\mathbf{1}}_3)\,, \tag{39}$$

where

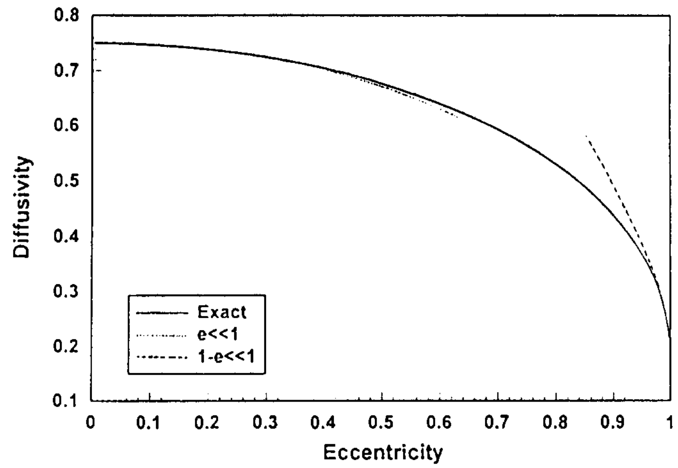

Fig. 2a. Longitudinal diffusivity in fixed beds of prolate spheroids as a function of the eccentricity.

$$D_l = \frac{3}{4\zeta}\left[\frac{1}{4}(Z_l + Z_t)^2 + \frac{1}{8}(Z_l - Z_t)^2\right], \tag{39a}$$

$$D_t = \frac{15}{128\zeta}(Z_l - Z_t)^2 . \tag{39b}$$

In Figs. 2a and 2b the values of the effective dispersion coefficients D_l and D_t are displayed as functions of the eccentricity e. Now consider the two limit cases where $e \ll 1$ and $1 - e \ll 1$. First, for the case of slightly deformed spheres, when $e \ll 1$, we have [27]

$$Z_l = 1 - \frac{2}{5}e^2 - \frac{17}{175}e^4 + O(e^6); \qquad Z_t = 1 - \frac{3}{10}e^2 - \frac{57}{700}e^4 + O(e^6),$$

leading to the following values of D_l and D_t:

$$D_l = \frac{3}{4}\left[1 - \frac{11}{30}e^2 - \frac{37}{168}e^4\right] + O(e^6); \qquad D_t = \frac{3}{2560}e^4 + O(e^6). \tag{40}$$

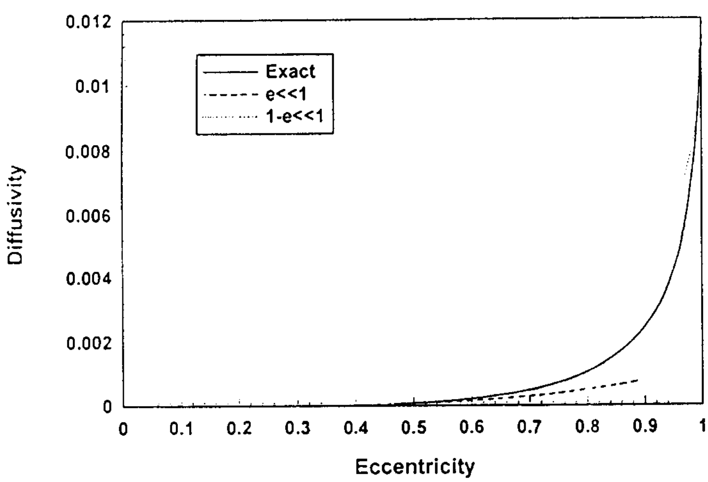

Fig. 2b. Transversal diffusivity in fixed beds of prolate spheroids as a function of the eccentricity.

Clearly, this result generalizes that of Koch and Brady [25] for a dilute fixed bed of spheres, when $e = 0$. On the other extreme, when the bed particles are slender bodies, i.e. $1 - e \ll 1$, we have:

$$Z_l = \frac{2}{3(\xi - 1/2)}; \qquad Z_t = \frac{4}{3(\xi + 1/2)},$$

where $\xi = \log(2a/b)$, so that we find:

$$D_l = \frac{3}{16}\frac{19\xi^2 - 9\xi + 11/4}{(5\xi - 3/2)(\xi^2 - 1/4)}; \qquad D_t = \frac{15}{64}\frac{(\xi - 3/2)^2}{(5\xi - 3/2)(\xi^2 - 1/4)}. \tag{41}$$

Note that at leading order this gives

$$\mathbf{D}^*/Va = \frac{3}{320\log(a/b)}[76\,\hat{\mathbf{1}}_3\hat{\mathbf{1}}_3 + 5(\mathbf{I} - \hat{\mathbf{1}}_3\hat{\mathbf{1}}_3)], \tag{41a}$$

showing that when $a \ll b$, $\mathbf{D}^*/Va$ tends to zero. This result is not obvious from Fig. 2, since D_l and D_t start to approach zero for values of $1 - e$ smaller than 0.001.

The case of oblate spheroids can be treated in the same way, finding again equation (39), with a denoting the longest, i.e. equatorial, radius of the spheroid, while the expression for Z_l and Z_t can be found in Happel and Brenner [26]. Figs. 3a and 3b show the value of the effective dispersivities D_l and D_t as a function of the eccentricity. In particular, when $e \ll 1$, i.e. the bed inclusions are slightly deformed spheres, we find:

$$D_l = \frac{3}{4}\left[1 - \frac{2}{15}e^2 - \frac{1343}{25200}e^4\right] + O(e^6); \qquad D_t = \frac{3}{2560}e^4 + O(e^6). \tag{42}$$

On the other extreme, when $1 - e \ll 1$, i.e. for beds of flat disks, we obtain

$$D_l = \frac{51}{28\pi}\left[1 + \frac{128}{357\pi}\epsilon\right] + O(\epsilon^2); \qquad D_t = \frac{5}{112\pi}\left[1 - \frac{256}{21\pi}\epsilon\right] + O(\epsilon^2), \tag{43}$$

where $\epsilon = (1 - e^2)^{1/2}$, so that at leading order we have

$$\mathbf{D}^*/Va = \frac{1}{112\pi}[204\,\hat{\mathbf{1}}_3\hat{\mathbf{1}}_3 + 5(\mathbf{I} - \hat{\mathbf{1}}_3\hat{\mathbf{1}}_3)]. \tag{43a}$$

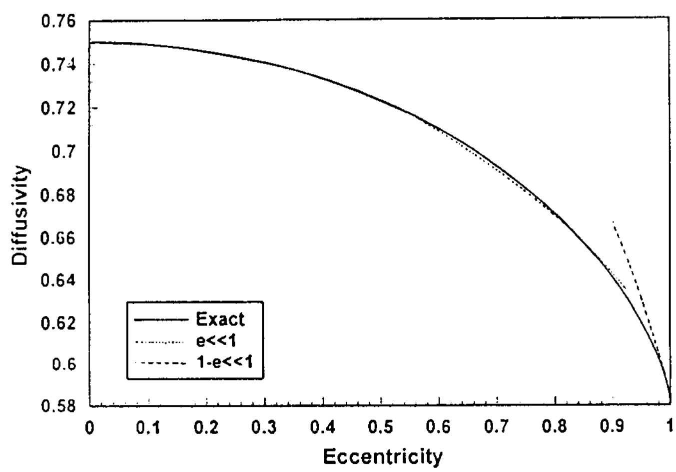

Fig. 3a. Longitudinal diffusivity in fixed beds of oblate spheroids as a function of the eccentricity.

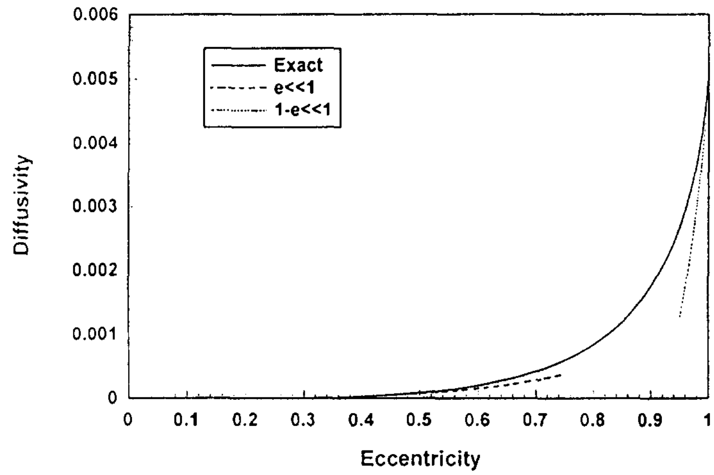

Fig. 3b. Transversal diffusivity in fixed beds of oblate spheroids as a function of the eccentricity.

6. Conclusions and final remarks

In this article we derived the effective transport equation of a Brownian passive tracer immersed in a random velocity field. This equation contains a convective and a diffusive term, which are expressed in terms of an average tracer velocity and an effective tracer diffusivity, respectively. The convective term, which is often much larger than the diffusive one, has a very predictable form, i.e. the mean tracer velocity equals the mean fluid velocity, and it can be accounted for by re-formulating the problem in a moving reference frame. On the other hand, the diffusive term is physically very interesting, with the effective diffusivity tensor given as a quadrature in terms of the fluid velocity random field. As an important example of application of our results, we studied the transport of Brownian solute particles convected through a dilute fixed bed of randomly distributed spheroids at high Peclet numbers. The main result of our work is equation (39), where the effective diffusivity tensor $\mathbf{D}^*$ is expressed as the product of the mean fluid velocity, the largest radius of the spheroids, and a non-dimensional function of the spheroid eccentricity. The two limit cases when the spheroids reduce to slender fibers and flat disks are particularly interesting, showing that [cf. Equations (41) and (43)] the effective diffusivity in the first case tends to zero, while in the second case it tends to a constant tensor. Finally, our results show that, unlike the case of spherical inclusions [25], where $\mathbf{D}^*$ has only the longitudinal component, in our case $\mathbf{D}^*$ does have a transversal component as well. In fact, keeping in mind the Lagrangian definition of the effective diffusivity tensor, $\mathbf{D}^* = \frac{1}{2}\, \mathrm{d}/\mathrm{d}t\, \langle (\mathbf{R} - \langle \mathbf{R} \rangle)^2 \rangle$, with $\mathbf{R} = \mathbf{R}(t)$ denoting the position of a tracer particle, we expect indeed that $\mathbf{D}^*$ should have both a longitudinal and a transversal component, since each 'collision' of the tracer with a spheroidal bed particle determines a transversal as well as longitudinal displacement. On the other hand, in the case of spherical bed particles, after each 'collision' the transversal net displacement of the tracer is identically zero, so that $\mathbf{D}^*$ will have only a longitudinal component.

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Note

[1]This condition is satisfied whenever $\sqrt{\phi} \ll b/a$.

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