Eddy diffusivities in scalar transport

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Standard and anomalous transport in incompressible flow is investigated using multiscale techniques. Eddy diffusivities emerge from the multiscale analysis through the solution of an auxiliary equation. From the latter it is derived an upper bound to eddy diffusivities, valid for both static and time-dependent flow. The auxiliary problem is solved by a perturbative expansion in powers of the Péclet number resummed by Padé approximants and a conjugate gradient method. The results are compared to numerical simulations of tracers dispersion for three flows having different properties of Lagrangian chaos. It is shown on a concrete example how the presence of anomalous diffusion in deterministic flows can be revealed from the singular behavior of the eddy diffusivity at very small molecular diffusivities. © *1995 American Institute of Physics.*

I. INTRODUCTION

The problem of passive scalars diffusion in incompressible velocity fields has a theoretical and practical importance in many fields of science and engineering, ranging from mass and heat transport in geophysical flows to chemical engineering and combustion.[1] The main interest is in the understanding of the mechanisms leading to transport enhancement. Taking into account the molecular diffusion, the motion of a fluid element can be described by the following Langevin equation:

$$\frac{d\mathbf{x}}{dt} = \mathbf{v}(\mathbf{x},t) + \boldsymbol{\eta}(t), \tag{1}$$

where $\mathbf{v}(\mathbf{x},t)$ is the Eulerian incompressible velocity field at position $\mathbf{x}$ and time t, and $\boldsymbol{\eta}$ is a Gaussian white noise with zero mean and correlation function

$$\langle \eta_i(t)\eta_j(t')\rangle = 2D_0\delta_{ij}\delta(t-t'). \tag{2}$$

The coefficient D_0 is the (bare) molecular diffusivity. If $\theta(\mathbf{x},t)$ denotes the concentration of tracers, the Fokker–Planck equation[2] associated to (1) is

$$\partial_t\theta + (\mathbf{v}\cdot\boldsymbol{\partial})\theta = D_0\partial^2\theta. \tag{3}$$

The incompressibility condition $\boldsymbol{\partial}\cdot\mathbf{v}=0$ is explicitly used in (3). Our interest will be mainly concentrated on the long-time behavior of (3). For time scales much longer than the characteristic microscopic time, the evolution of $\theta(\mathbf{x},t)$ is dominated by long-wave disturbances. The equation for these slow modes can be obtained by the usual "hydrodynamic" analysis[3]

$$\partial_t\langle\theta\rangle = D_{ij}^E\frac{\partial^2}{\partial x_i\partial x_j}\langle\theta\rangle + \cdots, \quad i,j=1,\ldots,d, \tag{4}$$

where $\langle\theta\rangle$ is the concentration field averaged locally over a volume of linear dimensions much larger than the typical length l of the velocity field and d is the space dimension. The corrections in (4) involve terms containing at least three derivatives of $\langle\theta\rangle$, which can be neglected in the weak gradients limit $|\boldsymbol{\partial}\langle\theta\rangle|/\langle\theta\rangle\ll l^{-1}$. Equation (4) then reduces to a diffusion equation, with an effective diffusion tensor D_{ij}^E (the eddy-diffusivity tensor). The latter has a direct practical importance since it measures the spreading for very long times of a spot of tracers:

$$D_{ij}^E = \lim_{t\to\infty}\frac{1}{2t}\langle(x_i(t)-\langle x_i\rangle)(x_j(t)-\langle x_j\rangle)\rangle,$$

$$i,j=1,\ldots,d. \tag{5}$$

where $\mathbf{x}(t)$ is the position of a tracer at time t and the average is taken over the initial positions or, equivalently, over an ensemble of test particles. Note that the existence of the limit in (5) ensures that the transport is a standard diffusion process, at least for a very large time. This is the typical situation, but there are also cases showing the so-called anomalous diffusion: the spreading of particles does not vary linearly with time but as a power law t^γ, with $\gamma\neq1$ (where $\gamma>1$ and $\gamma<1$ correspond to superdiffusive and subdiffusive behaviours, respectively). Transport anomalies indicate the presence of strong correlations in the dynamics, even at large time and space scales. An interesting possibility is the one discussed in Ref. 4. The flow is periodic, but the Lagrangian phase space is a complicated self-similar structure of islands and cantori. Particles are thus transported in a coherent way longer and longer as D_0 is decreased, finally leading to anomalous diffusion in the absence of any molecular diffusion.

The aim of this paper is using multiscale techniques[5] to study standard and anomalous diffusion. The multiscale formalism is discussed in Sec. II, where the calculation of eddy diffusivities is reduced to the solution of an auxiliary equa-

tion. From the latter, upper and lower bounds for eddy diffusivities are derived in the general case of time-dependent flows. The calculation of the exact analytical expression of the eddy diffusivity for parallel flows and random flows δ-correlated in time is also reviewed. Random flows with a short correlation time are discussed more thoroughly in the Appendix. Numerical methods are generally needed to solve the auxiliary equation leading to the eddy-diffusivity tensor for a generic flow. Two possibilities are discussed in Sec. III. The first one is to perform a Padé resummation of the series expressing the eddy diffusivity in powers of the Péclet number. The second is the use of a conjugate gradient algorithm. Both methods are used in Sec. IV to analyze three flows having a standard diffusive transport (the ABC,[6,7,8] the BC, and a two-dimensional time-dependent flow). The results are compared to numerical simulations of tracers dispersion, i.e., numerical integrations of (1). The flows have been chosen since they can be considered as prototypes for three very different situations with respect to Lagrangian chaos,[9,10] i.e., the chaotic properties of the deterministic equation obtained from (1) suppressing the noise. If the latter equation is integrable, as for the BC flow, the diffusion process is expected to be strongly sensitive to the detailed geometric structure of the Eulerian field and to the presence of molecular diffusion. For a nonintegrable flow we expect a competition between coherent transport in the nonchaotic regions (which turns out to be dominant in the ABC flow) and random advection. The limiting case is the one of a strongly turbulent flow, like the time-dependent flow, where molecular transport can be ignored on a large range of scales and chaotic advection is dominant. The study of anomalous diffusion is presented in Sec. V, where the flow introduced in Ref. 4 is analyzed. A singular behavior of the eddy diffusivity at high Péclet numbers is shown to be a signature of anomalous transport. A reliable procedure for predicting the presence of anomalous diffusion is thus provided.

II. THE MULTISCALE TECHNIQUE

A powerful method for studying transport processes is the so-called multiscale technique (also known as homogenization[5]). The general idea is to exploit the scale separation in the dynamics. In the specific case of passive scalars the use of the technique was proposed in Ref. 11 and it is recalled here for the sake of completeness. Specifically, let $\mathbf{v}(\mathbf{x},t)$ be an incompressible velocity field, periodic both in space and time. (The technique can be extended to handle the case of a random, homogeneous, and stationary velocity field with some nontrivial modifications in the rigorous proofs of convergence.[12]) The scalar field $\theta(\mathbf{x},t)$ evolves according to the Fokker–Planck equation (3). The units are chosen in such a way that the periodicities of $\mathbf{v}$ are $O(1)$. Note that by a Galilean transformation one can always reduce to the case with zero mean flow. Assume the original velocity field be $\mathbf{v}(\mathbf{x},t)=\mathbf{u}(\mathbf{x},t)+\mathbf{U}$, where $\mathbf{U}$ is the mean velocity and $\mathbf{u}$ has zero mean. In the new frame of reference $\mathbf{x}'=\mathbf{x}-\mathbf{U}t$, the velocity field becomes $\mathbf{u}(\mathbf{x}'+\mathbf{U}t,t)$. In particular, a flow which is static in the original frame becomes time dependent, possibly leading to nontrivial transport effects.[13] We shall be interested in the dynamics of the field θ on *large* scales as-

sumed to be $O(1/\epsilon)$, where $\epsilon \ll 1$ is the parameter controlling the scale separation. Because we expect the scalar field to have a diffusive dynamics, the associated time scale is $O(1/\epsilon^2)$.

The presence of the small parameter ϵ naturally suggests to look for a perturbative approach. The perturbation is, however, singular[14] since a constant field is a trivial solution of (3). The origin of this phenomenon can be grasped in the following simple situation. Let the large-scale field have a single wave number ϵ. Because of the advection term in (3), a small-scale field $\tilde{\theta}$ is produced and the wave numbers spaced from those of $\mathbf{v}$ by multiples of ϵ are generally excited. The interaction between the latter modes and those of $\mathbf{v}$, due again to the advection term, is responsible for the transport coefficients renormalization. The essential shift of order ϵ in the wave numbers of $\tilde{\theta}$ with respect to those of $\mathbf{v}$ is missed by regular perturbation expansions. Asymptotic methods, like multiscale techniques, are thus needed.

In addition to the *fast* variables $\mathbf{x}$ and t, let us then introduce *slow* variables as $\mathbf{X}=\epsilon\mathbf{x}$ and $T=\epsilon^2 t$. The prescription of the technique is to treat the two sets of variables as independent. It follows that

$$\partial_i \mapsto \partial_i + \epsilon\nabla_i; \quad \partial_t \mapsto \partial_t + \epsilon^2\partial_T, \tag{6}$$

where ∂ and ∇ denote the derivatives with respect to fast and slow space variables, respectively. The solution is sought as a perturbative series

$$\theta(\mathbf{x},t;\mathbf{X},T)=\theta^{(0)}+\epsilon\theta^{(1)}+\epsilon^2\theta^{(2)}+\ldots, \tag{7}$$

where the functions $\theta^{(n)}$ depend *a priori* on both fast and slow variables. By inserting (7) and (6) into (3) and equating terms having equal powers in ϵ, we obtain a hierarchy of equations. The solutions of interest to us are those having the same periodicities as the velocity field. The first equation, corresponding to $O(\epsilon^0)$, is

$$\partial_t \theta^{(0)}+(\mathbf{v}\cdot\partial)\theta^{(0)}=D_0\partial^2\theta^{(0)}. \tag{8}$$

By using Poincaré inequality, one can show[15] that for periodic solutions

$$-\partial_t\int(\theta^{(0)})^2 dV=D_0\int(\partial\theta^{(0)})^2 dV$$

$$\geq D_0\left(\frac{2\pi}{L}\right)^2\int(\theta^{(0)})^2 dV, \tag{9}$$

where L is the spatial periodicity length of $\mathbf{v}$ (supposed for simplicity to be the same in all directions) and the integral is over the periodicity box. The inequality (9) implies that the solution will relax to a constant with respect to fast variables, i.e.,

$$\theta^{(0)}(\mathbf{x},t;\mathbf{X},T)=\theta^{(0)}(\mathbf{X},T). \tag{10}$$

It can be also easily checked that the transient has no effect on the large-scale dynamics. The equations at order ϵ and ϵ^2 are

$$\partial_t\theta^{(1)}+(\mathbf{v}\cdot\partial)\theta^{(1)}-D_0\partial^2\theta^{(1)}=-\mathbf{v}\cdot\nabla\theta^{(0)}, \tag{11}$$

$$\partial_t\theta^{(2)}+(\mathbf{v}\cdot\partial)\theta^{(2)}-D_0\partial^2\theta^{(2)}$$

$$=-\partial_T\theta^{(0)}-(\mathbf{v}\cdot\nabla)\theta^{(1)}+D_0\nabla^2\theta^{(0)}+2D_0\partial\cdot\nabla\theta^{(1)}. \tag{12}$$

Since Eq. (11) is linear, its solution can be written as

$$\theta^{(1)}(\mathbf{x},t;\mathbf{X},T) = \theta^{(1)}(\mathbf{X},T) + \mathbf{w}(\mathbf{x},t) \cdot \nabla \theta^{(0)}(\mathbf{X},T), \quad (13)$$

where the first term on the right-hand side (RHS) is a solution of the homogeneous equation and the vector field $\mathbf{w}$ has a vanishing average over the periodicities and satisfies

$$\partial_t \mathbf{w} + (\mathbf{v} \cdot \boldsymbol{\partial}) \mathbf{w} - D_0 \partial^2 \mathbf{w} = -\mathbf{v}. \quad (14)$$

Due to the incompressibility of the velocity field, the average over the periodicities of the left-hand side (LHS) in (11) and (12) is zero. For the equations to have a solution, the average of the RHS should also vanish (Fredholm alternative). The resulting solvability conditions provide the equations governing the large-scale dynamics, i.e., the dynamics in the slow variables. From (12) we obtain

$$\partial_T \langle \theta^{(0)} \rangle = D_0 \nabla^2 \langle \theta^{(0)} \rangle - \langle \mathbf{v} \cdot \nabla \theta^{(1)} \rangle, \quad (15)$$

where the symbol $\langle \cdot \rangle$ denotes the average over the periodicities. The solvability condition for (11) is trivially satisfied, reflecting the absence of α-type effects.[16,17] By plugging (13) into (15) we obtain the diffusion equation

$$\partial_T \theta^{(0)}(\mathbf{X},T) = D_{ij}^E \nabla^2 \theta^{(0)}(\mathbf{X},T), \quad (16)$$

where the eddy diffusivity tensor is

$$D_{ij}^E = D_0 \delta_{ij} - \tfrac{1}{2}[\langle v_i w_j \rangle + \langle v_j w_i \rangle]. \quad (17)$$

Remark that the structure of the eddy-diffusivity tensor will reflect the rotational symmetries of $\mathbf{v}$ and is, in general, nonisotropic.

A. Inequalities for the eddy diffusivity

Two important inequalities can be derived from auxiliary equation (14) and expression (17) of the eddy-diffusivity. Let us consider the i-th and the j-th components of (14) and multiply by w_j and w_i, respectively. Taking the sum and averaging, the time derivative and the advective term vanish and we obtain

$$-\tfrac{1}{2}[\langle v_i w_j \rangle + \langle v_j w_i \rangle] = D_0 \langle \partial w_i \cdot \partial w_j \rangle. \quad (18)$$

From (18) and (17) it follows that

$$D_{ij}^E = D_0[\delta_{ij} + \langle \partial w_i \cdot \partial w_j \rangle]. \quad (19)$$

This expression of the eddy diffusivity clearly shows that the correction to the molecular contribution is positive definite. Large-scale scalar transport is therefore enhanced in the presence of a small-scale incompressible velocity field. This is related to the property of the advection–diffusion equation (3) that integrals of even powers of θ and the maximum of the field are decreasing functions of time. When the dynamics do not possess the latter property the large-scale transport can actually be depleted, rather than increased. For momentum transport in Navier–Stokes flow, the depletion can be so strong that the eddy viscosity becomes negative, i.e., the average flux is in the same direction as the large-scale gradient.[18,19]

The second inequality also is derived from (18) but it is an upper bound to eddy diffusivities. Because of incompress-

ibility, the velocity field can be expressed using a vector potential as $\mathbf{v} = \mathrm{rot}\,\mathbf{A}$. By taking the trace of (18) and integrating by parts, we obtain

$$0 \leqslant D_0 \langle \partial w_i \cdot \partial w_i \rangle = -\langle v_i w_i \rangle = -\langle \mathbf{A} \cdot \mathrm{rot}\,\mathbf{w} \rangle. \quad (20)$$

Application of the Schwartz inequality leads to

$$D_0 \langle \partial w_i \cdot \partial w_i \rangle \leqslant \langle A^2 \rangle^{1/2} \langle (\mathrm{rot}\,\mathbf{w})^2 \rangle^{1/2}$$
$$\leqslant \langle A^2 \rangle^{1/2} \langle \partial w_i \cdot \partial w_i \rangle^{1/2}, \quad (21)$$

whence

$$\frac{D_{ii}^E}{D_0} \leqslant d + \frac{\langle A^2 \rangle}{D_0^2} \equiv d + \mathrm{Pe}^2. \quad (22)$$

The Péclet number is denoted by Pe. The result (22), valid for time-dependent flows also, generalizes a similar inequality known for time-independent velocity fields.[12,20] The inequality (22) also provides an upper bound for each eigenvalue since the eddy-diffusivity tensor is positive definite.

B. Two exactly solvable cases

By using multiscale techniques, the calculation of eddy diffusivities has been reduced to the solution of auxiliary equation (14). Numerical methods are generally needed to solve it but there are a few cases where one can obtain the solution of (14) analytically. We shall briefly review here the case of parallel flows and random flows δ-correlated in time.

The peculiar property of parallel flows is that the velocity is everywhere in the same direction, e.g., in three dimensions,

$$\mathbf{v}(x,y,z;t) = [v_x(y,z;t),0,0], \quad (23)$$

and v_x cannot depend on x because of incompressibility. The advective nonlinearity $\mathbf{v} \cdot \partial \mathbf{v}$ is thus vanishing. Thanks to the latter, we can easily obtain the solution of auxiliary equation (14) as

$$\hat{w}(\mathbf{q},\omega) = \frac{\hat{v}(\mathbf{q},\omega)}{i\omega - D_0 q^2}. \quad (24)$$

The Fourier transforms of v_x and w_x are denoted by $\hat{v}$ and $\hat{w}$. If $F(\mathbf{q},\omega) = \langle |\hat{v}(\mathbf{q},\omega)|^2 \rangle$, it follows that the eddy-diffusivity is

$$D_{\|}^E = D_0 \left(1 + \int \frac{F(\mathbf{q},\omega)q^2}{\omega^2 + D_0^2 q^4} d\mathbf{q}\,d\omega \right); \quad D_{\perp}^E = D_0. \quad (25)$$

Here, $D_{\|}^E$ and $D_{\perp}^E$ are the components of the eddy-diffusivity tensor parallel and orthogonal to the direction of the velocity. Equation (25) is a simple generalization of a well-known result due to Zeldovich.[21]

Let us now consider random flows having a short correlation time τ. Neglecting the diffusion term in (14) we obtain a hyperbolic equation which can be formally integrated along the characteristics

$$\mathbf{w}[\mathbf{x}(\mathbf{a},t);t] = -\int_0^t \mathbf{v}[\mathbf{x}(\mathbf{a},s);s]\,ds + \mathbf{w}(\mathbf{a};0). \quad (26)$$

Here, $\mathbf{a}$ denotes the Lagrangian initial position and the Eulerian position at time t is

$$\mathbf{x}(\mathbf{a},t) = \mathbf{a} + \int_0^t \mathbf{v}[\mathbf{x}(\mathbf{a},s);s]ds. \tag{27}$$

From (26) Taylor's expression of the eddy-diffusivity tensor immediately follows

$$D_{ij}^E = \frac{1}{2} \int_0^\infty [\Gamma_{ij}^L(s) + \Gamma_{ji}^L(s)]ds, \tag{28}$$

where the Lagrangian correlation function is defined as

$$\Gamma_{ij}^L(t-s) = \langle v_i[\mathbf{x}(\mathbf{a},t);t]v_j[\mathbf{x}(\mathbf{a},s);s]\rangle. \tag{29}$$

The operation $\langle \cdot \rangle$ denotes either spatial or ensemble averaging which do coincide since the velocity field is supposed homogeneous, stationary and mixing. Note that the convergence of the integral (28) is not at all guaranteed. The role of a small, but nonzero, molecular diffusivity can be crucial in this respect.[1] In the limit where τ is small, the Lagrangian correlation Γ_{ij}^L tends to the Eulerian correlation $\langle v_i(\mathbf{x},t)v_j(\mathbf{x},s)\rangle$. For a signal δ-correlated in time

$$\langle v_i(\mathbf{x},t)v_j(\mathbf{x},s)\rangle = 2F_{ij}\delta(t-s), \tag{30}$$

the expression (28) reduces to

$$D_{ij}^E = D_0 \delta_{ij} + F_{ij}. \tag{31}$$

The corrections to this result due to a small, nonzero, correlation time will be studied in the Appendix.

III. NUMERICAL METHODS

Whenever the auxiliary equation (14) cannot be solved exactly, numerical methods are needed. In this section we shall discuss two different methods that we have used: a perturbative expansion and a conjugate gradient algorithm.

In the perturbative method, the solution $\mathbf{w}$ of auxiliary equation (14) is sought as a power series in the Péclet number $Pe \sim 1/D_0$:

$$\mathbf{w} = Pe \; \mathbf{w}^{(1)} + Pe^2 \; \mathbf{w}^{(2)} + \cdots . \tag{32}$$

We shall concentrate on the time-independent case for simplicity. By inserting the expansion (32) into (14) the following recursive relation is obtained:

$$\mathbf{w}^{(1)} = \partial^{-2} \frac{\mathbf{v}}{D_0 \; Pe}, \quad \mathbf{w}^{(2)} = \partial^{-2} \frac{\mathbf{v} \cdot \partial \mathbf{w}^{(1)}}{D_0 \; Pe},$$

$$\cdots \; \mathbf{w}^{(n)} = \partial^{-2} \frac{\mathbf{v} \cdot \partial \mathbf{w}^{(n-1)}}{D_0 \; Pe}, \cdots . \tag{33}$$

Expressions (33) and the calculation of the average value in (17) are conveniently handled in Fourier space, leading to

$$\frac{D_{ij}^E}{D_0} = \delta_{ij} + \sum_{n \geqslant 1} (c_n)_{ij} \; Pe^{2n}. \tag{34}$$

Here, the c_n's are numerical coefficients and the series turns out to be in Pe^2, rather than in Pe. The contribution of order $2n+1$ in $\langle v_i w_j \rangle$ is indeed antisymmetric, as can be easily checked by integrating n times by parts. The series (34) will in general converge for $Pe < Pe^*$ only, because of singularities in the complex plane. A reliable analytic continuation beyond the disc of convergence can however be performed.

In Ref. 22 it was indeed shown that the component of the eddy diffusivity in the arbitrary direction $\hat{\mathbf{n}}$ can be represented as a Stieltjes integral

$$\frac{D_{\hat{n}}^E}{D_0} = 1 + Pe^2 \int dz \; \frac{\rho_{\hat{n}}(z)}{1 + Pe^2 \; z^2}, \tag{35}$$

where $\rho_{\hat{n}}(z)$ is a positive definite function, possibly singular. The Stieltjes integral representation was recently generalized to the time-dependent case in Ref. 23. The poles of the eddy diffusivity, considered as a function of a complex variable, are all on the imaginary axis. Moreover, it follows from (35) that Padé approximants of (34) have some interesting peculiar properties (see, e.g., Ref. 14). Let us indeed denote by $P_n^n(Pe)$ the diagonal Padé approximant of order n for the series (34) and by $P_{n+1}^n(Pe)$ the Padé approximant having the numerator and the denominator of degree n and $n+1$, respectively. The following results hold for every value of the Péclet number: (i) The diagonal sequence P_n^n is monotonically increasing and has an upper bound; (ii) the sequence P_{n+1}^n is monotonically decreasing and has a lower bound; (iii) the exact value P^* of the Stieltjes integral satisfies

$$\lim_{n \to \infty} P_n^n \leqslant P^* \leqslant \lim_{n \to \infty} P_{n+1}^n. \tag{36}$$

The difference $(P_{n+1}^n - P_n^n)$ decreases monotonically in n and provides an upper bound to the error due to the finite order. The quality of the resummation by a finite order approximant can thus be checked self-consistently. Padé approximants are very sensitive to the precision in the computations when the series is extended well beyond its radius of convergence. For small values of the molecular diffusivity, the coefficients in the series (34) must be then known with very high precision. In our numerical calculations we used the FORTRAN multiple-precision package (MP), written by R. P. Brent.[24] It should be noted, however, that very high precision computations are quite expensive in computers memory costs (see the next section).

The second method that we have used to solve the auxiliary equation (14) is a conjugate gradient algorithm.[25] The components of the vector $\mathbf{w}$ are not coupled in Eq. (14), which is thus equivalent to a set of scalar equations. All of them can be written in Fourier space as

$$A_{i,j}x_j = b_i, \quad i,j = 1,...,V. \tag{37}$$

Here, V is the resolution, x_i and b_i are vectors having the V components equal to the Fourier transform of the relevant components of $\mathbf{w}$ and $-\mathbf{v}$, respectively. Conjugate gradient algorithms are widely used to minimize multidimensional functions when the number of dimensions is very large. The interested reader is referred to Ref. 26 for a comparison with other methods (Gauss-Siedel or Minimal-Residue[25]) in another stiff numerical problem, the inversion of the propagator in lattice quantum chromodynamics. The solution of the problem (37) is sought by minimizing the quantity $(Ax-b)^2$ over a sequence of directions orthogonal to the matrix A. In all the applications of the method that we have considered, the matrix A in (37) is sparse (quasidiagonal). Each iteration of the minimization algorithm can be then performed in

$O(V)$ operations, rather than $O(V^2)$. For a positive-definite matrix, the rate of convergence of the method can be shown to be exponential.[25] Our matrix A has actually one zero eigenvalue, corresponding to a constant field. The problem is nevertheless well-posed, since both the velocity field and the solution w are orthogonal to constants, i.e., have zero average. As in any other numerical scheme, the simulations are expected to become more and more demanding as the molecular diffusivity becomes smaller. An increasing number of excited scales requires indeed a greater resolution and the rate of convergence of the method decreases when V and the Péclet number are increased. It is also to be checked that no eigenvalue is equal to zero within the numerical accuracy because of round-off errors. In the next section it will turn out that the previous limitations are not very severe and do not forbid to perform high Péclet numbers simulations. Note finally that Eq. (14) could also be solved by other techniques, e.g., those used in Ref. 13 and 27.

We conclude this section by briefly describing the numerical scheme used for the numerical simulations of tracers dispersion. The latter are done by uniformly distributing N particles in the periodicity box and letting them evolve according to the Langevin equation (1). The ith diagonal element of the eddy-diffusivity tensor is then given by

$$\sigma_i^2(t) = \lim_{t \to \infty} \frac{1}{2Nt} \sum_{k=1}^{N} \left[x_i^{(k)}(t) - \frac{1}{N} \sum_{j=1}^{N} x_i^{(j)}(t) \right]^2. \quad (38)$$

The indices k and j label the N particles, whereas the index i denotes the spatial directions (x, y for the two-dimensional case and x, y, z for the three-dimensional case). The numerical integration of the Langevin equation was performed by a Runge–Kutta algorithm, modified to take into account the white noise term.[28] The integration step was $\Delta t = 0.01$ and the total number of integration steps was 10^6. This ensured a good convergence of the quantities (38) also for the lowest molecular diffusion coefficients D_0 used. The number of particles used was 1000 for the three-dimensional case and 2000 for the two-dimensional case.

IV. STANDARD DIFFUSION

The aim of this section is to apply the methods previously discussed to three flows showing standard diffusion. The criterion in the choice of the flows is to have different mechanisms of diffusion enhancement, highlighting the influence of Lagrangian chaos on transport at high Péclet numbers. Specifically, we have considered the following:

• The three-dimensional ABC flow:[6,7,8]

$$\dot{x} = A \sin(z) + C \cos(y),$$

$$\dot{y} = B \sin(x) + A \cos(z), \quad (39)$$

$$\dot{z} = C \sin(y) + B \cos(x).$$

with $A = B = C$. The ABC flow is a Beltrami time-independent solution of Euler's equations. Equation (39) shows Lagrangian chaos but the phase space is also made of regular regions, having roughly the shape of a tube parallel to one of the three axes (principal vortices).

• The two-dimensional BC flow

$$\dot{x} = C \cos(y),$$

$$\dot{y} = B \cos(x), \quad (40)$$

obtained by projecting the flow (39) onto the x-y plane and translating the x coordinate by $\pi/2$. Equation (40) is integrable and the streamlines form a closed structure made of four cells in each periodicity box.

• The two-dimensional time-dependent flow

$$\dot{x} = \cos(y) + \sin(y)\cos(t),$$

$$\dot{y} = \cos(x) + \sin(x)\cos(t). \quad (41)$$

This flow is not a solution of Euler's equations anymore but it is the superposition of the flow (40) with another flow of the same type oscillating with frequency $\omega = 1$. The motivation for introducing a time dependency is to destroy all possible "regular islands," like the vortices in (39).

Note that both the flows (39) and (40) have an isotropic eddy-diffusivity tensor. Let us indeed consider the latter for simplicity and perform the following two operations: translation by π and mirror inversion with respect to one of the axes (e.g., $x \mapsto \pi - x$ and $y \mapsto \pi - y$). From auxiliary equation (14) it follows that, under the previous operations, one of the components of w is odd and the other is even, in such a way that $\langle v_x w_y \rangle = \langle v_y w_x \rangle = 0$. The diagonal components are obviously equal because of the symmetry $x \leftrightarrow y$. For (39) the proof is similar, exploiting the fact that the group of symmetries of the flow is isomorphic to the cubic group.[8] The flow (41) possesses the symmetry $x \leftrightarrow y$, but it is not mirror symmetric. The diagonal components of the eddy diffusivity will then be equal but the nondiagonal component does not vanish. For molecular diffusivity 2×10^{-3} the components of the eddy-diffusivity tensor are, for example, $D_{11} = D_{22} = 1.34$ and $D_{12} = 1.27$. This implies that the eigendirections are rotated by an angle of roughly $\pi/4$ with respect to the axes, as clearly seen in Fig. 1. In Langevin simulations the previous symmetry properties are exploited to reduce the statistical fluctuations by averaging over the directions.

In Figs. 2–4 we present the results for the diagonal component of the eddy-diffusivity tensor of (39)–(41), respectively. The curves in each figure correspond to numerical simulations of the Langevin equation, the Padé method and the conjugate gradient algorithm. To attain the highest Péclet number the order of Padé approximants used is 54, 115, and 29 and the number of significant digits in the computations is 83, 203, and 40, respectively. Concerning the conjugate gradient algorithm, in Fig. 5 it is shown the power spectrum of the auxiliary field w for the flow (41) at $D_0 = 0.01$. It can be seen that the field is resolved enough to ensure the presence of a conspicuous exponentially decaying tail. The conjugate gradient algorithm turns out to be much more efficient at high Péclet numbers than the Padé method. The latter has the advantage of requiring the calculation of the coefficients of (34) only: once they are computed, the eddy diffusivities for all values of D_0 such that the method works are available. On the other hand, the memory costs for high precision arithmetics are a major drawback and practically restrict the method to moderate Péclet numbers.

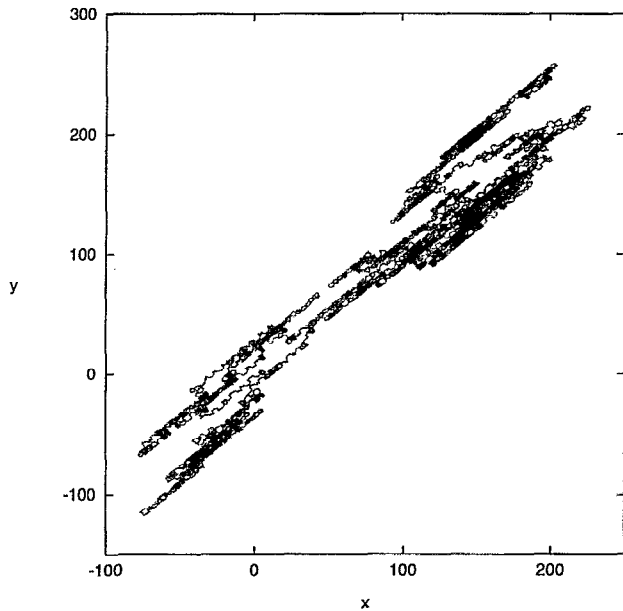Phys. Fluids, Vol. 7, No. 11, November 1995

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FIG. 1. A typical trajectory of a particle moving in the velocity field (41). Note the strong difference between transport in the $\hat{x}=\hat{y}$ and $\hat{x}=-\hat{y}$ directions.

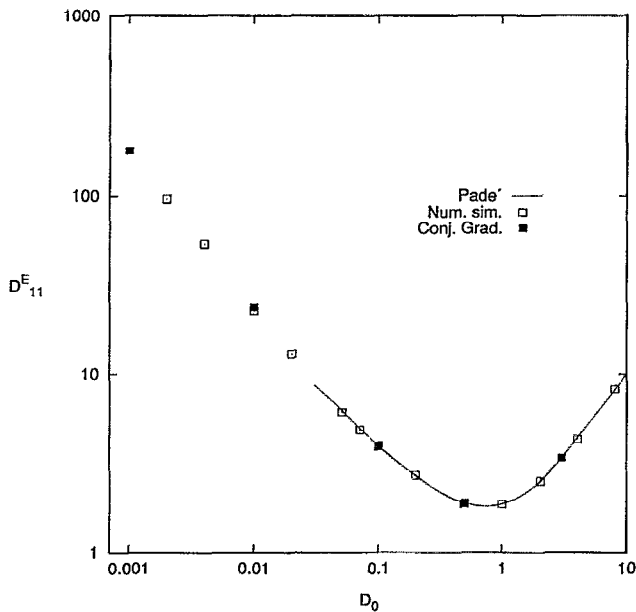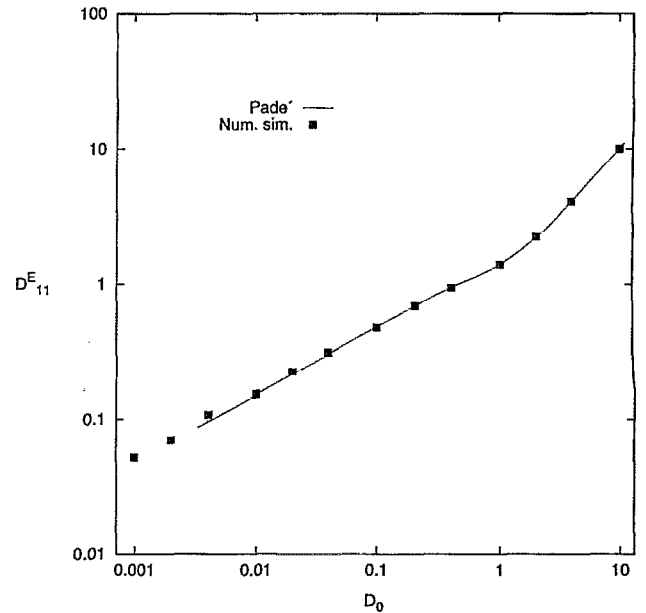FIG. 3. The diagonal component D_{11}^{E} as a function of the bare molecular diffusivity D_0 for the two-dimensional BC flow (40) with $B=C=1$. The continuous line is the result of the Padé method. The black squares are the results of the direct simulations.

From the high Péclet number behavior of the eddy diffusivities in the figures it is clear that the three flows have very different dynamics. The main contribution to diffusion in the flow (39) comes from the particles in the vortices, where the transport is almost ballistic, leading to the observed $1/D_0$ dependence. This is a simple example of maxi-

mally enhanced diffusion, as discussed in Ref. 29. Because of the presence of closed cells, a nonzero molecular diffusivity is needed to have an effective diffusion in the flow (40), as indicated by the $\sqrt{D_0}$ behavior in Fig. 3. The transport for small molecular diffusivities indeed occurs by jumps from one cell to another due to the white-noise term in the Lange-
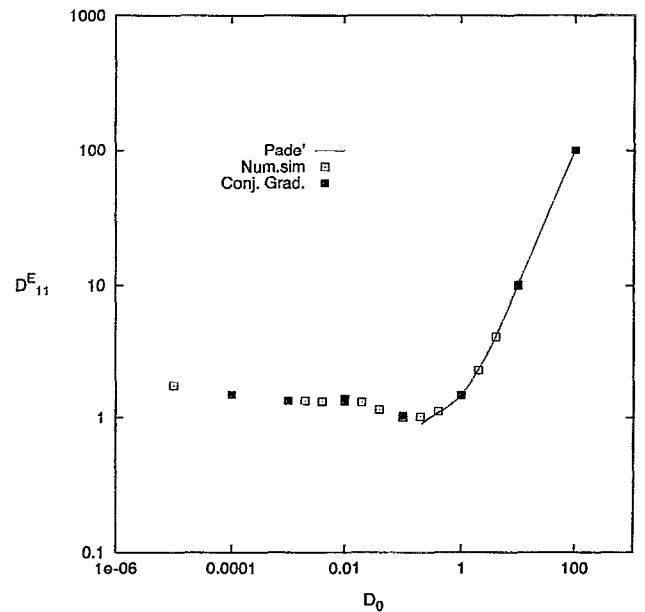

FIG. 2. The diagonal component D_{11}^{E} as a function of the bare molecular diffusivity D_0 for the three-dimensional ABC flow (39) with $A=B=C=1$. The continuous line is the result of the Padé method. The black and white squares are the results of the conjugate gradient method and direct simulations, respectively.
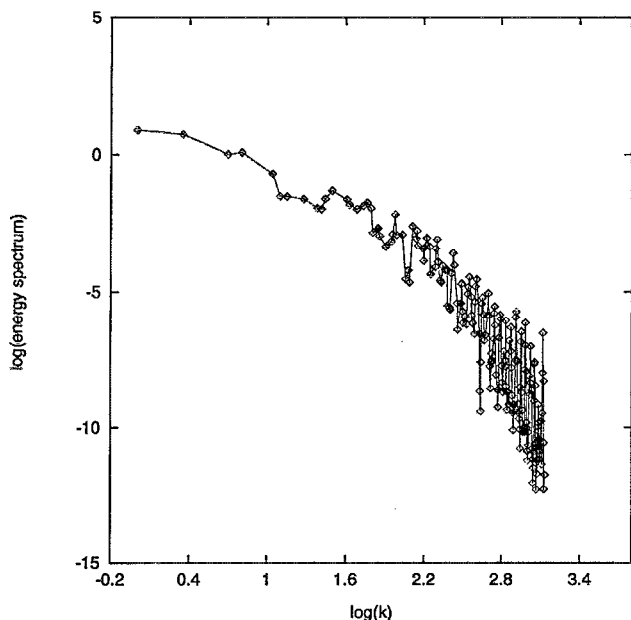

FIG. 4. The diagonal component D_{11}^{E} as a function of the bare molecular diffusivity D_0 for the two-dimensional time-dependent flow (41). The continuous line is the result of the Padé method. The black and white squares are the results of the conjugate gradient method and of direct simulations, respectively.

FIG. 5. Log–log plot of the energy spectrum of the auxiliary field **w** for the flow (41) at $D_0=0.01$.

vin equation.[30–32] The probability of jumping is controlled by the width of boundary layers located near the separatrices and gives the square-root law. The flow (41) is finally an example of strong Lagrangian turbulence. The particles can diffuse even in the absence of molecular diffusion, chaotic advection is dominant and the eddy diffusivity attains a finite value independent of the molecular diffusivity. The figures show that for all the flows considered, Langevin simulations and numerical solutions of auxiliary equation (14) do agree. Moreover, in the latter method no problem of finite statistics and simulation times must be overcome. We conclude that multiscale techniques combined with an efficient numerical scheme for the solution of the auxiliary equation (e.g., a conjugate gradient algorithm or a pseudospectral code[33]) provide a powerful tool for the calculation of eddy diffusivities and transport properties.

V. ANOMALOUS DIFFUSION

We shall discuss here how the multiscale formalism presented in the previous sections can be used for the problem of anomalous diffusion. At a first sight it would seem that multiscale techniques cannot be used anymore. Consider indeed a two-dimensional static parallel flow (23). If the power spectrum $F(q)$ defined in Sec. II B is such that

$$F(q) \sim q^\alpha, \quad \alpha \leqslant 1, \quad \text{for } q \ll 1, \tag{42}$$

then the integral in (25) diverges and the eddy diffusivity is not defined. The divergence is actually reflecting the fact that the transport in the direction of the flow is superdiffusive,[34–38] i.e.,

$$\langle x^2(t) \rangle \sim t^{2\nu}, \quad \nu > 1/2, \tag{43}$$

and it is not a standard diffusion. The particles are indeed coherently swept by large-scale modes having wavelengths

comparable (or even larger) to the typical length of the scalar field. Scale-separation breaks down and multiscale methods, heavily relying on this assumption, seem to become useless. However, a regularization procedure can be adopted in order to have standard diffusion. The anomalous behavior can then be captured by looking at the dependance of the eddy diffusivity on the regularization parameter.

For random flows with long-range correlations, as (42), a convenient regularization is provided by an infrared cutoff. The singular part in the integral (25) is cut out by introducing a regularized velocity field $\mathbf{v}_L$, such that

$$F_L(q) = \begin{cases} F(q), & \text{if } q > L^{-1}, \\ 0, & \text{if } q < L^{-1}. \end{cases} \tag{44}$$

The eddy diffusivity is now finite and exhibits a dependence

$$D_{\parallel}^E(L) \sim L^{1-\alpha}, \quad L \gg 1, \tag{45}$$

on the cutoff length L. A standard diffusion is however observed only for spatial and time lengths larger than L and $t^* \sim L^2/D_0$, respectively. For $t \sim t^*$ the system has indeed a crossover,[38] and for times shorter than t^* it shows the same behavior as in (43). By matching at t^* the two different regimes, we obtain

$$\nu = \frac{3-\alpha}{4} \geqslant 1/2. \tag{46}$$

For $\alpha=0$, i.e., a velocity field which is a white noise in space, (46) leads to $\nu=3/4$, the well-known result of Matheron and De Marsily.[34] Equation (46) had been rigorously obtained in Ref. 39.

In the previous example, the origin of superdiffusion was related to the spatial structure of the velocity field. We shall turn now to the interesting case of deterministic velocity fields with very long Lagrangian correlation times. The integral defining the eddy diffusivity in Taylor's expression (28) may then diverge, indicating the presence of anomalous transport for $D_0=0$. Note, however, that for any $D_0>0$ the transport is, in general, a standard diffusion [see (25) for an example of the role of a small molecular diffusivity]. The molecular diffusivity can be thus used as a regularization parameter, similarly to the cutoff length for parallel flows. As in the latter case, by studying the behavior of the eddy diffusivity close to the critical point (small D_0) one should be able to have some insights into the anomalous behavior at the critical point ($D_0=0$). Specifically, the examples of Sec. IV show that in the presence of ballistic channels the eddy diffusivity varies as the inverse of D_0 for small D_0, while for a system with strong Lagrangian chaos it tends to a constant. If $D_{\hat{n}}^E$ denotes the eddy diffusivity in the arbitrary direction $\hat{n}$, we are thus led to interpret a small D_0 behavior,

$$D_{\hat{n}}^E \sim D_0^{-\beta}, \quad 0 < \beta < 1, \tag{47}$$

as a mark of anomalous diffusion in the direction $\hat{n}$ for $D_0=0$.

For a practical application of the previous argument, we have considered the velocity field[4]

$$\begin{cases} \dot{x} = \partial_y \psi + \epsilon \sin z, \\ \dot{y} = -\partial_x \psi + \epsilon \cos z, \\ \dot{z} = \psi, \end{cases} \qquad (48)$$

where

$$\psi(x,y) = 2\left[\cos x + \cos\left(\frac{x+\sqrt{3}y}{2}\right) + \cos\left(\frac{x-\sqrt{3}y}{2}\right) \right]. \qquad (49)$$

Numerical simulations of (48) have led the authors of Ref. 4 to conclude that the flow exhibits anomalous diffusion in the x-y plane for some intervals of ϵ values in the range (0,5). In particular, $\epsilon = 1$ and $\epsilon = 2.3$ are such that the diffusion is standard and anomalous, respectively. In the anomalous transport case, the Lagrangian phase space is a complicated self-similar structure of islands and cantori. Particles are thus transported in a way similar to Lévy flights (see Fig. 6).

Let us now introduce a small molecular diffusivity and calculate the eddy diffusivity of the flow (48). The auxiliary equation is solved by the conjugate gradient method and the results for D_{xx} are presented in Figs. 7 and 8. It is evident that for $\epsilon = 1$ the eddy diffusivity tends to a constant for small D_0, while for $\epsilon = 2.3$ it is observed the behavior $D_{xx} \sim D_0^{-\beta}$ with $\beta \approx 0.7$. This value is in rough agreement with the numerical results of Ref. 4 using the dimensional relation $\beta = 2\nu - 1$ obtained by matching the diffusive behavior with the anomalous behavior (43) at the typical diffusive time $O(1/D_0)$. The criterion (47) is thus confirmed and we conjecture that its validity is not restricted to the flow (48) only. For a generic deterministic flow, anomalies in the zero-diffusivity dynamics could then be captured by introducing a small molecular diffusivity and looking for a singular behavior of transport coefficients. As shown in the previous section, the advantage with respect to simulations of the Lange-
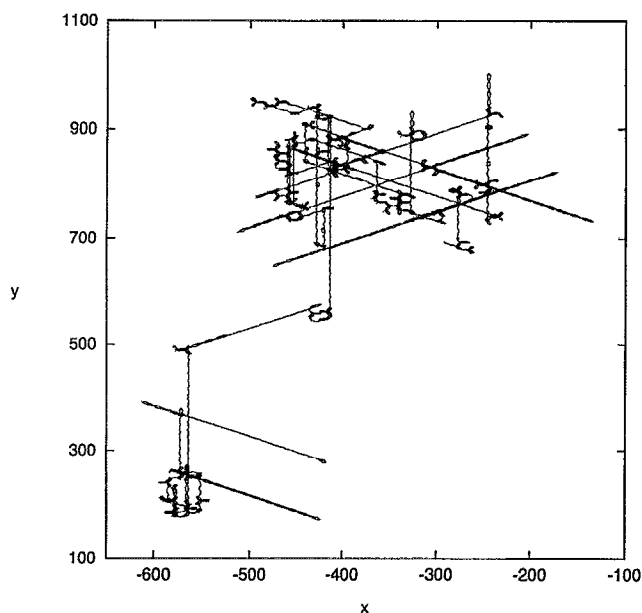
vin equation is that no problem of statistical fluctuations must be tackled. The previous procedure should then allow to make robust predictions on the presence of anomalous transport.
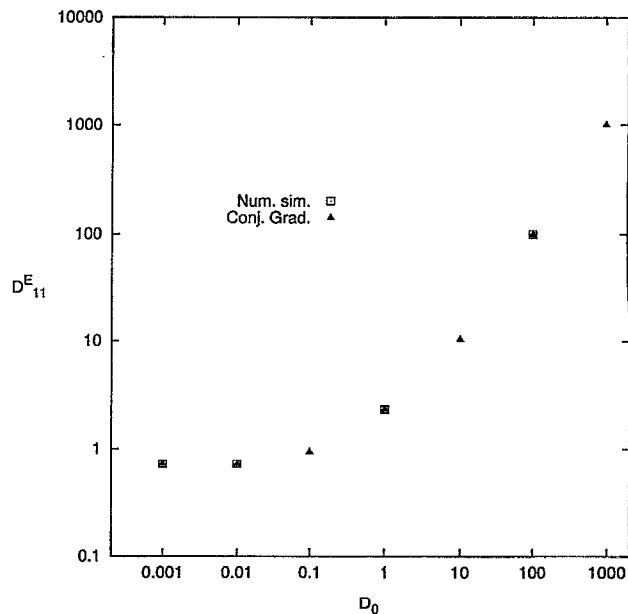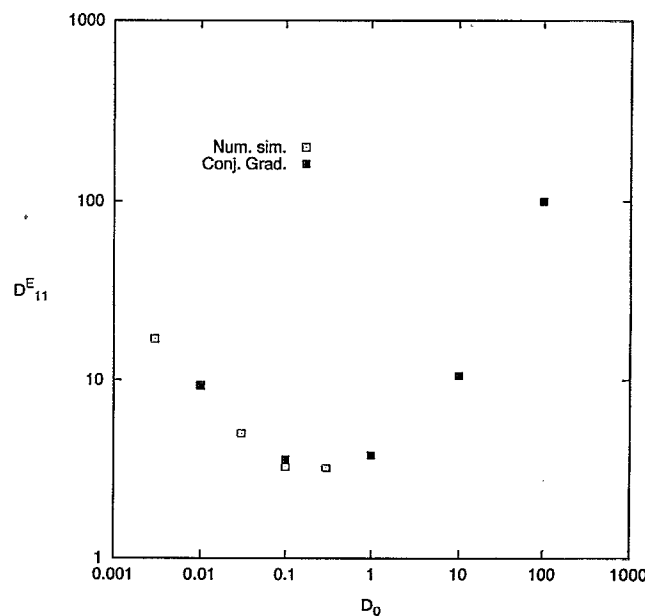
ACKNOWLEDGMENTS

FIG. 7. The diagonal component D_{11}^E as a function of the bare molecular diffusivity D_0 for the three-dimensional flow (48), (49) with $\epsilon = 1$ (standard diffusion).

FIG. 6. A typical trajectory of a particle moving in the velocity field (48) for $\epsilon = 2.3$ and $D_0 = 0.0003$.

FIG. 8. The diagonal component D_{11}^E as a function of the bare molecular diffusivity D_0 for the dimensional flow (48), (49) with $\epsilon = 2.3$ (anomalous diffusion).

APPENDIX: EDDY DIFFUSIVITY FOR INCOMPRESSIBLE FLOWS WITH SHORT CORRELATION TIME

We shall derive here the expression of the eddy diffusivity for incompressible flows having a short correlation time. Specifically, the ratio τ_c/τ_s between the correlation and the sweeping time (defined precisely later) is supposed to be small. We shall be particularly interested in three-dimensional isotropic flows. By the latter we mean velocity fields invariant under rotations, but not, in general, under parity transformations. When the correlation time tends to zero, we recover the case of flows δ-correlated in time. For a Gaussian flow, the first two corrections are shown to be proportional to $(\tau_c/\tau_s)^2$: one of them is related to the correlation length of the flow and the second is due to helicity. The former reduces, while the latter increases the eddy diffusivity, in agreement with Ref. 40.

Let $\mathbf{v}(\mathbf{x},t)$ denote a random, homogeneous, and stationary incompressible velocity field. We shall suppose the flow to be isotropic, Gaussian, and the correlation function

$$\langle v_i(\mathbf{x},t)v_j(\mathbf{y},s)\rangle = C(|t-s|)B_{ij}(\mathbf{x}-\mathbf{y}). \tag{A1}$$

The mean velocity is equal to zero. The temporal correlation function $C(t)$ decays on a time scale of order τ_c. The spatial correlation function is defined via its Fourier transform as

$$\hat{B}_{ij}(\mathbf{k}) = P_{ij}(\mathbf{k})\frac{E(k)}{4\pi k^2} - \frac{i}{2}\epsilon_{ijl}k_l\frac{H(k)}{4\pi k^4}, \tag{A2}$$

where $P_{ij}=\delta_{ij}-k_ik_j/k^2$ is the solenoidal projector and ϵ_{ijk} is the fundamental antisymmetric tensor. The functions $E(k)$ and $H(k)$ will be called the energy and the helicity spectrum, since

$$\frac{1}{2}\langle v^2\rangle = C(0)\int E(k)dk; \quad \langle \mathbf{v}\cdot\omega\rangle = C(0)\int H(k)dk. \tag{A3}$$

The helicity is a pseudoscalar and it is thus vanishing for flows having a center of symmetry (parity invariance). The helicity spectrum satisfies the inequality (see Ref. 41):

$$|H(k)| \leq 2kE(k). \tag{A4}$$

We shall be interested in the calculation of eddy diffusivities for very high Péclet numbers. The eddy diffusivity is given in this limit by Taylor's expression (28)

$$D_{ij}^E = \frac{1}{2}\int_0^\infty [\langle v_i[\mathbf{x}(\mathbf{a},t),t]v_j(\mathbf{a},0)\rangle + i\leftrightarrow j]dt. \tag{A5}$$

Let us now suppose the correlation time τ_c of the velocity field to be much smaller than the sweeping time τ_s. The latter is defined as

$$\tau_s = \frac{\lambda}{\langle v^2\rangle^{1/2}} = \left(\frac{1}{C(0)\int k^2E(k)dk}\right)^{1/2}, \tag{A6}$$

and it is roughly the average time it takes for a particle to travel a distance equal to the correlation length λ. The dominant contribution in (A5) will be given by Eulerian positions $\mathbf{x}(\mathbf{a},t)$ close to $\mathbf{a}$:

$$\mathbf{x}(\mathbf{a},t) = \mathbf{a} + \int_0^t ds\ \mathbf{v}(\mathbf{a},s) + \int_0^t ds(\nabla_l\mathbf{v})(\mathbf{a},s)$$
$$\times \int_0^s ds'\ v_l(\mathbf{a},s') + \cdots, \tag{A7}$$

and the velocity $\mathbf{v}[\mathbf{x}(\mathbf{a},t),t]$ in (A5) is

$$\mathbf{v}(\mathbf{x}(\mathbf{a},t),t) = \mathbf{v}(\mathbf{a},t) + (\nabla_l\mathbf{v})(\mathbf{a},t)\int_0^t ds\ v_l(\mathbf{a},s) + (\nabla_l\mathbf{v})(\mathbf{a},t)$$
$$\times \int_0^t ds(\nabla_m v_l)(\mathbf{a},s)\int_0^s ds'\ v_m(\mathbf{a},s')$$
$$+ \frac{1}{2}(\nabla_l\nabla_m\mathbf{v})(\mathbf{a},t)\int_0^t ds\ v_l(\mathbf{a},s)$$
$$\times \int_0^t ds'\ v_m(\mathbf{a},s') + \cdots. \tag{A8}$$

Equation (A8) can now be plugged into Taylor's expression (A5), leading to

$$D_{ij}^E = \frac{1}{2}\int_0^\infty dt\left[\langle v_i(\mathbf{a},t)v_j(\mathbf{a},0)\rangle\right.$$
$$+ \frac{1}{2}\int_0^t ds\int_0^t ds'\langle(\nabla_l\nabla_m v_i)(\mathbf{a},t)v_j(\mathbf{a},0)\rangle$$
$$\times\langle v_l(\mathbf{a},s)v_m(\mathbf{a},s')\rangle + \int_0^t ds\int_0^s ds'\langle(\nabla_l v_i)(\mathbf{a},t)$$
$$\left.\times v_m(\mathbf{a},s')\rangle\langle(\nabla_m v_l)(\mathbf{a},s)v_j(\mathbf{a},0)\rangle\right] + i\leftrightarrow j, \tag{A9}$$

where homogeneity, incompressibility, and the properties of Gaussian statistics have been exploited. Equation (A9) is valid for a generic Gaussian random flow and the next terms in the expansion are $O(\tau_c/\tau_s)^4$. Let us now specialize (A9) to the isotropic case. The eddy-diffusivity tensor is then proportional to δ_{ij} and its trace can be calculated by using (A1) and (A2):

$$\text{Tr}\ D_{ij}^E = 2\int E(k)dk\int_0^\infty dt C(t) - \frac{2}{3}\left(\int E(k)dk\right)$$
$$\times\left(\int k^2E(k)dk\right)\int_0^\infty dt\ C(t)\int_0^t ds\int_0^t ds'\ C(|s-s'|)$$
$$+ \frac{1}{6}\left(\int H(k)dk\right)^2\int_0^\infty dt\int_0^t ds\ C(s)\int_0^s ds'\ C(t-s'). \tag{A10}$$

In order to estimate the order of magnitude of the various terms in (A10) it is convenient to consider the case

$$C(|t|) = \frac{1}{2\tau_s} \chi_{\tau_s}(|t|); \quad \chi_{\tau_s}(|t|) = \begin{cases} 1, & \text{if } |t| \leqslant \tau_s; \\ 0, & \text{otherwise.} \end{cases}$$
(A11)

When $\tau_s \to 0$ a flow δ-correlated in time is obtained. In this limit, the only nonvanishing contribution in (A10) is the first one, which coincides with (31). Both corrections in (A10) are proportional to $(\tau_c/\tau_s)^2$, as can be checked by using (A4) and the Schwartz inequality. If the correlation function $C(t)$ is not (A11), the constants are changed but not the orders of magnitude, provided the condition $\int C(t)dt = 1$ is kept fixed.

Note that for the correlation function (A11) the helicity contribution in (A10) is clearly positive while the one related to the correlation length is negative. These results have a simple physical interpretation. It is convenient to consider the Lagrangian correlation time which is proportional to the eddy diffusivity. The first correction in (A10) is due to the fact that the presence of a spatial correlation length obviously reduces the Lagrangian correlation time. The second correction depends on the presence of helicity. The latter has the effect that particles move following a helix, instead of a straight line. The mean velocity is, however, the same since it depends on the energy spectrum only. It will then take a longer time for a particle to escape a strongly correlated region; the Lagrangian correlation time is longer and the eddy diffusivity is increased. An equivalent remark is that a path following a helix is discriminated against tightly bending back on itself.[40]

A Gaussian flow has been considered but the results can be easily generalized to the general case. If third-order moments do not vanish the first correction will, in general, be proportional to τ_c/τ_s. We finally note that the helical term is actually the only one in (A9) which needed to be symmetrized with respect to the indices i and j. The latter fact is related to Onsager's reciprocity theorem.[42] When the helicity does not vanish, the correlation function will indeed not satisfy the time-reversibility condition $B_{ij}(\mathbf{x}) = B_{ji}(\mathbf{x})$, and the velocity field has a preferred sense of rotation.[1] The lack of parity invariance can be thus interpreted as a lack of symmetry with respect to time reversal, which is responsible for the antisymmetry of transport coefficients.

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