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Effective Diffusion in a Stochastic Velocity Field

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Analytical results are derived for the effective dispersion of a passive scalar in a stochastic velocity field evolving in a fast time scale. These results are favorably compared with direct computer simulation of stochastic differential equations containing multiplicative space-time correlated noise.

KEY WORDS: Effective diffusion; stochastic velocity; multiplicative correlated noise.

Dispersion of a passive scalar convected by a moving fluid is certainly a problem of major interest in chemical reactions, mixing of fluids, and spreading of pollutants. It is therefore of fundamental and practical importance to understand how fluid flow affects dispersion. In particular, and since the pioneering work by Batchelor[1] in the late 1950s, this question has been extensively examined in the context of turbulent flows, where the concept of an eddy diffusivity has been commonly invoked to describe the effectiveness of turbulent mixing. For homogeneous flows and nonreactive scalar one expects that such a turbulent diffusion will essentially depend on the statistical properties of the turbulence.

Actually, the computation of an effective diffusion coefficient in terms of a turbulent velocity statistics is a problem with its own long history. Roberts[2] applied the direct interaction approximation (DIA) for one-particle diffusion to get an expression for a turbulent diffusion coefficient

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which has to be determined self-consistently using the solution of the scalar field itself. Kraichnan[3] confirmed numerically the consistency of that approach using a Lagrangian description appropriate to 2D and 3D prescriptions for the energy spectra of the turbulent field. This last author also applied the DIA formalism to evaluate the evolution of the spatial correlation function of the scalar field.[4] The abstract work by McLaughlin *et al.*[5] proves in a formal and mathematical way the existence of an effective diffusion coefficient in turbulent media. The closure result obtained by Saffman[6] with average and truncation procedures has been recently generalized by Lipscombe *et al.*[7] to account for Gaussian non-homogeneous velocity fields.

Here we present a derivation of the effective diffusion coefficient which finally depends only on the properties of the stochastic isotropic, homogeneous, and stationary random velocity field, in the limit of small correlation times. To this end we will make use of non-Markovian techniques appropriate to deal with Langevin equations involving multiplicative noise in spatially extended systems. Our predictions are favorably compared with direct computer simulations of a simple model performed using algorithms developed for stochastic partial differential equations, discretized in a lattice, and incorporating multiplicative space-time colored noise.

Our starting point is an equation of motion for a scalar variable $\psi(\mathbf{x}, t)$ in a turbulent velocity field $\mathbf{v}(\mathbf{x}, t)$

$$\frac{\partial\psi}{\partial t} = D\nabla^2\psi - \nabla\cdot(\mathbf{v}\psi) \tag{1}$$

D is the molecular diffusion coefficient. The velocity field is a homogeneous, stationary, and isotropic stochastic quantity defined by its cumulants. In particular, its mean value is zero and the second cumulant is given by[8]

$$\langle v_i(\mathbf{x}, t)\, v_j(x', t')\rangle = R_{ij}(\mathbf{x} - \mathbf{x}'; t - t') \tag{2}$$

Since $\mathbf{v}(\mathbf{x}, t)$ is the velocity of an incompressible fluid, $\nabla\cdot\mathbf{v} = 0$, and as a consequence[9]

$$\sum_j \frac{\partial R_{ij}}{\partial x_j} = 0 \tag{3}$$

Our interest here is to study the evolution of the mean value of the scalar field. Taking averages over the statistical distribution of $\mathbf{v}$ in Eq. (1), we get

$$\frac{\partial}{\partial t}\langle\psi\rangle = D\nabla^2\langle\psi\rangle - \sum_i \frac{\partial}{\partial x_i}\langle v_i(\mathbf{x}, t)\, \psi(\mathbf{x}, t)\rangle \tag{4}$$

Using now Novikov's theorem[10] to evaluate the last average, we obtain

$$\langle v_i(\mathbf{x}, t)\, \psi(\mathbf{x}, t)\rangle = \sum_j \int_0^t dt' \int d\mathbf{x}'\, R_{ij}(\mathbf{x}-\mathbf{x}'; t-t') \left\langle \frac{\delta\psi(\mathbf{x}, t)}{\delta v_j(\mathbf{x}', t')} \right\rangle \tag{5}$$

In deriving this last expression we have assumed that $\mathbf{v}$ is Gaussian. For a non-Gaussian field one should include higher-order cumulants in Eq. (5). In any case, Eq. (5) can be considered as a good approximation for a non-Gaussian $\mathbf{v}$ if higher-order cumulants are small enough in comparison with R_{ij}. Let R_{ij} be a rapidly decaying function in $t_0^{-1}(t-t')$, not necessarily a delta function, on a time scale t_0 which is a small quantity in comparison with other time scales of the system. In this circumstances we expand the response function in Eq. (5) around $t'=t$,

$$\frac{\delta\psi(\mathbf{x}, t)}{\delta v_j(\mathbf{x}', t')} = \left.\frac{\delta\psi(\mathbf{x}, t)}{\delta v_j(\mathbf{x}', t')}\right|_{t'=t} + \left.\frac{\partial}{\partial t'}\frac{\delta\psi(\mathbf{x}, t)}{\delta v_j(\mathbf{x}', t')}\right|_{t'=t} (t-t') + \cdots \tag{6}$$

Now the response function at equal times is evaluated from Eq. (1):

$$\left.\frac{\delta\psi(\mathbf{x}, t)}{\delta v_j(\mathbf{x}', t')}\right|_{t'=t} = -\frac{\partial}{\partial x_j}\,\delta(\mathbf{x}-\mathbf{x}')\,\psi(\mathbf{x}, t) \tag{7}$$

Substituting Eqs. (5)–(7) into Eq. (4) and after an integration by parts in the space coordinates and the use of Eq. (3), we obtain the equation of motion for the mean value

$$\frac{\partial}{\partial t}\langle\psi\rangle = D\nabla^2\langle\psi\rangle + \sum_{ij} \frac{\partial^2}{\partial x_i\,\partial x_j}\,\Delta D_{ij}\,\langle\psi(\mathbf{x}, t)\rangle + \theta(t_0^2) \tag{8}$$

where ΔD_{ij} is a new contribution to the molecular diffusivity D, which has the explicit expression

$$\Delta D_{ij} = \int_0^\infty R_{ij}(0; s)\, ds \equiv u_0^2 t_0 \delta_{ij} \tag{9}$$

where $u_0^2 = R_{ii}(0; 0)$. Actually, this result can be considered as an exactly correct limiting case of Roberts' analysis[2] for the diffusion of a scalar field by a rapidly varying random velocity field. The correction is of order t_0, and the next contribution of Eq. (6) is of order t_0^2, which we have discarded in this approximation. ΔD_{ij} can be evaluated from an experimental or analytical knowledge of R_{ij}. Nevertheless, we want to relate it to dispersion experiments, for example, of a small drop of a passive scalar in a turbulent fluid. This can be done by considering that the field $\langle \psi \rangle$ is like a probability density whose second moment, from Eq. (8), obeys[8]

$$\frac{d}{dt} M_{ij}(t) = 2(D\delta_{ij} + \Delta D_{ij}) \tag{10}$$

where M_{ij} is defined by

$$M_{ij}(t) = \langle x_i x_j \rangle = \int d\mathbf{x}\, x_i x_j \langle \psi(\mathbf{x}, t) \rangle \tag{11}$$

Since the first moment is zero, we have for the relative fluctuations of the density

$$\langle \Delta x_i \Delta x_j \rangle = 2(D\delta_{ij} + \Delta D_{ij})\, t \tag{12}$$

Dealing with isotropic turbulence, $\Delta D_{ii} = \Delta D_{jj} = \Delta D$, then the modulus of the relative fluctuations in two dimensions is given by

$$\langle \Delta r^2 \rangle = \langle \Delta x^2 \rangle + \langle \Delta y^2 \rangle = 4(D + \Delta D)\, t \tag{13}$$

In an experiment or in a simulation one can look at $\langle \Delta r^2 \rangle$ of the dispersed scalar and from its behavior in time one can obtain the effective diffusion

$$\bar{D}_{\text{eff}} = \frac{\langle \Delta r^2 \rangle}{4t} \tag{14}$$

which should be compared with the theoretical prediction

$$\bar{D}_{\text{th}} = D + \Delta D \tag{15}$$

In order to test our theoretical results, we have made computer simulations. We follow here a different approach from that of ref. 11, where the position of one Brownian particle is simulated. Here, instead, we simulate the stochastic partial differential equation (1) in a two-dimensional space.

The simulation takes place in a square lattice of 64×64 points with shifted periodic boundary conditions[12] and space steps of $\Delta x = \Delta y = 1$. Then the two-dimensional lattice is treated as a one-dimensional array in the computing simulation, so that the updating can be easily vectorized.

Our computer simulation of Eq. (1) has two main steps: first we construct a stochastic velocity field with prescribed properties, and then we simulate Eq. (1) by means of a first-order Euler algorithm. The first step involves the simulation of a scalar field $\eta(\mathbf{x}, t)$, by means of the Langevin equation

$$\frac{\partial \eta}{\partial t} = -\frac{1}{\tau}(1 - \lambda^2 \nabla^2)\,\eta + \frac{\xi(\mathbf{x}, t)}{\tau} \tag{16}$$

taken in the above-mentioned lattice. $\xi(\mathbf{x}, t)$ is a Gaussian white noise of correlation

$$\langle \xi(\mathbf{x}, t)\, \xi(\mathbf{x}', t') \rangle = 2\varepsilon \frac{\delta_{\mathbf{x},\mathbf{x}'}}{\Delta x \Delta y}\, \delta(t - t') \tag{17}$$

We have here three parameters, the intensity of the noise ε and the space and time correlation lengths λ and τ, respectively. These three independent parameters are conveniently related to the corresponding parameters which characterize the statistics of the turbulent field, i.e., its own intensity and space and time correlation lengths l_0 and t_0, respectively. Since Eq. (16) is linear, the scalar field η is also a Gaussian process. Now the velocity field is constructed by means of the discrete version of the definition

$$\vec{v}(\mathbf{x}, t) = (v_x(\mathbf{x}, t), v_y(\mathbf{x}, t)) = \left(-\frac{\partial \eta}{\partial y}, \frac{\partial \eta}{\partial x} \right) \tag{18}$$

which corresponds to an incompressible fluid.

The algorithm for Eqs. (16) and (17) is

$$\eta_{ij}(t + \Delta t) = \eta_{ij}(t) - \frac{\Delta t}{\tau}(1 - \lambda^2 \nabla^2)\, \eta_{ij}(t) + \left(\frac{2\varepsilon \Delta t}{\tau^2} \right)^{1/2} \alpha_{ij}(t) \tag{19}$$

where Δt is the time step integration, which is small enough to ensure the stability of the simulation results, ∇^2 is now the discrete version of the Laplacian operator, and $\alpha_{ij}(t)$ are Gaussian independent random numbers of zero mean and variance equal to one. Now Eq. (18) is discretized as

$$\vec{v}_{ij}(t) = \left(\frac{\eta_{i,j-1}(t) - \eta_{i,j+1}(t)}{2}, \frac{\eta_{i+1,j}(t) - \eta_{i-1,j}(t)}{2} \right) \tag{20}$$

The algorithm for the scalar field variable is now

$$\psi_{ij}(t + \Delta t) = \psi_{ij}(t) + \Delta t\, D \nabla^2 \psi_{ij}(t) - \Delta t \vec{\nabla} \cdot (\vec{v}_{ij}(t)\, \psi_{ij}(t)) \tag{21}$$

where we have used a symmetric form for the discrete gradient operator.[13] Then we proceed in the following way: we simulate $\eta(\mathbf{x}, t)$ during enough time to be sure that we are in an isotropic and homogeneous steady state.

Once this has been accomplished, we start the simulation of Eq. (21) with the initial condition

$$\psi(32, 32; 0) = 1$$
$$\psi(i, j; 0) = 0; \qquad i, j \neq 32 \tag{22}$$

Now under the influence of the molecular diffusion D and the velocity field, the scalar spreads over all the lattice. At different time intervals we measure the variance, Eq. (11), and from it we get $\bar{D}_{\text{eff}}$ using Eq. (14).

Actually some remarks are worth making in relation to the temporal evolution of the variance (Fig. 1). At the beginning the dispersed scalar needs a certain time to become effectively convected by the turbulent fluid. This gives rise to a transient behavior from an initial regime dominated by pure molecular diffusion to a later one where turbulent dispersion predominates. On the other hand, as time increases, finite-size effects begin to play a role and the dispersion of the passive scalar is bounded due to the periodic boundary conditions here prescribed. As a consequence, $\bar{D}_{\text{eff}}$ would artificially decrease to zero. Between these two regimes, $\bar{D}_{\text{eff}}$ is evaluated along the flattest part of the time evolution of the variance. In Fig. 1 we also show for the sake of comparison the onset of the pure molecular diffusive regime when convection is totally absent.

In Fig. 2 a log–log plot of $\Delta D = \bar{D}_{\text{eff}} - D$ versus $u_0^2 t_0$, this last quantity obtained through the simulation of the velocity field and using the rhs of Eq. (9), is presented for different values of the time scale t_0. The most important conclusion is that according to our theoretical predictions, the effective simulated diffusivity fits better the theoretical result as t_0 decreases. On the other hand, an important remark is worth making concerning the discrepancies observed at larger values of t_0. Actually these deviations

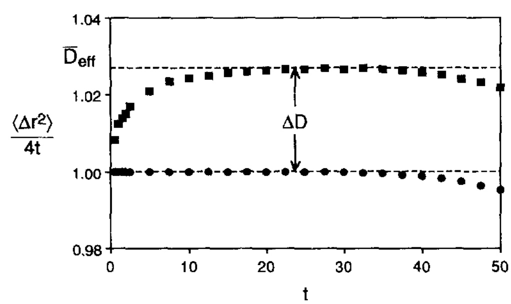

Fig. 1. Time evolution of the dispersion $\langle \Delta r^2 \rangle / 4t$ from direct numerical simulation of Eq. (21) with $D = 1.0$, $\varepsilon = 10.0$, $\tau = 0.1$, and $\lambda = 2.0$ (■). Circles stand for the pure molecular diffusion regime.

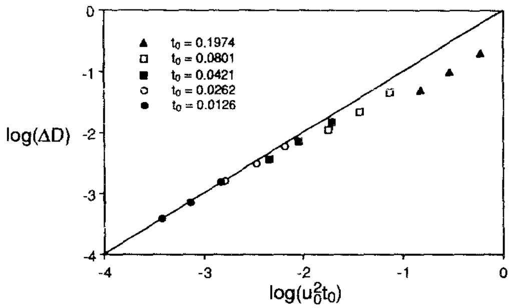

Fig. 2. A log–log plot of ΔD versus $u_0^2 t_0$ computed from direct numerical simulation of Eqs. (21) and (9), respectively, for different values of t_0. For all points, $D = 1.0$ and $\tau = 1.0$. (▲) $\lambda = 1.0$, (□) $\lambda = 2.0$, (■) $\lambda = 3.0$, (○) $\lambda = 4.0$, and (●) $\lambda = 6.0$. The three points for each symbol correspond to $\varepsilon = 5.0$, 10.0, and 20.0, respectively.

should be considered as somewhat spurious since according to the way our results have been plotted in Fig. 2, the largest values of t_0 correspond to the smallest values of λ, actually comparable to the pescribed lattice mesh in our spatial discretization procedure. An extended presentation of the work here reported, where this question will be properly addressed, and comprising a more detailed discussion of our results in relation to both the turbulent velocity field characterization and the dispersion experiments, will be published elsewhere.

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