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1990 J. Phys. A: Math. Gen. 23 3307

(http://iopscience.iop.org/0305-4470/23/14/027)

J. Phys. A: Math. Gen. **23** (1990) 3307-3315. Printed in the UK

Anisotropic diffusion in fluids with steady periodic velocity fields

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Received 11 December 1989

Abstract. We study the effective diffusivity tensor **D** for a contaminant carried by a steady periodic two-dimensional velocity field, in the limit of small molecular diffusivity χ. We discuss a generic model where the transport process is strongly anisotropic for the presence of channels (where, if one neglects Brownian motion, the motion is ballistic) among the convection cells. It is shown that for the longitudinal (along the channels direction) diffusivity one has: $D_{\parallel} \propto 1/\chi$, while for the transverse diffusivity: $D_{\perp} \propto \chi$. The behaviour $D_{\parallel} \sim D_{\perp} \propto \chi^{1/2}$, which is typical of the Rayleigh-Bénard system, is found to hold at intermediate values of χ. The scaling arguments are supported by extended numerical simulations.

1. Introduction

Transport in fluids is a complicated and fascinating phenomenon which moreover has a great interest from practical and applicative purposes [1]. Taking into account the molecular diffusion, it can be described by the following Langevin equation:

$$\frac{\mathrm{d}\boldsymbol{x}}{\mathrm{d}t} = \boldsymbol{u}(\boldsymbol{x}, t) + \boldsymbol{\eta}(t). \tag{1.1}$$

In (1.1) $\boldsymbol{u}(\boldsymbol{x}, t)$ is the velocity at the position $\boldsymbol{x}$ at the time t and $\boldsymbol{\eta}$ is a white noise such that

$$\langle \eta_i \rangle = 0 \qquad \text{and} \qquad \langle \eta_i(t)\eta_j(t') \rangle = 2\chi\delta_{ij}\delta(t-t')$$

where χ is the molecular diffusion coefficient. It is important to stress that transport and diffusion properties are affected by the presence of Lagrangian chaos [2], i.e. the chaotic behaviour in the motion of a fluid element described by the deterministic equation

$$\frac{\mathrm{d}\boldsymbol{x}}{\mathrm{d}t} = \boldsymbol{u}(\boldsymbol{x}, t). \tag{1.2}$$

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0305-4470/90/143307+09$03.50

The dispersion of a contaminant in a fluid is thus the result of two different effects: Lagrangian chaos and molecular diffusion. In general, it is much faster than expected by considering only the molecular effects. Let us recall that the Lagrangian chaos can be present even if the velocity field $\boldsymbol{u}(\boldsymbol{x}, t)$ is not chaotic [3]. Moreover a chaotic velocity field is neither a necessary nor a sufficient condition (although strange enough) for the Lagrangian chaos, as shown in the Lorenz model [4]. Real fluids practically always have a certain degree of Lagrangian chaos, e.g. in 2D one just needs that the stream function be time dependent. The understanding of the diffusion process thus is a very hard task, since it may depend in a complicated way on the detailed structure of the velocity field.

Two limit situations have nowadays been treated:

(i) fully developed turbulence, where the molecular effect can be ignored on a large range of scales;

(ii) fluids where (1.2) is quasi-integrable and the degree of Lagrangian chaos is very small.

It is clear that the latter case can be highly non-trivial. For this reason, it is important to study simple integrable velocity fields (in 2D corresponding to time-independent stream functions), with the addition of a noise term.

The main object of our paper is the effective diffusivity given by the covariance tensor:

$$D_{ij} = \lim_{t\to\infty} \frac{1}{2t} [\langle (x_i(t) - \langle x_i \rangle)(x_j(t) - \langle x_j \rangle) \rangle]. \tag{1.3}$$

Here $\boldsymbol{x}$ is the position of the passive impurity and the average $\langle \ldots \rangle$ is taken over an ensemble of test particles. The indices $i, j = 1, \ldots, d$ label the components of $\boldsymbol{x}$. We want to focus our attention to the study of transport in the presence of convection rolls and molecular diffusion.

A widely studied flow, in the context of 3D Lagrangian chaos is the Arnold-Beltrami-Childress (ABC) flow [3, 5], described by the velocity field:

$$\boldsymbol{u} = (B \cos y + C \sin z, A \sin x + C \cos z, A \cos x + B \sin y). \tag{1.4}$$

This flow is one of the first examples of 3D Lagrangian chaos which, in addition, satisfies the Beltrami condition $\nabla \times \boldsymbol{u} = \text{constant} \cdot \boldsymbol{u}$.

We have analysed a steady and periodic in space velocity field obtained by projecting the ABC flow on the xy plane with $C = 0$, since in the recent literature the case $|A| = |B|$ has been widely discussed. Its qualitative behaviour models the Rayleigh-Bénard convection as the phase space consists of square cells separated by lines (separatrices) where the rotation period diverges. The dispersion of a passive impurity on large scale is impossible without the molecular diffusion that allows the jumping among different rolls. The relevant non-dimensional parameter is therefore the Peclet number which measures the relative importance of advection over diffusion

$$P_e = \frac{VL}{\chi}$$

where V and L are the typical rotation velocity and size of a cell. The Peclet number can be regarded as the ratio between the diffusive time L^2/χ and the turnover time $T_r \sim L/V$ in a cell. The limit $\chi \to 0$ is thus singular. For a large Peclet number, which is the physical interesting situation, the effective diffusivity has been found (theoretically

[6] and experimentally [7]) to scale as:

$$D_{ij} \propto \chi P_e^{1/2} = (VL)^{1/2} \chi^{1/2} \tag{1.5}$$

and thus to be larger than χ.

When $|A| \neq |B|$, narrow channels arise among the convection cells, in a direction which depends on the relative magnitude of $|A|$ and $|B|$. The motion of a test particle inside a channel appears to be ballistic and this enormously enhances the transport along the channels direction. The process is strongly anisotropic and can be regarded as due to long runs in the channels interrupted by trapping periods inside the rolls. The effect of a small noise (i.e. a small diffusivity χ), is responsible for the jumping in the direction transversal to the channels.

Our main result, supported by numerical simulations, is that the effective diffusion coefficients $D_\parallel$ (along the channels direction) and $D_\perp$ (along the direction transversal to the channels) are given, in the limit of small molecular diffusion, by

$$D_\parallel \propto \frac{L^2}{V} ||A| - |B||^3 \chi^{-1} \qquad \text{and} \qquad D_\perp \propto V ||A| - |B||^{-1} \chi. \tag{1.6}$$

The anisotropy enhancement seems to disappear for (not too large) values of χ where one recovers the $|A| = |B|$ scaling (1.5)

$$D_\parallel \sim D_\perp \propto (VL)^{1/2} \chi^{1/2}. \tag{1.7}$$

In section 2, we analyse the model in some detail, and give the arguments which lead to the scaling behaviour (1.6) and (1.7) of the covariance tensor as a function of the Peclet number and channel width (i.e., as a function of χ and $|A| - |B|$). In section 3, we describe the numerical simulations which support our rough perturbative arguments. In section 4, the reader can find the conclusions and a discussion on the relevance of our model for the description of the dispersion in some situations.

2. The model and the scaling arguments

We study the Langevin equation (1.1) in two dimensions with $\boldsymbol{u}$ the velocity field obtained by projecting the ABC flow with $C = 0$ on the x-y plane:

$$\boldsymbol{u} = (B \cos y, A \sin x) \qquad \boldsymbol{x} = (x, y). \tag{2.1}$$

By a suitable choice of length and time units, we have $L = O(1)$ and $V = O(1)$; so we can set $B = 1$ and $A = -(1 + \delta)$. In the following in all the relations among quantities with dimensions we omit multiplicative factors $O(1)$, such as L and V. The stream function becomes $\psi = -\sin y + (1 + \delta) \cos x$. For $\delta = 0$ the field (2.1) describes convection cells of width 2π where the motion of a test particle is always periodic in the absence of a noise term. The separatrices are the lines where the stream function is zero (for $\delta = 0$) and they cross in the unstable hyperbolic fixed points of the flow (see figure 1(a)). When $\delta > 0$ the border lines between cells do not coincide and there appear channels along the y direction (see figure 1(b)). By simple perturbative calculations one finds that for small δ the width of a channel is $\sim \delta$, although the maximum distance between the separatrices increases up to $\sim \delta^{1/2}$ near the unstable fixed points. Note that $\delta < 0$ corresponds to channels along the x axis. The motion of a particle inside the channels, if one neglects Brownian motion, is ballistic and the velocity field changes sign between neighbouring channels. The basic mechanism of

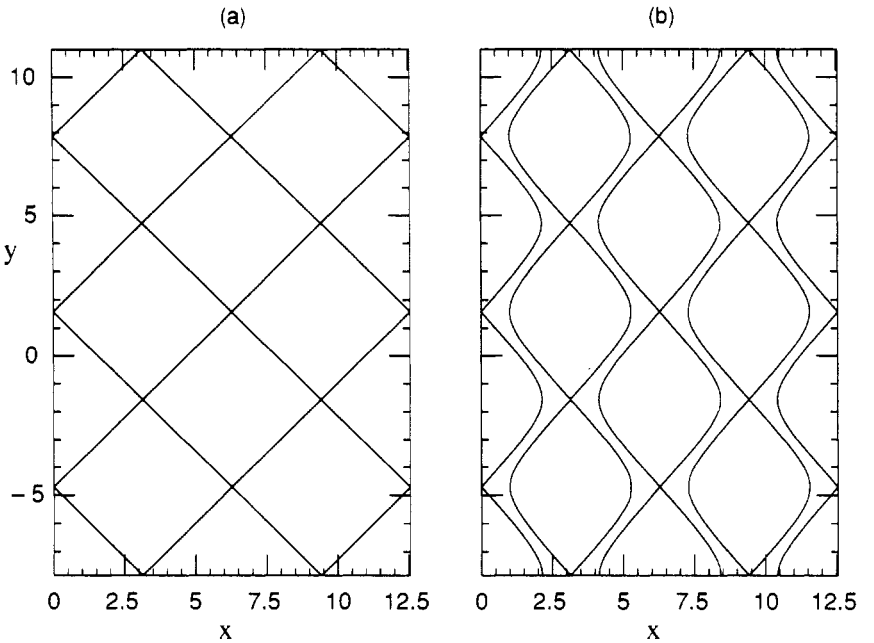

Figure 1. Structure of the separatrices for equation (1.2), with the field (2.1) and: (*a*) $A=-1$, $B=1$; (*b*) $A=-1.3$, $B=1$.

the transport is illustrated in figure 2. For small χ, a test particle can jump into a channel, because of molecular diffusion. Then, one has a ballistic motion inside the channel (with velocity $V_c \sim O(1)$ either in the up or in the down y direction) stopped by a capture from a cell after a time $T_c \sim \delta^2/\chi$, and so on. Let us consider the case for which the ratio

$$T_c/T_r \gg 1 \qquad \text{i.e.} \qquad \delta^2/\chi \gg 1$$

since $T_r \sim O(1)$. This dimensional estimate of the diffusive times in the channels allows us to compute the effective diffusivity tensor, that in our coordinates is diagonal with

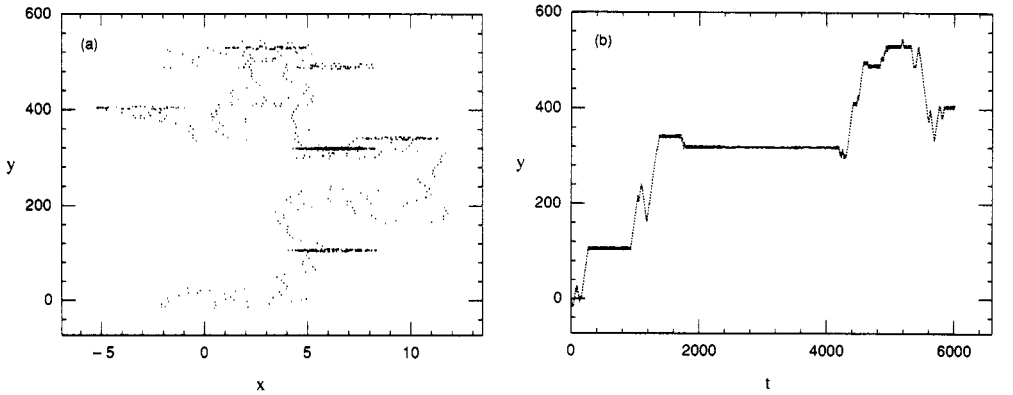

Figure 2. (*a*) 1000 positions (recorded every 6 units of time) of one particle driven by equation (1.1) with the field of figure 1(*b*) and $\chi = 0.001$. (*b*) y against t for the same particle.

$D_\perp = D_{11}$ and $D_\parallel = D_{22}$. The typical length run along a channel is easily seen to be

$$L_c \sim T_c V_c \sim \delta^2/\chi. \tag{2.2}$$

The probability p to find a particle in a channel is proportional to its width $\sim\delta$, and thus we obtain:

$$D_\parallel \sim p\frac{L_c^2}{T_c} \sim \frac{\delta^3}{\chi}. \tag{2.3}$$

On the other hand, the transport in the x direction can be described as a random walk where the timestep is T_c and the length step is the cell width $\sim 2\pi$. This leads to

$$\frac{\langle (x(t)-\langle x\rangle)^2\rangle}{4\pi^2} \propto p\frac{t}{T_c} \tag{2.4}$$

so that one obtains

$$D_\perp \sim \frac{\chi}{\delta}. \tag{2.5}$$

We remark that the presence of the ballistic channels produces strong changes in the diffusion coefficients: from $D_\parallel = D_\perp \sim \chi^{1/2}$ to $D_\parallel \sim \delta^3/\chi$ and $D_\perp \sim \chi/\delta$.

Let us stress that these arguments are valid only in the limit of large T_c/T_r. By this we mean that the time spent in the channels should be large with respect to the circulation time T_r, i.e., $\chi \ll \delta^2$. When T_c/T_r becomes smaller than unity, a particle has not enough time to perform a significant run along a channel between two successive trappings. Practically, the transport process can be described as if there were no channels. In this limit ($\chi \to 0$, $\delta \to 0$, with $T_c/T_r \sim 1$), the anisotropy disappears and, using the analysis developed by Pomeau and other authors [6] for a two-dimensional cellular structure without channels (case $\delta = 0$), one expects $D_\perp \sim D_\parallel \propto \chi^{1/2}$.

3. Numerical study of the model

We have verified our simple dimensional argument, by a numerical analysis of the model. We let $N = 1000$ test particles evolve, uniformly distributed in the square $(0, 2\pi) \times (0, 2\pi)$, and computed the covariance

$$\sigma_i^2(t) = \frac{1}{N}\sum_{k=1}^{N}\left[x_i^{(k)}(t) - \frac{1}{N}\sum_{j=1}^{N} x_i^{(j)}(t)\right]^2. \tag{3.1}$$

The indices k and j label the particles and $i = 1, 2$ indicate the x, y component of the vector $\boldsymbol{x}$. The effective diffusivity tensor is thus given by:

$$D_\perp = \frac{1}{2}\lim_{t\to\infty}\frac{1}{t}\sigma_1^2(t) \qquad D_\parallel = \frac{1}{2}\lim_{t\to\infty}\sigma_2^2(t). \tag{3.2}$$

The numerical integration of the Langevin equation has been performed by the Runge-Kutta algorithm, modified in order to take into account the white noise term [8], with an integration step $\Delta t = 0.01$. In order to get the limits in (3.2) stabilised, we had to follow the ensemble evolution for $\sim 20\,000$ time units (i.e. 2×10^6 integration steps), when $\chi > 10^{-4}$, and for $\sim 80\,000$ time units when $\chi < 10^{-4}$. The point with $\chi = 1 \times 10^{-6}$ has been obtained with $t = 340\,000$. In figure 3 we show the longitudinal

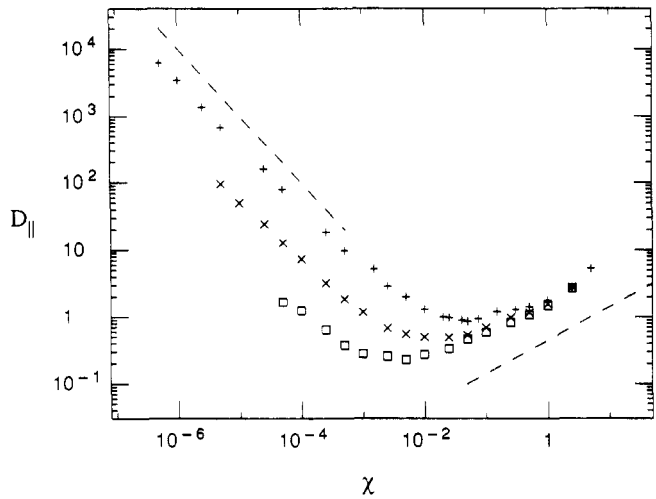

Figure 3. The longitudinal diffusion coefficient against the molecular diffusion coefficient for the field (2.1) and: $|A|-|B|=0.30$ (+), 0.15 (×), 0.075 (□). The (broken) lines with slopes −1 and 1/2 are drawn for comparison. The numerical errors bar are comparable with the symbols size.

diffusivity $D_{\|}$ as a function of the molecular diffusivity χ. At large $T_c/T_r \simeq \delta^2/\chi$, which is the control parameter in our model, we observe the expected scaling $D_{\|} \propto 1/\chi$, while at larger molecular diffusion ($\chi > \delta^2$) one recovers the standard scaling law for cell convection $D_{\|} \propto \chi^{1/2}$. Let us stress that, following our arguments, one expects a minimum of the longitudinal diffusivity $D_{\|}$ at the transition between the two scaling regimes. By assuming $D_{\|} \sim \delta^3/\chi \sim \chi^{1/2}$, one thus sees that the transition takes place when the control parameter T_c/T_r becomes O(1), that is for $\chi \sim \delta^2$. Finally, figure 4(*a*) shows that for large T_c/T_r, as predicted by equation (2.3), the longitudinal diffusivity $D_{\|}$ scales as δ^3/χ. In the same region the transverse diffusivity $D_{\perp}$ exhibits the scaling behaviour δ/χ, in accord with equation (2.5) (see figure 4(*b*)). Let us note that the agreement between the numerical data and the results of section 2 is rather

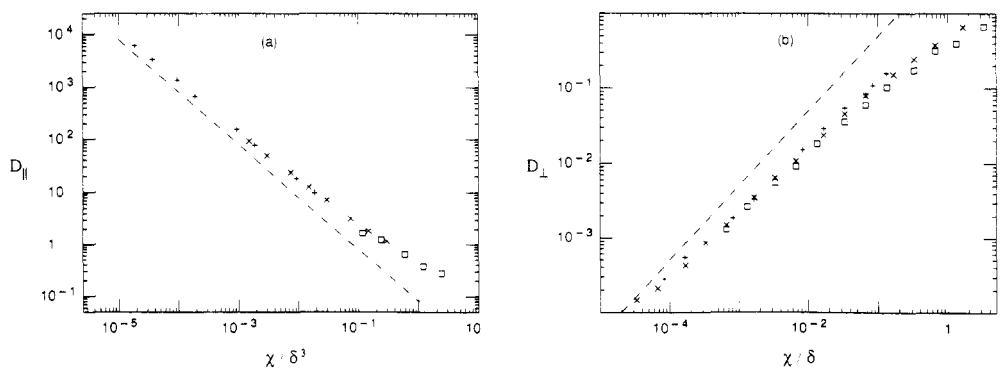

Figure 4. (*a*) The longitudinal diffusion coefficient against χ/δ^3 (together with a dashed line of slope −1). (*b*) The transverse diffusion coefficient against χ/δ (together with a broken line of slope 1). The symbols refer to $\delta = |A|-|B| = 0.30$ (+), 0.15 (×), 0.075 (□). The numerical errors bar are comparable with the symbol size.

good for $D_{\parallel}$, but only fair for $D_{\perp}$. This is because our scaling arguments of section 2 do not consider in (2.3) and (2.5) an additional linear term in χ due to the bare molecular diffusion. This is negligible for $D_{\parallel}$ but not for $D_{\perp}$ if δ is not very small.

We have also computed the value of the kurtosis

$$K_i(t) = \frac{1}{N\sigma_i^4(t)} \sum_{k=1}^{N} \left[x_i^{(k)}(t) - \frac{1}{N} \sum_{j=1}^{N} x_i^{(j)}(t) \right]^4 \tag{3.3}$$

in order to have a quantitative indication of the flatness of the spreading distributions in the x and y directions. For large t the kurtosis seems to tend to the Gaussian value $K_i = 3$. Let us stress that in spite of the apparently 'anomalous' diffusion process (long runs interrupted by trappings), the diffusion is standard and Gaussian.

4. Concluding remarks

We have proposed a simple mechanism of anisotropic contaminant transport which is quite general in two- and three-dimensional steady periodic flows. The presence of ballistic channels is indeed a common feature of a large class of transport phenomena. We thus believe that our model can be a useful tool in many cases. In fact this model presents the same behaviour of the dispersion of a contaminant for laminar flows in long straight tubes or channels. By the direct analysis of the equation for a scalar field θ passively advected

$$\partial_t \theta + \nabla \cdot (\boldsymbol{u}\theta) = \chi \Delta \theta. \tag{4.1}$$

Taylor [9] has shown that there is a strong enhancement of the longitudinal diffusivity $D_{\parallel}$, while the radial inhomogeneities are smoothed out:

$$D_{\parallel} = \frac{\hat{\delta}^2}{\chi} \frac{U^2}{48} + \chi \tag{4.2}$$

where $\hat{\delta}$ is the radius of the tube, and U the average velocity of the flow. Note that (4.1) is the Fokker–Planck equation related to the Langevin equation (1.1). The first term of the RHS of (4.2) always dominates, because $\hat{\delta}^2 U^2/\chi^2$ is very large ($\gg 1$), except for the case of very slow flows and/or extremely fine capillaries. The presence of transverse velocity gradients causes the sharp increase of $D_{\parallel}$. It is worth stressing that the larger the molecular diffusion the smaller the longitudinal dispersion. It is not difficult to understand that the leading term in (4.2) can be obtained by the arguments discussed in section 2. The dependence on $\hat{\delta}^2$ instead of δ^3 is due to the fact that here all the particles contribute to the diffusion, while in the case studied in section 2 only a fraction $p \sim \delta$ contributes to $D_{\parallel}$.

We now briefly discuss the connection of our work with the study of the transport properties of chaotic deterministic systems (i.e. without molecular diffusion).

Let us remark that we have described a picture for the transport which is very similar to the scenario which has been actually observed in the truncated 2D Navier–Stokes equations [10]. Near the critical Reynolds number Re_c, for which the stream function $\psi(x, t)$ becomes time dependent via a Hopf bifurcation (a general mechanism for the onset of Lagrangian chaos in 2D systems), one has, if $\mathrm{Re} = \mathrm{Re}_c + \varepsilon$, $\psi(x, t) = \psi_0(x) + \varepsilon^{1/2} f(x, t) + O(\varepsilon)$ where $f(x, t)$ is periodic in time. The separatrices structure given by $\psi_0(x)$ is qualitatively equal to the one shown in figure 1(*b*) (see figure 3 of reference [4]). Chaotic layers appear around the separatrices and the diffusion takes place for $\varepsilon > \varepsilon_c$. The test particle is thus trapped for long times in a small limited

region (where it performs an irregular motion) and then escapes along ballistic channels until a subsequent trap. The qualitative behaviour of the tensor **D** is found to be the same as the one given by the Langevin equation: the longitudinal diffusivity diverges approaching ε_c, $D_{\parallel} \propto (\varepsilon - \varepsilon_c)^{-1/2}$; while the transversal diffusivity vanishes as $D_{\perp} \propto (\varepsilon - \varepsilon_c)^{1/2}$. In a rough way, equation (1.1) with an integrable velocity field can be regarded as a crude approximation of a Lagrangian chaotic system described by equation (1.2). In this sense, the perturbation strength $(\varepsilon - \varepsilon_c)^{1/2}$ plays the role of the noise variance χ.

We must note that Lagrangian chaos is also possible in 3D steady space-periodic flows. One then may conclude that a contaminant is dispersed by the flow. However, regular trajectories along ballistic directions appear for 3D generic chaotic flows. For instance, figure 5 shows the positions of 1000 particles, which are initially uniformly distributed in the cube $(0, 2\pi) \times (0, 2\pi) \times (0, 2\pi)$, after a time $t = 10\,000$ for the full 3D ABC flow (1.4) with parameters $A = 1.15$, $B = 1$, $C = 0.1$. One sees that some particles (spots very far from the origin) have run ballistic trajectories. This provides evidence that, for every initial condition, Lagrangian chaos without molecular diffusion is not sufficient to disperse a contaminant in 3D steady velocity fields, such as those describing convection roll structures. On the contrary, without a molecular diffusion mechanism, the dispersion of contaminants is obtained for all initial conditions only when velocity fields are time-dependent, both in 2D and 3D. We want to note, finally, that in the case of 2D time-dependent velocity field an anomalous diffusion (i.e. $\sigma_i^2(t)$ not linear with t) has also been observed [11].

After the completion of this paper we received reference [12] in which similar results have been obtained by a different method.

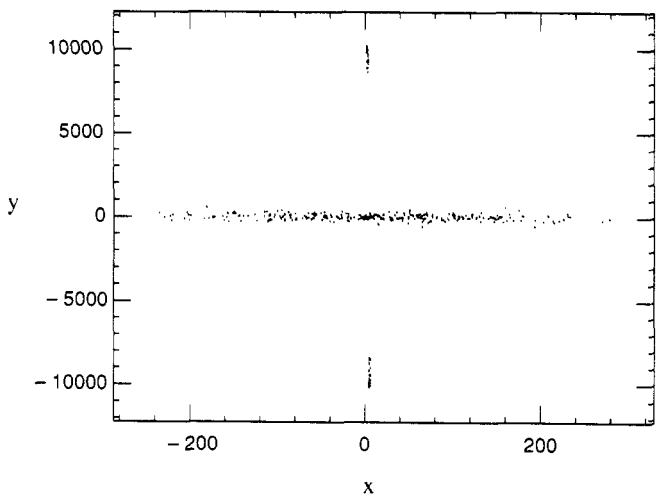

Figure 5. The positions in the x-y plane of 1000 particles, initially in a cube of side 2π at the origin of the axes, after they evolved for 10 000 units of time according to the 3D ABC flow.

Acknowledgments

We thank S Childress and A M Soward for sending us reference [12].

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