Applications of stochastic particle models to oceanographic problems

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Abstract

Three Markovian particle models are reviewed, providing a hierarchy of increasingly detailed descriptions of particle motion and dispersion. Model 1 assumes that the scales of turbulent motion are infinitesimal, and it is equivalent to the advection-diffusion equation. Model 2 introduces a finite scale T for the turbulent velocity,, and model 3 introduces an additional scale for the acceleration, $T_a < T$. The models are compared with oceanographic data from drifting buoys, which satisfactorily approximate the motion of ideal particles in mesoscale turbulent fields. Model 2 appears to provide a satisfactory description of the second order particle statistics in the upper ocean. Model 3 appears to be applicable to deep ocean data with some questions still remaining open. Some examples of analytical calculations of dispersion using the models are shown for some simple oceanographic flows. The results indicate that the introduction of finite scales of turbulence plays an important role not only at initial times, $t < T$, but also for dispersion at longer times if the mean flow is strongly dependent on space and time, so that the scales of the mean flow and of the turbulence are of the same order. In these situations, which are characteristics of important current systems in the ocean, the advection-diffusion equation is not accurate, and the use of stochastic models such as 2 and 3 is especially indicated. Two different classes of applications for the models are reviewed: "direct" applications, where the models are directly integrated to compute dispersion, and "inverse" applications where the models are used to extract information about the velocity field from the Lagrangian data. A discussion is also provided on future applications of the models to study more general classes of oceanic flows including coherent structures.

1. Introduction

The use of stochastic particle models has a long history in dispersion studies (e.g. Chandrasekhar, 1943). Here we focus on some examples of models which are useful in the study of the ocean. The specific nature of the oceanic processes is discussed, a review of recent progress is provided, and a number of open questions is pointed out, which can lead to new areas of research and applications.

The main difficulty in the study of the ocean is the infinite number of scales participating in the motion, ranging from the planetary scales of the general circulation (thousands of km) to the scales of molecular motion. Analytical and numerical treatments involving all these scales are not feasible, so that the oceanographic problems are usually approached isolating first the scales of interest (characterized by the mean flow $\mathbf{U}$) and deriving approximated equations for them. In order to obtain a closed formulation for the scales of the mean field, the smaller scales, (usually indicated as turbulence $\mathbf{u}$), have to be parameterized in terms of the mean field.

In the study of tracer dispersion, the simplest parameterization is obtained using the same "scale separation" arguments that are used for molecular diffusion, i.e. by assuming that the scales of the turbulence are infinitesimal compared with the scales of the mean field (Taylor, 1921). Under this assumption, the equation which describes the evolution of the mean tracer concentration C is the same as for molecular diffusion, i.e. it is the advection-diffusion equation (5) with the molecular diffusivity coefficient replaced by an "eddy-diffusivity" coefficient K. The eddy-diffusion coefficient is several orders of magnitude larger than the molecular diffusivity and it parameterizes the action of the turbulent vortices (eddies) on the mean field. In the following, we focus on applications valid for mesoscale dispersion, i.e. for dispersion due to eddies with scales of 50-100 km acting on the large scales of the general circulation.

As noticed by a number of authors (e.g. Davis, 1987; Holloway, 1989; Zambianchi and Griffa, 1994), the applicability of the advection-diffusion equation is often questionable for oceanographic problems, because in most flows there is no clear gap betweeen scales, so that the scale separation hypothesis does not strictly hold. Despite this problem, the advection-diffusion equation is widely used in oceanography, mainly because it is simple and straightforward to implement. Generalizations of the advection-diffusion equation (generalized "K-models"), where the scale separation hypothesis is relaxed, are available in the literature (e.g. Davis, 1987) , but they are not frequently used in practical applications because of the difficulties in their implementation.

In this paper an alternative class of models for dispersion is discussed, based on the use of stochastic equations for particle motion. These models

combine the advantage of being generalizable to less stringent assumptions than the advection-diffusion equation, while maintaining a simple implementation. The models describe the motion of "single" particles, i.e. of ensembles of particles independently launched in different realizations of the turbulent flow. Since the particles can be thought of as belonging to a tracer, their concentration corresponds to the (normalized) ensemble average concentration C of the tracer itself (e.g. Csanady, 1980).

We remark that the particle models can also be used as a diagnostic tool for the interpretation of data from Lagrangian (i.e. current followers) instruments. These instruments, which have become increasingly popular in the last two decades, play a major role in providing oceanographic data at global scales. They consist of drifing buoys designed to follow the currents at the ocean surface or in the interior, reporting their position at discrete times either acoustically or via satellite (for a review on Lagrangian measurements the reader is referred to Davis, (1991a)). They provide, at least in the mesoscale range in which we are interested, a satisfactory approximation of the motion of ideal particles, so that they are perfectly suitable to be interpreted and explained in terms of particle models.

In this paper, three Markovian models are discussed in some depth, providing a hierarchy of increasingly detailed descriptions of particle motion. The first model (model 1) corresponds to the classic "random walk" model, and it assumes that the particle position $\mathbf{x}$ is a Markov variable. This model assumes that the scales of the turbulence velocity are infinitesimal and it is equivalent to the advection-diffusion description (5). Model 2, which is sometimes referred to as a "random flight" model (van Dop et al., 1985), assumes that the particle position $\mathbf{x}$ and the turbulent velocity $\mathbf{u}$ are jointly Markovian. Finally, model 3 (Sawford, 1991) assumes that $\mathbf{x}$, $\mathbf{u}$ and the turbulent acceleration $\mathbf{a}$ are jointly Markovian. Physically, models 2 and 3 correspond to the introduction of a finite scale for the velocity and the acceleration, respectively. Extensive literature is available for these models, including a number of meterological applications focused on dispersion at relatively small scales (discharges in local regions and valleys, e.g. Thomson, 1986). Here we focus on those aspects of the models that are relevant for oceanographic applications and in particular for applications at the scales of the general circulation and of the mesoscale. We stress the comparison of the models with the data, and illustrate typical oceanographic scales and situations where the use of models 2 and 3 is especially indicated.

In Section 2, a review of the general characteristics of the three models is given, while the details for Model 1, 2, 3 are given in Section 3, 4, 5 respectively. A comparison between the performance of the advection-diffusion equation and model 2 is shown in Section 6, whereas in Section 7 a discussion is presented of the practical applications of the models. A summary and a general discussion are provided in Section 8.

2. General characteristics of the models 1, 2, 3.

The three models 1, 2 and 3 describe the motion of single particles. Each particle is independently launched in a different realization of $\mathbf{u}$, and the statistics are computed by averaging over ensembles of particles launched from the same position in space. In these models, since the particles are independent, $\mathbf{u}$ can be considered as a purely time-dependent process, which represents the turbulent velocity encountered by the particle during its motion. This allows for a substantial simplification compared with the space-dependent representation of $\mathbf{u}$ necessary to study two-particles or higher order statistics.

The three models are Markovian, i.e. they describe processes whose conditional probability density at time t_n depends only on the process value at the earlier time t_{n-1}. The Markov property is valid for a wide class of physical processes. It represents the generalization to probabilistic systems of the deterministic property of unique dependence on the initial conditions, which is characteristic of all the systems obeying first-order differential equations. Considered in this light, the assumption of Markovian turbulent velocity appears motivated and natural. The real velocity field, in fact, obeys the Navier Stokes equations, which are of first order in time. As a consequence, the time evolution of the velocity is uniquely determined by the initial conditions, and in the presence of a stochastic forcing or pertubation, it is a Markovian process.

The models 1, 2 and 3 are simple examples of a general class of stochastic models called generalized Langevin equations (e.g. Risken, 1989), which can be nonlinear and have arbitrary dimensions N:

$$ds_i = h_i(\mathbf{s}, t)dt + g_{i,j}(\mathbf{s}, t)d\mu_j \tag{1}$$

where $i = 1, N$, $d\mu_i$ is a random increment, and h_i and $g_{i,j}$ are continuous functions. The behaviour of stochastic processes such as $\mathbf{s}$ is characterized by their probability density function P. The evolution equation for the probability density P of a Markovian process as (1) is called the Fokker-Planck equation (or forward Kolmogorov equation). The Fokker-Plank equation, which has the form of a partial differential equation, can be derived from the stochastic equations (1) using a procedure which is conceptually quite difficult, but by now well known and standadized (e.g. Risken, 1989). The Fokker-Plank equations for our specific models will be introduced and discussed in the following.

We terminate this Section remarking that the main discussion of the three models in Sections 3, 4 and 5 will be done using some simplifyng assumptions. More general forms of the models valid for more general conditions are available (a discussion is included in Section 4), but the simplyfing assumptions allow for a clear presentation of the fundamental properties of the models and of their relationships, while maintainig a general physical

validity. The assumptions can be summarized as follows:

1) the velocity field is 2-dimensional and on an infinite domain. The assumption of 2-dimensional motion is appropriate for mesoscale phenomena (e.g. Davis, 1991b), since the particles move mainly on isodensity surfaces (e.g. on the ocean surface or on interior isopycnals). The simplification of an infinite domain is acceptable for the description of the ocean interior, away from the boundaries,

2) the turbulent velocity field is homogeneous in space and stationary in time. The condition of homogeneity can be verified, at least partially, in selected regions of the ocean, typically in the subtropical interior regions, away from the boundaries and from the equatorial regions. The stationarity assumption is more difficult to satisfy, because the presence of low frequency variability makes the ocean circulation an essentially red spectrum process. This is a problem for any statistical description or analysis concerned with the description of average quantities or "typical" aspects of the ocean. This difficulty is usually overcomed acknowledging that the mean quantities are in reality only "averages over some finite time, representing a particular ocean climate" (Davis, 1991b). Notice that we allow inhomogeneity and nonstationarity to occur in the mean flow $\mathbf{U}(\mathbf{x}, \mathbf{t})$. This a suitable choice, since the main sources of inhomogeneity and nonstationarity in the ocean are indeed given by the mean flow.

3) the two components of the velocity are independent. This condition is the least essential of the three, and it is introduced solely in order to simplify the notation in the following. Since each component is independent, in fact, the models can be written in 1-dimensional form, for each component separetely.

3. Model 1. Markovian x

Under the assumptions stated in Section 2, the equations that describe the particle motion for Model 1 can be written, for a single component, in incremental form as

$$dx = U dt + d\hat{x} \tag{2}$$
$$d\hat{x} = (K)^{1/2} dw \tag{3}$$

with

$$K = \sigma T, \tag{4}$$

and $x(0) = 0$. In the above expressions, for the selected component, dx is the total displacement of the particle during the time dt; $d\hat{x}$ is the displacement due only to the turbulent velocity; $U(\mathbf{x}, t)$ is the mean flow; K is the diffusion coefficient; σ is the turbulent velocity variance; T is the turbulent time scale; $dw(t)$ is a random increment from a normal distribution with zero mean and second order moment $< dw \cdot dw >= 2dt$. Notice that the turbulent time scale T in (4) must be $T = dt/2$ in order to have the correct turbulent velocity variance from (3), $< (d\hat{x}/dt)^2 >= \sigma$.

Physically, the equations (2)-(3) describe the displacement of a particle as resulting from two contributions. The first one is due to the mean flow and it is represented deterministically by the increment $U dt$, the second one, $d\hat{x}$, is due to the turbulence and it is represented as a stochastic process uncorrelated from one time step to the next. This means that the particle moving through the fluid receives at each time step a random impulse due to the action of the incoerent turbulent motions, and it "loses memory" of its previous turbulent momentum.

Another way of saying this is that the model describes a turbulent motion whose typical scale T is infinitesimal (of order dt) with respect to the other time scales of the problem. This means that T is small with respect to the scales of U, and it is also small with respect to the actual time t. In other words, the initial transient, $t < T$ is not described by the model (2)-(3) which applies only for asymptotic times $t >> T$.

The Fokker-Planck equation associated with model 1, in 2-dimensions and for an incompressible flow ($\nabla \cdot \mathbf{U} = 0$) is

$$\partial P/\partial t = -\mathbf{U} \cdot \nabla P + \nabla(\mathbf{K}\nabla P) \tag{5}$$

with $P(x_1, x_2, 0) = \delta(x_1)\delta(x_2)$. In (5), $P(x_1, x_2, t)$ is the probability density function that a particle launched at $(0,0)$ at time 0 is found at (x_1, x_2) at time t, and $\mathbf{K}$ is a diagonal tensor with non zero elements given by (4).

Notice that in the case of a tracer released at time $t = 0$ from a point source located at $\mathbf{x} = (0,0)$, the average tracer concentration C at $(\mathbf{x}, t)$ is connected to P in the following way:

$$C(\mathbf{x}, t) = QP(\mathbf{x}, t)$$

where Q is the total tracer mass released (see, e.g. Csanady, 1980). As a consequence, (5) is also the advection-diffusion equation for the average concentration C, with the eddy-diffusion coefficient K defined by (4). To have an idea of the order of magnitude of K for mesoscale motion, consider that T is of the order of 2-10 days, and σ is of the order of $10 - 10^2\ cm^2/sec^2$, so that K is of the order of $10^6, 10^7 cm^2/sec$.

4. Model 2. Joint Markovian x and u

The incremental equations for particle motion for Model 2 under the same assumptions as before are

$$\begin{aligned} dx &= (U+u)dt \qquad (6)\\ du &= -(1/T)u dt + (\hat{K})^{1/2} d\hat{w} \qquad (7) \end{aligned}$$

with

$$\hat{K} = \sigma/T = K/T^2 \tag{8}$$

and $x(0) = 0, u(0) = \hat{u}$, where $\hat{u}$ are drawn from a Gaussian distribution with mean zero and variance σ. In (7) and (8), $\hat{K}$ is the diffusion coefficient, and $d\hat{w}$ is a random increment with the same statistical characteristics as dw in (3).

Model 2 differs from Model 1 in the treatment of the turbulent velocity, which is not assumed to be uncorrelated from one time step to another. Rather, the turbulent velocity obeys the classical Langevin equation (7), stating that at each time step the particle loses only a fraction of its momentum, $U(dt/T)$, and in turn receives a random impulse $d\hat{w}$. As a consequence, the particle "conserves the memory" of its initial turbulent velocity during a finite time of order T. The autocorrelation function of u decays exponentially (e.g. Risken, 1989),

$$R(\tau) = \frac{< u(t)u(t+\tau) >}{\sigma} = e^{-\tau/T} \tag{9}$$

From (9) the time scale of the memory of the turbulent velocity T turns out to be also the integral time scale. T is arbitrary in the model (6)-(7), and it can be of the same order or larger than the other time scales in the problem, i.e. of the scales of U and of the actual time t.

Notice that, even though model 2 introduces the scale for the velocity which is absent in model 1, the acceleration is still assumed to have an infinitesimally small scale, as it is shown by (7) where the acceleration has a discontinuity at each time step dt. This limitation is physically more acceptable than the limitation of small velocity scales, since in real flows the time scales over which the acceleration is correlated are usually much shorter than the velocity time scales. In the following, a comparison with data will be performed to verify for which flows in the ocean the assumptions of infinitesimal acceleration scales are indeed acceptable.

The Fokker-Planck equation associated with model 2, in 2-dimensions is (van Dop et al., 1985):

$$\partial P/\partial t = -(\mathbf{U}+\mathbf{u}) \cdot \nabla P + \nabla_u(\mathbf{u}P/T) + \nabla_u(\hat{\mathbf{K}}\nabla_u P) \tag{10}$$

with $P(x_1, x_2, u_1, u_2, 0) = M\delta(x_1)\,\delta(x_2)\, e^{-\frac{u_1^2}{\sigma_1}} e^{-\frac{u_2^2}{\sigma_2}}$ where M is a normalization factor. In (10) ∇_u represents the gradient with respect to $\mathbf{u}$ and $\hat{\mathbf{K}}$ is a diagonal tensor with nonzero elements given by (8).

Notice that the probability density function $P(x_1, x_2, u_1, u_2, t)$ is now a function not only of the space variables $\mathbf{x}$ but also of the turbulent velocities $\mathbf{u}$. This is because the particle "remembers" the value of $\mathbf{u}$ for a finite time, so that the motion at each instant depends not only on the previous position but also on the turbulent velocity. Equation (10) can effectively describe also the transient processes occurring at time $t < T$, unlike equation (5) which is valid only for $t > T$.

4.1 Comparison of model 2 with numerical and oceanographic data. Model 2 describes a process with a turbulent velocity characterized by the exponential autocorrelation (9) and by an associated spectrum with normalized density

$$S(\omega) = (\frac{1}{\pi})\frac{1/T}{1/T^2 + \omega^2}. \tag{11}$$

The spectrum (11) is approximately white for frequencies lower than the cutoff frequency, $1/T$, and it decreases as ω^{-2} for higher frequencies.

A simple way to test the applicability of model 2 (at least for second order statistics) for real flows consists in verifying whether or not the autocorrelation (9) and the spectrum (11) are present in simulated and experimental data of turbulent motion.

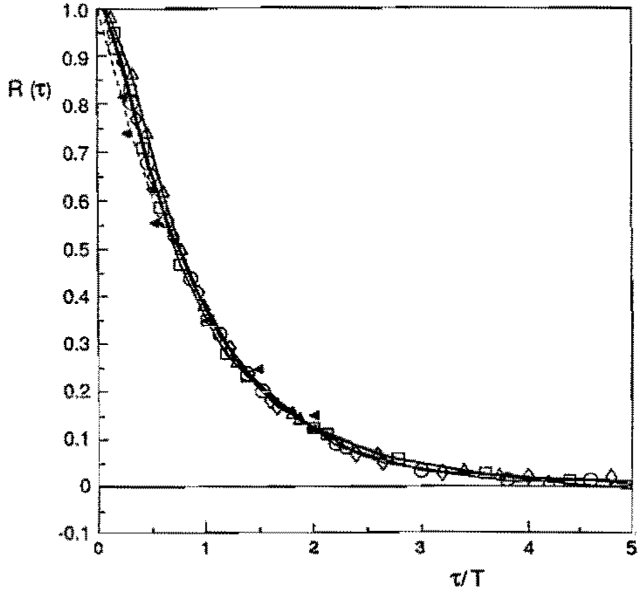

Figure 1. Velocity autocorrelations from particle simulations in isotropic turbulence (from Yeung and Pope, 1989). The dashed line is the exponential autocorrelation of model 2; the open symbols and lines are the Direct Numerical Simulations of Yeung and Pope (1989); the full symbols are from the experiments of Sato and Yamamoto (1987).

Tests in this direction have been done in the framework of 3-dimensional isotropic turbulence, considering the statistics of ensembles of particle trajectories in simulated velocity fields (Sato and Yamamoto, 1987; Yeung and Pope, 1989). For high Reynolds number, the results show that the autocorrelation is well represented by the exponential shape (9), except at very short time lags where the scale of the acceleration cannot be neglected (Fig. 1). For these scales, close to the origin $\tau \approx 0$, the autocorrelation computed from the simulated trajectories is smoother than the exponential curve predicted by model 2. For all the other lags, the exponential approximation appears to be very satisfactory. Positive results have also been found in numerical simulation (Verron and Nguyen, 1989; Davis, 1991b) reproducing mesoscale turbulent flows in the upper ocean. The exponential shape is found to represent very accurately a wide class of flows of this type, characterized by various wavenumber spectra.

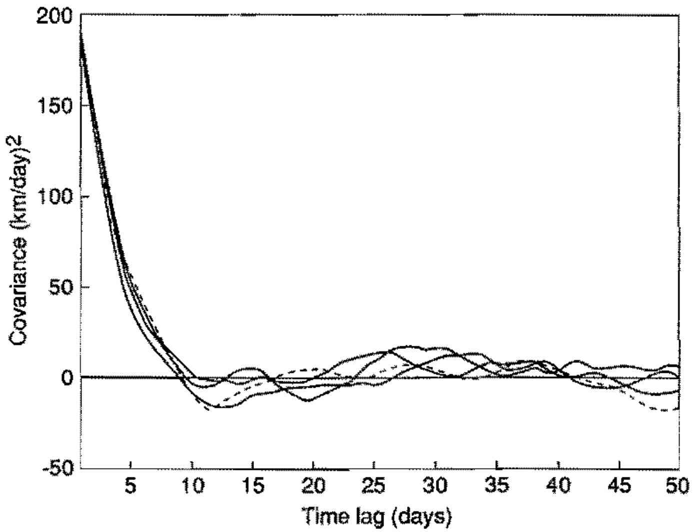

Figure 2. Velocity covariance from drifting buoys in the Brazil Malvinas Current (dashed line) and from particle simulations using model 2 (continuous lines) (from Griffa et al., 1995).

Concerning the experimental oceanographic data, a good agreement is found with model 2 for upper ocean mesoscale flows in approximately homogeneous regions (e.g. Krauss and Boning, 1987; Colin de Verdiere, 1983). Most data of this type, in fact, are characterized by spectra with a ω^{-2} slope at frequencies higher than a cutoff value, and the corresponding autocorrelations have a shape qualitatively similar to the exponential curve. A closer inspection of the autocorrelations shows some additional interesting features. First of all, the autocorrelations computed from the oceanographic data usually do not deviate significantly from the exponential shape at small time lags (unlike the simulated isotropic turbulence data) (Fig. 2). This can be understood by considering that for these flows the scale of the velocity T is of the order of 2-10 days, whereas the scale of the acceleration is of the order of one day or less. Motions at scales less than one day are usually filtered out and neglected in mesoscale studies, because they are characterized by different dynamics, such as inertial and tidal oscillations. In the mesoscale range, then, the scales of the acceleration are not considered and the exponential approximation for the autocorrelation holds, even close to the origin. At longer time lags ($\tau > T$), on the other hand, the experimental autocorrelations usually show some deviations from exponential, characterized by zero crossings, negative lobs and oscillations (Fig. 2). An important question is whether these deviations are significant (indicating that the dynamics are indeed different from the description of model 2), or whether they are simply due to the relatively small number of data points available that do not allow the proper resolution of the longer time lags.

A first step in the direction of addressing this question in a quantitative way has been taken by Griffa et al. (1995, GOPR), and applied to the analysis of a set of surface drifting buoys in the Brazil Malvinas current. GOPR have tested whether or not the measured data can be considered as a specific realization of model 2, characterized by a given length and a sampling interval. Their procedure can be summarized in the following way. First they use the data to estimate the model parameters σ and T (with a method that is reviewed in Section 7.2), and then they integrate the model forward, using the estimated values of σ and T in (6)-(8). A set of realizations of simulated velocities are generated, with the same number of measurements and the same sampling interval as for the data. The data and the simulations are then compared by plotting together the autocorrelation functions (examples for three realizations are shown in Fig. 2) The results strongly suggest that the data are indeed consistent with the model, since data and simulations appear to be essentially indistinguishable, with the data correlation falling right into the envelope of the simulated ones. Even though this test is still qualitative, it certainly indicates that the model is a reasonable and valid starting point. Similar results have been obtained also with data in the California Current (Zambianchi, private communication) and in the Equatorial Pacific. An interesting future development can be envisioned involving more accurate and quantitative statistical tests of the model along this line.

All the results summarized so far indicate that model 2 is well suited to describe mesoscale particle motion in the upper ocean. An important remark, though, is that model 2 does not appear equally suited for deep

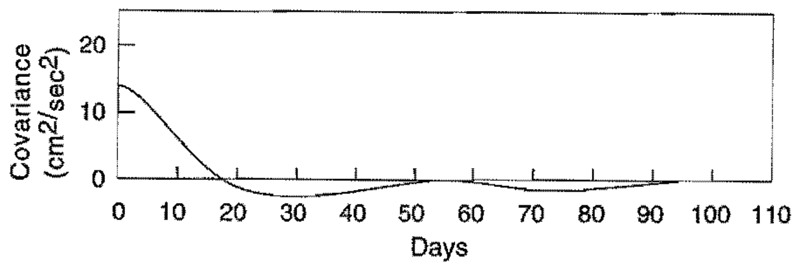

Figure 3. Velocity covariance from particle simulations in the lower layer of a 2 layer quasi-geostrophic model of the ocean circulation (from Verron and Nguyen, 1989).

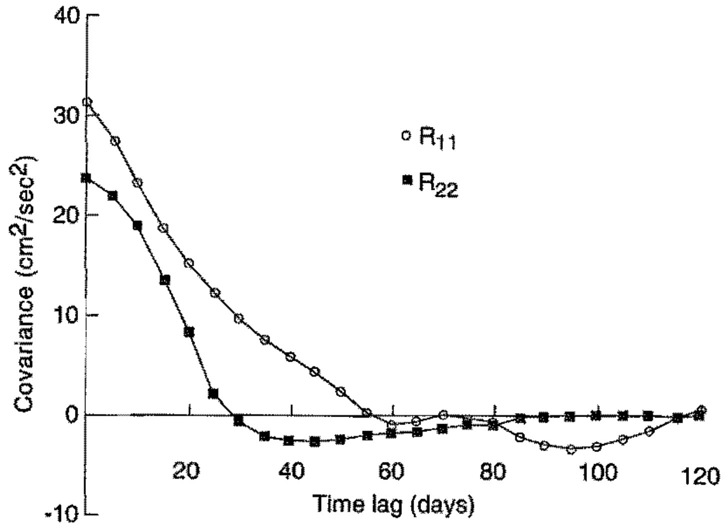

Figure 4. Velocity autocorrelation from subsurface floats in the Western Atlantic at 700 mt. R11 indicate the east-west component and R22 the north-south component (from Riser and Rosby, 1983).

ocean flows (see Fig. 3, Fig. 4). Deep flows (e.g. Riser and Rossby, 1983), in fact, are characterized by much longer time scales of evolution (T is of the order of 10 days or more), so that the scale of the acceleration cannot generally be neglected. We will come back on this point in Section 5. In addition to this, we also notice that model 2 is not appropriate when the motion is dominated by strong coherent structures or waves. As an examples, if the particles move in a ring with a very long life, the model is not suited to describe them. This can be easily understood considering that the autocorrelation in coherent structures is characterized by more complex and persistent patterns than the exponential decay. Also this point will be discussed in more detail in the following.

4.2 Generalization of model 2 to inhomogeneous and nonstationary turbulence. The results presented so far have been obtained under the assumption of homogeneous and stationary turbulence. As discussed in Section 2, this assumption is acceptable in midlatitude regions and in the interior of the ocean. When considering regions close to the western boundary currents and their extensions or close to the equatorial currents, this assumption breaks down. The intense shears and the associated instabilities, in fact, generate intensifications of the turbulent activity in well defined geographical regions. Also, when considering coastal regions, the dependence of the turbulent flows on the distance from the coast plays an important role and it cannot be neglected. For practical applications which include these type of flows, then, it appears very important to relax the assumption and to study the stochastic models in the presence of inhomogeneous turbulence.

The generalization of stochastic particle models such as model 1 and 2 to the case of inhomogenous and nonstationary flows is not completely straightforward, because the basic Langevin equation is incorrect in presence of inhomogeneity and nonstationarity. When the turbulent parameters are space and time dependent, $\sigma(\mathbf{x}, \mathbf{t})$ and $T(\mathbf{x}, \mathbf{t})$, eq. (2)-(3) and (6)-(7) predict an incorrect particle distribution, characterized by unphysically high concentrations in regions of lower variance (e.g. van Dop et al., 1985). The problem of adequately correcting the stochastic models has been addressed by several authors in the past decade (e.g. Legg and Raupach, 1982; Thomson, 1984). The main motivation for these type of studies has been provided by atmospherical applications, such as studies of dispersion from point sources close to the ground, where the spatial dependence of the turbulent parameters in the boundary layer is very important. The studies show that model 1 is fundamentaly unable to produce the correct disributions in presence of inhomogeneity, whereas model 2 can be satisfactorily modified. Several modified forms of model 2 have been proposed in the literature, and a certain number of criteria have been indicated in order to identify the "good" models (e.g. Janicke, 1983; Durbin, 1984). The relationships between the various models and criteria have been finalized by Thomson (1987), with the introduction of a generalized "well mixed" criterium, which unify the previous results and guarantees that the particles have the correct distribution.

The simplest form of model 2 for inhomogeneous and nonstationary turbulence obeying the "well mixed" condition, and having a Gaussian distribution for the turbulent velocity, is a direct generalization of (6)-(7),

and can be written as

$$dx = (U+u)dt \qquad (12)$$

$$du = -(1/T(x,t))u\,dt + \left(\frac{\partial \sigma(x,t)}{\partial x}\right)dt + (\hat{K})^{1/2}d\hat{w} \qquad (13)$$

Dop !

with $\hat{K}$ and $d\hat{w}$ defined as in (6-8).

Equation (13) differs from the homogeneous model (7) by the term $\frac{\partial \sigma}{\partial x}dt$ on the r.h.s.. This term describes a mean acceleration acting on the particles and directed toward the regions of larger variance. This acceleration counterbalances the tendency of the particles to spend more time in the lower variance regions. As a result, the particle distribution remains well mixed, with no formation of unphysical concentrations in the lower variance regions.

We conclude remarking that, in order to correctly use (12)-(13) in practical applications, the time and space dependence of σ and T has to be known with accuracy. In mesoscale oceanographic applications, the geographic distribution of σ and T is approximately known in some regions of the ocean, but more information is needed in order to have a reliable and detailed description. Concerning smaller scale, e.g. coastal applications, not much is known on the characteristics of the coastal boundary layer. Specific experiments focused on these aspects are presently underway (Olson, private communication) and hopefully they will provide sufficient insights for a correct application of the model.

5. Model 3. Joint Markovian x, u and a

The equations for model 3, written in incremental form and under the assumptions in Section 2, are

$$dx = (U+u)dt \qquad (14)$$

$$du = a\,dt \qquad (15)$$

$$da = -\left(1+\frac{T_a}{T}a\right)\frac{dt}{T_a} - \frac{u}{T}\frac{dt}{T_a} + (K^*)^{1/2}dw^* \qquad (16)$$

with

$$K^* = \frac{1}{T_a}\left(\sigma_a\left(1+\frac{T_a}{T}\right)\right), \qquad (17)$$

$$\sigma_a = \frac{\sigma}{T_a T}$$

and $x(0)=0, u(0)=\hat{u}, a(0)=\hat{a}$ where $\hat{u}$ and $\hat{a}$ are drawn from a Gaussian distribution with mean zero and variance σ and σ_a respectively. In (14-17), K^* is the diffusion coefficient, σ_a is the acceleration variance, and dw^* is a random increment with the same statistical characteristics as dw in (3) and $d\hat{w}$ in (7).

Model 3 assumes that the turbulent acceleration a obeys the first order autoregressive equation (16), and it is characterized by the finite scale T_a. The model has then two distinct time scales: T which characterizes the velocity, and T_a which characterizes the acceleration. The quantity da/dt, i.e. the time rate of change of the acceleration, is instead considered infinitesimal in the model. Since the changes in the acceleration are characterized by shorter scales than the acceleration itself, model 3 is expected to be more accurate than model 2.

In order to understand the basic characteristics of model 3, it is useful to consider the form of the autocorrelation for the velocity (e.g. Pope, 1994)

$$R(\tau) = (e^{-\tau/T} - \frac{T_a}{T}e^{-\tau/T_a})/(1 - \frac{T_a}{T}) \tag{18}$$

For simplicity, we discuss the case where there is a complete separation between the scale of the velocity T and the scale of the acceleration T_a, $T_a << T$. For time lags $\tau >> T_a$, R reduces to $R(\tau) \approx e^{-\tau/T}$, as (9) for model 2. This corresponds to a spectrum having an ω^{-2} slope for $\omega T_a << 1$. For time lags of the order of T_a, instead, R has a different shape than in model 2 and is characterized by a quadratic behaviour at $\tau \approx 0$. This is the correct behaviour, expected in a real flow. The autocorrelation for the acceleration, R_a, has an approximately exponential shape for small lags, $R_a(\tau) \approx e^{-\tau/T_a}$, and correspondinly, the velocity spectrum has a ω^{-4} slope at high frequencies, $\omega T_a >> 1$

Concerning the physical interpretation of model 3 and in particular of the acceleration time scale T_a, we note that Model 3 has been first introduced (Sawford, 1991) in the framework of isotropic turbulence to correct the small scale behaviour of model 2 in the description of flows at high but finite Reynolds number. In the isotropic turbulence context, the velocity time scale T is the scale of the energy containing eddies, and the acceleration scale T_a is determined by the dissipation. In the mesoscale oceanographic context we are interested in, the molecular dissipation range is too removed to be able to play a direct role, but eddy dissipation by internal waves and other "subgrid-scales" processes might be a posible candidate. If model 3 has to be applied to oceanographic problems, then, the interpretation of the acceleration time scale T_a has to be rethought and redefined. It might help to consider that the system of equations (15),(16) in model 3 is equivalent to a Langevin equation for u with an exponentially correlated noise instead of white noise (Krasnoff and Peskin, 1971; Sawford, 1991). The acceleration time scale, then, could be physically dependent on the nature of the forcing represented by the correlated noise.

As a last remark on model 3, we notice that even though the model appears to be in principle generalizable also to inhomogeneous turbulence

problems, applications of this type have not been done yet, at least to the author's knowledge.

5.1 Comparison of model 3 with numerical and oceanographic data Model 3 has been tested with results of direct numerical simulations of 3-dimensional isotropic turbulence at high but finite Reynolds number (Sawford, 1991). The model appears to represent very well the second-order statistics of the simulated particles. There are of course some differences between the model and the simulations, such as for instance the form of the acceleration autocorrelation at the origin, which is not analytical in the model, but altogether the ability of the model to describe the second order Lagrangian statistics is definitely impressive.

Regarding oceanographic simulations and data, a close comparison with model 3 has not yet been performed, so that only a preliminary and qualitative discussion can be done. In the following, we focus on oceanographic flows in the deep ocean which, as noted in Section 4.1, have long acceleration time scales and which are not correctly represented by model 2 (see Fig. 3, Fig. 4). Model 3 is a possible candidate to describe them. At first inspection, Model 3 seems suitable to represent the simulated and measured velocity autocorrelations at small time lags, $\tau \approx 0$, since it is characterized by the correct quadratic behaviour. The interesting (and hard) question to address, though, is whether or not the model can adequately describe the oceanographic autocorrelations at longer times, $\tau > T$. The data and the simulations of the deep flows, in fact, show pronounced oscillations and negative lobes at $\tau > T$, which are not present in the model autocorrelation (18) characterized by the exponential decay. As already stated in Section 4.1 for the upper ocean flows, the question is whether or not the oscillations are significant, given the finite number of data available. With respect to the upper ocean flows, the lobes and the oscillations of the deep flows seem more pronounced, but on the other hand the time scales T are much longer so that the resolution is harder to acheive from the data. Only a direct statistical comparison of the model and the data will enable one to answer this question.

The question of significance of the oscillations in the autocorrelation is conceptually very important. If they are found to be significant, in fact, this is a clear indication that the deep velocity field is dominated by coherent structures or waves. If instead the oscillations are not significant, it is justified to hypothize that the deep ocean has a similar, random structure as the upper ocean, except that the dominant time scales are much longer. In both cases, the results will open further questions which are of fundamental interest in oceanography, such as what is the link between time scales and generation mechanisms, and what is the persistence and the relevance of coherent structures in the ocean.

6. Dispersion estimates from the models. Accuracy of the eddy-diffusion parameterization.

The advection-diffusion equation (5) with the eddy-diffusion parameterization (4) is commonly used in oceanography, even in situations where the basic assumption of infinitesimal scales of turbulence is questionable, and the exact limits of its applicability have been the object of many debates in the literature (e.g. Holloway, 1989). A simple way to quantitatively define the accuracy of the advection-diffusion parameterization is to compare estimates of dispersion obtained with the advection-diffusion equation (5) (or equivalently with model 1) with estimates obtained using the stochastic models 2, 3 which are not based on the assumption of infinitesimal turbulent scales. Model 2 and 3 are not completely realistic, but, as shown in Sections 4 and 5, they describe satisfactorily the second order statistics of a vast class of flows. For these flows, the results of the models can be used as a valid approximation of the real turbulent dispersion.

In the following we focus mainly on the comparison between the results of model 1 and 2 for some simple flows at oceanographic scales. This comparison has been analyzed in a recent paper by Zambianchi and Griffa (1994, ZG in the following), and it will be summarized in the following. The results apply to mesoscale turbulent flows in the upper ocean, where model 2 has been shown to provide an accurate description. When considering flows with longer acceleration scales, the dispersion estimates should be corrected, for instance using model 3, and this could cause modifications to the presented results (Sawford, 1991).

ZG compute analytically the first two moments of particle displacements, i.e. the mean displacement $< x >$ and the "dispersion" $S =< (x- < x >)^2 >$, for the two models 1 and 2, using the method of moments applied on the Fokker-Planck equations (5) (the advection-diffusion equation) and (10). In all the cases considered by ZG, the mean displacement $< x >$ is the same in both models, whereas the dispersion S is different. In order to quantify this difference, ZG compute the normalized difference

$$\Delta = \frac{\mid S_1 - S_2 \mid}{\mid S_1 \mid} \tag{19}$$

where the subscripts 1 and 2 indicate the model which is used to compute the dispersion. Δ is used as a measure of the action of finite scales of turbulence, and therefore of the accuracy of the advection-diffusion equation.

Three simple and idealized mean flows $\mathbf{U}$ are considered by ZG: a constant mean flow ($\mathbf{U} = \mathbf{C}$), a linear shear ($\mathbf{U} = \mathbf{C} + \mathbf{Bx}$), and a linear shear oscillating in time ($\mathbf{U} = (\mathbf{C} + \mathbf{Bx})\mathbf{sin}\omega_s \mathbf{t}$). In all the cases, the turbulent field $\mathbf{u}$ superimposed to the mean shear is considered homogeneous and stationary. The first case, i.e. the flow with constant mean, corresponds

to the classic and well known case of purely homogeneous turbulence (e.g. Taylor, 1921). We briefly review it first, because it provides a good basis for the understanding of more complex situations.

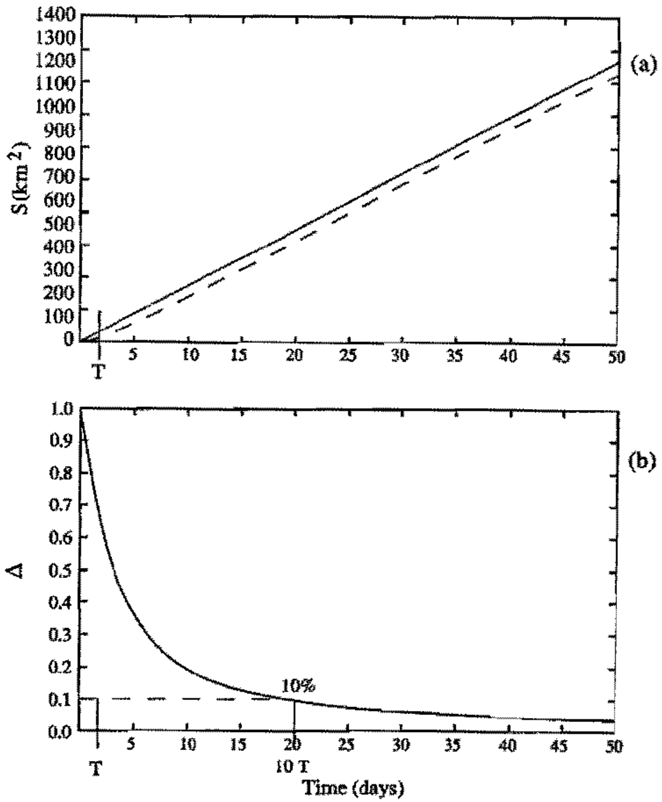

Figure 5. a) Dispersion versus time for homogeneous turbulence with constant mean flow. The solid line represents the result from model 1, S_1; the dashed line represent the result from model 2, S_2. b) Relative difference between the results from the two models, $\Delta = \frac{|S_1 - S_2|}{|S_1|}$ (from Zambianchi and Griffa, 1994).

The dispersion S computed for $\mathbf{U} = \mathbf{C}$ is, (in one direction),

$$S_1 = 2Kt \tag{20}$$

for model 1, and

$$S_2^* = 2Kt - 2KT(1 - e^{-\gamma t}) \tag{21}$$

for model 2, where $\gamma = 1/T$ is the inverse of the turbulent velocity time scale. As expected, the two models differ in a transient term which is not present in model 1, and it has an exponential form in model 2. Expanding the exponential in (21) for $t << T$ we obtain

$$S_2 \sim \sigma t^2 \tag{22}$$

which is the classical result of Taylor (1921) for initial time dispersion, with the quadratic behaviour due to the initially high correlation of the turbulent velocity u. Comparing the linear expression (20), rewritten as $2\sigma Tt$, with the quadratic expression (22), it is clear that model 1 overestimates the dispersion for initial times $t < T$. This behaviour is shown in Fig. 5a. The initial overestimate of model 1 influences the dispersion also for $t > T$ producing an offset $2KT$ between the two curves S_1 and S_2 (Fig. 5a). The relative importance of this offset is illustrated by the quantity Δ (19) at the limit $\lim_{t\to\infty}$

$$\Delta_\infty = \frac{2KT}{2Kt} = \frac{T}{t}, \tag{23}$$

which shows how the results converge as t goes to infinity, as expected (see Fig. 5b). Quantitatively, the overestimate of model 1 is less than 10% for $t > 10T$, which for oceanographic values of T, $T \simeq 2-10$ days, corresponds to $t > 20 - 100$ days.

The previous results suggest that the use of model 1, and equivalently the use of the advection-diffusion equation (5), are appropriate in homogeneous situations in the ocean for dispersion studies at scales of one month or more (i.e. at the scales of the mesoscale and of the general circulation), while caution should be used in studies over shorter times.

When a linear shear mean flow $\mathbf{U}$ is considered, the behaviour of the dispersion S changes (Taylor, 1953), but the relative difference Δ still behaves asymptotically as T/t. This suggests that for mean flows with weak spatial dependence, the accuracy of the advection-diffusion equation is the same as for purely homogeneous flows.

Very different results are found, instead, when the time-dependence is introduced in the mean flow $\mathbf{U}$ (Okubo, 1987). For the oscillating linear shear with frequency ω_s, the relative difference Δ between the two models does not converge to zero in the asymptotic limit $\lim_{t\to\infty}$, but rather it converges to the oscillating function

$$\Delta_\infty = \frac{{\omega_s}^2}{(\gamma^2 + {\omega_s}^2)} \frac{1}{(2 + \cos 2\omega_s t)}, \tag{24}$$

with constant average and constant extrema. The graphs of the dispersion estimates from the two models and the corresponding Δ are shown in Figs (6a) and (6b).

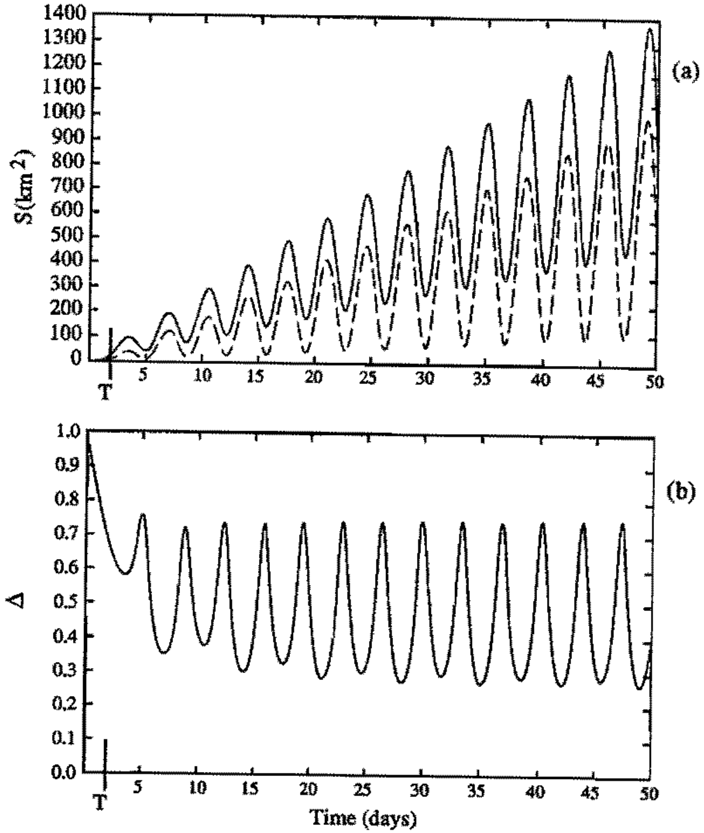

Figure 6. As in Figure 5, but for dispersion with oscillating linear shear. The time scales of the turbulence and of the shear are comparable, $T \sim \frac{T_s}{2\pi}$.

As it is shown from (24), the value of Δ depends on the ratio between the turbulent time scale $T = \frac{1}{\gamma}$ and the time scale of the shear $T_s = \frac{2\pi}{\omega_s}$. When

$$\gamma^2 >> {\omega_s}^2, \qquad \Delta_\infty \sim 0,$$

which indicates that the two estimates essentially coincide when the current oscillation is slow compared with the turbulent correlation time. In the other limit

$$\gamma^2 \leq {\omega_s}^2, \qquad \Delta_\infty \sim O(1),$$

which indicates that when the two time scales are comparable, $T \geq T_s/2\pi$, the estimates are significantly different at all times. In this case the use of the advection-diffusion equation (5) can lead to an order one error in the estimate of the dispersion even for asymptotically large times. Intuitively, this arises because each reversal of the mean velocity results in a change of regime in the dispersal flow. During each regime, for time $t < T$, the motion of the particles is described differently by the two models, with model 2 being characterized by a correlation between particle position and turbulent velocity which is absent in model 1. If the reversals occur at time intervals of the same order of T, this initial time difference in particle behaviour becomes permanent, and the dispersion between the two models is different at all times.

Examples of flows which can be idealized as oscillating mean shears and for which $T \sim T_s$ are along-shore coastal currents characterized by fluctuations with a period of few days and cross-stream turbulent motion with similar time scales (Kundu and Allen, 1976), and tidal currents with highly variable cross-stream motion.

The results obtained analytically by ZG for oscillating linear shear are likely to be generalizable to a much wider class of flows, including shear flows with complex spatial structure. Unfortunately analytical calculations using the method of moments are not feasible for such flows in the framework of model 2, so that more detailed results will have to rely either on future numerical studies or on analytical studies using different techniques. By now, only a qualitative discussion can be given. It appears reasonable to assume that in the presence of strong inhomogeneity in the shear flows, the interplay of the space scales of turbulence and shear (L and L_s respectively) can introduce an additional mechanism for permanent differences between the two models. Classical examples of flows of this type are the intense western boundary currents and their open ocean extensions (e.g. the Gulf Stream, the Kuroshio Current, the Brazil Current), characterized by strong meandering currents. For flows of this type, even though the impact of finite scales of turbulence cannot be clearly assessed at this point, the previous arguments suggest that caution should be used in applying the advection-diffusion equation with the eddy-diffusion parameterization.

7. Practical applications.

As discussed in Section 6, the introduction of finite scales for the turbulence plays an important role in the study of dispersion for initial times, $t < T$, and also for longer times, provided that the mean flow is strongly space or time dependent so that the scales of the mean flow and of the turbulence are of the same order. In these situations, that are characteristics of important current systems in the ocean, the eddy-diffusion parameterization is likely to be inaccurate, while its generalizations (generalized K-models) are usually not simple to implement. The stochastic particle models 2 and 3, instead, provide a convenient and valid tool of investigation. Two main classes of

applications of the models can be identified in this general framework.

The first class includes the "direct" applications, where the stochastic particle models are used to study and simulate dispersion problems in mean velocity fields that can have arbitrarily complex space and time dependence. The equations for single particle motion are directly integrated in time to simulate ensemble of tracer particles in the prescribed mean velocity fields, and the concentration of the particles corresponds to the ensemble average concentration of the tracer. The models 2 and 3 are especially suitable to study dispersion from localized sources, since the statistics have to be computed over a large number of particles (of the order of thousands) for each release point. An example of an application of model 2 to a dispersion study in an idealized model of the Gulf Stream is reviewed in Section 7.1 (Dutkiewicz et al., 1993).

An other class of promising applications of the stochastic particle models is related to the "inverse" problem of extracting information about the velocity field from Lagrangian data from drifting buoys. The Lagrangian data are usually available only for relatively short intervals of time, so that their statistics are often satisfactory only for times of the order of T. As a consequence, as noticed by Davis (1991b), the Lagrangian data should be studied in the framework of a model that describes satisfactorily the behaviour of turbulent particles at scales of the order of T. Davis (1987) suggests to use an elaborated form of the advection-diffusion equation with time-dependent diffusivity. We, instead, advocate the use of the stochastic particle models as a more natural and simple tool. An example of an application of model 2 to surface drifter data to estimate turbulence parameters is summarized in Section 7.2 (GOPR).

7.1 Diffusion in a meandering jet. A direct problem. Dutkiewicz et al. (1993) have performed a numerical study on the turbulent mixing across an ideal model of a meandering Gulf Stream extension, using model 2 to simulate the turbulent motion. This is an important problem from both the physical and biological point of view, because the Gulf Stream divides two bodies of water (the Sargasso Sea and the Slope Water) which differ in physical characteristics such as temperature and salt, and in biological properties such as zooplankton and nekton species.

In the study of Dutkiewicz et al., (as in other previous studies such as Bower 1991), the Gulf Stream extension is crudely represented by a meandering jet (see Fig. 7), steadily propagating eastward with velocity c. Dutkiewicz et al. consider the distribution of ensemble of particles, simulated using model 2 and launched in several regions of the jet, over typical mesoscale times of the order of one month. The particle distribution patterns turn out to depend crucially on the initial conditions. Particles launched in the meander bends, where the flow is recirculating, tend to be trapped in the bends and the distribution tends to homegenize. Particles launched in the jet core (defined as the region where the local velocity U is higher than the meander phase speed c, $U > c$) tend to be lost from the jet in plumes at the extrema of the meanders and to be entrained in successive recirculating regions (Fig. 7).

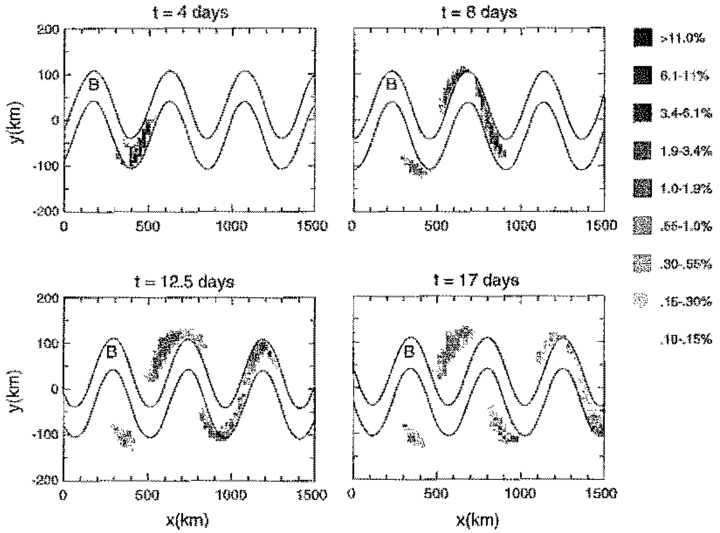

Figure 7. Evolution of the concentration of particles in a meandering jet propagating eastward (toward the right) at constant speed c. The solid lines indicate the core of the jet (defined as the region where the particle velocity U is greater than c). The particles are launched at point B, inside the jet core, and their concentration is indicated by the shading as in the right panel (from Dutkiewicz et al., 1993)

The net result is thus a buildup of homogenized particle distributions in the meander regions. This has important biological consequences, as it has been tested by Dutkiewicz et al. incorporating a simple biological model in the particle model. The biological model, which represent the interaction of two species, one dominant in the Sargasso Sea and the other in the Slope Water, shows the observed tendency to produce patches of species in the recirculating meander regions, on the side of the jet each species favors.

7.2 Estimates of turbulence parameters from Lagrangian data. An inverse problem. GOPR have proposed a method based on model 2 to study Lagrangian data and to estimate turbulence parameters from the data. The method, which is based on a "parametrical" approach, consists of assuming that the data obeys the model, so that the velocity autocorrelation is assumed to have the known exponential shape which depends on the two turbulent parameters σ and T. The classical method of moments is then used to estimate from the data the parameters σ and T, together with the mean value of the velocity U. Also an estimate of the diffusivity parameter K is obtained using (4)

The main advantage of this approach is that it provides more accurate parameter estimates than other existing methods (e.g. Figueroa and Olson, 1989), by using the a-priori knowledge of the model. In particular, the estimates of T and K depend on the slope of the autocorrelation and are computed using only the first two time lags. The other estimates in the literature, instead, are based on the integration of the autocorrelation and turn out to depend on subjective procedures of truncation of the long time lags of the correlation. By contrast the GOPR estimates are "objective" (in the sense that, given the model assumption, the method provides unique values for the estimates) and have a well defined associated error. The method, in fact, provides a complete error analysis of the estimates and is valid in the presence of observational errors. On the other hand, the validity of the a-priori assumptions has to be checked before the application of the method in order to obtain reliable estimates. As discussed in Section 4, model 2 appears to be generally appropriate for mesoscale upper ocean flows, so that the method is expected to have a large applicability for these type of flows.

Note that, even though the results obtained by GOPR are valid for the specific model 2, and in the additional assumption of homogeneous turbulent flows with constant mean U, the methodology is very general and can be applied to more complete and less restrictive models. Work is presently underway to generalize the model in the case of space and time dependent U. Also, the identification of a suitable model for deep ocean flows is under consideration. Once the model is identified, the same method of moments used by GOPR can be used to estimate the parameters.

8. Summary and discussion.

In this paper we discuss a hierarchy of three Markovian particle models. Model 1 assumes that the scales of turbulent motion are infinitesimal, and it is equivalent to the advection-diffusion equation with the eddy-diffusion parameterization. Model 2 introduces a finite scale T for the turbulent velocity, still neglecting the acceleration scales. The particle velocity obeys the classical Langevin equation, and its autocorrelation is characterized by an exponential behaviour. Model 3 introduces in addition a scale for the acceleration, $T_a < T$, while assuming infinitesimal scales for the acceleration derivatives. The velocity autocorrelation is exponential as in model 2 at time lags $> T_a$, and it has a quadratic behaviour near the origin.

A comparison of model 2 with oceanographic Lagrangian data shows that the model gives a satisfactory description of mesoscale turbulent flows in the upper ocean. For these flows, the velocity autocorrelation following particles is typically exponential as in model 2. The exponential behaviour is found to hold even at small time lags, suggesting that the acceleration scales are small and can be neglected. The typical velocity time scale T is of the order of 2-10 days.

Model 2, on the other hand, is not appropriate for deep ocean flows, where the time scales are much longer (T is of the order of 10 days or more). The acceleration scales are not negligible for these flows, and the autocorrelation is characterized by a smoother, quadratic behaviour at the origin. Model 3 reproduces correctly the autocorrelation behaviour for small lags, but, on the other hand, the data autocorrelations show strong oscillations at longer lags, which are not present in the model. Specific statistical tests on the data have not been performed yet, so that it is not clear at this stage whether the oscillations signal a significant deviation from model 3, or whether they are only due to the relatively short record lengths available.

A comparison between dispersion estimates performed with the three stochastic models shows that the introduction of finite scales of turbulence plays an important role not only for dispersion at initial times, $t < T$, but also for dispersion at longer times, $t > T$, if the mean flow is characterized by scales of the same order than T. This suggests that model 1, and therefore the advection-diffusion equation with the eddy-diffusion parameterization, is not accurate when used in higly variable mean flows where the scales of the mean flow and of the turbulence are comparable. Flows of this type are quite common in oceanography. They range from tidal or shelf oscillating currents, to large scale meandering jets such as the Gulf Stream or other western boundary currents, which play a major role in the distribution of properties in the ocean. For these type of flows, the use of stochastic models such as 2 or 3 appears more indicated and accurate than the advection-diffusion equation.

Two main classes of applications of the stochastic particle models are indicated. The first one consists of "direct" problems, where the models are directly integrated in time to study dispersion problems in flows with high space and time complexity. An example of a study on an idealized Gulf Stream model is discussed in some detail. The other class of applications involve "inverse" problems, where the models are used to infer information on the statistics of the velocity field from Lagrangian oceanographic data. An example of an application of model 2 to the estimate of turbulence parameters from surface drifting buoys is discussed. New applications and problems are suggested, that can be addressed with a combination of physical and statistical modeling.

The summarized results show that the particle models provide a valuable and flexible tool which can be used in a wide range of problems in oceanography. It is important to recognize, though, that Markovian models such as 2 or 3 are limited to ergodic processes where the autocorrelation decays exponentially to zero, and thus they cannot explain phenomena

related to the presence of strong coherent structure with more complex autocorrelations. The presence and the importance of coherent structures in the ocean have been the object of works and discussions in the literature (e.g. Mc Williams, 1984). Oceanographic data, and in particular Lagrangian data in mid and deep ocean, show a remarkable incidence of eddies persisting for a long time (Richardson, 1993). On the other hand, a clear assessment of their impact on the statistical properties of the oceanic flows, and in particular on the dispersion, is not yet avaiable, and work is in progress on this subject.

We believe that the particle models discussed here can provide, at least indirectly, some contributions to this investigation. The comparison between the oceanographic data and model 2, for instance, suggests that the coherent structures do not play an important role in the upper ocean, whereas in the deep ocean the question is still open. As previously noted, an accurate statistical analysis is necessary to establish whether or not the data significantly deviate from model 3 at long times, $t > T$. If they do, this strongly suggests that coherent structures or waves dominate the flow. If they do not, instead, it is possible that the deep ocean has a random structure similar to the upper ocean, but with longer time scales. The question of how the time scales are connected to different forcing and generation mechanisms in the upper and deep ocean is still open.

We conclude remarking that, even though we have confined our discussion to the three models 1,2 and 3, an extremely interesting and challenging question is how to formulate more general particle models that can include the presence of coherent strucures (e.g. Bennett, 1986; Carnevale et al., 1990). Contributions to this problem, which is still unsolved in the literature, are expected to help improve our understanding of turbulent mechanisms and transport.

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