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A Scheme for Simulating Particle Pair Motions in Turbulent Fluid

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A technique is developed for simulating the random motion of particles in turbulent fluid. The technique is applicable to single particles or to pairs of particles whose motions are correlated. The method is intended for use in determining one or two-particle Lagrangian turbulence statistics either from instantaneous velocity fields generated by turbulence simulation models or from Eulerian statistics of the turbulence acquired either from observations, from theory, or from a turbulence closure model. In the latter capacity the scheme provides a basis for Monte Carlo type models of turbulent diffusion. The scheme requires as inputs the probability density of the Eulerian velocity, or at least its mean and variance; the autocorrelation of the Eulerian velocity, or at least its integral time scale; and the energy dissipation rate of the turbulence.

I. INTRODUCTION

One of the classical problems of turbulence is relating the Eulerian and Lagrangian statistical properties of the fluid velocity field (the Euler–Lagrange problem). The Eulerian (fixed reference frame) statistics are readily measurable and significant advances have been made in recent years in solving their governing equations numerically. However, it is the Lagrangian (fluid particle reference frame) statistics that are required to analyze the dispersion of material substances in turbulent fluid. Unfortunately, the Lagrangian statistics are very difficult to measure and their governing equations have received only cursory attention (see Monin and Yaglom [1]). Thus, all fields of applied science that treat problems of turbulent diffusion would benefit greatly from the ability to predict mean properties of material concentrations given measured or numerically simulated profiles of Eulerian statistical properties of the flow.

To cast the problem in more specific terms let us consider the Lagrangian form of the equation for the ensemble mean concentration $\langle c \rangle$ of a substance at a specific point $\mathbf{x}$ and time t [1]:

$$\langle c(\mathbf{x}, t) \rangle = \int_0^t \int p(\mathbf{x}, t \mid \mathbf{x}', t')\, S(\mathbf{x}', t')\, d\mathbf{x}'\, dt'. \tag{1}$$

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Here p is the probability density that a material particle released at the point $\mathbf{x}'$ at time t' will be found at $\mathbf{x}$ at time t, S is the time rate of emission of material per unit volume at $(\mathbf{x}', t')$, and the integration with respect to $\mathbf{x}'$ is over all space. Under the assumption that the material substance does not affect the fluid motions, the so-called passive scalar assumption, p is a Lagrangian property of the turbulence. It is independent of both S and c. Within this context the Euler–Lagrange problem is simply that of expressing p in terms of the fixed point statistical moments of the fluid velocity.

Due to formidable mathematical difficulties, attempts to derive analytical solutions to the Euler–Lagrange problem have failed to produce any results of significant practical value (see Lumley [2]). Numerical solutions are the only recourse, yet to date relatively few numerical studies have been performed. The numerical approach is rather straightforward:

(1) Create an ensemble of pseudo-random velocity fields $\mathbf{u}_n(\mathbf{x}, t)$, $n = 1, 2, \ldots, N$ whose statistics are equivalent to the available Eulerian statistics of the turbulence. The given statistics may be obtained from measurements, from theory, or from a turbulence model that predicts Eulerian statistics directly, such as that described by Lewellen and Teske [3].

(2) Transform the ensemble of velocity fields into an ensemble of particle trajectories,

$$\mathbf{x}_n(t \mid \mathbf{x}_0) = \mathbf{x}_0 + \int_0^t \mathbf{u}_n(\mathbf{x}(t' \mid \mathbf{x}_0), t')\, dt', \qquad n = 1, 2, \ldots, N. \tag{2}$$

(3) Calculate p from the ensemble of trajectories.

Patterson and Corrsin [4] used this procedure to estimate some of the low-order moments of p. Kraichnan [5] performed a similar study except he created the random velocity ensemble in wave number space and transformed it into physical space at only those points required to solve (2).

The approach that we have just outlined (which we shall call Eulerian based) is not well suited to most applied studies because it requires a considerable amount of computer time to generate the ensemble of velocity fields and large amounts of computer memory to store them, especially in studies of 3-D flows. Both problems can be avoided by generating an ensemble of particle (Lagrangian velocities $v_n(t \mid \mathbf{x}_0)$, $n = 1, 2, \ldots, N$, rather than Eulerian velocities. In this case the ensemble of trajectories is given simply by

$$\mathbf{x}_n(t \mid \mathbf{x}_0) = \mathbf{x}_0 + \int_0^t \mathbf{v}_n(t' \mid \mathbf{x}_0)\, dt'. \tag{3}$$

This appraoch seems paradoxical at first because it is the *Lagrangian* properties of the flow that we are seeking to determine. Consider, though, that quite good theoretical–empirical descriptions are available of the relationships among the

lowest–order Eulerian and Lagrangian statistics in stationary, homogeneous flows. Thus, if all flows behave as though they are *locally* stationary and homogeneous, then we could use the available information to simulate particle motions in general situations. This is the basic premise behind the Lagrangian based methods. Thompson [6] and Jonas and Bartlett [7] performed studies using this approach. In both cases the $\mathbf{v}_n$ ensemble was created using an algorithm of the form

$$\mathbf{v}_n(t \mid \mathbf{x}_0) = \alpha \mathbf{v}_n(t - \Delta t \mid \mathbf{x}_0) + \beta \boldsymbol{\rho}_n(t), \tag{4}$$

where α and β are constants and $\boldsymbol{\rho}_n$ is a computer generated normally distributed random vector with zero mean and unit variance.

A basic limitation of all numerical approaches to the Euler–Lagrange problem is that only a finite set of the infinite group of stochastic moments required to describe the turbulence can be taken into account. Consequently, the random velocities $\mathbf{u}_n$, or $\mathbf{v}_n$, that the numerical schemes generate are not unique and Lagrangian statistics derived from them can differ significantly from those of the turbulence modeled unless key Eulerian moments are taken into account. In many instances one does know in advance which of the Eulerian moments are most important and often the values of the moments themselves are not available. In these cases the accuracy of the Lagrangian statistics calculations is greatly improved by using a turbulence model that predicts instantaneous grid cell averaged velocities to create the ensemble of Eulerian velocity fields. A notable example of a turbulence model of this kind is that developed by Deardorff [8] of the convective planetary boundary layer. The grid dimensions ($\Delta x = \Delta y = 125$ m, $\Delta z = 50$ m) in his model are sufficiently small that the dominant, energy containing eddies of the turbulence are described explicitly. However, as with all discrete grid models, velocity fluctuations with spatial scales smaller than the grid dimensions Δ, say, are unresolvable. Thus, using a model such as Deardorff's to create the velocity ensemble one would have

$$\mathbf{u}_n(\mathbf{x}, t) = \hat{\mathbf{u}}_n(\mathbf{x}, t) + \mathbf{u}'_n(\mathbf{x}, t), \qquad n = 1, 2, \ldots, N, \tag{5}$$

where $\hat{\mathbf{u}}$ is the velocity field derived from the model, i.e., a component representing the large scale ($>\Delta$) features of the flow; and $\mathbf{u}'$ is a random component representing the unresolvable, subgrid scales of motion. With this appraoch it is necessary to represent only the small scale features of the flow by pseudo-random functions (either Eulerian or Lagrangian based). This is advantageous because if Δ falls within the equilibrium subrange of the turbulence, as it does in Deardorff's model, the Eulerian statistics of $\mathbf{u}'$ can be specified with much more confidence than those of the entire velocity field $\mathbf{u}$. In fact, if Δ is small enough that the total kinetic energy contained in the subgrid scale eddies is a small fraction of the total turbulent energy, then single particle Lagrangian statistics such as p can be determined ignoring $\mathbf{u}'$ altogether. Deardorff and Peskin [9] and Riley and Patterson [10] have computed moments of p using (2) and (5) with u' neglected.

While it is true that the effects of $\mathbf{u}'$ on the displacement statistics of a single particle are small if $\mathbf{u}'$ constitutes only a small fraction of the total energy spectrum of fluid motion, the subgrid scale velocity component $\mathbf{u}'$ plays a dominant role in determining the joint displacement statistics of a pair of particles separated initially by a distance smaller than the dimensions of the grid on which the model data $\hat{\mathbf{u}}$ are available. This is true even when $\mathbf{u}'$ represents only a small fraction of the total fluid kinetic energy. Thus, to calculate two or more particle Lagrangian statistics for particles separated initially by distances smaller than Δ, one must retain the subgrid scale velocity term $\mathbf{u}'$ in (5) regardless of the size of Δ. Particle pair trajectory simulations are needed to determine the two-particle displacement probability density

$$p_2(\mathbf{x}, t; \mathbf{x}', t' \mid \mathbf{x}_{10}, t_1; \mathbf{x}_{20}, t_2)$$

that a pair of particles released at the space–time points $(\mathbf{x}_{10}, t_1)$, $(\mathbf{x}_{20}, t_2)$ will be found at $(\mathbf{x}, t)$, $(\mathbf{x}', t')$, respectively. The function p_2 is required to calculate second moments such as the mean square concentration $\langle c^2(\mathbf{x}, t)\rangle$, viz.,

$$\langle c^2(\mathbf{x}, t)\rangle = \int_0^t \int_0^t \iint p_2(\mathbf{x}, t; \mathbf{x}, t \mid \mathbf{x}', t'; \mathbf{x}'', t'')\, S(\mathbf{x}', t')\, S(\mathbf{x}'', t'')\, d\mathbf{x}'\, d\mathbf{x}''\, dt'\, dt''$$

(see [11]). Shu *et al.* [12] have used this equation in conjunction with p_2 estimates derived from (2) and (5) (with $\hat{\mathbf{u}}$ from Deardorff's [8] model and $\acute{\mathbf{u}}$ from Kraichnan's [5] technique) to model nonlinear chemical reactions among the constituents of a point source plume and species in the ambient, turbulent fluid. Simulations of $\langle c^2\rangle$ are also needed in air pollution studies to estimate "peak" concentrations.

An experience gained in the study conducted by Shu *et al.* [12] was that Eulerian based techniques (i.e., those using Eq. (2)) for simulating particle and particularly particle pair motions in turbulence are cumbersome and expensive to use and they do not provide the degree of control over the particle separation rates that is desired. The Lagrangian type schemes are much easier to use but none of those developed to date is applicable to particle pair simulations.

The purpose of this paper is to develop a Lagrangian based methodology for generating particle and particle pair velocities that can be used to simulate either the dispersive effects of the entire spectrum of velocity fluctuations, as is done in Monte Carlo type models, or the perturbations in particle motion induced by only a portion of the velocity spectrum, as is required to parametrize subgrid scale turbulence in diffusion simulations performed with numerical turbulence models. In our analyses we will work exclusively with ensemble averages, which we denote by the angle brackets $\langle\ \rangle$. Whether the velocities $\mathbf{u}'$ that we treat represent subgrid scale turbulence or the entire spectrum of velocity fluctuations, they constitute stochastic variables whose ensemble statistics are well defined. The ensemble mean and mean square concentrations $\langle c\rangle$ and $\langle c^2\rangle$ that one might derive from simulated Lagrangian statistics can be related to time- or space-averaged values using the ergodic theorem if the flow is statistically stationary.

II. Design of the Parameterization Scheme

As we noted in the Introduction, Lagrangian based schemes assume locally stationary homogeneous conditions. For simplicity we will invoke the further assumption of isotropy. In a later section we will discuss the conditions under which this scheme is applicable to generalized flows.

Let x_1 and x_2 denote the locations of a pair of particles in a coordinate system moving with the mean speed U of the fluid. Under the conditions assumed above, if the particles are released from the points x_{10} and x_{20}, their mean displacements are

$$\langle x_n(t)\rangle = x_{n0}, \qquad n = 1, 2. \tag{6}$$

Here x represents any one of the three vector components of position. We will represent the variance of the single particle displacement by

$$\sigma^2(t) \equiv \langle (x_n - x_{n0})^2\rangle, \qquad n = 1, 2 \tag{7a}$$

(in homogeneous turbulence σ is independent of the release point x_{n0}); and we will denote the mean square particle separation by

$$\langle l^2\rangle \equiv \langle (x_1 - x_2)^2\rangle - (x_{10} - x_{20})^2. \tag{7b}$$

There are an infinite number of joint moments of x_1 and x_2 and all of them would have to be specified to describe these two stochastic variables uniquely. In practice, only the first- and second-order moments given by (6) and (7) are of interest or are practical to measure, and hence these are the only moments that will be of conern to us in this study.

The type of problem to which we intend the scheme we develop to be applied is that in which one has knowledge of certain statistics of the Eulerian velocity field u and wishes to use it to estimate the Lagrangian statistics σ and $\langle l^2\rangle$. The Eulerian information that we shall assume is available is the probability density $p_u(u)$, or at least the variance σ_u; the autocorrelation $R_u(t)$, or at least some idea of its general form and its integral time scale; and the energy dissipation rate of the turbulence, ε. The first two pieces of information are adequate to generate an ensemble of pseudo-random particle trajectories from which the single particle displacement variance σ can be estimated. The energy dissipation rate constrains the evolution of $\langle l^2\rangle$ relative to that of σ. Thus, the starting point in the mathematical formulation of our scheme must be an expression for generating (x_1, x_2) that allows $\langle l^2\rangle$ to be specified in terms of σ^2.

Through experimentation we have found that the desired control can be achieved using an algorithm of the form

$$x_n - x_{n0} = a\xi + b\chi_n, \qquad n = 1, 2, \tag{8}$$

where a and b are deterministic functions of travel time t and ξ and χ_n are computer generated random numbers. To satisfy (6) we require that

$$\langle \xi \rangle = \langle \chi_n \rangle = 0 \tag{9}$$

and to facilitate the task of generating ξ and χ_n we require that they be statistically independent. In this case we have as a result of (9)

$$\langle \chi_1 \chi_2 \rangle = \langle \chi_1 \rangle \langle \chi_2 \rangle = 0, \tag{10a}$$

$$\langle \xi \chi_n \rangle = \langle \xi \rangle \langle \chi_n \rangle = 0, \qquad n = 1, 2. \tag{10b}$$

Squaring and averaging (8) we obtain with the aid of (10)

$$\langle (x_n - x_{n0})^2 \rangle = a^2 \langle \xi^2 \rangle + b^2 \langle \chi_n^2 \rangle \tag{11}$$

and by squaring the difference of (8) for the cases of $n = 1$ and $n = 2$ we get

$$\langle (x_1 - x_2)^2 \rangle - (x_{10} - x_{20})^2 = b^2 (\langle \chi_1^2 \rangle + \langle \chi_2^2 \rangle). \tag{12}$$

Now if we generate the variables ξ, χ_1, and χ_2 so that their variances are all equal to σ^2, i.e.,

$$\langle \xi^2 \rangle = \langle \chi_1^2 \rangle = \langle \chi_2^2 \rangle = \sigma^2(t), \tag{13}$$

we can force the ratio $\langle l^2 \rangle / \sigma^2$ of the simulated particle displacements to have the desired form (a function of the dissipation rate ε, which we discuss later) by choosing

$$a^2 = 1 - \langle l^2 \rangle / 2\sigma^2, \tag{14a}$$

$$b^2 = 1 - a^2. \tag{14b}$$

In order to use the scheme eventually in inhomogeneous flows, we must configure it to produce particle velocities rather than displacements. We can transform (8) into a velocity generator that retains the properties cited above by differentiating:

$$v_n = a\dot{\xi} + \dot{a}\xi + b\dot{\chi}_n + \dot{b}\chi_n, \tag{15}$$

where the over dot denotes a first-order time derivative. The next task is to formulate a rule for generating the velocities $\dot{\xi}$ and $\dot{\chi}_n$ that is compatible with requirement (13).

As we noted earlier, we do not know the exact form of $\sigma^2(t)$ and $\langle l^2(t) \rangle$ in advance. Indeed, it is partly these functions that we are attempting to determine. We have only certain information about the Eulerian velocities (listed above) from which we can construct an ensemble of particle trajectories whose statistics σ^2 and $\langle l^2 \rangle$ are as close to the true values as possible. Thus, we must assume some relationship between the Eulerian and Lagrangian velocities to guide the formulation of the particle velocity generator. We shall adopt the following conventional assumptions: (1) the probability density of the Lagrangian velocity is identical to that of the Eulerian velocities $p_u(u)$

at the release time; (2) the Lagrangian and Eulerian velocity autocorrelations $R_v(v)$ and $R_u(u)$ have similar shapes; and (3) the integral times scale $\mathscr{T}$ of R_v is larger than that of R_u by a constant factor.

We can incorporate all of these assumptions into the particle velocities $\dot{\xi}$ and $\dot{\chi}_n$ by assigning them the general forms

$$\dot{\xi}(t_n) = \sum_{m=1}^{M} \alpha_m \dot{\xi}(t_{n-m}) + \alpha_0 \rho_\xi(t_n), \tag{16a}$$

$$\dot{\chi}_k(t_n) = \sum_{m=1}^{M} \alpha_m \dot{\chi}_k(t_{n-m}) + \alpha_0 \rho_k(t_n), \tag{16b}$$

where $t_n = n\,\Delta t$, Δt is the time step used in the particle simulation, α_m are time-dependent deterministic variables, and ρ_ξ and ρ_k are random variables with the following properties:

$$p(\rho_\xi) = p_u(\rho_\xi), \tag{17a}$$

$$\begin{aligned} \langle \rho_\xi(t_n)\, \dot{\xi}(t_m) \rangle &= 0, \qquad n \neq m, \\ \langle \rho_\xi(t_n)\, \rho_\xi(t_m) \rangle &= 0, \qquad n \neq m. \end{aligned} \tag{17b}$$

Similar properties are possessed by ρ_k. In fact, since the statistics of ξ and χ_n are identical, we shall restrict attention to ξ in the analyses that follow.

Equations (16) constitute Markov-M sequences. Note that Eq. (4), which some previous investigators have used to simulate single particle motions, is Markov-1. This lowest-order sequence is limited in its applicability because it is incapable of producing autocorrelations that are not positive definite. The band-limited spectrum of subgrid scale turbulence and the damping action of stably stratified flows both give rise to oscillatory velocity autocorrelations whose integral times scales are vanishingly small. To reproduce these types of stochastic velocities requires Markov-2, or higher, sequences. From here on we will restrict attention to the case $M = 2$.

For notational purposes it is convenient at this point to dispense with the subscripts on the coefficients α in (16) and to use them instead to denote the time step. Thus, for the case $M = 2$ we will write (16a) in the form

$$\dot{\xi}_{n+1} = \alpha \dot{\xi}_{n-1} + \beta \dot{\xi}_n + \gamma \rho_\xi. \tag{18}$$

For notational simplicity, we will not carry a time subscript on ρ_ξ because it is immaterial except in analytical manipulations of (18) that produce joint moments, such as those specified in (17). Squaring (18), averaging, and making use of (17) we obtain

$$\langle \dot{\xi}_{n+1}^2 \rangle = \alpha^2 \langle \dot{\xi}_{n-1}^2 \rangle + \beta^2 \langle \dot{\xi}_n^2 \rangle + 2\alpha\beta \langle \dot{\xi}_{n-1} \dot{\xi}_n \rangle + \gamma^2 \langle \rho_\xi^2 \rangle. \tag{19}$$

By virtue of (17a)

$$\langle \rho_\xi^2 \rangle = \sigma_u^2. \tag{20}$$

Furthermore, in stationary homogeneous turbulence, which we are considering here, we have $\langle v_n^2 \rangle = \sigma_u^2$, $n = 1, 2, \ldots, \infty$. From (14)–(17) and (20) we find that this condition is satisfied if

$$\langle \dot{\xi}_n^2 \rangle + \langle \xi_n^2 \rangle \dot{b}^2/a^2 = \sigma_u^2. \tag{21a}$$

As we discuss later, in applications of this scheme to subgrid scale turbulence, we can represent the parameters a and b by constants without significant loss of accuracy. The same assumption can be adopted to treat particle motion in boundary layer flows up to the time that one of the particles strikes a boundary. After that point we set $a = \xi = 0$, $b = 1$. Thus, in the remainder of this paper we restrict attention to the case where $\dot{a} = \dot{b} = 0$. In these situations, (21a) reduces to

$$\langle \dot{\xi}_n^2 \rangle = \sigma_u^2 \tag{21b}$$

for all n, and the autocorrelation $\langle v_n v_m \rangle$ becomes

$$\langle v_n v_m \rangle = \langle \dot{\xi}_n \dot{\xi}_m \rangle = \sigma_u^2 R_{n-m} \qquad (R_{n-m} \equiv R_v((n-m)\,\Delta t)). \tag{22}$$

That is, the velocity autocorrelation is a function only of the time interval between the two observations. In view of (19), conditions (20)–(22) place a constraint on the values of α, β, and γ—

$$\alpha^2 + \beta^2 + \gamma^2 + 2\alpha\beta R_1 = 1. \tag{23}$$

Multiplying (18) by ξ_n and averaging we get

$$R_1 = \beta/(1-\alpha) \tag{24}$$

and in general

$$R_n = \alpha R_{n-2} + \beta R_{n-1}, \qquad n \geqslant 2. \tag{25}$$

An important characteristic of the autocorrelation function, and one that we wish to control in simulations, is its integral time scale, which in the present instance we define by

$$\mathscr{T} \equiv \Delta t \sum_{n=0}^{\infty} R_n. \tag{26}$$

Using (24) and (25) we obtain

$$\mathscr{T}/\Delta t = 1 + \beta/(1-\alpha) + \alpha \sum_{n=2}^{\infty} R_{n-2} + \beta \sum_{n=2}^{\infty} R_{n-1}. \tag{27}$$

Expressing the two summations in this equation in terms of $\mathscr{T}$ we find

$$\mathscr{T}/\Delta t = \frac{(1-\alpha+\alpha\beta)}{(1-\alpha)(1-\alpha-\beta)}. \tag{28}$$

It is evident from this result that the coefficients α and β, but not γ, affect the form of the velocity autocorrelation and that by selecting them properly we can achieve a desired integral time scale and autocorrelation form. Once α and β have been selected, γ is fixed by Eq. (23).

Figure 1a is a plot of Eq. (28). It shows that with the Markov-2 sequence, integral times scales in the range $0.5 < \mathscr{T}/\Delta t \leqslant \infty$ can be achieved. (As a point of reference, $\mathscr{T}/\Delta t = 1$ corresponds to a white noise process, i.e., one in which the particle velocity at any given time is independent of its values at all previous times.) The shaded region in Fig. 1a delineates the "working space" of the coefficients α and β. Outside this space, γ, under the constraint of (23), is complex.

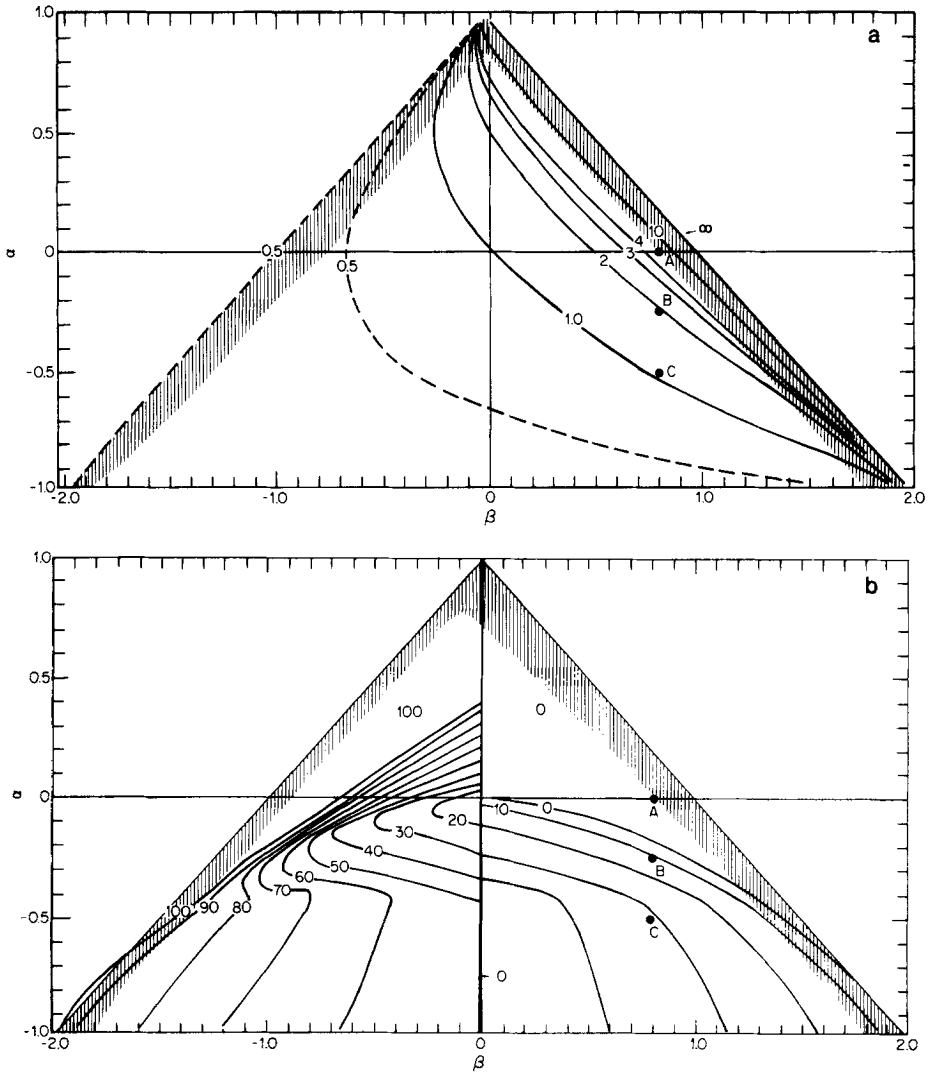

FIG. 1. (a) The integral time scale $\mathscr{T}/\Delta t$ of the simulated particle velocities as a function of the parameters α and β (see Eqs. (18), (22), and (26)). Values of α and β outside the shaded triangular region are not permissible because they force the parameter γ to be complex. (b) Isolines of the number of zero crossings of the velocity autocorrelation (Eq. (22)) in the lag interval $0 \leqslant t \leqslant 100\Delta t$.

A general picture of how the joint values of α and β affect the shape of the autocorrelation R_n (defined by (22)) is provided by Fig. 1b. Plotted there are isolines of the number of times the autocorrelation R_n crosses the zero line in the time lag interval $0 \leqslant n \leqslant 100$. Further details are available from Fig. 2 which shows the actual autocorrelations for the three sets of parameter values (α, β) indicated by the points labeled A, B, and C in Fig. 1. It appears that, in general, as the frequency of oscillation of R_n increases, the damping of the amplitude of R_n decreases. Thus, for $(\alpha, \beta) \simeq (-1, -1)$ the autocorrelation function oscillates virtually undamped between values of $+1$ and -1 at each successive lag interval $n\,\Delta t$ as $n \to \infty$.

By definition of $\dot{\xi}$ we have

$$\xi(t_N) = \xi(0) + \Delta t \sum_{n=1}^{N} \dot{\xi}_{n-1} \tag{29}$$

which yields for the case $\xi(0) = 0$

$$\langle \xi^2(t_N) \rangle = \Delta t^2 \sigma_u^2 \left(N + 2 \sum_{n=1}^{N} (N-n) R_n \right). \tag{30}$$

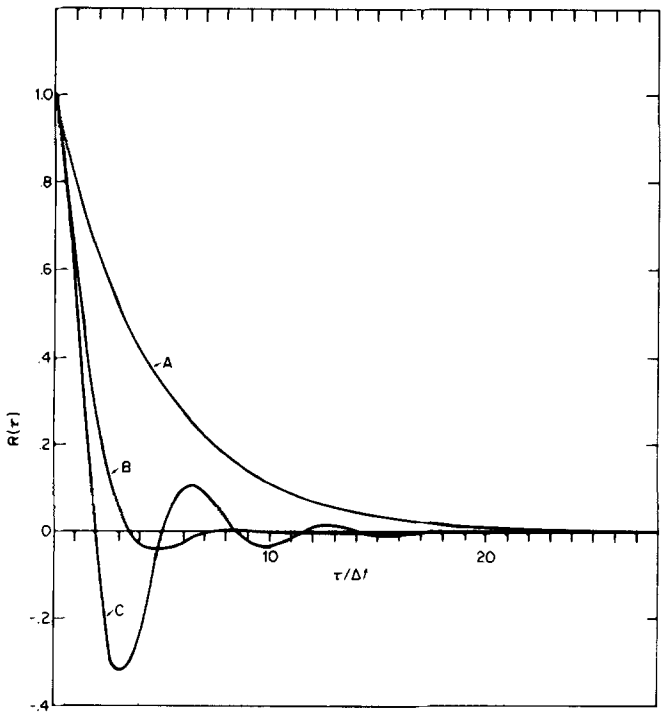

FIG. 2. The velocity autocorrelation produced by the (α, β) values denoted by the points labeled A, B, and C in Fig. 1. The corresponding values of γ are given by Eqs. (23) and (24).

Since it is $\langle \xi^2 \rangle$ that represents the single particle displacement variance (see (13)), it is imperative that α and β be selected to make R_n as accurate a representation of the true particle velocity autocorrelation as possible.

We have already specified in (17a) that the probability density of the computer generated random numbers ρ_ξ be identical to that of the Eulerian velocities. In neutrally stratified, homogeneous turbulence, velocity fluctuations are normally distributed (Batchelor [13];, but in other conditions, e.g., convective turbulence, it may be distinctly non-Gaussian. Methods exist for generating random variables with any distribution. Perhaps the simplest is to use a uniform random number generator to index a table of numbers configured in such a manner that the values retrieved have the desired distribution. We have found this technique to be very effective and to require minimum machine time.

All of the steps described above for generating $\dot{\xi}$ and ξ pertain to χ_1 and χ_2 as well. The only difference is that the random numbers ρ_1 and ρ_2, which are the counterparts of ρ_ξ, should have the proper joint distribution. In practice this information is rarely available and it is necessary to assume that these are statistically indepent variables. Their marginal densities are the same as that of ρ_ξ.

III. Initialization of the Scheme

In order to preserve the constancy of $\langle \dot{\xi}^2 \rangle$ and $\langle \dot{\chi}^2 \rangle$ in simulations of stationary, homogeneous turbulence, care must be taken in generating the initial values of these velocities. From (18) and analyses like those that follow that equation it is easy to show that the initial values of $\dot{\xi}$ should be

$$\dot{\xi}_0 = \rho_\xi(t_0), \tag{31a}$$

$$\dot{\xi}_1 = R_1 \dot{\xi}_0 + (1 - R_1^2)^{1/2} \rho_\xi(\Delta t). \tag{31b}$$

Subsequent values are then obtained from (18). Similar expressions apply to $\dot{\chi}_1(t_0)$ and $\dot{\chi}_2(t_0)$.

IV. Application of the Scheme to Nonstationary, Inhomogeneous Flows

Our methodology has been based on the premise that any turbulent flow can be treated as though it is locally stationary, homogeneous, and isotropic. These assumptions create at least two basic problems in attempting to apply it to situations where the flow does not possess these properties everywhere. The first is that some of the mathematical relationships that we used to develop the scheme no longer hold; and the second is that it is not clear how a particle velocity acquires the local properties of a flow as it moves through regions possessing spatially and temporally variable flow properties. For example, if a particle leaves a point where the integral time scale of the Eulerian velocity autocorrelation has one value and moves into a

region characterized by a wholly different value, at what rate is this change manifest in the particle's motion. This is a very basic question that we cannot answer at this point. Perhaps studies performed with numerical turbulence models can resolve it.

The problems associated with the mathematical structure of the scheme can be minimized by making the simulation time step Δt sufficiently small. In inhomogeneous turbulence the velocity variance $\langle \dot{\xi}_n^2 \rangle$ will depend on where the particle is in the fluid in the mean at time step $n\,\Delta t$. If σ_u is taken as a characteristic particle velocity scale and $(\sigma_u^{-1} |\nabla \sigma_u|)^{-1}$ as a characteristic length scale of the inhomogeneity of the flow, then we can expect that $\langle \dot{\xi}^2 \rangle$ will vary little within any interval of three time steps (as we assumed earlier in our manipulation of (19)) provided that

$$\Delta t \ll |\nabla \sigma_u|^{-1}. \tag{32}$$

The time step should also be small compared to the smallest period of non-stationarity of the flow statistics.

In order for the definition (22) of R_n that we used in the scheme development to remain meaningful, we require in addition that

$$\mathscr{E} \ll |\nabla \sigma_u|^{-1}. \tag{33}$$

There is no way to estimate accurately the magnitude of error that would be incurred by applying our scheme to problems in which (33) is not satisfied.

V. Modifications of the Scheme near Reflective Boundaries

The Markov form of the velocity parameterization imparts a "memory" of approximate length $\mathscr{E}$ to the motion of each particle. Consequently, a particle that has a positive velocity, say, just prior to its striking a reflective boundary, is more likely to have a positive value again after impact than a negative one. Hence, on average, each particle will bounce against barriers several times before finally its velocity is reversed and it moves away. This phenomenon is manifest in diffusion simulations by anomalously large particle concentrations adjacent to all reflective surfaces.

In actuality, turbulent eddies that carry particles toward a wall usually have a circulatory motion that soon carries them back away, and consequently the toward-the-wall memory is lost. We can approximate this effect in our scheme by reinitializing ξ, $\dot{\xi}$, χ_n, and $\dot{\chi}_n$ (using (31)) immediately following each reflection from a surface. We have tested this modification of the scheme and have found that it eliminates the bouncing phenomenon. We might add that if the toward-the-wall memory is reversed after collision with walls, rather than erased, the particles rebound so strongly that they spend too little time near reflective surfaces.

In applications of the scheme to simulation of subgrid scale turbulence, the probability density of ρ_ξ (and ρ_n) can be skewed either positively or negatively during

post reflection reinitializations to account for the presence of resolvable scale updraft or downdraft motions in the grid cell directly over the particle.

VI. Applications

In this final section we will discuss some of the steps involved in applying the scheme we have developed to simulating subgrid scale turbulence and to modeling dispersion in the atmospheric boundary layer. Before proceeding it is convenient to summarize the complete scheme.

$$v_k = a\dot{\xi} + \dot{a}\xi + b\dot{\chi}_k + \dot{b}\chi_k, \qquad k = 1, 2,$$

$$\dot{\xi}(t_{n+1}) \equiv \dot{\xi}_{n+1} = \alpha\dot{\xi}_{n-1} + \beta\dot{\xi}_n + \gamma\rho_\xi$$

($\dot{\xi}_n$ is reinitialized, see (31), after each particle reflection from walls)

$$\dot{\xi}_0, \dot{\xi}_1 \qquad \text{see (31)},$$

$$\xi(t_n) \equiv \xi_n = \Delta t \sum_{m=1}^{n} \dot{\xi}_{m-1},$$

where ρ_ξ is a computer generated random number with properties (17) and α and β are time-dependent variables chosen to yield a given integral time scale $\mathscr{E}$ (see Eq. (28)) and velocity autocorrelation shape (see Figs. 1 and 2)

$$\gamma^2 = 1 - \alpha^2 - \beta^2 - 2\alpha\beta^2/(1-\alpha),$$

$$\dot{\chi}_k(t_{n+1}) = \alpha\dot{\chi}_k(t_{n-1}) + \beta\dot{\chi}_k(t_n) + \gamma\rho_k(t_{n+1}),$$

$$\chi_k(t_n) = \Delta t \sum_{m=1}^{n} \dot{\chi}_k(t_{m-1}) \qquad (\chi_k(t_n) = 0 \text{ after reflection})$$

$\dot{\chi}_k(t_0)$ and $\dot{\chi}_k(t_1)$ are the same as (31) except ρ_ξ is replaced by ρ_k. $\rho_k\,(k = 1, 2)$ are computer generated random numbers with properties analogous to (17);

$$a^2 = 1 - \langle l^2 \rangle / 2\sigma^2,$$

$$b^2 = 1 - a^2,$$

$$\dot{a} = \frac{da}{dt}, \qquad \dot{b} = \frac{db}{dt}.$$

Specification of the particle separation $\langle l^2 \rangle$ needed to determine the coefficient a is discussed below.

A. *Subgrid Scale Turbulence Parameterization*

When the flow fields from numerical turbulence models are used to derive Lagrangian turbulence statistics, the effects on particle motion of subgrid scale velocity fluctuations must be taken into account. This was discussed in the introduction (see Eq. (5) and the ensuing discussion). Here we will discuss how the scheme we have developed could be used in this role in applications of Deardorff's [8] turbulence model.

His model provides, in addition to other quantities, 3-D wind components and subgrid energy E at time intervals of 8 sec on a network of 64000 grid points of resolution $\Delta = (\Delta x\, \Delta y\, \Delta z)^{1/3} \simeq 100$ m. Under the conditions of his simulations, Δ lies in the inertial subrange.

Assuming that the subgrid scale velocities are isotropic and have a Gaussian distribution, we would use in accordance with (17a) normally distributed random numbers for ρ_ξ (and ρ_1, ρ_2) with zero mean, and variance (see (20)

$$\langle \rho_\xi^2 \rangle = \sigma_u^2 = \tfrac{2}{3}E, \tag{34}$$

where E is evaluated at the instantaneous particle position.

The band-limited spectrum of subgrid scale turbulence implies that the autocorrelation of the Eulerian velocities has a zero integral time scale [14]. Whether the same is true for the Lagrangian velocity is not known, but it is probably safe to assume that its time scale $\mathscr{T}$ is much smaller than $E^{-1/2}\Delta$. The smallest time scale that can be simulated by our scheme is $\mathscr{T} = 0.5\Delta t$. Thus, if we select values for α and β that yield this minimum time scale (see Eq. (28) and Fig. 1a), and if we assume that the time scale $\mathscr{T}$ of subgrid turbulence is $\mathscr{T} = 0.1E^{-1/2}\Delta$, then we would require a time step

$$\Delta t \leqslant 0.2E^{-1/2}\Delta$$

in the simulation of the subgrid turbulence.

Figure 1a shows that there is a sizable region of (α, β) space in which the corresponding integral time scale $\mathscr{T}$ has its minimum value $0.5\,\Delta t$. To decide which point in this space to use to simulate subgrid scale turbulence, we recommend that (α, β) be selected to yield an autocorrelation function that is consistent with the energy spectrum of the subgrid scale turbulence. In this regard we point out that a homogeneous stochastic process with the band-limited spectrum

$$S(k) = \begin{cases} A, & k_0 - B/2 \leqslant k \leqslant k_0 + B/2 \\ 0 & \text{otherwise} \end{cases} \tag{35}$$

has the autocorrelation

$$R(\delta) = AB\left(\frac{\sin B\delta}{B\delta}\right)\cos k_0\delta. \tag{36}$$

Here k is wave number,

$$R(\delta) = \langle u(x)\, u(x+\delta)\rangle, \tag{37}$$

and B is the bandwidth. If we assume that the spectrum of subgrid scale turbulence can be approximated by (35), then the spectrum amplitude A and the band width B are related to the variance σ_u^2 of the subgrid turbulence by

$$\sigma_u^2 = AB. \tag{38}$$

If we use as a measure of A the amplitude of the spectrum at the grid cutoff wave number π/Δ (the Nyquist wave number), then the effective bandwith is

$$B = 2E/3S(\pi/\Delta) \tag{39}$$

(cf. (34) and (38)). The amplitude of S at π/Δ might be approximated by extrapolating the resolvable scale velocity spectrum down to this wave number or by making use of inertial subrange theory, if appropriate. Thus, with B given by (39), $A = S(\pi/\Delta)$, and

$$k_0 = \pi/\Delta + B/2, \tag{40}$$

we have in (36) an approximation of the form of the spatial correlation of the subgrid scale turbulence. The corresponding form of the Lagrangian time autocorrelation may be grossly different: but if we assume for now that the two correlation functions have at least similar shapes, we can use (36) to guide the choice of (α, β) values for use in the velocity parameterization above. Note, for example, that if the bandwidth B is small, the damping factor (in parentheses) in (36) has approximately unit value for sufficiently small values of δ and the resulting function $R(\delta)$ is an undamped cosine wave. Our scheme yields autocorrelations with this property as is revealed by the plot in Figure 1b of the number of zero crossings of the correlation as a function of (α, β). The larger the number of zero crossings, the less damped the oscillatory component of the simulated autocorrelation is.

For large bandwidths, the damping factor in (36) is more dominant, leading to functions $R(\delta)$ that, for sufficiently small δ, resemble that plotted in Fig. 2 for the (α, β) pair denoted by the point C in Fig. 1.

The guidelines we have just outlined for selecting values of α and β for simulating subgrid scale turbulence are obviously not definitive. Further studies of the Lagrangian characteristics of band-limited turbulence are needed to achieve reliable parameterizations of subgrid turbulence. Our guidelines should be viewed only as a suggested criterion, in addition to that of minimizing the integral time scale $\mathscr{T}$, for selecting (α, β).

The fact that Δ lies in the inertial subrange greatly facilitates the task of formulating an expression for the parameter a for use in simulating the subgrid scale motions of a pair of particles separated initially by a distance $l_0 < \Delta$. Using

Kolmogorov's similarity hypothesis, Batchelor [15] showed that if l_0 lies in the inertial subrange, then for small times

$$\langle l^2 \rangle = \tfrac{10}{3} C_1 l_0^{2/3} \varepsilon^{2/3} t^2, \qquad t \ll l_0^{2/3} \varepsilon^{-1/3}, \tag{41}$$

where C_1 is a constant of order one, ε is the energy dissipation rate of the turbulence, and t is travel time. The single particle displacement variance σ^2 is initially

$$\sigma^2 = \sigma_u^2 t^2. \tag{42}$$

This follows immediately from the relationship $x = ut$, which is valid only for travel times t small enough that $R_u(t) \simeq R_u(0)$.

Deardorff [16] suggests for ε the semi-empirical expression

$$\varepsilon = E^{3/2}(0.7G/\Delta), \tag{43a}$$

where

$$G = 1 + 2((z/\Delta z + 3/2)^2 - 3.3)^{-1}, \qquad z > \Delta z/2, \tag{43b}$$

and z is elevation above ground. Combining (41)–(43) with (14a), we obtain an expression for the initial value of the scheme parameter a—

$$a_0 = a(t_0) = 1 - (0.7G)^{2/3} (l_0/\Delta)^{2/3}. \tag{44}$$

To obtain this expression we set $C_1 = 2/5$.

Earlier we pointed to evidence that the time scale $\mathscr{E}$ of subgrid scale turbulence is very small. It can be shown [14] that if $\mathscr{E} = 0$, σ^2 increases from an initial value of zero to some finite constant value that it retains for all later time. The corresponding behavior of $\langle l^2 \rangle$ when $l_0 \ll \Delta$ is not known. Based on the points just raised we propose that a reasonable interim aproximation is

$$\langle l^2 \rangle \propto \sigma^2$$

from which it follows that

$$a(t) = a_0. \tag{45}$$

Any errors introduced into the scheme by this simple expression will not grow indefinitely because once the particle separation exceeds Δ, its subsequent evolution is dominated by the resolvable scales of motion.

In summary, in simulations of subgrid scale turbulence, our recommended particle pair velocity parameterization is

$$v_k = a_0 \dot{\xi} + (1 - a_0^2)^{1/2} \dot{\chi}_k, \qquad k = 1, 2,$$

where a_0 is given by (44) and

$$\dot{\xi}(t_{n+1}) \equiv \dot{\xi}_{n+1} = \alpha \dot{\xi}_{n-1} + \beta \dot{\xi}_n + \gamma \rho_\xi .$$

Here ρ_ξ is a Gaussian (computer generated) random number with zero mean and variance

$$\langle \rho_\xi^2 \rangle = \tfrac{2}{3}E.$$

It must also have the properties given by Eq. (17).

The parameters α and β should be chosen such that (1) $\mathscr{E}/\Delta t \simeq 0.5$ (see Eq. (28) and Fig. 1), and (2) the shape of the autocorrelation function R_n (see (25)) is consistent with the energy spectrum of the subgrid turbulence (see Eqs. (35) and (36) and the discussions that follow them). The time step Δt used in the scheme should be

$$\Delta t \simeq 0.2E^{-1/2}\Delta .$$

The expressions for γ and $\dot{\chi}_k$ are given in the introduction of Section VI (the random variables ρ_1 and ρ_2 used to generate $\dot{\chi}_k$ have properties identical to ρ_ξ). Refer to Sections III and V for instructions on initialization, and modifications near boundaries.

B. *Modeling Dispersion in the Atmospheric Boundary Layer*

The mathematical details of applying the scheme developed here in conjunction with Eq. (1) to predict mean concentration is presented in Lamb *et al.* [17]. The use of the velocity simulation scheme in this role is the same as in the parameterization of subgrid scale motion described above, except similarity profiles of σ_u, σ_w, ε, etc., are used in place of E, and profiles of the horizontal flow $\bar{u}(z)$ gotten either from similarity theory or observations are used in place of the model generated $\hat{u}$ values to determine mean transport. In this type of application the stochastic velocity has an indefinitely broad spectrum, rather than just the high-frequency fluctuations rejected by the grid cell averaging employed in numerical turbulence models. Thus, the integral time scale $\mathscr{E}$ is significantly larger than zero and empirical data are available from which it can be estimated (see [17]). The dispersion model presented in Ref. [17] is tested against an extensive set of concentrations data and found to provide quite accurate estimates of the mean concentrations produced by sources in the atmospheric boundary layer under a wide range of wind speed and stability conditions.

VII Conclusion

We have developed a method of generating pairs of random velocity fields suitable for simulating particle pair motions in turbulent fluid. The scheme can be used to simulate the effects of subgrid scale turbulence where one in interested in determining

Lagrangian turbulence statistics from instantaneous velocity fields obtained from a numerical turbulence model; or the scheme can be used as the basis of a Monte Carlo model of turbulent dispersion, where one attempts to simulate dispersion from given Eulerian statistics of the turbulence. The inputs to the scheme include the profiles of mean wind and variances of the turbulence velocities, the Lagrangian integral time scale, and the energy dissipation rate of the turbulence. With very simple modifications, the scheme can be used to simulate buoyant particles, particles with nonzero settling velocities, and particles that are absorbed or resuspended from boundary surfaces.

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