Stochastic Differential Equations and Turbulent Dispersion

Paul A. Durbin

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Paul A. Durbin
Lewis Research Center
Cleveland, Ohio

PREFACE

This report introduces aspects of the theory of continuous stochastic processes that seem to contribute to an understanding of turbulent dispersion. It is expected that the reader has a knowledge of basic probability theory and some exposure to turbulence theory and the phenomena of turbulent transport.

The report is addressed to researchers in the subject of turbulent transport, especially those with an interest in stochastic modeling. However, the material presented herein deals with the theory and philosophy of modeling, rather than treating specific practical applications. The book by Csanady (ref. 1) is a good place to begin an exploration of applications, as well as to obtain a background to the contents of the present report.

CONTENTS

CHAPTER I: OBJECTIVES AND INTRODUCTION

The transport, or dispersion, of contaminant by turbulent convection is an archetypal continuous stochastic process. The theory of stochastic differential equations evolved, from early studies on Brownian motion, as a mathematical theory of continuous stochastic processes. It is natural to look to the theory of stochastic differential equations for insight into the phenomenon of turbulent transport. Indeed, some comprehension of the theory of continuous stochastic processes seems prerequisite to a basic understanding of turbulent dispersion. This report introduces aspects of stochastic differential equations that seem to bear on turbulent dispersion theory.

The problem of turbulent dispersion can be posed as follows:
Given a statistically prescribed field of turbulent velocity, describe statistically the evolution of a contaminant field from a known initial state.

In this formulation of the problem the velocity field is given in whatever degree of minuteness is requested. From this information one wants to describe statistically the concentration field $C(x,t)$ of a contaminant, knowing it initially to be $C_0(x)$. This report is addressed entirely to the problem of determining either the mean value of this contaminant field $\overline{C}(x,t)$ or the spatial moments of this mean contaminant field - the latter as functions of time alone.

Two approaches can be taken to the analysis of turbulent dispersion, the Eulerian approach and the Lagrangian approach. In the Eulerian approach one formulates model conservation equations for fixed control volumes in the fluid; in the Lagrangian approach one formulates a random trajectory model of the motion of parcels of contaminated fluid. This latter approach will be followed herein. However, there is a close relation between the Eulerian and Lagrangian formulations: the Eulerian conservation equations determine the probability density function (pdf) of the random, Lagrangian, trajectories. For example, when the Eulerian model consists simply of an eddy diffusion equation (ref. 1, section 5.5), the Lagrangian model for which it determines the pdf represents trajectories by a continuous Markov process (chapter III). How could the evolution of mean concentration from an initial state be calculated from the statistics of random trajectories?

Suppose one knows the initial distribution of contaminant to be $C_0(y)$. Also, one knows an ensemble of random trajectories of fluid particles, each trajectory originating at some point y_0. If it is assumed that fluid particles retain their initial concentration $C_0(y_0)$, then the mean concentration at the point (y,t) is just the probability that a parcel observed at position y at time t originated at some arbitrary point y_0, times the concentration at that point $C_0(y_0)$, summed over all possible origins:

$$\overline{C}(y,t) = \int_{-\infty}^{\infty} P(y,t; y_0)\, C_0(y_0)\, dy_0 \qquad (I-1)$$

This equation uses the definition that the probability of a particle originating at y_0 (actually, between $y_0 - dy_0/2$ and $y_0 + dy_0/2$) is

$$P(y,t; y_0)dy_0 \qquad\qquad (I-2)$$

Note that in equation (I-1) the final position of the random trajectories is fixed at y, while the initial position y_0 is the random variable. (The random position y_0 would be calculated by following a trajectory from the known position y backwards in time to y_0.)

The derivation of equation (I-1) required that fluid particles conserve their initial contaminant concentration. To what extent is this valid? For any contaminant with finite molecular diffusivity κ, fluid particles will not totally conserve their initial concentration. However, equation (I-1) describes only the average transport of contaminant; so this loss of contaminant by molecular diffusion may not be important. Let us consider the relative contributions of molecular and turbulent transport to mean dispersion.

Molecular diffusion transports contaminant down concentration gradients. Hence, it acts primarily on small-scale features of the contaminant distribution, which have the largest gradients. These small-scale features are produced by an interaction between molecular diffusion and convection of contaminant by the small eddies of the turbulent velocity field. It follows that the length scale relevant to these small-scale features is the turbulence microscale λ_κ (ref. 2, p. 67; the subscript κ here indicating that the microscale is based on molecular diffusivity instead of on viscosity). Molecular diffusion, by smoothing these small-scale features, transports contaminant a distance of order λ_κ. Turbulent convection, on the other hand, transports contaminant a distance comparable to the turbulence integral scale ℓ (ref. 2, p. 20). The ratio of transport by molecular diffusion to that by turbulent dispersion is thus of order λ_κ/ℓ or of order $(Pe)^{-1/2}$ (ref. 2, p. 68). The turbulent Peclet number is defined by

$$Pe = u'\ell/\kappa \qquad\qquad (I-3)$$

where u' is the variance of the turbulent velocity. Hence, it can be concluded that equation (I-1) is formally valid when $(Pe)^{-1/2} \ll 1$. This report is concerned with high-Peclet-number and high-Reynolds-number turbulence, so equation (I-1) is justified.

The problem of mean dispersion has been reduced by equation (I-1) to that of determining $P(y,t;y_0)$, or equivalently, to modeling the random trajectories for which $P(y,t;y_0)$ is the pdf. This can be done by representing the dynamics of fluid particles in turbulent flow by simple stochastic processes. The criterion such models must satisfy is that they reproduce certain statistical features of the turbulent velocity field. As the problem of turbulent dispersion was posed above, the statistics of the velocity field are considered to be known in their entirety. However, the statistics most crucial to turbulent transport are the macroscopic length and time scales and the variance of the turbulent velocity and, in the case of nonhomogeneous turbulence, their spatial distribution. To make progress, models are based on only these restricted properties of the turbulence; for example, the eddy diffusion model requires knowledge only of the product $u'\ell$ of the length scale and velocity variance, which has the dimensions of diffusivity. The

present report is a discussion of concepts pertinent to stochastic modeling of turbulent dispersion.

This report is not meant to be comprehensive, either in its treatment of stochastic differential equations or in its description of turbulent dispersion. Stochastic differential equations are introduced in reference 3 and treated more comprehensively in reference 4; for accounts of turbulent dispersion see references 1, 2, and 5. In chapter II a very nonrigorous review of the theory of stochastic differential equations is provided, touching on those aspects of this theory that seem relevant to understanding and analyzing turbulent dispersion. Chapters III and IV deal specifically with models for the random trajectories of fluid particles through turbulent flow. If these trajectories are considered at times that are long compared with the macroscopic time scale T_L of the turbulence, they can be modeled by continuous Markov processes, or as they are alternatively called, by diffusion processes. Chapter III discusses eddy diffusion models; chapter IV discusses dispersion at times comparable to T_L and uses the Langevin equation for a random trajectory model.

To avoid later confusion, this introduction ends with a discussion of some notation to be used in this report. When a letter such as y is used as a dependent variable to denote a random trajectory, it will be written as a capital $Y(t)$, with or without explicit indication of time dependence. When it is used as an independent variable, denoting a spatial coordinate, it will be written as a lower case y. The average of a random variable is signified by an overbar: $\overline{Y}(t)$ is the mean trajectory of $Y(t)$. Of course, averaging can be carried out by integrating over a probability density if necessary:

$$\overline{Y}(t) = \int_{-\infty}^{\infty} y\, P(y,t)\, dy \qquad (I-4)$$

This illustrates the use of upper- and lower-case letters. The function $P(y,t)$ is the pdf of observing a particle at various points y at a certain t; y and t vary independently here. However, if at each time the mean position of particles is computed, the result is the mean trajectory $\overline{Y}(t)$.

In chapter II a time-dependent stochastic process, called the Wiener process, is introduced and denoted by W_t. By convention the time dependence here is indicated with a subscript: W_t is synonymous with $W(t)$. It might be added that if the randomness in Y is due to a dependence on the Wiener process, the average value of Y could formally be computed as

$$\overline{Y}(t) = \int_{-\infty}^{\infty} Y(w_t,t) P(w_t,t)\, dw_t \qquad . \qquad (I-5)$$

In equation (I-5) the lower-case w_t is used to indicate the independent variable of integration; the subscript is for identification with W_t, not to indicate time dependence.

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CHAPTER II: REVIEW OF STOCHASTIC DIFFERENTIAL EQUATIONS

The theory of stochastic differential equations was developed in the first half of this century by physicists and mathematicians. The physicists trace the origin of their research to Einstein's work on Brownian motion and include Langevin, Fokker, Planck, Smoluchowski, Ornstein, and Uhlenbeck (refs. 6 and 7). This line of research had as its impetus the use of continuous stochastic processes to model random physical systems. The mathematicians' line of approach was to investigate formally the nature of continuous stochastic processes, including their relation to properties of partial differential equations. This body of work originated with Bachelier (who incidentally was investigating the fluctuation of stockmarket prices) and includes contributions by Wiener, Kolmogorov, Ito, and others (ref. 4).

It might be supposed that a stochastic differential equation is any differential equation containing random terms or coefficients. However, the body of theory referred to above is more restrictive in its definition: randomness may only be introduced via a white-noise process. Our review starts naturally with a discussion of white noise and its integral, the Wiener process.

The Wiener Process

Consider the proverbial "drunkard's walk," in which the drunkard moves in one dimension by independent random steps, the nth such step being denoted $\Delta W_{n\Delta t}$. Each step is taken after a fixed time interval Δt. After N steps his position is

$$W_{N\Delta t} = \sum_{n=1}^{N} \Delta W_{n\Delta t}$$

In addition to being independent of one another, the drunkard's steps all have the same statistical properties. For modeling random dynamical systems one would like to replace this discrete random walk by a continuous random process.

A continuous random walk might be constructed by introducing a continuous independent variable $t = N \Delta t$ and letting $N \to \infty$ while $\Delta t \to dt \to 0$. If the resulting W_t is to be continuous, it must further be required that the steps become infinitesimal: $\Delta W_{n\Delta t} \to dW_t$, and of course, the above equation is now $W_t = \int_0^t dW_{t'}$. With these stipulations W_t may be called the continuous drunkard's walk, although it is known more formally as the Wiener process.

Since W_t is the sum of a large number of identically distributed independent random variables, by the central limit theorem (ref. 8) it has a

Gaussian probability density. The Gaussian distribution is fully character-ized by its mean and its variance. Our drunkard will not be allowed any preference in the direction of his walk, so W_t has mean zero.

Now, we return to the discrete drunkard's walk and compute its variance, $\overline{W_{N\Delta t}^2}$. The steps of the drunkard's walk are statistically independent, so $\overline{\Delta W_{n\Delta t}\, \Delta W_{m\Delta t}} = 0$ if $n \neq m$ and $\overline{\Delta W_{n\Delta t}^2}$ has a value, say σ_Δ^2, which is inde-pendent of n since the steps are statistically identical. (The overbar here denotes an average over an ensemble of realizations of the random walk, see equation (I-4).) Thus

$$\overline{W_{N\Delta t}^2} = \overline{\left(\sum_{n=1}^{N} \Delta W_{n\Delta t}\right)^2} = \sum_{n=1}^{N} \overline{\Delta W_{n\Delta t}^2} = N\sigma_\Delta^2 \tag{II-1}$$

Remember that in the continuous walk, $N\,\Delta t$ becomes t. But $\overline{W_t^2}$ can be a function only of t, and this will be the case in equation (II-1) only if σ_Δ^2 is proportional to Δt; indeed, after suitable normalization σ_Δ^2 can be set equal to Δt and equation (II-1) tends to

$$\overline{W_t^2} = t \tag{II-2}$$

as $N \to \infty$ and $\Delta t \to dt$. Thus W_t is Gaussian with mean zero and variance as given in equation (II-2), so its pdf is

$$P(w_t, t) = \frac{e^{-w_t^2/2t}}{\sqrt{2\pi t}} \tag{II-3}$$

(ref. 8, p. 107; see the introduction for a description of the use of upper- and lower-case letters).

The pdf $P(w_t)$ is required to be Gaussian by the central limit theorem, irrespective of the distribution of the increments dW_t. However, it is natural to require $P(dw_t)$ also to be Gaussian; clearly, with mean zero. The variance of dW_t is known too because dW_t is the limit of $\Delta W_{n\Delta t}$ and the latter has variance $\sigma_\Delta^2 = \Delta t$. Thus $\overline{(dW_t)^2} = dt$ and

$$P(dw_t) = \frac{e^{-(dw_t)^2/2dt}}{\sqrt{2\pi\, dt}} \tag{II-4}$$

By their derivation equations (II-3) and (II-4) are consistent with

$$W_t = \int_0^t dW_t .$$

As an aside, note that although W_t is continuous in t, it strictly is not differentiable with respect to t. This can be seen from an order-of-magnitude analysis: $\overline{dW_t^2} = dt$, so $dW_t = O(dt^{1/2})$ and $dW_t/dt = O(dt^{-1/2})$. Therefore dW_t/dt becomes infinite (almost surely) as $dt \to 0$. However, white noise dW_t/dt can be defined as a generalized stochastic process: it gets its name from the fact that its covariance $\overline{dW_t \, dW_{t'}}/dt \, dt'$ is a delta function of $t - t'$. Although the incremental Wiener process dW_t divided by dt is usually called white noise, dW_t itself may be thought of as a white-noise process; of course, its variance is a factor of dt^2 smaller than the usual white noise.

Equation (II-2) gives the variance of the Wiener process at a particular time t. The two-time covariance is also readily determined from the properties of W_t. Because the increments in our drunkard's walk were assumed to be uncorrelated, W_t has independent increments; that is,

$$\overline{dW_t \, dW_\tau} = \begin{cases} 0 & \tau \neq t \\ dt & \tau = t \end{cases} \tag{II-5}$$

(Since dW_t is Gaussian, equation (II-5) ensures complete independence of dW_t and dW_τ, $\tau \neq t$.) Covariances of W_t follow directly from equation (II-5) and the definition of W_t as the integral of dW_t:

$$\overline{W_t W_\tau} = \int_0^t \int_0^\tau \overline{dW_{t'} \, dW_{t''}} = \iint_0^{\min(t,\tau)} \overline{dW_{t'} \, dW_{t''}}$$

$$= \int_0^{\min(t,\tau)} dt' = \min(t,\tau) \tag{II-6}$$

The first step uses the fact that $\int_0^t dW_{t'} = W_t$ and $\int_t^{t+\Delta} dW_{t'} = W_{t+\Delta} - W_t$ are uncorrelated when $\Delta \neq 0$. This follows directly from equation (II-5); indeed, it is an alternative statement of the fact that the increments of which W_t is composed are independent. Multiple-time moments can similarly be determined from equations (II-4) and (II-5).

The property of being composed of independent increments is a crucial property of the Wiener process. This makes it a continuous Markov process - our next topic.

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Continuous Markov Processes

A Markov process can be described as a time-dependent stochastic process in which the future is determined by the present, independently of the past. In deterministic dynamical systems this is the natural state of affairs; but a random system usually has a finite correlation time scale, which is the memory time of the system. Thus it is only in the special case where this correlation time becomes negligible that one obtains a Markov process. A continuous Markov process is also called a diffusion process (for reasons that should become clear later). Thus when describing turbulent transport we only refer to turbulent diffusion when we have in mind a Markovian model of fluid trajectories (eddy diffusion), but in general we refer to turbulent dispersion.

The Wiener process is Markovian, for given its present value as W_t, its future is determined as $W_{t+\Delta} = W_t + \int_t^{t+\Delta} dW_t$, where the integral is independent of the past. The objective of the present study of continuous stochastic processes is to model the random trajectories of fluid particles in turbulent flow. If we call the trajectory of a fluid particle $Y(t)$, the trajectory generated by the Wiener process is the solution to

$$dY/dt = dW_t/dt \qquad (II-7)$$

subject to an initial condition on Y. Clearly, the correlation time of the random velocity in equation (II-7) is zero (see eq. (II-5)), and this makes $Y(t)$ a Markov process. Since dW_t/dt does not really exist, equations like (II-7) will hereinafter be written

$$dY(t) = dW_t$$

The random velocity on the right side of equation (II-7) is a function of time but not of particle position. Thus it describes diffusion in a homogeneous medium. In an inhomogeneous medium a natural generalization of equation (II-7) would be

$$dY(t) = a[Y(t)]dW_t \qquad (II-8)$$

where $a(\cdot)$ is some prescribed function of particle position and without loss of generality $a(y) \geq 0$ for all y. Now the random velocity varies with position. (We will not consider unsteady media, where $a(\cdot)$ is also a function of t, although most of our discussion would remain valid.)

Unfortunately, the interpretation of equation (II-8) is ambiguous unless the idea of a nonanticipating function is introduced. To see this, consider finite-difference approximations to equation (II-8). Compare

$$Y_{n+1} = Y_n + a(Y_n) [W_{(n+1)\Delta t} - W_{n\Delta t}] \qquad (II-9a)$$

to

$$Y_{n+1} = Y_n + a\left(\frac{Y_n + Y_{n+1}}{2}\right)[W_{(n+1)\Delta t} - W_{n\Delta t}] \qquad (II-9b)$$

observing that Y_n depends only on $W_{m\Delta t}$ for $m \leq n$. Thus the right side of equation (II-9a) depends only on $W_{m\Delta t}$, $m \leq n$, and on the increment $W_{(n+1)\Delta t} - W_{n\Delta t}$. But the Wiener process has independent increments, so $W_{(n+1)\Delta t} - W_{n\Delta t}$ is independent of $W_{m\Delta t}$, $m \leq n$. Therefore the statistical average of $a(Y_n)[W_{(n+1)\Delta t} - W_{n\Delta t}]$ over an ensemble of Wiener processes is

$$\overline{a(Y_n)[W_{(n+1)\Delta t} - W_{n\Delta t}]} = \overline{a(Y_n)} \; \overline{[W_{(n+1)\Delta t} - W_{n\Delta t}]} = \overline{a(Y_n)} \times 0 = 0$$

so $\overline{Y}_{n+1} = \overline{Y}_n$. Thus, equation (II-9a) gives rise to no mean particle velocity. The second form does not have this property. In fact, if the truncated Taylor expansion

$$a\left(\frac{Y_{n+1} + Y_n}{2}\right) = a(Y_n) + a'(Y_n)\left(\frac{Y_{n+1} - Y_n}{2}\right) + O(Y_{n+1} - Y_n)^2$$

is substituted, equation (II-9b) can be solved for Y_{n+1}:

$$Y_{n+1} = Y_n + a(Y_n)[W_{(n+1)\Delta t} - W_{n\Delta t}]$$

$$+ \frac{1}{2}a(Y_n)a'(Y_n)[W_{(n+1)\Delta t} - W_{n\Delta t}]^2$$

$$+ O(W_{(n+1)\Delta t} - W_{n\Delta t})^3 \qquad (II-10)$$

Averaging equation (II-10), using $\overline{[W_{(n+1)\Delta t} - W_{n\Delta t}]^2} = \Delta t$, gives

$$\overline{Y}_{n+1} = \overline{Y}_n + \frac{1}{2}\overline{a(Y_n)\,a'(Y_n)}\Delta t$$

Thus equation (II-9b) gives rise to the mean velocity

$$d\overline{Y}/dt = \frac{1}{2}\overline{a(Y)a'(Y)}$$

on letting $\Delta t \to dt$.

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In the continuous limit of equation (II-9a), $a[Y(t)]$ is independent of dW_τ, $\tau \geq t$. A function defined in this way is called nonanticipating because it depends neither on future values of W_t nor on the increment dW_t. This is a convenient way to define $a[Y(t)]$, and it will be adopted hereinafter. Practically, this has the effect that any function of $Y(t)$ is independent of dW_t, as in equation (II-9a). Thus equation (II-8) has zero mean velocity:

$$\overline{dY(t)} = \overline{a[Y(t)]dW_t} = \overline{a[Y(t)]} \times \overline{dW_t} = 0 \qquad (II-11)$$

In general, particles in nonhomogeneous turbulence can have nonzero mean velocity. Such a velocity can be added to equation (II-8) to get the general form for a (one dimensional) diffusion process

$$dY = b(Y)dt + a(Y)dW_t \qquad (II-12)$$

By equation (II-11), equation (II-12) has average

$$d\overline{Y} = \overline{b(Y)}dt$$

Thus $\overline{b(Y)}$ is the mean particle velocity.

Fokker-Planck Equation

A diffusion process of the form of equation (II-12) describes the random trajectories of fluid particles through turbulent flow. The description of fluid motion in terms of particle trajectories is called a Lagrangian description, as mentioned in chapter I. The alternative description discussed there is called Eulerian. The Eulerian analysis is based on a partial differential equation that governs the evolution of the probability density function (pdf) for the random process (eq. (II-12)). The pdf is a function of position in the fluid and of time and determines the probability of a trajectory passing infinitesimally close to a given point. Or, as an alternative physical description, if a large number of marked particles are initially released into the fluid, the pdf gives the fraction of these that at some later time will lie in a small volume around a given point.

We now turn our attention to a derivation of the partial differential equation governing the pdf. In this equation y and t are the independent variables. Hence, it becomes necessary to define an average that can be evaluated at an arbitrary point in the fluid. Such an average is called a conditional average: we wish to calculate the moments of the increment $dY(t)$ on the condition that only trajectories passing through y at time t are considered. However, once subject to $Y(t) = y$, the only randomness remaining in equation (II-12) is dW_t; hence averaging is carried out readily. Making use of $\overline{dW_t} = 0$, $\overline{(dW_t)^2} = dt$, and $\overline{(dW_t)^n} = 0(dt)^{n/2}$, we get

$$\overline{dY} = b(y)dt + a(y)\overline{dW_t} = b(y)dt$$

$$\overline{(dY)^2} = \overline{(b(y)dt + a(y)dW_t)^2} = a^2(y)dt + O(dt^2) \qquad\text{(II-13)}$$

$$\overline{(dY)^n} = O(dt^{n/2}) \ , \ n > 2$$

For later purposes it is only necessary to keep the terms in equation (II-13) that are of order dt.

By definition, the future of a Markov process is determined by its present state alone. Thus the probability density at time t is determined by that at time t – dt and by a transition probability:

$$P(y,t) = \int_{\substack{\text{all} \\ dY}} P(y - dY, t - dt)dP_T(dY; y - dY) \qquad\text{(II-14)}$$

Here $P(\cdot,\cdot)$ is the pdf for fluid particle positions and $dP_T(\cdot,\cdot)$ is the transition probability that a particle moves from $y - dY$ to y in time dt. The integral is over all possible jumps dY. The Fokker-Planck equation is derived from equation (II-14) as follows: The right side of equation (II-14) is expanded in a Taylor series in dY and dt, and the following definitions of the moments of dY:

$$\int dP_T (dY;y) \equiv 1$$

$$\int (dY)^n \ dP_T(dY;y) = \overline{(dY)^n}(y) \qquad\text{(II-15)}$$

$$\int (dY)^n \ \frac{\partial \ dP_T(dY;y)}{\partial y} = \frac{\partial}{\partial y}\int (dY)^n \ dP_T(dY,y) = \frac{\partial \overline{(dY)^n}(y)}{\partial y}$$

are then substituted. The $(dY)^n$ are given explicitly by equation (II-13). If they are substituted, keeping only terms up to order dt, one finds from equation (II-14)

$$P(y,t) = P(y,t) - \overline{dY} \frac{\partial P(y,t)}{\partial y} + \frac{1}{2} \overline{(dY)^2} \frac{\partial^2 P(y,t)}{\partial y^2} - dt \frac{\partial P(y,t)}{\partial t}$$

$$- \frac{\partial \ \overline{dY}}{\partial y} P(y,t) + \frac{1}{2} \frac{\partial^2 \overline{(dY)^2}}{\partial y^2} P(y,t) + \frac{\partial \overline{(dY)^2}}{\partial y} \frac{\partial P(y,t)}{\partial y} + O(dt^2)$$

$$= P(y,t) + dt \left[\frac{1}{2} \frac{\partial^2 [a(y)P(y,t)]}{\partial y^2} - \frac{\partial P(y,t)}{\partial t} - \frac{\partial [b(y)P(y,t)]}{\partial y} \right] + O(dt^2)$$

The last equation can be written as

$$\frac{\partial P(y,t)}{\partial t} + \frac{\partial[b(y)P(y,t)]}{\partial y} = \frac{1}{2}\frac{\partial^2[a(y)P(y,t)]}{\partial y^2} \qquad (II-16)$$

Equation (II-16) is called the Fokker-Planck equation for equation (II-12); clearly, it is a diffusion equation for $P(y,t)$. Indeed, if $a^2(y)/2$ is defined as the eddy diffusivity, $a^2(y)/2 = K(y)$, then equation (II-16) can be put into the form

$$\frac{\partial P}{\partial t} + \frac{\partial}{\partial y}\left[\left(b - \frac{\partial K}{\partial y}\right)P\right] = \frac{\partial}{\partial y}\left(K\frac{\partial P}{\partial y}\right) \qquad (II-17)$$

which is the conservation equation form of an eddy diffusion equation. In equation (II-17) $[b(y) - \partial K(y)/\partial y]$ plays the role of an Eulerian mean convection velocity. When the latter is zero, $b(y) = \partial K(y)/\partial y$ and equation (II-17) becomes

$$\frac{\partial P}{\partial t} = \frac{\partial}{\partial y}\left(K\frac{\partial P}{\partial y}\right)$$

with the corresponding form of equation (II-12) being

$$dY = \frac{\partial K}{\partial y}(Y)dt + \sqrt{2\,K(Y)}\,dW_t \qquad (II-18)$$

(since $a^2 = 2K$ and $b = \partial K/\partial y$). Averaging equation (II-18) over an ensemble of trajectories gives the Lagrangian mean velocity

$$\frac{d\overline{Y}}{dt} = \overline{\frac{\partial K}{\partial y}(Y)} \qquad (II-19)$$

Hence, in a nonhomogeneous medium (where K is a function of y) the Lagrangian mean velocity of fluid particles may be nonzero, even though their Eulerian mean velocity is zero. More will be said about equations (II-18) and (II-19) in chapter III.

Ito's Theorem

We return from our excursion into Eulerian analysis to equation (II-12) and investigate its calculus. Because the functions in equation (II-12) were defined to be nonanticipating, certain peculiarities arise; it is necessary to derive a calculus consistent with the nonanticipating property.

Consider the following example: In equation (II-12) let $b = 0$ and $a = Y$,

$$dY = Y\,dW_t \qquad (II-20)$$

One is inclined to integrate this as

$$Y = Ce^{W_t} \tag{II-21}$$

where C = constant. However, on averaging equation (II-20), using the non-anticipating property to write $\overline{Y\,dW_t} = \overline{Y}\ \overline{dW_t} = \overline{Y} \times 0$, one finds $d\overline{Y} = 0$ or $\overline{Y} = C$. But by equations (II-3) and (I-5), equation (II-21) has the average

$$\overline{Ce^{W_t}} = \frac{C}{\sqrt{2\pi t}} \int_{-\infty}^{\infty} \exp\left(W_t - W_t^2/2t\right) dW_t = Ce^{t/2}$$

Hence equation (II-21) is not a nonanticipating solution to equation (II-20) Clearly $Y = C\exp(W_t - t/2)$ has the correct mean, and in fact it is the non-anticipating solution to equation (II-20). How does one know this?

The derivative of a function $f(W_t)$ of W_t can be defined as df in the relation

$$f(W_t,t) = \int df(W_t,t) + \text{constant}$$

Expanding the integrand in a Taylor series, to order dt, gives

$$\int df = \int \frac{\partial f}{\partial W_t}\, dW_t + \frac{1}{2}\int \frac{\partial^2 f}{\partial W_t^2}\,(dW_t)^2 + \int \frac{\partial f}{\partial t}\, dt + o(dt) \tag{II-22}$$

It can be shown that (ref. 3, p. 98)

$$\int \frac{\partial^2 f}{\partial W_t^2}\,(dW_t)^2 = \int \frac{\partial^2 f}{\partial W_t^2}\, dt \tag{II-23}$$

using equality in a statistical sense. (Roughly, the equality (II-23) is shown as follows: In mean square, upon averaging over dW_t with W_t fixed

$$\left[\int \frac{\partial^2 f}{\partial W_t^2}\,(dW_t)^2 - \int \frac{\partial^2 f}{\partial W_t^2}\, dt\right]^2 = \iint \frac{\partial^2 f}{\partial W_t^2}\frac{\partial^2 f}{\partial W_{t'}^2}\overline{(dW_t)^2\,(dW_{t'})^2}$$

$$-2\iint \frac{\partial^2 f}{\partial W_t^2}\frac{\partial^2 f}{\partial W_{t'}^2}\, dt\ \overline{(dW_{t'})^2} + \iint \frac{\partial^2 f}{\partial W_t^2}\frac{\partial^2 f}{\partial W_{t'}^2}\, dt\, dt'$$

$$= \iint \frac{\partial^2 f}{\partial W_t^2}\frac{\partial^2 f}{\partial W_{t'}^2}\,(dt\, dt' - 2dt\, dt' + dt\, dt') = 0$$

$$\tag{II-24}$$

having used $\overline{(dW_t)^2} = dt$ and $\overline{(dW_t)^2(dW_{t'})^2} = dt\, dt'$, $t \neq t'$. Since the square of a number is nonnegative, the fact that the mean value of the left side of equation (II-24) is zero implies equation (II-23) (except on a set of measure zero.)

Substituting equation (II-23) into equation (II-22) and equating quantities under the integrals in that equation give

$$df(W_t, t) = \frac{\partial f(W_t, t)}{\partial W_t}\, dW_t + \left[\frac{1}{2} \frac{\partial^2 f(W_t, t)}{\partial W_t^2} + \frac{\partial f(W_t, t)}{\partial t} \right] dt \qquad (II-25)$$

As an example of the formula (II-25) for differentiation, if
$f = \exp(W_t - t/2)$

$$df = f\, dW_t + \frac{1}{2} f\, dt - \frac{1}{2} f\, dt = f\, dW_t$$

This shows $\exp(W_t - t/2)$ to be a solution to equation (11-20), as was claimed previously.

The formula analogous to equation (II-25) for functions of $Y(t)$ is called Ito's theorem. If in equation (II-22) the function is $f[Y(t), t]$, then

$$\int df = \int \left[\frac{\partial f}{\partial Y}\, dY + \frac{1}{2} \frac{\partial^2 f}{\partial Y^2} (dY)^2 + \frac{\partial f}{\partial t}\, dt \right] + o(dt)$$

$$= \int \left[\frac{\partial f}{\partial Y}\, b(Y) dt + \frac{\partial f}{\partial Y}\, a(Y) dW_t + \frac{1}{2} \frac{\partial^2 f}{\partial Y^2}\, a^2(Y)(dW_t)^2 + \frac{\partial f}{\partial t}\, dt \right] + o(dt)$$

having used equation (II-12) for dY. Again, we use equation (II-23) and equate integrands to find

$$df = \left[b(Y) \frac{\partial f}{\partial Y} + \frac{1}{2} a^2(Y) \frac{\partial^2 f}{\partial Y^2} + \frac{\partial f}{\partial t} \right] dt + a(Y) \frac{\partial f}{\partial Y}\, dW_t \qquad (II-26)$$

This is Ito's theorem.

Attainability of Boundaries

As an application of theorem (II-26), consider a turbulent flow between boundaries at y_+ and y_-. Consider a trajectory that originates at some point y_0 in the fluid and strikes one of the boundaries at some arbitrary later time. We will determine the probability that this trajectory strikes the boundary y_+ (or y_-). If this probability is zero for one of the boundaries, that boundary (almost surely) cannot be reached from within the fluid and is called nonattainable.

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Let

$$f(y) = \int_{y_0}^{y} \exp\left[-2 \int_{y_0}^{y'} \frac{b(x)}{a^2(x)} dx\right] dy' \qquad (II-27)$$

where $f(y)$ is the solution to $d^2f/dy^2 + (2b/a^2)\, df/dy = 0$, satisfying $f(y_0) = 0$; thus by equation (II-26)

$$df(Y) = a(Y) \exp\left[-2 \int_{y_0}^{Y} \frac{b(x)}{a^2(x)} dx\right] dW_t$$

Averaging this gives $\overline{df[Y(t)]} = 0$ (cf. eq. (II-11)); hence $\overline{f[Y(t)]}$ is a constant. But $f(y_0) = 0$, so $\overline{f[Y(t)]} = 0$ independently of t.

Consider trajectories that at some time strike a boundary y_+ or y_-. There is a probability P_+ that a given trajectory strikes y_+, and P_- that it strikes y_-. These are the probabilities that we wish to determine.

Since $\overline{f(Y)} = 0$ is true at any time, it is true at the particular time when the boundary is struck. At that time, Y is at either y_+ or y_-, so

$\overline{f(Y)} = f(y_+)P_+ + f(y_-)P_- = 0$. Or, because $P_+ + P_- = 1$,

$$P_{\pm} = \frac{- f(y_{\mp})}{[f(y_{\pm}) - f(y_{\mp})]} \qquad (II-28)$$

Equation (II-28) gives $P_{\pm}$ explicitly in terms of the integral (II-27) with a nonrandom upper limit of y_+ or y_-. In particular if the integral does not converge at y_- (say), then $f(y_-) = -\infty$ and $P_- = 0$ and thus y_- is nonattainable.

In the case of equation (II-18), $a^2(y) = 2K(y)$ and $b(y) = K'(y)$, and equation (II-27) becomes simply

$$f(y) = \int_{y_0}^{y} \frac{K(y_0)}{K(y')} dy'$$

Then $f(y_-)$ is infinite if K tends linearly to zero at y_-. Such a boundary has $P_- = 0$ and it cannot be struck by a typical fluid trajectory. Generally, if $b(y) \geq K'(y)$ and $K(y) \to 0$ as $y \to y_-$, y_- is not attainable. In the inhomogeneous turbulent flow near a surface it is usually the case that $K \to 0$ at the surface.

Numerical Methods for Stochastic Differential Equations

Often closed-form solutions to equation (II-12) cannot be found and one wants to solve it numerically. This requires replacing dt by Δt and dW_t by a Gaussian random variable with mean zero and variance Δt. Two considerations present themselves in connection with approximating equation (II-12) consistently: first, dW_t becomes $O(\Delta t^{1/2})$ so that an approximation to $O(\Delta t^n)$ requires retaining terms to $O(dW_t^{2n})$; second, the approximation must preserve the nonanticipating property of the coefficients $a(Y)$ and $b(Y)$.

Consistent finite-difference approximations to Ito differential equations are derived in references 9 and 10; here the method of reference 9 is followed. This method consists of integrating equation (II-12) between times t_n and t_{n+1}, separated by Δt

$$Y_{n+1} = Y_n + \int_{t_n}^{t_{n+1}} [b(Y)dt + a(Y)dW_t] \qquad (II-29)$$

and approximating the integral by successive approximations. Thus, to $O(\Delta t^{1/2})$

$$Y_{n+1} = Y_n + a(Y_n)\Delta W$$

where $\Delta W = W_{(n+1)\Delta t} - W_{n\Delta t}$ is a (computer generated) Gaussian random variable with $\overline{\Delta W} = 0$ and $(\Delta W)^2 = \Delta t$. The preceding first approximation can be generalized to $Y(t) = Y_n + a(Y_n)(W_t - W_{n\Delta t})$; $t > t_n$. Using this in equation (II-29), to $O(\Delta t)$, yields

$$Y_{n+1} = Y_n + b(Y_n)\Delta t + \int_{t_n}^{t_{n+1}} a[Y_n + a(Y_n)(W_t - W_{n\Delta t})]dW_t$$

$$= Y_n + a(Y_n)\Delta W + b(Y_n)\Delta t + a(Y_n)a'(Y_n) \int_{t_n}^{t_{n+1}} (W_t - W_{n\Delta t}) dW_t$$

$$= Y_n + a(Y_n)\Delta W + b(Y_n)\Delta t + a(Y_n)a'(Y_n) \left(\int_{t_n}^{t_{n+1}} W_t dW_t - W_{n\Delta t}\Delta W \right) \qquad (II-30)$$

Now, according to Ito's theorem (eq. (II-26))

$$\frac{dW_t^2}{2} = W_t dW_t + \frac{dt}{2}$$

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and thus

$$\int_{t_n}^{t_{n+1}} W_t \, dW_t = \frac{1}{2} \left(W^2_{(n+1)\Delta t} - W^2_{n\Delta t} - \Delta t \right)$$

Substituting this into equation (II-30) gives, to $O(\Delta t)$,

$$Y_{n+1} = Y_n + a(Y_n)\Delta W + b(Y_n)\Delta t + \frac{a(Y_n)a'(Y_n)}{2} [(\Delta W)^2 - \Delta t] \qquad (\text{II-31})$$

Mil'shtein's (ref. 10) method for deriving equation (II-31) consists of showing that it approximates Y_{n+1} with a mean square error of $O(\Delta t^3)$. Higher order finite difference schemes are derived in references 9 and 10. Mil'shtein also notes that it may often be convenient to replace equation (II-31) by a Runge-Kutta scheme with the same order of accuracy:

$$Y_{n+1} = Y_n + b(Y_n)\Delta t + p_1 \, a(Y_n)\Delta W$$

$$+ p_2 \, a\left[Y_n + \alpha_1 \, a(Y_n)\Delta W + \alpha_2 \, a(Y_n) \frac{\Delta t}{\Delta W} \right]\Delta W \qquad (\text{II-32})$$

where $p_1 + p_2 = 1$ and $p_2\alpha_1 = -p_2\alpha_2 = 1/2$. Expanding the last term to $O(\Delta t)$ recovers equation (II-31). Formula (II-32) has the advantage of not requiring a derivative of $a(Y)$.

Types of Boundary Conditions

When dispersion takes place in a bounded fluid, one must impose boundary conditions, and these conditions must be compatible with the stochastic differential equation. Numerical formulas such as (II-31) and (II-32) also must be supplemented with boundary conditions.

Reference 4 classifies the types of boundary that can occur and the boundary conditions compatible with them; the appendix to this chapter describes this classification. In the present context the most important consideration is whether or not the boundary is attainable (eqs. (II-27) and (II-28)). If a boundary is not attainable, no boundary condition can be imposed on it; stated otherwise, it automatically satisfies a no-normal-flux condition. An attainable boundary will usually be reflecting or absorbing. Other variants could be conceived: for instance a trajectory could remain at the boundary some time before leaving, modeling an initially absorbing boundary that saturates; or the boundary could be an interface to a region with different properties, modeling an impedance condition. Here only reflecting, absorbing, and nonattainable boundaries are considered.

Nonattainable Boundaries

Although in principle these boundaries cannot be reached, when a finite-difference approximation is made, it becomes possible for a trajectory to

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reach a nonattainable boundary. Such a trajectory must return to the interior in a suitable way. The following scheme might be used in a numerical calculation to handle this eventuality.

If on one time step a trajectory reaches the "nonattainable" boundary $y = 0$, at the next time step it may be considered a trajectory originating at $y = 0$. Its position then can be chosen from the probability distribution for particles originating on the boundary; the relevant pdf is derived next. (To avoid confusion, it should be remarked that a nonattainable boundary can be the __origin__ of particle trajectories. Its property is that once these trajectories move into the interior, they cannot __return__ to the boundary.)

Suppose $K(y) \to \alpha y$ and $b(y) \to \beta$ near the boundary, where α and β are constants with $\beta \geq \alpha$ (if $\beta < \alpha$, the boundary is attainable). Then equation (II-17) becomes

$$\frac{\partial P}{\partial t} + \beta \frac{\partial P}{\partial y} = \alpha \frac{\partial^2}{\partial y^2} (yP)$$

The pdf at time Δt for trajectories originating at the boundary $y = 0$ is the solution to this at $t = \Delta t$, subject to $P(y, t = 0) = \delta(y)$:

$$P(y, \Delta t) = \left(\frac{y}{\alpha \Delta t}\right)^{(\beta - \alpha)/\alpha} \frac{e^{-y/\alpha \Delta t}}{\Gamma(\beta/\alpha)\alpha \Delta t} \tag{II-33}$$

where it is assumed that $\alpha \Delta t \ll 1$. ($\Gamma(\cdot)$ here is the gamma, or factorial, function.)

In a numerical calculation, if a trajectory reaches the boundary on some time step, its position at the next time step should be a random variable Y chosen from the distribution (II-33). At subsequent time steps its position is determined by equation (II-31) or by equation (II-32), until the boundary is again reached.

Next, we consider attainable boundaries at which $K(y) \neq 0$. This is the case where the turbulent eddy diffusivity is nonzero at the boundary.

Reflecting Boundaries

If the boundary is at $y = 0$ and the flow domain is in the region $y > 0$, reflection is achieved by replacing Y by $|Y|$ as soon as Y becomes negative. Equivalently, the condition of reflection is imposed by placing a particle, which at the end of a time step has passed a distance through the boundary, an equal distance above the boundary.

An analysis of the reflection boundary condition proceeds through consideration of the case where the flow domain is the entire region $y > 0$. In this case a solution $Y(t)$ to

$$dY = b(Y)dt + a(Y)dW_t \tag{II-34}$$

satisfying $Y(t) > 0$, and being reflected at $y = 0$ is required. It will be assumed that $a(0) > 0$. Note that as formulated, equation (II-34) governs $Y(t)$ only when $Y(t) > 0$; $Y(t)$ at $y = 0$ is governed by the boundary condition. What we will do is find another process $Y^+(t)$ defined on the entire

y-axis, and hence not subject to any boundary condition, but which satisfies equation (II-34) in $y > 0$. The process $Y^+(t)$ also will have the property that $|Y^+(t)|$ satisfies equation (II-34) for all nonzero values of $Y^+(t)$; $|Y^+|$ satisfies the reflection condition and hence is the required solution $Y(t) = |Y^+(t)|$.

In equation (II-34) $b(Y)$ and $a(Y)$ are defined only for $Y > 0$. Their definitions will be extended to all Y by letting $b(-Y) = -b(Y)$ and $a(-Y) = a(Y)$; that is, $b(Y) = sgn(Y)b(|Y|)$ and $a(Y) = a(|Y|)$. It will be seen that these extended definitions give Y^+ the properties required of it in the last paragraph.

Let $Y^+(t)$ satisfy

$$dY^+ = b(Y^+) + a(Y^+)dW_t^+ \qquad \text{(II-35a)}$$

Then by Ito's theorem (eq. (II-26))

$$d|Y^+| = b(Y^+)sgn(Y^+)dt + a(Y^+)sgn(Y^+)dW_t^+ + \frac{1}{2}\delta(Y^+)a^2(0)dt$$

But dW_t and $-dW_t$ are statistically equivalent, so we may replace $sgn(Y^+)dW_t^+$ by dW_t and use the extended definitions of $a(Y)$ and $b(Y)$ to rewrite this last equation as

$$d|Y^+| = b(|Y^+|)dt + a(|Y^+|)dW_t + \frac{1}{2}\delta(|Y^+|)a^2(0)dt \qquad \text{(II-35b)}$$

Thus $|Y^+|$ satisfies all of the criteria that were set for it: it is determined by the equation (II-35a), on which no boundary conditions need be imposed, and it is a solution to equation (II-34) irrespective of whether $Y^+(t)$ is positive or negative. Thus, $Y(t) = |Y^+(t)|$.

Equation (II-35b) shows that when the boundary condition is incorporated into the dynamical equation, it takes the form of an impulsive velocity at the boundary – the δ-function term. This impulsive velocity accomplishes the reflection of the trajectory. It will be shown below equation (II-43) that a consequence of the δ-function in equation (II-35b) is to make the pdf for Y satisfy the boundary conditions $\partial P(y,t)/\partial y = 0$ on $y = 0$.

The reflection condition is illustrated clearly by the simple case $b = 0$, $a = \sigma = $ constant. In this case equation (II-35a) is easily integrated to

$$Y^+ = y_0 + \sigma W_t$$

where y_0 is the integration constant. Therefore $Y = |Y^+| = |y_0 + \sigma W_t|$. A given value of Y occurs when $y_0 + \sigma W_t = Y$ and when $y_0 + \sigma W_t = -Y$. Therefore the probability (density) of observing a given Y is

$$P(y,t) = P\left(W_t = \frac{y - y_0}{\sigma}\right) + P\left(W_t = \frac{-y - y_0}{\sigma}\right) \qquad \text{(II-36)}$$

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But $P(w_t) = e^{-w_t^2/2t}/\sqrt{2\pi t}$ (eq. (II-3)), so

$$P(y,t) = \frac{1}{\sigma \sqrt{2\pi t}} \left\{ \exp\left[-\frac{(y - y_0)^2}{2\sigma^2 t}\right] + \exp\left[-\frac{(y + y_0)^2}{2\sigma^2 t}\right] \right\} H(y) \qquad (II-37)$$

(The Heaviside function $H(y)$ times $1/\sigma$ arises on transforming from w_t to $y = |y^+|$ as the independent variable.) Equation (II-37) is the pdf for y, subjected to a reflection boundary condition, given that, at $t = 0$, $y = y_0$.

Absorbing Boundaries

It is shown in the appendix to this chapter that some boundaries are naturally absorbing, in the sense that once a trajectory reaches such a boundary it cannot escape from it. If the boundary is not naturally absorbing but is attainable, one can still impose the condition that, once the boundary is reached, the trajectory stops. As might be expected, the formal analysis of absorption (provided by ref. 4) shows that the absorption condition corresponds to imposing the boundary condition $P(y,t) = 0$ at $y = 0$ on the Fokker-Planck equation (II-16). This is discussed further in the next section.

Again this boundary condition is readily illustrated through the case $b = 0$, $a = \sigma$. Since trajectories terminate upon hitting the boundary, the probability (density) of observing a particle at y at time t is the probability of observing a particle at y in the absence of a boundary, minus the probability of the particle's trajectory reaching $y = 0$ at some time prior to t. Now, dW_t is statistically equivalent to $-dW_t$, and dW_t is uncorrelated with $dW_{t+\tau}$ if $\tau \neq 0$. Thus if we take a trajectory $dY = \sigma\,dW_t$ that reaches y at time t, having crossed $y = 0$ at some prior time, and from the first time that trajectory reaches $y = 0$ onward replace dW_t by $-dW_t$, we obtain an equally likely trajectory that arrives at $-y$ at time t. Hence there is a one-to-one correspondence between trajectories that reach y having crossed $y = 0$ and trajectories that reach $-y$. This correspondence can be used to derive the pdf for $Y(t)$. Thus as described

$P[Y(t) = y \mid$ absorbing boundary$]$
    $= P[Y(t) = y \mid$ no boundary$] - P[Y(t) = y \mid$ no boundary and
        $Y(t') = 0$ for some $t' < t]$
    $= P[Y(t) = y \mid$ no boundary$] - P[Y(t) = -y \mid$ no boundary$]$

$$(II-38)$$

Here the vertical bars are to be read "given the condition to the right."
Since $Y(t) - y_0 = \sigma W_t$ and $P(W_t,t)$ is given by equation (II-3), $P[Y(t) = y \mid$ no boundary$]$ is

$$\exp\left[-(y - y_0)^2/2\sigma^2 t\right]/\sigma \sqrt{2\pi t}$$

With this, equation (II-38) is

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$$P(y,t) = \frac{1}{\sigma \sqrt{2\pi t}} \left(\exp\left[-(y - y_0)^2/2\sigma^2 t\right] - \exp\left[-(y + y_0)^2/2\sigma^2 t\right] \right) H(y) \qquad \text{(II-39)}$$

In equation (II-39) $P(y = 0,t) = 0$ as expected from the first paragraph of this section.

Application to Mean Concentration

Having now summarized the theory of continuous Markov processes, it is time to return to our starting point, equation (I-1), and see how all of this relates to it. The mean concentration of contaminant at y,t is determined from any initial distribution of concentration by equation (I-1). The averaging in this equation is over random initial positions $Y(0)$, given the final position $Y(t) = y$. In the overbar notation of equation (I-4), equation (I-1) is

$$\bar{C}(y,t) = \overline{C_0[Y(0)]} \qquad \text{(II-40)}$$

Thus calculation of $\bar{C}(y,t)$ requires trajectories to be integrated backward in time from their known position y at time t to their random position $Y(0)$ at time zero. The known initial concentration is then evaluated at the random initial position, and $C(y,t)$ is the average of all such evaluations, as in equation (II-40).

To calculate the requisite reversed trajectories, the reversed time s is introduced: $ds = -dt$. As time runs from 0 to t, s runs from t to 0. In terms of s, equation (II-12) becomes

$$dY(s) = -b[Y(s)]ds + a[Y(s)]dW_s \qquad \text{(II-41)}$$

with $Y(0) = y$. We next show that the calculation involving this reversed diffusion does indeed give the solution to the actual forward diffusion process.

Let $C_0(y,s)$ satisfy

$$\frac{\partial C_0(y,s)}{\partial s} = b(y) \frac{\partial C_0(y,s)}{\partial y} + \frac{1}{2} a^2(y) \frac{\partial^2 C_0(y,s)}{\partial y^2} \qquad \text{(II-42)}$$

with initial condition $C_0(y,s = 0) = \bar{C}(y,t)$. (Recall that $s = 0$ corresponds to time t.) Then by Ito's theorem, substituting $-\partial/\partial s$ for $\partial/\partial t$, we get

$$dC_0(Y,s) = a(Y) \frac{\partial C_0(Y,s)}{\partial Y} dW_s$$

Integrating this between $s = 0$ and t yields

$$C_0(y, s = 0) = C_0(y, s = t) - \int_0^t a(Y) \frac{\partial C_0(Y,s)}{\partial Y} dW_s \qquad (II-43)$$

After averaging and reverting to forward time, so that $s = 0$ is replaced by time t and $s = t$ is replaced by time 0, equation (II-43) becomes $\overline{C}(y,t) = \overline{C_0[Y(0)]}$, which is equation (II-40). Here the initial condition $C_0(y, s = 0) = \overline{C}(y,t)$ is used.

Thus equation (II-40) is obtained provided that C_0 satisfies equation (II-42). Equation (II-42) is quite similar to the Fokker-Planck equation (II-16). Indeed, it is called the backward Fokker-Planck equation (ref. 3, p. 159). (Note that we have let s increase in the direction of negative t; usually ds is taken as positive in the direction of forward time so the first term in eq. (II-42) is $-\partial C_0/\partial s$.) It is easily shown that this equation with fixed final time t and variable initial time s corresponds to exactly the same diffusion process as does equation (II-16), where the initial time is fixed and the final time is variable (refs. 3 and 4). Therefore the correctness of equation (II-40) as calculated by reversed diffusion has been demonstrated.

As an addendum, it is now clear why, when a reflecting boundary is present, $C_0(y,s)$ must satisfy $\partial C_0(y,s)/\partial y = 0$ on the boundary. The delta function in equation (II-35b) adds a term

$$\frac{1}{2} a^2(0) \int_0^t \frac{\partial C_0(Y,s)}{\partial Y} \delta(Y) dt$$

to the right side of equation (II-43). In deriving equation (II-35b), it was assumed that $a(0) \neq 0$, so $\partial C_0(0,s)/\partial y$ must equal zero if equation (II-40) is to obtain. Thus, calculation of $\overline{C}(y,t)$ from the Fokker-Planck equation with a zero normal derivative gives the same result as expression (II-40) for reflected trajectories.

A similar line of reasoning can be followed in the case of absorbing boundaries. Let $C_0(y,s)$ be as above and satisfy equation (II-42). Let $Y(s)$ be the solution to equation (II-41), now subjected to the constraint that if, at any $s < t$, Y reaches the boundary $y = 0$, the trajectory subsequently remains there. For trajectories that do not reach the boundary, equation (II-43) will apply; but for a trajectory that reaches the boundary and remains there, $Y(s = t) = 0$, with the effect that equation (II-43) becomes

$$C_0(y, s = 0) = C_0(0, s = t) - \int_0^t a(Y) \frac{\partial C_0(Y,s)}{\partial Y} dW_s$$

Consequently, if the indicator function

$$X = \begin{cases} 0 & \text{if the trajectory reaches the boundary} \\ 1 & \text{otherwise} \end{cases}$$

is introduced, averaging equation (II-43) gives

$$\overline{C}(y,t) = \overline{(1 - x)C_0(0, s = t)} + \overline{x C_0[Y(s = t), s = t]} \qquad (II\text{-}44)$$

Only if $C_0(0) = 0$, so that the first term in equation (II-44) vanishes, will equation (II-40) obtain. (It should be realized that the factor of x multiplying the second term in eq. (II-44) only indicates that averaging is carried out over those trajectories that are not absorbed at the boundary.)

APPENDIX: CLASSIFICATION OF BOUNDARIES

Gikhman and Skorohod (ref. 4, chapter 5) classify four types of boundary, according to the convergence of

$$L_1 = \int_{y_-}^{y_+} \exp\left[-2\int_{y_+}^{y} \frac{b(x)}{a^2(x)}\,dx\right]dy$$

$$L_2 = \int_{y_-}^{y_+} \exp\left[-2\int_{y_+}^{y} \frac{b(x)}{a^2(x)}\,dx\right]\left\{\int_{y}^{y_+} \frac{\exp\left[2\int_{y_+}^{z} \frac{b(x)}{a^2(x)}\,dx\right]}{a^2(z)}\,dz\right\}dy \qquad (II-A1)$$

$$L_3 = \int_{y_-}^{y_+} \frac{\exp\left[2\int_{y_+}^{y} \frac{b(x)}{a^2(x)}\,dx\right]}{a^2(y)}\,dy$$

where the boundary is at $y = y_-$, trajectories originate at $y = y_0 > y_-$ and $y_+ > y_0$ is an arbitrary interior point of the fluid. Their classifications of the boundary are

$$\left.\begin{array}{l} (1)\quad \text{Nonattainable:}\ L_1 = \infty \\ (2)\quad \text{Asymptotic:}\ L_1 < \infty,\ L_2 = \infty \\ (3)\quad \text{Absorbing:}\ L_1 < \infty,\ L_2 < \infty,\ L_3 = \infty \\ (4)\quad \text{Normal:}\ L_1 < \infty,\ L_2 < \infty,\ L_3 < \infty \end{array}\right\} \qquad (II-A2)$$

A nonattainable boundary is one that cannot be reached from the interior of the fluid. An asymptotic boundary is one that trajectories can only reach asymptotically as $t \to \infty$. An absorbing boundary is one that is attainable but from which trajectories cannot escape in finite time. A normal boundary is attainable and not absorbing. Clearly, no boundary conditions can be imposed on boundaries of types 1 or 2. Continuous trajectories can only satisfy an absorption boundary condition on type 3 although, since this boundary can be reached in finite time, one can impose the condition that, having reached the boundary, trajectories jump from it to a random position within the fluid. On boundaries of type 4 one can arbitrarily impose a condition such as reflection or absorption. We will give a brief derivation of this boundary classification.

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The function L_1 is equivalent to the function $f(y_+) - f(y_-)$ in equation (II-28); the fact that $L_1 = \infty$ implies that the boundary is unattainable is explained in the main text.

To explain type 2 and 3 boundaries, it is necessary to introduce the idea of a stopping time τ_{y_0}. This is simply the (random) time at which a a trajectory originating at y_0 reaches a boundary of the interval (y_-, y_+). Applying Ito's theorem (eq. (II-26)) to

$$f(y) = 2 \frac{\int_y^{y_+} \varphi(x)dx}{\int_{y_-}^{y_+} \varphi(x)dx} \int_{y_-}^{y_+} \left[\varphi(x) \int_x^{y_+} \frac{dz}{\varphi(z)a^2(z)} \right] dx$$

$$- 2 \int_y^{y_+} \left[\varphi(x) \int_x^{y_+} \frac{dz}{\varphi(z)a^2(z)} \right] dx \qquad (\text{II-A3})$$

where

$$\varphi(x) = \exp\left[-2 \int_{y_+}^x \frac{b(z)}{a^2(z)} dz \right]$$

gives

$$df = -dt + a(Y) \frac{df(Y)}{dY} dW_t$$

Integrating from $t = 0$ to $t = \tau_{y_0}$, noting that $Y(\tau_{y_0}) = y_\pm$ by definition and that $f(y_+) = f(Y_-) = 0$, gives

$$f(y_0) = \tau_{y_0} - \int_0^{\tau_{y_0}} a(Y) \frac{df(Y)}{dY} dW_t \qquad (\text{II-A4})$$

Averaging this gives

$$f(y_0) = \overline{\tau}_{y_0} \qquad (\text{II-A5})$$

Since y_+ is an arbitrary point, it generally can be reached in a finite time. Hence τ_{y_0} can be infinite only if (on average) it takes an infinite time for trajectories to reach $y = y_-$. (Ref. 4 shows that "on average" in the last sentence can be changed to "with probability 1.") Thus $f(y_0) = \infty$

implies that the boundary is of type 2. But it is clear from equation (II-A3) that $f(y_0)$ is infinite if and only if L_2 is infinite.[1]

If a boundary is attainable in finite time, $L_1 < \infty$ and $L_2 < \infty$, a third possibility exists: having attained the boundary, a particle may be unable to escape it in finite time. To derive the condition for this to occur, we consider the stochastic process in which a particle is released at y_0 and each time it reaches the boundary of the interval (y_-, y_+) it immediately returns to y_0. Then we let $y_0 \to y_-$ and determine whether there is nonzero probability that after a finite time the particle will have reached y_+. If this probability is zero, the particle (almost surely) cannot escape from y_- because y_+ can be taken arbitrarily close to y_-.

After a sufficiently long time t, it is expected that the number of times the boundary has been reached in the preceding stochastic process will be

$$N = t/\bar{\tau}_{y_0} \tag{II-A6}$$

---

[1]The mean stopping time $\bar{\tau}_{y_0}$ can be decomposed into the mean stopping times $\bar{\tau}^+_{y_0}$ for particles reaching $y_\pm$ and $\bar{\tau}^-_{y_0}$ for those reaching y_-. (This does not seem to be discussed in ref. 4.) Let $P_\pm$ be as in eq. (II-28). Then, the stopping time is decomposed as

$$\bar{\tau}_{y_0} = \bar{\tau}^+_{y_0} P_+ + \bar{\tau}^-_{y_0} P_-$$

The mean stopping time $\bar{\tau}^-_{y_0}$ is computed as follows: Let

$$g(y) = \int_y^{y_+} \varphi(x)dx \left/ \int_y^{y_+} \varphi(x)dx \right.$$

with $\varphi(x)$ defined below eq. (II-A3). Note that $g(y_+) = 0$, $g(y_-) = 1$, and $g(y_0) = P_-$. Let

$$h(y) = 2g(y) \int_{y_-}^{y_+} \varphi(x) \left[\int_x^{y_+} \frac{g(z)}{a^2(z)\varphi(z)} dz \right] dx - 2 \int_y^{y_+} \varphi(x) \left[\int_x^{y_+} \frac{g(z)}{a^2(z)\varphi(z)} dz \right] dx$$

(For computing $\bar{\tau}^+_{y_0}$ replace $g(z)$ by $1 - g(z)$ in the innermost integral.) Note that $h(y_+) = h(y_-) = 0.$ Then by Ito's theorem

$$d[h(Y) + tg(Y)] = a(Y)[h'(Y) + tg'(Y)]dW_t$$

Integrating this from time zero to the stopping time and averaging give $h(y_0) = P_- \bar{\tau}^-_{y_0}$ or

$\bar{\tau}^-_{y_0} = h(y_0)/P_-.$ Since $g(y_-) = 1$, the condition for convergence of $h(y_0)$ is the same as that for eq. (II-A3), confirming that $L_2 = X$ means y_- can only be approached asymptotically.

where it is understood that N is the integer part of the right side of equation (II-A6). The probability that the boundary struck is y_+ on any one of these times is P_+ as given in equation (II-28). In N releases the probability that y_- is struck every time is P_-^N. Hence the probability that y_+ is struck at least once is

$$1 - P_-^N = 1 - (1 - P_+)^N \qquad \text{(II-A7)}$$

Now, by equations (II-A5) and (II-A3), as y_0 tends to y_-, $\bar{\tau}_{y_0}$ and P_+ tend to zero. Therefore $N \to \infty$ and $P_+ \to 0$ in equation (II-A7) and it becomes

$$1 - \exp\left[- t \lim_{y_0 \to y_-} \left(\frac{P_+}{\bar{\tau}_{y_0}}\right)\right] \qquad \text{(II-A8)}$$

This will be greater than zero only if

$$\lim_{y_0 \to y_-} \left(\frac{\bar{\tau}_{y_0}}{P_+}\right) < \infty$$

A direct calculation using equation (II-A5) for τ_{y_0} and equation (II-28) for P_+ yields

$$\lim_{y_0 \to y_-} \left(\frac{\bar{\tau}_{y_0}}{P_+}\right) = 2L_1 \int_{y_-}^{y_+} \frac{\exp\left[2 \int_{y_+}^{y} \frac{b(x)}{a^2(x)} dx\right]}{a^2(y)} dy - 2L_2 \qquad \text{(II-A9)}$$

Since L_1 and L_2 were assumed to be finite, this last equation shows that equation (II-A8) is nonzero if and only if $L_3 < \infty$.

CHAPTER III: EXAMPLES OF EDDY DIFFUSION

In this chapter, three examples illustrating the statistical approach to turbulent dispersion theory are considered. These examples serve also to make the theory of the previous chapter more concrete. The examples considered have been dealt with in various publications; however, they are analyzed here entirely through consideration of the solutions to stochastic ordinary differential equations, rather than the more usual treatments based on the diffusion equation. Because the Fokker-Planck equation relates stochastic ordinary differential equations to the diffusion equation, there clearly must be an equivalence between the present methods and those based on the diffusion equation. For the most part the second and third examples are treated more easily by analysis of the Fokker-Planck equation than by the approach used in this chapter. Our purpose here, however, is to show that statistical reasoning can be used equally in these examples. In doing so we hope to make clear that the often-made distinction between "statistical" theory and "eddy diffusion" theory is fictitious: eddy diffusion theory is really just a Markovian statistical theory; the eddy diffusion equation is just the Fokker-Planck equation for the pdf of a Markovian random process. The following examples show, furthermore, that by analyzing the random process itself one can obtain the same results obtainable from its Fokker-Planck equation. In fact, for example 1 the present analysis seems simpler than the diffusion equation analysis.

Aside from their pedantic value the statistical methods used in this chapter will be useful in chapter IV, where a slightly more complex stochastic model of turbulent dispersion is considered. It is hoped these methods will also provide an insight that will be of use to others who wish to formulate and analyze stochastic models.

As a further word of preface to these examples of eddy diffusion, it should be observed that the eddy diffusion approximation is only justified in an asymptotic sense. It applies at times that are long compared with the correlation time (the Lagrangian time scale) of the turbulence. This is discussed further in connection with example 2 and in chapter IV.

In the following examples dispersion takes place in the y-direction and is governed by a stochastic equation of the form

$$dY(t) = K'[Y(t)] + \sqrt{2K[Y(t)]}dW_t \qquad (III-1)$$

where $K'(y) = dK(y)/dy$. However, we will consider two-dimensional flows, with a mean shear in the x-direction. The turbulent velocity in this direction will be ignored with respect to this mean velocity; thus

$$dX(t) = U[Y(t)]dt \qquad (III-2)$$

where $U(y)$ is a known mean velocity, such as the log profile

$$U(y) = \frac{u_*}{2.5} \ln\left(\frac{y}{y_0}\right) \qquad \text{(III-3)}$$

In this, u_* is the friction velocity and y_0 is the surface roughness. The Fokker-Planck equation for equations (III-1) and (III-2) is, in analogy to equation (II-16),

$$\frac{\partial P(x,y,t)}{\partial t} + \frac{\partial [U(y)P(x,y,t)]}{\partial x} = \frac{\partial}{\partial y} K(y) \frac{\partial P(x,y,t)}{\partial y} \qquad \text{(III-4)}$$

(refs. 3 and 4). Equation (III-4), of course, is the diffusion equation usually used in analyses of the following examples.

Example 1: Shear Dispersion

In this first example we consider diffusion in homogeneous turbulence, so K in equation (III-1) is a constant:

$$dY(t) = \sqrt{2K}\, dW_t \qquad \text{(III-5)}$$

If the turbulence is homogeneous, to be consistent, any mean shear ought also to be homogeneous; that is, the rate of shear should be a constant. If this rate of shear is η, then $U(y) = \eta y$ and equation (III-2) becomes

$$dX(t) = \eta Y(t)dt \qquad \text{(III-6)}$$

This example of homogeneous turbulence in uniform shear might approximately describe horizontal dispersion in a horizontally infinite boundary layer. For instance, it might represent dispersion in the atmosphere when horizontal variations of the wind are present.

It is sufficiently general to use the initial condition $Y(0) = 0$. Then equation (III-5) integrates to

$$Y(t) = \sqrt{2K}\, W_t \qquad \text{(III-7)}$$

From the properties of W_t (eqs. (II-2) and (II-3)) $Y(t)$ is a Gaussian random variable with mean zero and variance $\overline{Y^2} = 2K\overline{W_t^2} = 2Kt$:

$$P(y,t) = \frac{1}{2\sqrt{\pi Kt}}\, e^{-y^2/4Kt} \qquad \text{(III-8)}$$

The function $X(t)$, subject to $X(0) = 0$, is found by integrating equation (III-6)

$$X(t) = \eta \sqrt{2K} \int_0^t W_{t'}\, dt' \qquad \text{(III-9)}$$

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Since the sum of a number of Gaussian random variables is a Gaussian random variable, $\int W_t \, dt$ is Gaussian. Hence X is also Gaussian, and from the properties of W_t (eq. (II-6))

$$
\left.
\begin{aligned}
\overline{X} &= 0 \\[2ex]
\overline{X^2} &= 2\eta^2 K \int_0^t \int_0^t \overline{W_{t'}, W_{t''}} \; dt' \; dt'' \\[2ex]
&= 2\eta^2 K \int_0^t \int_0^t \min(t', t'') \; dt' \; dt'' \\[2ex]
&= \frac{2\eta^2 K t^3}{3}
\end{aligned}
\right\}
\qquad \text{(III-10)}
$$

Thus

$$
P(x,t) = \frac{1}{2\sqrt{\pi K\eta^2 t^3/3}} \; e^{-3x^2/4K\eta^2 t^3}
\qquad \text{(III-11)}
$$

Clearly, X and Y are jointly Gaussian random variables, so their joint distribution is given by reference 8 (eq. (5.1.28)). This joint distribution requires that we evaluate $\overline{X(t)Y(t)}$:

$$
\overline{XY} = 2K\eta \overline{W_t \int_0^t W_{t'} \; dt'} = 2K\eta \int_0^t t' \; dt' = K\eta t^2
\qquad \text{(III-12)}
$$

Substituting equations (III-10) and (III-12) and $\overline{Y^2} = 2Kt$ into equation (5.1.28) of reference 8 gives

$$
P(x,y,t) = \frac{\sqrt{3}}{2\pi K\eta t^2} \exp\left[-\frac{3x^2}{K\eta^2 t^3} + \frac{y^2}{Kt} - \frac{3xy}{K\eta t^2} \right]
\qquad \text{(III-13)}
$$

Physically, $P(x,y,t)$ is the concentration distribution that would evolve from an instantaneous point release of contaminant at $x = 0$, $y = 0$, $t = 0$.

Conditional x-moments. — Expression (III-10) is the second moment of this contaminant cloud in the x-direction (cf. eq. (I-4))

$$
\overline{x^2}(t) = \iint_{-\infty}^{\infty} x^2 \; P(x,y,t) dx \; dy
$$

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It is a moment of the entire cloud. Sometimes one is interested in the x–moments at fixed y, rather than in the moments of the entire cloud. These are usually calculated in terms of the conditional pdf, $P(x|y)$:

$$\overline{x^2}(y,t) = \int_{-\infty}^{\infty} x^2\, P(x\ y,t)\,dx$$

The conditional pdf is the pdf of observing a particle at a random point x, given that its other coordinate is y. This pdf is given by

$$P(x|y,t) = \frac{P(x,y,t)}{P(y,t)} \tag{III-14}$$

If written $P(x,y) = P(x|y)P(y)$, equation (III-14) is intuitively clear: the unconditional pdf is just the probability of observing a particle at x, given its y-position, times the probability of observing a particle at that y-position.

From equations (III-8), (III-13), and (III-14)

$$P(x|y,t) = \sqrt{\frac{3}{\pi K_\eta^2 t^3}} \exp\left[-\frac{3}{K_\eta^2 t^3}(x - \eta t y/2)^2\right] \tag{III-15}$$

That is, x here is a Gaussian random variable with mean $\eta y t/2$ and variance $K_\eta^2 t^3/6$; these are the first and second moments of x at fixed y.

Wiener process with fixed end points. – Another way the problem of determining moments of x at fixed y can be approached is through consideration of a Wiener process with given end points. That is, we consider the subset of all random trajectories $W_{t'}$, $0 \leq t' \leq t$ that satisfy $W_0 = 0$ and $W_t = y$. This stochastic process will be denoted by $W_{t'}^t$; thus $W_0^t = 0$ and $W_t^t = y$. The processes W_t and $W_{t'}^t$ are illustrated in figure III-1 by schematic drawings of ensembles of trajectories. Because of the stationarity
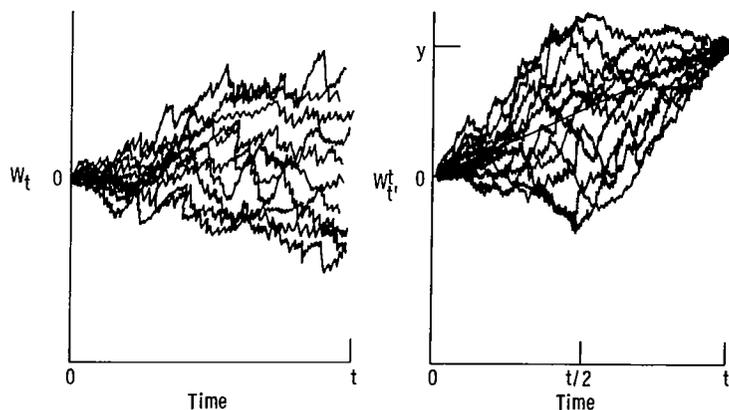

Figure III-1. – Schematic comparison of Wiener process W_t and process with fixed end points $W_{t'}^t$. In the former the cloud of trajectories spreads monotonically from the origin. In the latter the cloud spreads and then collapses about the mean trajectory.

of the increments of W_t, on average $W_{t'}^t$ ought to move linearly between 0 and y; that is, $\overline{W_{t'}^t} = t'y/t$. A stochastic process with this average, and which satisfies the end conditions is

$$W_{t'}^t = \frac{t'}{t} y + W_{t'} - \frac{t'}{t} W_t \qquad \text{(III-16)}$$

Because $W_{t'}$ and W_t are Gaussian, this is a Gaussian random process with variance

$$\overline{\left(W_{t'}^t\right)^2} - \overline{W_{t'}^t}^2 = \overline{\left(W_{t'} - \frac{t'}{t} W_t\right)^2} = t' \left(1 - \frac{t'}{t}\right) \qquad \text{(III-17)}$$

Another consequence of the increments of W_t being stationary is that the variance of $W_{t'}^t$ should be symmetric about $t/2$; that is, if t' is replaced by $t - t'$, equation (III-17) retains its value. (To see that this must be so, consider the case where $y = 0$. Then trajectories originating at ($y = 0$, $t' = 0$) and ending at ($y = 0$, $t' = t$) must be statistically equivalent to trajectories originating at ($y = 0$, $t' = t$) and ending at ($y = 0$, $t' = 0$), after reversing the direction of time.)
  Introducing a turbulent diffusivity into equation (III-16) yields the trajectory

$$Y(t') = \frac{t'}{t} y + \sqrt{2K} \left(W_{t'} - \frac{t'}{t} W_t\right)$$

For this trajectory

$$X(t) = n \int_0^t Y(t') dt'$$

has mean

$$\overline{X}(t) = n \int_0^t \frac{t'}{t} y \, dt' = \frac{nyt}{2}$$

and variance

$$\overline{(X - \overline{X})^2} = 2n^2 K \int_0^t \int_0^t \overline{\left(W_{t'} - \frac{t'}{t} W_t\right)\left(W_{t''} - \frac{t''}{t} W_t\right)} dt' \, dt''$$

$$= 2n^2 K \int_0^t \int_0^t \min(t',t'') - \frac{t't''}{t} \, dt' \, dt'' = \frac{Kn^2 t^3}{6}$$

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This mean and variance agree with those of equation (III-15), showing process (III-16) to be the correct form of a Wiener process with two fixed end points.

There is an advantage to approaching the calculation of conditional moments via prescription of this modified Wiener process. The stochastic process (III-16) contains more information than the pdf (eq. (III-15)), for the latter describes the stochastic process only at a single time. The joint distributions at multiple times can be inferred from the process (eq. (III-16)). Or more generally, its description as a continuous dynamical process makes $W_{t'}^t$, amenable to analysis.

Reflecting boundary. - The case where a reflecting boundary is inserted at $y = 0$ can also be dealt with. This has already been discussed in chapter II (eq. (II-37)). When boundaries are present in turbulent flow, they make the turbulence inhomogeneous; so it is not entirely consistent to take K constant and apply a reflection boundary condition. However, for illustrative purposes it is an interesting case to consider.

As mentioned in chapter II the reflection condition is incorporated by taking an absolute value. Thus the stochastic process

$$Y(t) = \left| y_0 + \sqrt{2K}\, W_t \right| \qquad (III-18)$$

satisfies a reflection condition at $y = 0$. For convenience in equation (III-18) the source y_0 of the trajectories will be put at the boundary $y_0 = 0$. Then equation (II-37) gives the pdf for the process (III-18) as

$$P(y,t) = \frac{1}{\sqrt{\pi K t}}\, e^{-y^2/4Kt}\, H(y) \qquad (III-19)$$

From this the moments

$$\bar{y} = 2\sqrt{Kt/\pi}$$

$$\qquad (III-20)$$

$$\overline{y^2} = 2Kt$$

are computed as in equation (I-4).

By equations (III-18) and (III-6)

$$X(t) = \eta\, \sqrt{2K} \int_0^t |W_{t'}|\, dt' \qquad (III-21)$$

Because $|W_t|$ is not Gaussian distributed, X is also no longer Gaussian; but its moments can be computed from the known properties of W_t. For example,

$$\overline{X} = \eta \ \sqrt{2K} \int_0^t \overline{|W_{t'}|} \ dt'$$

$$= 2\eta \ \sqrt{K/\pi} \int_0^t \sqrt{t'} \ dt' = \frac{4}{3} \eta \ \sqrt{K/\pi} \ t^{3/2} \qquad (III-22)$$

and $\overline{X^2}$ is given by

$$\overline{X^2} = 2\eta^2 K \int_0^t \int_0^t \overline{|W_t, W_{t''}|} \ dt'' \ dt' = 4\eta^2 K \int_0^t \int_{t'}^t \overline{|W_t, W_{t''}|} \ dt'' \ dt' \qquad (III-23)$$

To evaluate the average occurring inside this double integral, the pdf of $W_{t'}$ and $W_{t''}$ for $t'' \geq t'$ is required. Since $W_{t'}$ and $W_{t''}$ are

jointly Gaussian with $\overline{W_{t'}^2} = t'$, $\overline{W_t^2} = t''$, and $\overline{W_{t'}W_{t''}} = t'$, this pdf is

$$P(W_{t'}, W_{t''}) = \frac{\exp\left\{\frac{-t''}{2t'(t'' - t')} \left[W_{t'}^2 + \frac{t'}{t''}\left(W_{t''}^2 - 2W_{t''}W_{t'}\right)\right]\right\}}{2\pi \ \sqrt{t'(t'' - t')}} \qquad (III-24)$$

(eq. (5.1.28) of ref. 8). From equation (III-24) and the definition

$$\overline{|W_{t'}, W_{t''}|} = \iint_{-\infty}^{\infty} |W_{t'}, W_{t''}| P(W_{t'}, W_{t''}) dW_{t'} \ dW_{t''}$$

it is found that

$$\overline{W_{t'}W_{t''}} = t' + \frac{2t'^{1/2}(t'' - t')^{3/2}}{\pi t''}$$

$$\times \frac{\sin\left(\cos^{-1} \sqrt{t'/t''}\right) - \sqrt{t'/t''} \cos^{-1} \sqrt{t'/t''}}{\sin^3\left(\cos^{-1} \sqrt{t'/t''}\right)} \qquad (III-25)$$

which is a comparatively complex formula. Substituting this into equation (III-23) and changing variables of integration to θ and φ where

$$\cos \theta = \sqrt{t'/t''} \quad \text{and} \quad \cos \varphi = \sqrt{t'/t}$$

give

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$$\overline{X^2} = \frac{n^2 K t^3}{\pi} \left(\frac{2\pi}{3} + 32 \int_0^{\pi/2} \int_0^{\varphi} \frac{\sin\theta - \theta\cos\theta}{\cos^4\theta} \sin\theta \sin\varphi \cos^5\varphi \, d\theta \, d\varphi \right)$$

$$= 3n^2 K t^3 / 4 \qquad\qquad\qquad\qquad (III-26)$$

The corresponding variance is

$$\overline{X^2} - \overline{X}^2 = n^2 K t^3 \left(\frac{3}{4} - \frac{16}{9\pi} \right)$$

Clearly, the reflection condition could also be imposed on the process with two fixed end points (eq. (III-16)). In this case

$$Y(t') = \left| \frac{t'}{t} y + \sqrt{2K} \left(W_{t'} - \frac{t'}{t} W_t \right) \right|$$

or, evaluating this on $y = 0$ for simplicity,

$$Y(t') = \sqrt{2K} \left| W_{t'} - \frac{t'}{t} W_t \right| \qquad\qquad (III-27)$$

Corresponding to the stochastic process (III-27),

$$X(t) = \sqrt{2K} \; n \int_0^t \left| W_{t'} - \frac{t'}{t} W_t \right| dt' \qquad\qquad (III-28)$$

Since $W_{t'} - W_t t'/t$ is a Gaussian random variable with variance $t'(1 - t'/t)$ (eq. (III-17)), the mean value of $\left| W_{t'} - W_t t'/t \right|$ is computed to be $\sqrt{2t'(1 - t'/t)/\pi}$. Hence

$$\overline{X} = 2n \sqrt{\frac{K}{\pi}} \int_0^t \sqrt{t' \left(1 - \frac{t'}{t} \right)} \, dt' = \frac{\sqrt{\pi K} \, n t^{3/2}}{4} \qquad (III-29)$$

This result, as well as the value of the variance $\overline{X^2} - \overline{X}^2$, is given in reference 1 (eq. (5.103)).

Example 2: The Surface Layer

Criterion for eddy diffusion. - Generally, the condition for turbulent dispersion to be described by a diffusion process is that the correlation time T_L of turbulent velocity fluctuations can be treated as being negligible. In most cases this is possible at times that are long compared with

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T_L, but in the early stages of dispersion this will only be possible if T_L is negligible at the position of the contaminant source.

Now, a vanishing correlation time is associated with a vanishing correlation length ℓ of turbulent eddies. In turn, ℓ is determined by a length scale of the geometry within which the turbulence exists. Near a plane wall, since distant regions of the flow do not affect the near-wall turbulence, the only geometric scale is distance from the wall. Thus the correlation length here is proportional to distance from the wall; in particular it tends linearly to zero at the wall. This near-surface region, in which $\ell \propto y$, with the wall at $y = 0$, is called the surface layer.

The conclusion to be drawn from the two paragraphs above is that eddy diffusion is valid at short times only for sources located at the wall: the argument being that the diffusion approximation is valid when $t \gg T_L$, and because $T_L \to 0$ at the wall, this criterion is satisfied by surface sources for all time. The effects of finite correlation time (or, the case of elevated sources) are discussed in chapter IV.

The surface layer. - The surface layer will be analyzed as a semi-infinite field of turbulence above a plane wall, in which the eddy diffusivity increases linearly with height. This form of diffusivity follows from dimensional analysis, for the only velocity scale for wall turbulence is the surface friction velocity u_* and the only length scale is y. Thus

$$K(y) = \beta u_* y \qquad (III-30)$$

where the constant of proportionality β is usually written as $\beta = 0.4/(Pr)_T$, $(Pr)_T$ being the turbulent Prandtl number (ref. 2, p. 51). Our analysis is simplified by introducing as the independent variable

$t = \beta u_* \tilde{t}$, where $\tilde{t}$ is actual time and t has the dimension of length. Then equation (III-1) with diffusivity (III-30) becomes

$$dY = dt + \sqrt{2Y}\, dW_t \qquad (III-31)$$

and, for a surface source, $Y(0) = 0$. By equation (III-31) and Ito's theorem

$$dY^n = nY^{n-1}\, dt + n(n - 1)Y^{n-1}\, dt + nY^{n-1}\, dW_t$$

which, after averaging, gives

$$\overline{dY^n} = n^2\, \overline{Y^{n-1}}\, dt \qquad (III-32)$$

for the nth moment of Y. By induction on n, the solution to equation (III-32) satisfying $\overline{Y^n}(0) = 0$ is

$$\overline{Y^n} = \Gamma(n + 1)t^n \qquad (III-33)$$

where Γ is the gamma function: $\Gamma(n + 1) = n!$ when n is an integer.

A knowledge of all of the moments of a random variable is as good as a knowledge of its pdf; in principle one determines the other. Because

$$\Gamma(n + 1) = \int_0^\infty x^n e^{-x} \, dx$$

it is clear by inspection that the pdf having the moments (III-33) is

$$P(y,t) = \frac{1}{t} e^{-y/t} H(y) \qquad\qquad (III-34)$$

(As previously, $H(y)$ is the Heaviside unit function.) This is the one and only probability density function, all of whose moments are given by equation (III-33).

The general method for determining a pdf from its moments is to note that the Fourier transform of $P(y,t)$ is (if the sum converges)

$$\int_{-\infty}^\infty e^{iky} P(y,t) dy = \sum_{n=0}^\infty \frac{(ik)^n}{n!} \overline{Y^n}(t) \qquad\qquad (III-35)$$

so, by inverting the transform,

$$P(y,t) = \frac{1}{2\pi} \int_{-\infty}^\infty e^{-iky} \sum_{n=0}^\infty \frac{(ik)^n}{n!} \overline{Y^n}(t) dk \qquad\qquad (III-36)$$

In the case of equation (III-33)

$$\sum_0^\infty \frac{(ik)^n}{n!} \overline{Y^n} = \frac{1}{(1 - ikt)}$$

which has the pdf (III-34) as its inverse transform. Formula (III-36) is used later in our analysis.

The streamwise mean velocity of a turbulent boundary layer near a plane wall has a logarithmic form

$$U(y) = 0.4 \, u_* \, \ln\left(\frac{y}{y_0}\right) \qquad\qquad (III-37)$$

where the constant y_0 is the effective surface roughness height. Equation (III-31) follows, again, from dimensional arguments (ref. 2, p. 155). As in the last example, we will next calculate $\overline{X}$ and $\overline{X^2}$ from equation (III-2).

Since $dX = U(Y) \, d\tilde{t}$,

$$\overline{X} = \frac{1}{\beta u_*} \int_0^t \overline{U(Y)} \, dt = (Pr)_T \int_0^t \overline{\ln Y} - \ln y_0 \, dt \qquad (III-38)$$

The value of $\overline{\ln Y}$ is easily determined. Equation (III-33) is valid for all real values of n, so by differentiating it with respect to n and setting $n = 0$

$$\left. \frac{\overline{dY^n}}{dn} \right|_{n=0} = \overline{\ln Y} = \ln t - \gamma \qquad (III-39)$$

where

$$\gamma = 0.5772156\ldots = -\left. \frac{d\Gamma(x)}{dx} \right|_{x=1}$$

is Euler's constant. Thus (for convenience, from here on we set $(Pr)_T = 1$).

$$\overline{X} = t \left[\ln \frac{t}{y_0} - 1 - \gamma \right] \qquad (III-40)$$

The variance of X is

$$\overline{X^2} - \overline{X}^2 = \iint_0^t \overline{\ln Y(t') \ln Y(t'')} - \overline{\ln Y(t')} \; \overline{\ln Y(t'')} \, dt'' \, dt'$$

$$= 2 \int_0^t \int_0^{t'} \overline{\ln Y(t') \ln Y(t'')} - \overline{\ln Y(t')} \; \overline{\ln Y(t'')} \, dt'' \, dt' \qquad (III-41)$$

The integrand of equation (III-41) can be evaluated analogously to equation (III-39); an expression for

$$f_{nm}(t',t'') = \overline{Y^n(t') \, Y^m(t'')} - \overline{Y^n(t')} \; \overline{Y^m(t'')} \qquad (III-42)$$

is derived and differentiated with respect to n and m, setting $n = m = 0$ in the result. Details of this procedure are given in appendix A of this chapter. The result

$$\overline{X^2} - \overline{X}^2 = t^2 \left(\frac{\pi^2}{6} - 1 \right) \qquad (III-43)$$

was derived by reference 11 through an analysis of the Fokker-Planck (i.e., diffusion) equation (III-4).

Conditional mean of X. - As in the previous example the mean value of X at fixed y can be determined (cf. eq. (III-15)). Recall that this mean is calculated from $P(x|y)$:

$$\bar{X}(y,t) = \int_{-\infty}^{\infty} P(x|y,t)x \, dx \tag{III-44}$$

Because $X(t) = \int_{0}^{t} \ln[Y(t')/y_0]dt'$, equation (III-44) can alternatively be written

$$\bar{X}(y,t) = \int_{0}^{t}\int_{-\infty}^{\infty} P(y',t'|y,t)\ln\left(\frac{y'}{y_0}\right)dy' \, dt'$$

It is convenient to use the fact that $P(y'|y)P(y) = P(y',y)$ and calculate $[\bar{X}(y,t) - \bar{X}(t)]P(y,t)$, where $\bar{X}(t)$ is as in equation (III-38). This quantity is given by

$$[\bar{X}(y,t) - \bar{X}(t)]P(y,t) = \int_{0}^{t}\int_{-\infty}^{\infty} P(y',t',y,t)(\ln y' - \ln t + \gamma)dy' \, dt'$$

$$\tag{III-45}$$

But, by expanding the y-dependence as in equation (III-36), the right side of this last equation becomes

$$\frac{1}{2\pi}\int_{0}^{t}\int_{-\infty}^{\infty} e^{-iky}\sum_{n=0}^{\infty}\frac{(ik)^n}{n!}\overline{Y^n(t)\ln Y(t')} - \overline{Y^n(t)}\,\overline{\ln Y(t')}dk \, dt'$$

$$= \frac{1}{2\pi}\int_{0}^{t}\int_{-\infty}^{\infty} e^{-iky}\sum_{n=0}^{\infty}\frac{(ik)^n}{n!}\frac{d}{dm}f_{nm}(t,t')\Big|_{m=0} dk \, dt' \tag{III-46}$$

with f_{nm} defined in equation (III-42) and given explicitly in appendix A by equation (III-A7). In appendix B equation (III-46) is evaluated to show that

$$\bar{X}(y,t) - \bar{X}(t) = t[e^{\xi}E_1(\xi) + \ln \xi + \gamma - 1] \tag{III-47}$$

where $\xi = y/t$ and $E_1(\xi) = \int_{\xi}^{\infty} e^{-x}/x \, dx$ is the exponential integral. Expression (III-47) was derived by Chatwin (ref. 11). His approach is simpler

than that used here, but our purpose is to illustrate the analysis of stochastic processes without resort to the diffusion equation (which is not available for non-Markov processes). For Markov processes the diffusion equation is available, so analysis can be based either on it or on the corresponding stochastic differential equation. The present example shows the equivalence of these analyses. In a sense this can be called an equivalence of the Lagrangian and Eulerian approaches to turbulent transport.

Streamwise dispersion. - In most experiments the surface layer consists of the near-wall region of a turbulent boundary layer. In these experiments the source of contaminant is steady and dispersion takes place in the cross-stream direction y as a function of streamwise distance x from the source at $x = 0$. Thus these experiments should be modeled by a stochastic process $Y(x)$ with x the independent variable. When $dt = dx/U(y)$ is used to change from t- to x-dependence, equation (III-31) becomes

$$dY(x) = \frac{dx}{U[Y(x)]} + \sqrt{\frac{2Y(x)}{U[Y(x)]}} \, dW_x \qquad (III-48)$$

The corresponding Fokker-Planck equation is (cf. eq. (II-16) with x replacing t)

$$\frac{\partial P(x,y)}{\partial x} = \frac{\partial}{\partial y} \, y \, \frac{\partial}{\partial y} \left[\frac{P(x,y)}{U(y)} \right] \qquad (III-49)$$

One usually defines a normalized concentration $C(x,y)$ by $P(x,y) = U(y)C(x,y)$, which shows the probabilistic meaning of $C(x,y)$. The concentration $C(x,y)$ satisfies

$$U(y) \, \frac{\partial C(x,y)}{\partial x} = \frac{\partial}{\partial y} \, y \, \frac{\partial C(x,y)}{\partial y} \qquad (III-50)$$

If $U(y)$ is given by a power law, $U(y) \propto y^p$, then a change of independent variable to $Y^{p+1}(x)$ transforms equation (III-48) to the form of equation (III-31), and it can be solved as above. However, when the more correct logarithmic form (III-37) is used for $U(y)$, equations (III-48) and (III-49) can no longer be solved in closed form. In this case a finite-difference version of equation (III-48) can be solved with relatively little computational effort by the methods described in chapter II. Reference 12 numerically solves an equation like equation (III-48) downstream of a line source located on the wall below a turbulent boundary layer. From an ensemble of solutions, statistical moments of $Y(x)$ are evaluated. Data on plume moments downstream of a source in a boundary layer are provided in reference 13. The plume moment is defined as

$$Y_p(x) = \int_0^\infty y \, C(x,y) dy = \int_0^\infty \frac{y}{U(y)} \, P(x,y) dy = \overline{\left(\frac{Y(x)}{U[Y(x)]} \right)} \qquad (III-51)$$

Numerical results of reference 12 for $Y_p(x)$ are shown in figure III-2, along with measurements of $Y_p(x)$. It can be seen that the eddy diffusion model does a good job of describing the evolution of Y_p.
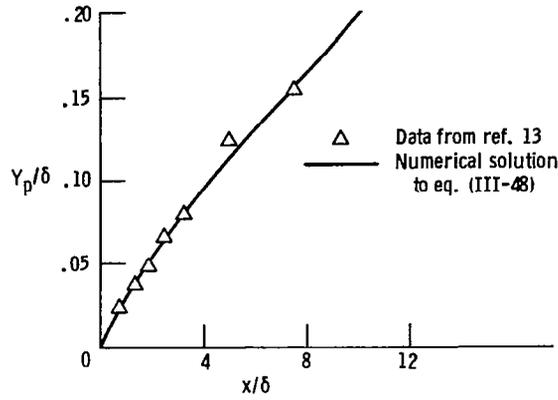
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Figure III-2. - Increase of plume moment with distance downstream of wall source in turbulent boundary layer. Distances are normalized by boundary layer thickness δ.

Example 3: Channel Flow

We analyse this example in considerably less detail than the previous two.

Consider the turbulent flow through a channel with walls at $y = 0$ and at $y = 1$. A diffusivity suitable to this flow is

$$K(y) = u_* \beta y(1 - y) \qquad \text{(III-52)}$$

with β as in example 2. Again if we let $t = u_* \beta \tilde{t}$, $Y(t)$ satisfies

$$dY = (1 - 2Y)\, dt + \sqrt{2Y(1 - Y)}\, dW_t \qquad \text{(III-53)}$$

The Fokker-Planck equation corresponding to equation (III-53) is

$$\frac{\partial P}{\partial t} = \frac{\partial}{\partial y}\left[y(1 - y)\, \frac{\partial P}{\partial y} \right] \qquad \text{(III-54)}$$

For the reasons given at the beginning of the previous example the eddy diffusion model, equation (III-53) or (III-54), of dispersion is only suitable for wall sources. Hence, we consider the initial condition $Y(0) = 1$ to equation (III-53). The corresponding condition to equation (III-54) is $P(y,0) = \delta(1 - y)$, where $\delta(\cdot)$ is the Dirac delta function.

By Ito's theorem

$$\frac{\overline{dY^n}}{dt} = -n(n + 1)\overline{Y^n} + n^2\, \overline{Y^{n-1}} \qquad \text{(III-55)}$$

subject to $\overline{Y^n}(0) = 1$, determines the moments of Y. These moments are readily seen to be

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$$\overline{Y} = \frac{1}{2}(1 + e^{-2t})$$

$$\overline{Y^2} = \frac{1}{3} + \frac{e^{-2t}}{2} + \frac{e^{-6t}}{6}$$

$$\overline{Y^n} = (n!)^2 \sum_{m=0}^{n} \frac{2m + 1}{n - m!\ n + m + 1!}\ e^{-m(m+1)t}$$

(III-56)

That $\overline{Y^n}$ satisfies equation (III-55) is seen by substitution; that the initial condition is satisfied is seen by writing $\overline{Y^n}$ (0) as

$$(n!)^2 \sum_{m=0}^{n} \frac{(n + m + 1) - (n - m)}{n + m + 1!\ n - m!}$$

$$= (n!)^2 \left\{ \sum_{m=0}^{n} \frac{1}{n + m!\ n - m!} - \sum_{m=1}^{n} \frac{1}{n + m!\ n - m!} \right\}$$

$$= 1$$

The expression for $\overline{Y(t)}$ is shown in figure III-3 with data from Sullivan (ref. 14). He measured the trajectories of neutrally bouyant particles in turbulent channel flow, from which $\overline{Y(t)}$ was determined directly.
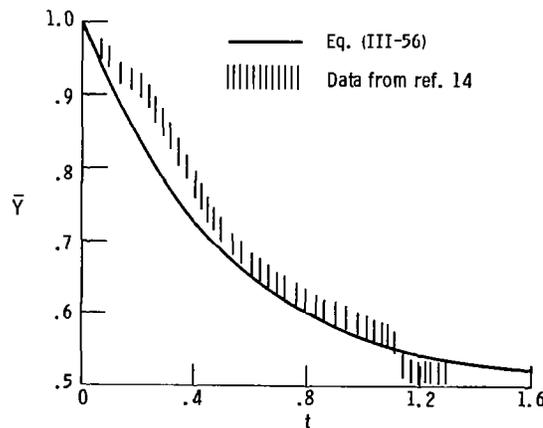
Figure III-3. - Mean trajectory in turbulent channel flow of particles released at wall.

The probability density for this example is obtained most simply by solving equation (III-54):

$$P(y,t) = \sum_{n=0}^{n} e^{-n(n+1)t} \mathscr{P}_n(2y - 1)(2n + 1) \qquad \text{(III-57)}$$

where $\mathscr{P}_n(\cdot)$ is the nth Legendre polynomial. The moments (III-56) follow from the pdf (III-57), showing the equivalence of the moment and pdf representations of the statistical properties of Y.

APPENDIX A: EVALUATION OF X-VARIANCE FOR EXAMPLE 2

The procedure for determining the variance of X consists first of finding an expression for f_{nm} with n and m real, then differentiating with respect to n and m (cf. eq. (III-41) et seq.). Because of the non-anticipating property of $Y(t)$, $Y(t'')$ is uncorrelated with $dW_{t'}$ when $t'' < t'$. Therefore multiplying

$$dY^n(t') = n^2 Y^{n-1}(t')dt' + nY^{n-1}(t')dW_{t'} \qquad \text{(III-A1)}$$

by $Y^m(t'')$ and averaging give

$$\frac{d}{dt'} \overline{Y^n(t')Y^m(t'')} = n^2 \overline{Y^{n-1}(t')Y^n(t'')} \qquad \text{(III-A2)}$$

where t'' is treated as constant and $t' > t''$. Since $\overline{Y^n(t')}$ satisfies equation (III-32) with respect to t', $f_{nm}(t',t'')$ as defined in equation (III-42) satisfies

$$\frac{df_{nm}(t',t'')}{dt'} = n^2 f_{n-1m}(t',t'') \qquad \text{(III-A3)}$$

Because $t' > t''$ in equation (III-A3), f_{nm} must satisfy an initial condition at $t' = t''$; clearly

$$f_{nm}(t'',t'') = \overline{Y^{n+m}(t'')} - \overline{Y^n(t'')}\ \overline{Y^m(t'')} \qquad \text{(III-A4)}$$

with the moments of Y given by equation (III-33), is this condition. Also, the recurrence relation (III-A3) starts from

$$f_{0m}(t',t'') = 0 \qquad \text{(III-A5)}$$

When n and m are integers, it can be seen that

$$f_{nm} = (n!)^2 \sum_{p=0}^{n} \frac{(t'')^{m+p}(t' - t'')^{n-p}}{p!^2 n - p!} (m + p! - m!p!) \qquad \text{(III-A6)}$$

satisfies equations (III-A3), (III-A4), and (III-A5).

Expression (III-A6) can be extended to noninteger n and m by re-expressing it as a contour integral:

$$f_{nm} = \frac{\Gamma^2(n + 1)}{2\pi i} \int_C \frac{(t'')^{m-s}(t' - t'')^{n+s}(-1)^s \Gamma(s)}{\Gamma(n + 1 + s)\Gamma(1 - s)}$$

$$\times \ [\Gamma(m - s + 1) - \Gamma(m + 1)\Gamma(1 - s)]ds \qquad \text{(III-A7)}$$

The contour of integration envelopes the poles on the negative real axis as shown below.
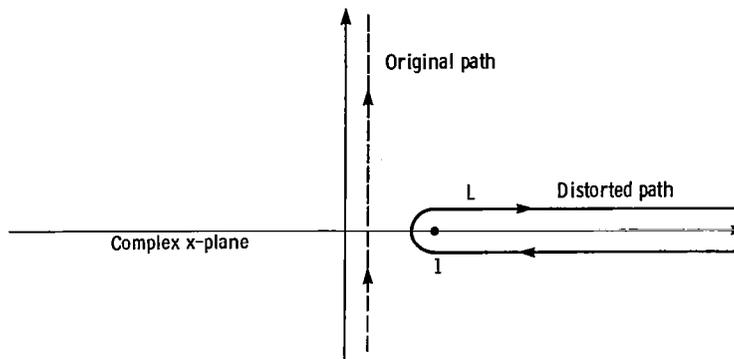
(This contour is appropriate when t" < t'/2. We appeal to analytic continuation to make equation (III-A10) valid for all t" < t'.)
    As described in the text below equation (III-41),

$$\overline{x^2} - \overline{x}^2 = 2 \int_0^t \int_0^{t'} \left.\frac{d^2 f_{nm}}{dn\ dm}\right|_{n=m=0} dt''\ dt' \qquad (III-A8)$$

Differentiating equation (III-A7) gives

$$\left.\frac{d^2 f_{nm}}{dn\ dm}\right|_0 = \frac{i}{2\pi} \int_C \left(\frac{t'' - t'}{t''}\right)^s \frac{\Gamma(s)\Gamma'(1 + s)}{\Gamma^2(1 + s)} [\psi(1 - s) + \gamma] ds \qquad (III-A9)$$

where $\Gamma'(x) = d\Gamma(x)/dx$, $\psi(x) = \Gamma'(x)/\Gamma(x)$ and $\gamma = -\psi(1)$. Upon evaluating the residues of equation (III-A9), the right side becomes

$$-\sum_{p=1}^{\infty} \left(\frac{t''}{t'' - t'}\right)^p \frac{\psi(1 + p) + \gamma}{p} = -\sum_{p=1}^{\infty} \sum_{r=1}^{p} \frac{1}{pr} \left(\frac{t''}{t'' - t'}\right)^p$$

$$= -\sum_{r=1}^{\infty} \sum_{p=r}^{\infty} \frac{1}{pr} \left(\frac{t''}{t'' - t'}\right)^p$$

$$= \int_0^{t''/(t'-t'')} \frac{\ln(1 + x)}{x(1 + x)} dx \qquad (III-A10)$$

where use has been made of the identity

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$$\psi(1 + p) + \gamma = \sum_{r=1}^{p} \frac{1}{r}$$

for integer p. Equation (III-A10) is the integrand of equation (III-A8), which therefore becomes

$$\overline{x^2} - \overline{x}^2 = 2 \int_0^t \int_0^{t'} \int_0^{t''/(t'-t'')} \frac{\ln(1 + x)}{x(1 + x)} \, dx \, dt'' \, dt'$$

$$= 2t^2 \int_0^1 \int_0^{\tau} \int_0^{\tau/\Delta - 1} \frac{\ln(1 + x)}{x(1 + x)} \, dx \, d\Delta \, d\tau \qquad (\text{III-A11})$$

where $\tau = t'/t$, $\Delta = (t' - t'')/t$. This triple integral is quite harmless: after integrating by parts with respect to Δ it becomes

$$2 \int_0^1 \int_0^{\tau} \frac{\ln(\tau/\Delta)}{\tau/\Delta - 1} \, d\Delta \, d\tau = - \int_0^1 \frac{x \ln x}{1 - x} \, dx$$

$$= \int_0^1 \ln x \, dx - \int_0^1 \frac{\ln x}{1 - x} \, dx = \frac{\pi^2}{6} - 1 \qquad (\text{III-A12})$$

The substitution $x = \Delta/\tau$ was made in the first step. Equation (III-43) is thus obtained.

APPENDIX B: EVALUATION OF $\bar{X}(y,t)$ FOR EXAMPLE 2

We wish to evaluate expression (III-46) with f_{nm} given by equation (III-A7). Differentiating equation (III-A7) with respect to m and setting $m = 0$ give

$$\left.\frac{df_{nm}(t,t')}{dm}\right|_{m=0} = \frac{\Gamma^2(n+1)}{2\pi i} \int_C \frac{(t-t')^{n+s}(-t')^s \Gamma(s)}{\Gamma(n+1+s)} [\psi(1-s) + \gamma] ds$$

$$= (n!)^2 \sum_{p=1}^{n} \frac{(t-t')^{n-p} t'^p}{p! \, n-p!} [\psi(1+p) + \gamma] \qquad (III-B1)$$

By substituting this and exchanging orders of integration, equation (III-46) becomes

$$\frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-iky} \sum_{n=1}^{\infty} n!(ik)^n \sum_{p=1}^{n} \frac{\psi(1+p) + \gamma}{p! \, n-p!} \int_0^t (t-t')^{n-p} t'^p \, dt' \, dk$$

$$(III-B2)$$

Because the last integral is equal to $t^{n+1} (n-p)! p!/(n+1)!$, this expression equals

$$\frac{t}{2\pi} \int_{-\infty}^{\infty} e^{-iky} \sum_{n=1}^{\infty} \sum_{p=1}^{n} \frac{\psi(p+1) + \gamma}{n+1} (ikt)^n \, dk \qquad (III-B3)$$

but

$$\sum_{p=1}^{n} \psi(p+1) + \gamma = \sum_{p=1}^{n} \sum_{r=1}^{p} \frac{1}{r} = \sum_{r=1}^{n} \sum_{p=r}^{n} \frac{1}{r} = (n+1)(\psi(n) + \gamma) - n$$
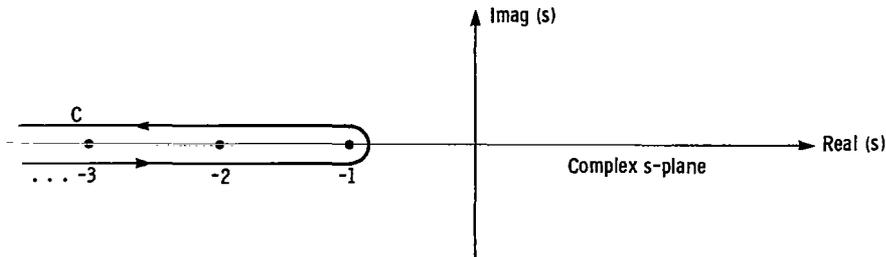
so expression (III-B3) equals

$$\frac{t}{2\pi} \int_{-\infty}^{\infty} e^{-iky} \sum_{n=1}^{\infty} (ikt)^n \left[\psi(n) + \gamma - \frac{n}{n+1}\right] dk$$

$$= \frac{-1}{2\pi i} \int_{-\infty i}^{\infty i} e^{-xy/t} \left[\frac{\ln(1-x)}{x(1-x)} + \frac{1}{1-x}\right] dx \qquad (III-B4)$$

where $x = ikt$. The residue for the $1/(1 - x)$ in square brackets is just

$$e^{-\xi} \qquad\qquad\qquad (III-B5)$$

where $\xi = y/t$. The first term can be evaluated by distorting the path of integration to envelope the part of the positive real axis greater than 1, as shown in the following sketch:

Then this term becomes

$$\frac{i}{2\pi} \int_L e^{-\xi x} \frac{\ln(1 - x)}{x(1 - x)} \, dx$$

Since $\ln(-x) = \ln|x| - \pi i$ above the real axis and $\ln(-x) = \ln|x| + \pi i$ below the real axis, this last integral equals

$$\int_1^\infty \frac{e^{-\xi x}}{x(1 - x)} \, dx = \int_1^\infty \frac{e^{-\xi x}}{x} \, dx - e^{-\xi} \int_0^\infty \frac{e^{-\xi x}}{x} \, dx \qquad (III-B6)$$

provided the integrals are interpreted in the generalized sense (ref. 15); that is,

$$\int_0^\infty \frac{e^{-\xi x}}{x} \, dx = \xi \int_0^\infty e^{-\xi x} \ln x \, dx = - \ln \xi - \gamma \qquad (III-B7)$$

The first integral in equation (III-B6) is just the exponential integral $E_1(\xi)$. Thus, collecting the results (III-B5), (III-B6), and (III-B7) gives

$$e^{-\xi} (\ln \xi + \gamma - 1) + E_1(\xi) \qquad\qquad (III-B8)$$

for the value of the expression (III-46). As given in equation (III-34), $P(y,t)$ is $e^{-\xi}/t$ and expression (III-B8) is the right side of equation (III-45). Thus we obtain equation (III-47).

INTERLUDE: A POINT CONCERNING MODELING

In examples 2 and 3 of chapter III it is noted that the eddy diffusion model can only be used for dispersion from surface sources. For elevated sources this model is incorrect in principle and in practice. It is sometimes suggested that a time-dependent diffusivity could be used to rectify this failure (ref. 1, section 5.8). In this procedure, time must be referred to an origin at the contaminant source. However, the justification for this suggestion is usually based on a false identification of diffusion processes and stochastic processes with Gaussian pdf's. The Gaussian distribution solves a diffusion equation with time-dependent diffusivity, as a matter of fact, but this does not make Gaussian processes diffusion processes. In nonhomogeneous turbulence the pdf is not Gaussian, so the failure of eddy diffusion there certainly cannot be rectified by a time-dependent diffusivity.

An illuminating discussion of the irrationality of time-dependent diffusivities is given by Taylor (ref. 16). He remarks that a diffusivity which is a function of time violates the principle of superposability: if two sources of contaminant start at different times, then where their clouds overlap it becomes necessary to assume that the diffusivity has two values, each referred to a different origin at the appropriate source time. This is nonsensical since the material emitted by each source is indistinguishable from that emitted by the other.

However, this scheme for dealing with elevated sources is illogical for another reason, which has to do with a general principle of turbulence modeling. Namely, the coefficients in a dispersion model can only be functions of the turbulence and not of the contaminant distribution (which, after all, is what is to be predicted.) Hence in stationary turbulence these coefficients cannot be functions of time; for example, in chapter III it would be incorrect to let $K(y)$ be a function of time. Even when the turbulence is not stationary, the coefficients should be referred to the time origin of the turbulence and not to any source time. The next chapter describes a model of dispersion from elevated sources in stationary turbulence that abides by this principle of modeling.

CHAPTER IV: DISPERSION WITH FINITE TIME SCALE

In chapter III examples in which particle trajectories are modeled by Markov processes were considered. In such processes the random component of the velocity is represented by white noise (recall that the white-noise process is dW_t/dt). Because white noise has a zero correlation time scale (cf. eq. (II-5)), by representing the randomness in this way one is assuming that the correlation time of velocity fluctuations T_L can be regarded as negligible. In examples 2 and 3 of chapter III it was noted that the Markovian eddy diffusion model was appropriate for dispersion from surface sources. The reason is that in the nonhomogeneous turbulence above a wall the velocity time scale tends to zero as the surface is approached. However, away from the surface this time scale is not negligible: dispersion from elevated sources must be modeled by a process with a finite correlation time for velocity fluctuations.

At high Reynolds numbers $(Re \equiv u'\ell/\nu)$ the time scale of acceleration fluctuations is of order $(Re)^{-1/2}$. This is so because acceleration has its rms value determined primarily by those components of turbulence that have a short time scale compared with the velocity time scale T_L. Analysis in reference 5, section 18.3, shows that the acceleration time scale T_a is of order $(Re)^{-1/2}T_L$. Thus, while T_L is of order 1, T_a tends to 0 like $(Re)^{-1/2}$ at high Reynolds numbers. Consequently it is suitable to model acceleration by a white-noise process; indeed, in writing equation (I-1), terms of order $(Re)^{-1/2}$ were ignored, so letting $T_a \sim 0$ is consistent with that equation.

An equation in which acceleration is modeled by white noise is the Langevin equation (ref. 7):

$$dV(t) = \frac{-V(t)dt}{T_L} + \sigma_v \sqrt{\frac{2}{T_L}}\, dW_t \qquad (IV-1)$$

Here σ_v and T_L are constants and $V(t)$ is velocity. The initial condition for equation (IV-1) is that $V(0)$ is a Gaussian random variable with mean zero and variance σ_v^2. The Langevin equation has its origin in the theory of Brownian motion, but it was used in a discretized form by Taylor (ref. 17) as a model of turbulent dispersion. Application of the analysis in this chapter to environmental dispersion can be made along the lines of reference 1, chapters III and V.

Langevin Model for Homogeneous Turbulence

Equation (IV-1) is a Markovian differential equation of the type discussed in chapter II, except that now it determines particle velocities $V(t)$. The trajectory $Y(t) = \int_0^t V(t')\, dt'$ is not a Markov process

(although V and Y jointly are a Markov process in phase space, ref. 3). Because the turbulent velocity has a finite time scale, particle trajectories must be nonMarkovian. But, by retaining the Markovian property at a higher level - that is, by making the velocity be a Markov process - the dispersion model remains tractable. There is no general theory for completely nonMarkov stochastic processes, so it is useful (for numerical as well as theoretical analysis) to maintain this connection to Markov processes at some level of modeling.

Equation (IV-1) is a linear equation for $V(t)$. Because dW_t is Gaussian and equation (IV-1) is linear, $V(t)$ is also Gaussian; thus $V(t)$ is characterized by its mean and its variance. Averaging equation (IV-1) gives

$$\frac{d\overline{V}}{dt} = \frac{-\overline{V}}{T_L}$$

But $\overline{V}(0) = 0$, so the mean of $V(t)$ is zero. By Ito's theorem

$$\frac{1}{2} \frac{d\overline{V^2}}{dt} = \frac{\sigma_v^2 - \overline{V^2}}{T_L}$$

Because $V(0)$ is Gaussian with variance σ_v^2,

$$\overline{V^2(t)} = \sigma_v^2 \qquad \text{(IV-2)}$$

is the solution of this equation for the variance $V(t)$. Thus $V(t)$ is Gaussian with constant mean and variance; in fact, it is a statistically stationary random process. The pdf of v is

$$P(v) = \frac{e^{-v^2/2\sigma_v^2}}{\sigma_v \sqrt{2\pi}} \qquad \text{(IV-3)}$$

In stationary, homogeneous turbulence the particle velocity is statistically independent of particle position; hence it is a stationary random process. For this reason equation (IV-1) is a model of dispersion in homogeneous turbulence: the constancy of σ_v and T_L makes it a model of homogeneous turbulence.

Carrying the analysis of second moments of V one step further, we calculate the correlation function $R(\tau) = \overline{V(t + \tau)V(t)}/\sigma_v^2$, $\tau \geq 0$. With t fixed and τ variable, $V(t + \tau)$ satisfies (cf. eq. (IV-1))

$$dV(t + \tau) = \frac{-V(t + \tau)}{T_L} d\tau + \sigma_v \sqrt{\frac{2}{T_L}} dW_{t+\tau} \qquad \text{(IV-4)}$$

By the nonanticipating property, $\overline{V(t)dW_{t+\tau}} = 0$, $\tau \geq 0$. Hence multiplying equation (IV-4) by $V(t)$, dividing by σ_v^2, and averaging give

$$\frac{dR(\tau)}{d\tau} = \frac{-R(\tau)}{T_L}$$

This has the solution

$$R(\tau) = e^{-\tau/T_L} \qquad\qquad (IV-5)$$

which satisfies the initial condition $R(0) = 1$. Thus the role of T_L as a correlation time scale is clear. Here it could be an integral time scale,

$$T_L = \int_0^\infty R(\tau)d\tau$$

but it is more natural to regard it as a scale for instantaneous decorrelation rate:

$$T_L = \left| \frac{1}{R(\tau)} \frac{dR(\tau)}{d\tau} \right|_{\tau=0}^{-1} \qquad\qquad (IV-6)$$

The reason for the interpretation (IV-6) of T_L is that when the turbulence is stationary but nonhomogeneous, $V(t)$ is not a stationary process; in this case an integral time scale is neither clearly defined nor a property of the turbulence. (Remember that $V(t)$ is the velocity of a particle. When the turbulence is not homogeneous, this will be statistically dependent on particle position and consequently will not be stationary. A time-dependent integral scale could be defined, but it would not be a property of the stationary turbulence.) Equation (IV-6) defines an instantaneous property of $V(t)$; therefore in nonhomogeneous turbulence it defines a local property of the fluid flow. If we wish to use equation (IV-1) for nonhomogeneous turbulence, equation (IV-6) must be used to define a local $T_L(y)$; similarly $\sigma_v(y)$ would then be related to the local value of the turbulent velocity variance. Later the application of the Langevin equation to non-homogeneous turbulence will be considered; first we explore the case of homogeneous turbulence further. As in example I of chapter III, we consider dispersion in a uniform shear flow but now allow for the finite time scale of the turbulence.

Shear Dispersion

The random trajectories of fluid particles are given by

$$\left.\begin{aligned} dY(t) &= V(t)dt \\ dX(t) &= \eta Y(t)dt \end{aligned}\right\} \qquad\qquad (IV-7)$$

(cf. eq. (III-6)) with V(t) determined by equation (IV-1) and the mean x-velocity being $U(y) = \eta y$. The turbulent velocity in the x-direction is ignored with respect to the mean; it could easily be included as a random process analogous to, but independent of V(t) – or, to model Reynolds stresses, it could be correlated with V(t).

Because V(t) is Gaussian and equations (IV-7) are linear, X(t) and Y(t) are Gaussian. Furthermore, if they are subject to the initial conditions $X(0) = Y(0) = 0$, then $\overline{X} = \overline{Y} = 0$. We proceed to analyze the second moments of X and Y.

Integrating the first equation (IV-7) with $Y(0) = 0$ gives

$$Y(t) = \int_0^t V(t')dt'$$

so

$$\overline{Y^2} = \iint_0^t \overline{V(t')V(t'')}dt'' \, dt'$$

$$= 2 \int_0^t \int_0^{t'} \overline{V(t')V(t'')}dt'' \, dt' \tag{IV-8}$$

By equation (IV-5) $\overline{V(t')V(t'')} = \sigma_v^2 \exp[-(t' - t'')/T_L]$, for $t' \geq t''$. After this is substituted, the integrals in equation (IV-8) can be evaluated:

$$\overline{Y^2}(t) = 2\sigma_v^2 T_L^2 \left(\frac{t}{T_L} - 1 + e^{-t/T_L} \right) \tag{IV-9}$$

As has been said previously, when $t \gg T_L$, the Markovian models of chapter III ought to be valid. When $t \gg T_L$, equation (IV-9) reduces to

$$\overline{Y^2} = 2\sigma_v^2 T_L t$$

Comparing this to the Markovian example 1 of chapter III, where $\overline{Y^2} = 2Kt$, we find that

$$K = \sigma_v^2 T_L \tag{IV-10}$$

is the eddy diffusivity of the Markov process to which equations (IV-1) and (IV-7) reduce as $t/T_L \to \infty$. Because Y(t) is Gaussian, the fact that its variance tends to that of example 1 of chapter III shows that it asymptotically has the Markovian pdf. At short times, $\overline{Y^2} \to \sigma_v^2 t^2$.

The variance of X is

$$\overline{X^2} = 2\eta^2 \int_0^t \int_0^{t'} \overline{Y(t')Y(t'')} dt' \, dt'' \tag{IV-11}$$

in which

$$\overline{Y(t')Y(t'')} = \int_0^{t'} \int_0^{t''} \overline{V(x')V(x'')} dx' \, dx''$$

$$= \sigma_v^2 \int_0^{t'} \int_0^{t''} e^{-|x' - x''|/T_L} dx' \, dx''$$

$$= \sigma_v^2 T_L^2 \left(e^{-t'/T_L} + e^{-t'/T_L} - e^{(t''-t')/T_L} - 1 + \frac{2t''}{T_L} \right) \tag{III-12}$$

and $t'' \leq t'$. Substituting equation (IV-12) into equation (IV-11) and integrating give

$$\overline{X^2} = 2\eta^2 \sigma_v^2 T_L^4 \left(\frac{t^3}{3T_L^3} - \frac{t^2}{2T_L^2} + 1 - e^{-t/T_L} - \frac{te^{-t/T_L}}{T_L} \right) \tag{IV-13}$$

As $t/T_L \to \infty$ this reduces to equation (III-10) with K given by equation (IV-10). As $t/T_L \to 0$, $\overline{X^2} \to \sigma_v^2 \eta^2 t^4/4$, so initially $\overline{X^2}$ grows quite slowly compared with $\overline{Y^2}$, although ultimately it grows more rapidly than $\overline{Y^2}$. The covariance $\overline{XY}$ is readily computed:

$$\overline{XY} = \eta \int_0^t \overline{Y(t)Y(t')} dt'$$

$$= \eta \sigma_v^2 T_L^2 t \left(\frac{t}{T_L} - 1 + e^{-t/T_L} \right) \tag{IV-14}$$

having used equation (IV-12). Because X and Y are jointly Gaussian

$$P(x,y) = \frac{\exp\left[\dfrac{-x^2 \overline{Y^2} - y^2 \overline{X^2} + 2xy\overline{XY}}{2(\overline{X^2}\,\overline{Y^2} - \overline{XY}^2)} \right]}{2\pi \sqrt{\overline{X^2}\,\overline{Y^2} - \overline{XY}^2}} \tag{IV-15}$$

(ref. 8, eq. (5.1.28)) with $\overline{X^2}$, $\overline{Y^2}$, and $\overline{XY}$ given by equations (IV-9), (IV-13), and (IV-14). The function P can be regarded as the concentration of a contaminant released initially by a point source at $x = y = 0$. The numerator of the exponential in equation (IV-15) is constant on ellipses in the x,y-plane: these ellipses are the surfaces of constant concentration. At short times their major axis is nearly along the y-axis; at long times it is nearly along the x-axis.

The pdf (IV-15) corresponds to the pdf (III-13), and

$$P(x|y) = P(x,y)/P(y)$$

$$= \sqrt{\frac{\overline{Y^2}}{2\pi(\overline{X^2}\ \overline{Y^2} - \overline{XY^2})}}\ \exp\left[\frac{-\overline{Y^2}}{2(\overline{X^2}\ \overline{Y^2} - \overline{XY^2})}\left(x - \frac{\overline{XY}}{\overline{Y^2}}\,y\right)^2\right] \quad \text{(IV-16)}$$

corresponds to equation (III-15). Equation (IV-16) is the probability density for the x-position of those trajectories that at time t are at a given y-position. It is also the normalized streamwise distribution, at fixed cross-stream position, of contaminant released by a point source.

From equation (IV-16) the first and second moments of $X(t)$ for those trajectories that have the fixed end point $Y(t) = y$ are

$$\overline{X}(y,t) = y\,\frac{\overline{XY}}{\overline{Y^2}} = \frac{n\,y\,t}{2} \quad \text{(IV-17)}$$

exactly as was true for equation (III-15), and

$$\overline{X^2}(y,t) - \overline{X}^2(y,t)$$

$$= \overline{X^2} - \frac{\overline{XY^2}}{\overline{Y^2}}$$

$$= 2n^2\sigma_v^2 T_L^4\left[\frac{t^3}{12T_L^3} - \frac{t^2}{4T_L^2} + 1 - \left(1 + \frac{t}{T_L} + \frac{t^2}{4T_L^2}\right)e^{-t/T_L}\right] \quad \text{(IV-18)}$$

As previously, $\overline{X^2}(y,t) - \overline{X}^2(y,t)$ is independent of the end point y. When $t/T_L \to 0$, expression (IV-18) tends to $n^2\sigma_v^2 t^5/60T_L$, which is much smaller than the unconditional variance $n^2\sigma_v^2 t^4/4$ (cf. eq. (IV-13)). The reason for the conditional variance being smaller than the unconditional variance is that the conditional variance is the spread of contaminant about the mean (eq. (IV-17)), while the unconditional variance is the spread of these spreads.

The preceding analysis of dispersion by a linear shear in homogeneous turbulence describes <u>horizontal</u> dispersion in a boundary layer. As mentioned in chapter III, this model is not suitable for <u>vertical</u> dispersion near a boundary because the turbulence is not homogeneous in that direction. Thus, while a reflection boundary condition could be imposed, following the approach of chapter III, example 1, such analysis is not strictly justified and will not be pursued here. Instead we proceed directly to a discussion of dispersion with finite time scale in a nonhomogeneous medium.

Dispersion in Nonhomogeneous Turbulence

In nonhomogeneous turbulence the coefficients in equation (IV-1) must be made functions of Y. For the present consider the case with T_L a function of y and σ_v constant; later we will consider the case in which σ_v is also a function of y.

Now equation (IV-1) has the form

$$dV = - \frac{V}{T_L(Y)} dt + \sigma_v \sqrt{\frac{2}{T_L(Y)}} dW_t \qquad \text{(IV-19)}$$

Along with $dY = V\, dt$ the model (IV-19) describes trajectories through nonhomogeneous turbulence. Equation (IV-19) is to be solved subject to the conditions that $Y(0) = h$ and that $V(0)$ is Gaussian with mean zero and variance σ_v for a source located at $y = h$. (The initial condition on V follows from the requirement that contaminant particles move with the fluid. At the point of release the fluid velocity is assumed by equation (IV-19) to be Gaussian with mean zero and variance σ_v.) Generally equation (IV-19) must be solved numerically (refs. 12 and 18); however, here it will be solved by asymptotic analysis.

It is obvious that at sufficiently short times T_L can be considered to be constant with value $T_L(h)$. During this initial period, dispersion takes place as described previously for homogeneous turbulence. To delimit and go beyond the initial stage, one might construct a solution to equation (IV-19) as a power series in t and W_t. However, a different, though similar, approach will be followed here: we consider dispersion in a slowly varying medium (ref. 19); that is, we assume T_L can be written as a function of εy where $\varepsilon \ll 1$. Our objective is to determine how inhomogeneity affects the solution to equation (IV-19).

With the functional form $T_L(\varepsilon y)$, equation (IV-19) reduces to the equation for a homogeneous medium when $\varepsilon = 0$. For small but nonzero ε the solution to equation (IV-19) can be expanded in a power series

$$\left.\begin{aligned} V(t) &= V_0(t) + \varepsilon V_1(t) \ldots \\[2mm] Y(t) &= Y_0(t) + \varepsilon Y_1(t) \ldots \end{aligned}\right\} \qquad \text{(IV-20)}$$

The terms with subscript 1 (and greater) are due to the inhomogeneity of the turbulence.

The equations solved by V_0 and V_1 are found by substituting the expansion (IV-20) along with the Taylor series

$$T_L(\epsilon Y) = T_L(0) + \epsilon T_L'(0)Y_0 \cdots \tag{IV-21}$$

where $T_L' = dT_L/dy$, into equation (IV-19). Without loss of generality the source height h has been set to zero. Equation (IV-19) then can be separated into a set of equations by equating to zero the coefficient of each power of ϵ. To order ϵ this results in

$$dV_0 = -\frac{V_0}{T_L(0)}\, dt + \sqrt{\frac{2}{T_L(0)}}\, \sigma_v\, dW_t \tag{IV-22}$$

and

$$dV_1 = -\frac{V_1}{T_L(0)}\, dt + \frac{T_L'(0)}{T_L^2(0)}\, Y_0 V_0\, dt - \frac{\sigma_v T_L'(0) Y_0}{2 T_L^{3/2}(0)}\, dW_t \tag{IV-23}$$

where $dY_0 = V_0\, dt$ and $dY_1 = V_1\, dt$. Clearly the solution to equation (IV-22) is that given in the previous section; in particular

$$\left.\begin{aligned}
\overline{Y_0} &= 0 \\[2mm]
\overline{Y_0^2} &= 2\sigma_v^2 T_L^2\left(\frac{t}{T_L} - 1 + e^{-t/T_L}\right)
\end{aligned}\right\} \tag{IV-24}$$

where it is understood that T_L is evaluated at $y = 0$.

At order ϵ the mean value of Y is no longer zero. Upon averaging, equation (IV-23) becomes

$$\frac{d\overline{V_1}}{dt} = -\frac{\overline{V_1}}{T_L} + \frac{1}{2}\frac{T_L'}{T_L^2}\frac{d\overline{Y_0^2}}{dt}$$

In this equation $\overline{Y_0 V_0}$ has been written in the equivalent form $\frac{1}{2}\, d\overline{Y_0^2}/dt$. Substituting equation (IV-24) and solving this, subject to $V_1(0) = 0$, gives

$$\overline{V_1} = \sigma_v^2 T_L'\left(1 - e^{-t/T_L} - \frac{t}{T_L}e^{-t/T_L}\right) \tag{IV-25}$$

Correspondingly

$$\overline{Y_1} = \sigma_v^2 T_L T_L'\left(\frac{t}{T_L} - 2 + 2e^{-t/T_L} + \frac{t}{T_L}e^{-t/T_L}\right)$$

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Thus the effect of inhomogeneity is to cause a nonzero mean vertical velocity. In physical terms the source of this mean velocity is that particles moving in a direction of increasing T_L maintain their direction of motion longer on average than particles moving in a direction of decreasing T_L; thus particles drift up gradients of T_L.

As $t/T_L \to \infty$, the velocity (IV-25) becomes $\sigma_v^2 T_L'$. If K is given by equation (IV-10) with T_L a function of y, this velocity is

$$\frac{d\overline{Y}}{dt} = \frac{\overline{dK}}{dy} \qquad (IV-26)$$

In the eddy diffusion model, equations (III-1) and (II-19), $d\overline{Y}/dt$ is also $\overline{dK/dy}$; therefore as $t/T_L \to \infty$, equation (IV-25) again reduces to the eddy diffusion result. In the next section it will be shown more completely that the stochastic process $Y = Y_0 + \epsilon Y_1$ tends asymptotically to an eddy diffusion process.

Although $d\overline{Y}/dt$ tends asymptotically to the formula (IV-26), it must initially be zero, for $\overline{V}(0) = 0$. The effect of the finite correlation time scale is that particles "remember" that they had this zero initial velocity, and their mean velocity only gradually becomes nonzero, tending eventually to the velocity (IV-26). In the eddy diffusion model the memory time scale is zero, so random trajectories immediately obtain the mean velocity (IV-26).
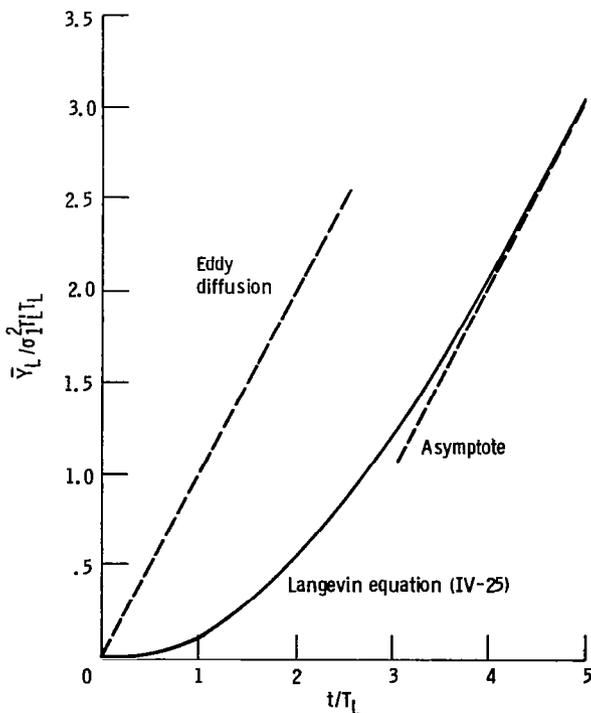

Figure IV-1. - Comparison of mean rise of particles as given by equation (IV-25) with that given by eddy diffusion model.
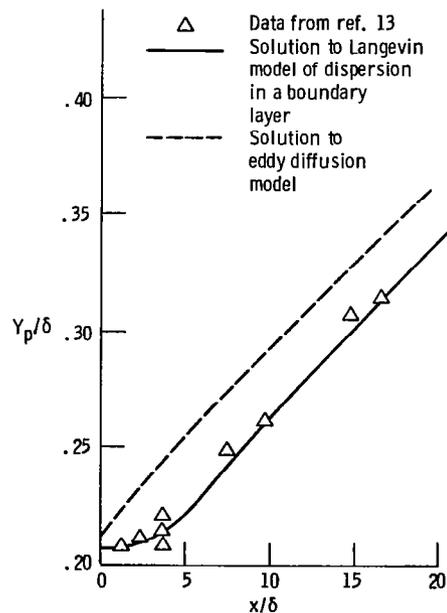
Figure IV-2. - Behavior of plume moment with distance downstream of elevated source in turbulent boundary layer. Distances are normalized by boundary layer thickness δ.

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This is illustrated in figure IV-1 by a comparison of the expression for $\overline{Y}_1$ with the diffusion result $\overline{Y} = \sigma_v^2 T_L' t$.

Shown in figure IV-2 is a numerical solution given in reference 12 of a model like equation (IV-19) for $\overline{Y}(x)$ (actually, for $Y_p(x)$, see eq. (III-51) et seq.) in a turbulent boundary layer; for comparison, data from reference 14 are included. Here downstream distance x plays the role of t in the preceding. In both theory and experiment, $d\overline{Y}/dx$ initially is zero and $\overline{Y}(x)$ only gradually becomes parallel to the eddy diffusion asymptote shown by the dashed line.

Next consider the mean squared value of Y: it will be shown that $\overline{Y^2}$ is unaltered to order ϵ. Since $\overline{Y^2} = \overline{Y_0^2} + \epsilon \overline{Y_1 Y_0} + O(\epsilon^2)$ and

$$\overline{Y_0 Y_1} = \iint_0^t \overline{V_0(t')V_1(t'')}\, dt'\, dt''$$

we need only show that $\overline{V_0(t')V_1(t'')} = 0$. When $t' > t''$, multiply equation (IV-22) by $V_1(t'')$ to find

$$\frac{d\overline{V_0(t')V_1(t'')}}{dt'} = -\frac{\overline{V_0(t')V_1(t'')}}{T_L}$$

and when $t' < t''$, multiply equation (IV-23) by $V_0(t')$ to find

$$\frac{d\overline{V_0(t')V_1(t'')}}{dt''} = -\frac{\overline{V_0(t')V_1(t'')}}{T_L} + \frac{T_L'}{2T_L^2}\frac{d\overline{Y_0^2(t'')V_0(t')}}{dt''}$$

That $\overline{Y_0^2(t'')V_0(t')} \equiv 0$ is clear from symmetry: Y_0^2 is symmetric with respect to reversal of the sign of W_t in equation (IV-22), while V_0 is antisymmetric. However, the processes W_t and $-W_t$ are equally likely, so $\overline{Y_0^2(t'')V_0(t')} = 0$. It now follows that $\overline{V_0(t')V_1(t'')} = \overline{V_0(\tau)V_1(\tau)}$ $\exp(-|t' - t''|)$, where $\tau = \min(t',t'')$. But it also can now be seen that, when $t' = t'' = \tau$,

$$\frac{d\,\overline{V_1(\tau)V_0(\tau)}}{d\tau} = -\frac{\overline{V_1(\tau)V_0(\tau)}}{T_L}$$

Since $V_1(0) = 0$, $\overline{V_1(\tau)V_0(\tau)} = 0$ and consequently $\overline{V_0(t')V_1(t'')} = 0$ – as was to be shown.

The asymptotic moments for which the lowest order terms were given are

$$\overline{Y} = \epsilon\overline{Y}_1 + O(\epsilon^3)$$

$$\overline{Y^2} = \overline{Y_0^2} + O(\epsilon^2)$$

Note, however, that to this order Y is not Gaussian distributed. This is the case because the right side of equation (IV-23) is a nonlinear function of Gaussian random variables.

Asymptotic Behavior of Langevin Model for Nonhomogeneous Turbulence

In studies of turbulent dispersion the eddy diffusion model has repeatedly been shown to be a good model where it is valid; that is, when in some sense $t \gg T_L$. The two comparisons between eddy diffusion and data for wall sources in chapter III support this observation. However, eddy diffusion generally is not valid at times that are short compared with T_L; figure IV-2 illustrates this. On the other hand, the discussion leading to the Langevin model was based only on an assumption of high turbulence Reynolds number; no restrictions were made on time. Therefore the Langevin model is uniformly valid in time.

Because the eddy diffusion model agrees well with those experimental data to which it is applicable, our confidence in the Langevin model will be bolstered if it can be shown that this model reduces asymptotically to eddy diffusion when $t \gg T_L$. If this can be shown, then eddy diffusion will be seen to be a special case of a high-Reynolds-number model. The Langevin model also will then seem to be the natural extension of eddy diffusion to the many situations where the latter is unsuitable.

For the purpose of examining the asymptotic behavior of the Langevin model of dispersion in nonhomogeneous turbulence, we again consider the case of a slowly varying medium. Thus we consider the asymptotic behavior of equations (IV-22) and (IV-23) as $t/T_L \to \infty$. This asymptote can be obtained conveniently by letting $T_L \to 0$. In the appendix to this chapter it is shown that the asymptotic behavior of equations (IV-22) and (IV-23) is obtained formally by equating the right sides of these equations to zero. By doing so and substituting $dY = V\,dt$, they become

$$dY_0 = \sqrt{2T_L}\,\sigma_v\,dW_t \qquad\qquad (IV-27a)$$

$$dY_1 = \frac{T_L'}{2T_L}\,dY_0^2 - \frac{\sigma_v T_L'}{\sqrt{2T_L}}\,Y_0\,dW_t \qquad\qquad (IV-27b)$$

Here it is necessary that $Y_0 V_0 \, dt = dY_0^2/2$ be substituted into equation (IV-23) before the asymptotic limit is taken.

The solution to equation (IV-27b) subject to $Y_0(0) = 0$ is

$$Y_0 = \sqrt{2T_L} \; \sigma_v W_t \qquad \text{(IV-28)}$$

Hence $\overline{Y_0^2} = 2T_L \sigma_v^2 t$, in agreement with the equation above equation (IV-10). When we substitute equation (IV-28), the equation for Y_1 becomes

$$dY_1 = \sigma_v^2 T_L' \; dW_t^2 - \sigma_v^2 T_L' W_t \; dW_t$$

$$= \frac{\sigma_v^2}{2} T_L' \; d\left(W_t^2 + t\right)$$

where Ito's theorem is used to write $W_t \, dW_t = \left(dW_t^2 - dt\right)/2$. Hence

$$Y_1 = \frac{\sigma_v^2}{2} T_L' \left(W_t^2 + t\right) \qquad \text{(IV-29)}$$

Averaging gives $\overline{Y_1} = \sigma_v^2 T_L' t$, in agreement with equation (IV-26). Also $\overline{Y_0 Y_1} = 0$ (since $\overline{W_t^3} = \overline{W_t} = 0$), as was shown to be true generally for equations (IV-22) and (IV-23).

Since $Y = Y_0 + \epsilon Y_1 + \ldots$, if equations (IV-28) and (IV-29) are added and the result differentiated, we find

$$dY = \epsilon \sigma_v^2 T_L' \; dt + \sigma_v \left(\sqrt{2T_L} + \epsilon T_L' W_t \right) dW_t + 0(\epsilon^2)$$

$$= \epsilon \sigma_v^2 T_L' \; dt + \sigma_v \left(\sqrt{2T_L} + \frac{\epsilon T_L'}{\sqrt{2T_L}} Y_0 \right) dW_t + 0(\epsilon^2) \qquad \text{(IV-30)}$$

But

$$\sqrt{2T_L(\epsilon y)} = \sqrt{2T_L(0)} + \frac{\epsilon T_L'(0)}{\sqrt{2T_L(0)}} Y_0 + 0(\epsilon^2)$$

which is the bracketed expression in equation (IV-30). Hence to order ϵ^2 equation (IV-30) can be written

$$dY = \sigma_v^2 T_L'[Y(t)]dt + \sqrt{\sigma_v^2 T_L[Y(t)]} dW_t \qquad \text{(IV-31)}$$

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This is just equation (III-1) for the eddy diffusivity

$$K = \sigma_v^2 T_L(y) \qquad \text{(IV-32)}$$

Thus we have achieved our objective of showing that the Langevin model (IV-19) tends asymptotically to the eddy diffusion model (III-1). It follows that the Langevin model is a plausible extension of eddy diffusion to dispersion with finite time scale. Of course, our demonstration was limited to the case of slowly varying T_L and was carried out only to order ϵ; reference 19 carries out the demonstration to order ϵ^2 and also shows that the asymptote (IV-31) is generally correct.

Case with Variable σ_v

In equation (IV-19) σ_v was taken to be constant, but it was promised that later σ_v would be allowed to be a function of y. We now have a criterion for determining the form equation (IV-19) takes when σ_v is a function of y: the model (IV-19) must tend asymptotically to the diffusion model (IV-31) when $T_L \rightarrow 0$.

It can be seen by following the procedure just used to derive equation (IV-31) that the form (IV-19) is not correct if σ_v is a function of y. However, since σ_v is constant there, that equation may be divided by σ_v^2 and written

$$d\left(\frac{V}{\sigma_v^2}\right) = -\frac{V}{\sigma_v^2 T_L} \, dt + \sqrt{\frac{2}{\sigma_v^2 T_L}} \, dW_t$$

In this form $\sigma_v^2 T_L$ plays the role that T_L played in equation (IV-19), and it can be shown that equation (IV-31) follows (ref. 19). Hence, for variable σ_v an appropriate Langevin model is[2]

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[2]Since writing this report I have been told that Legg and Raupach (to appear in Boundary Layer Meteorology) use

$$dV = -\frac{V}{T_L} \, dt + \sigma_v \sqrt{\frac{2}{T_L}} \, dW_t + \frac{d\sigma_v^2}{dy} \, dt$$

to obtain the correct asymptotic behavior when σ_v is variable. Both this and equation (IV-33) are incorrect when the turbulence is homogeneous but nonstationary [$\sigma_v(t)$].
    The equation

$$d(V/\sigma_v) = -\frac{V}{\sigma_v T_L} \, dt + \sqrt{\frac{2}{T_L}} \, dW_t + \frac{\partial \sigma_v}{\partial y} \, dt$$

appears to be correct for nonhomogeneous and nonstationary turbulence. Clearly the issue is not finally resolved.

$$d\left[\frac{V}{\sigma_v^2}(Y)\right] = -\frac{V}{K(Y)}\,dt + \sqrt{\frac{2}{K(Y)}}\,dW_t \qquad (IV\text{-}33)$$

where $K(y) = \sigma_v^2(y)T_L(y)$.

An analysis of this model can be carried out for a slowly varying medium, as was done for the case with varying time scale. Define $\mathscr{V}(t)$ by

$$\mathscr{V}(t) = \frac{V(t)}{\sigma_v^2[Y(t)]} \qquad (IV\text{-}34)$$

and expand

$$\mathscr{V}(t) = \mathscr{V}_0(t) + \epsilon\,\mathscr{V}_1(t) \cdots$$

$$\sigma_v^2 = \sigma_v^2(0) + 2\epsilon\sigma_v(0)\sigma_v'(0)Y_0 \cdots$$

with Y and T_L expanded as before in equations (IV-20) and (IV-21). Again Y_0 is the solution to the constant-coefficient Langevin model. Its variance is given by equation (IV-24) with T_L and σ_v^2 evaluated at $y = 0$.

To order ϵ we now have

$$\frac{d\overline{\mathscr{V}_1}}{dt} = -\frac{\overline{\mathscr{V}_1}}{T_L} + \frac{T_L'}{2T_L^2}\frac{d\overline{Y_0^2}}{dt} \qquad (IV\text{-}35)$$

for the mean value of $\mathscr{V}_1$ (see equation following eq. (IV-24)). Because of the definition (IV-34), $dY = \sigma_v^2(Y)\mathscr{V}\,dt$. Hence

$$dY_1 = \left(\sigma_v^2\mathscr{V}_1 + 2\sigma_v\sigma_v'\mathscr{V}_0 Y_0\right)dt$$

and

$$\frac{d\overline{Y_1}}{dt} = \sigma_v^2\overline{\mathscr{V}_1} + \frac{\sigma_v'}{\sigma_v}\frac{d\overline{Y_0^2}}{dt} \qquad (IV\text{-}36)$$

it being understood that σ_v is evaluated at $y = 0$. The factor $\sigma_v^2\overline{\mathscr{V}_1}$ in equation (IV-36) is given by equation (IV-25). However, an additional term associated with the inhomogeneity of σ_v appears in equation (IV-36). Upon substituting equations (IV-24) and (IV-25), equation (IV-36) can be integrated, subject to $Y_1(0) = 0$. Thus it is found that

$$\overline{Y}_1 = \left(\sigma_v^2 T_L\right)' T_L\left(\frac{t}{T_L} - 1 + e^{-t/T_L}\right) + \sigma_v^2 T_L T_L'\left(e^{-t/T_L} - 1 + \frac{t}{T_L}e^{-t/T_L}\right) \qquad (IV\text{-}37)$$

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By design, when $t \gg T_L$ this reproduces equation (IV-26) with the eddy diffusivity $K = \sigma_v^2 T_L$. As $t/T_L \to 0$, $\overline{Y}_1 \to \left(\sigma_v^2\right)' t^2/2$. Thus at short times the mean drift is due to variation of σ_v^2 and not to variation of T_L; the variation of T_L enters at order t^3/T_L^3.

Perhaps this discussion of the Langevin model for nonhomogeneous dispersion should conclude with the observation that this model has not been widely exploited. It seems a promising model for many problems involving dispersion with a finite time scale.

APPENDIX: ASYMPTOTE OF LANGEVIN EQUATION

Derivations of the asymptotic behavior of the Langevin equation are available in references 20 and 6. Essentially, a derivation is as follows: Since T_L is constant in equation (IV-1), it can be integrated as

$$V(t) = V(0) e^{-t/T_L} + \int_0^t e^{(t'-t)/T_L} \sigma_V \sqrt{\frac{2}{T_L}} \, dW_{t'} \qquad \text{(IV-A1)}$$

Because we are taking the limit $t/T_L \rightarrow \infty$, the first term can be dropped. Then

$$Y(t) = \int_0^t V(t') \, dt'$$

$$= \int_0^t \int_0^{t'} \frac{e^{(t''-t')/T_L}}{T_L} \sigma_V \sqrt{2T_L} \, dW_{t''} \, dt' \qquad \text{(IV-A2)}$$

As $T_L \rightarrow 0$

$$\frac{e^{-|t'-t''|/T_L}}{T_L} \rightarrow \delta(t' - t'')$$

so equation (IV-A2) tends to

$$Y(t) = \int_0^t \sigma_V \sqrt{2T_L} \, dW_{t'}$$

or

$$dY(t) = \sigma_V \sqrt{2T_L} \, dW_t \qquad \text{(IV-A3)}$$

Equation (IV-A3) is called the Smoluchowsky equation[3]. Equation (IV-22) is

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[3] A simpler and more rigorous derivation of $Y(t) \rightarrow \sigma_V \sqrt{2T_L} W_t$ as $t/T_L \rightarrow \infty$ makes use of theorem 1, p. 8 of ref. 4. That theorem says that any continuous stochastic process $X(t)$ that is independent of future events and has $\overline{X(t) - X(t')} = 0$ and $[X(t) - X(t')]^2 = t - t'$ $(t > t')$ for arbitrary t, t' is a Wiener process. But if $X(t) = Y(t)/\sigma_V \sqrt{2T_L}$ with $Y(t)$ the solution to the Langevin equation, the properties of $Y(t)$ derived in the text (eqs. (IV-9) and (IV-12) show that, as $t/T_L \rightarrow \infty$, $X(t)$ has the required properties.

the same equation as equation (IV-1), so equation (IV-27a) follows immediately, while equation (IV-23) can be integrated as

$$V_1(t) = \int_0^t e^{(t'-t)/T_L} \left[\frac{T_L'}{2T_L^2} \, dY_0^2(t') - \frac{\sigma_v T_L'}{\sqrt{2} \, T_L^{3/2}} \, Y_0(t') dW_{t'} \right] \quad (IV\text{-}A4)$$

and equation (IV-27b) can be obtained by the argument leading to equation (IV-A3). Note that V_0 does not have a proper asymptote. (Its asymptote is **not** $\sigma_v \sqrt{2T_L} \, dW_t/dt$, as one might suggest from equation (IV-A3), for it was shown in the text after equation (IV-1) that V_0 is statistically stationary with variance σ_v^2, while $\overline{(\sigma_v \sqrt{2T_L} \, dW_t/dt)^2} = 2\sigma_v^2 T_L/dt$.) This is why it was necessary to write $Y_0 V_0 \, dt$ as $dY_0^2/2$ before taking the asymptotic limit of equation (IV-A4).

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15. Supplementary Notes

16. Abstract

This report introduces aspects of the theory of continuous stochastic processes that seem to contribute to an understanding of turbulent dispersion. It is expected that the reader has a knowledge of basic probability theory and some exposure to turbulence theory and the phenomena of turbulent transport. The report is addressed to researchers in the subject of turbulent transport, especially those with an interest in stochastic modeling. However, the material presented herein deals with the theory and philosophy of modeling, rather than treating specific practical applications. The book by Csanady (ref. 1) is a good place to begin an exploration of applications, as well as to obtain a background to the contents of the present report.

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