LA-UR -82-3240

Conf-830307--5

LA-UR--82-3240

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SUBMITTED TO: American Meteorological Society
Sixth Symposium on Turbulence and Diffusion
Boston, MA
March 22-25, 1983

SUPPORTED BY: United States Army Atmospheric Sciences Laboratory
White Sands Missile Range, New Mexico 88002
Contract Monitor: William Ohmstede

AND

U. S. Department of Energy

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EULERIAN-LAGRANGIAN RELATIONSHIPS IN MONTE CARLO SIMULATIONS OF TURBULENT DIFFUSION*

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1. INTRODUCTION

Monte Carlo techniques have been used in a number of studies to simulate turbulent diffusion in the atmosphere. In these studies the Lagrangian velocity autocorrelation function was used to calculate the trajectories of a large number of tracer particles through a turbulent flow field. One difficulty in applying this method is determining the Lagrangian integral time scale, especially for nonhomogeneous flows such as the planetary boundary layer. Scaling relationships and theoretical results have been used to relate the Lagrangian time scale to the local Eulerian properties of the turbulence which can be measured directly.

In this paper we present a Monte Carlo technique which uses the Eulerian space-time velocity autocorrelation function to calculate particle trajectories. This method is shown to be equivalent to the Lagrangian approach in homogeneous turbulence, and its extension to nonhomogeneous conditions appears to be straightforward. We also derive an analytic relationship between the Lagrangian time scale and the Eulerian space and time scales.

2. THEORETICAL ANALYSIS

We consider one-dimensional diffusion in a stationary, homogeneous field of turbulence. A typical particle trajectory is illustrated schematically in Fig. 1 where t is the time after release of the particle, y is the cross-wind coordinate, and v is the cross wind component of the turbulent velocity. A large number of particle trajectories are used to calculate particle displacement statistics such as $\overline{y^2}(t)$, where the overbar denotes an ensemble average.

In the Lagrangian approach particle trajectories are calculated in a step by step manner using the relations

$$\Delta y = v(t)\delta t \qquad (1)$$

$$v(t + \delta t) = v(t)\, R_L(\delta t) + v' \qquad (2)$$

*This work was supported by the U.S. Army Atmospheric Sciences Laboratory and the U.S. Dept. of Energy. We gratefully acknowledge useful discussions with Sumner Barr, Frank Gifford, and William Clements.

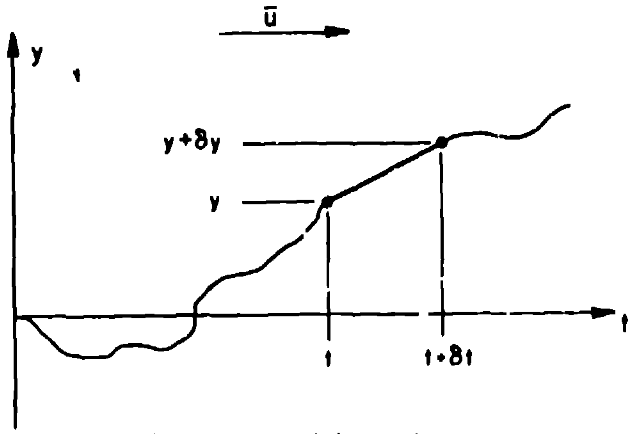

Fig. 1. Particle Trajectory

where R_L is the Lagrangian velocity autocorrelation function which depends only on the time separation τ, $R_L(\tau) = \overline{v(t)v(t+\tau)}/\overline{v^2}$. This definition of $R_L(\tau)$ is valid for arbitrary values of τ, but Eq. (1) is valid only for a small time step δt. The velocity v' is a normal random variable which is statistically independent of $v(t)$. The mean of v' is zero, and the variance must satisfy the relation

$$\overline{v'^2} = \overline{v^2}\,(1 - R_L^2(\delta t)) \qquad (3)$$

In order for the variance of the particle velocities to equal the field variance $\overline{v^2}$. The Markov process defined by Eq. (2) produces an exponential autocorrelation function, $R_L(\tau) = \exp(-\tau/t_L)$, where t_L is the Lagrangian integral time scale. This process converges to a solution that is independent of the step size δt for $\delta t \ll t_L$. The numerical result for the mean square particle displacement $\overline{y^2}(t)$ for a point source agrees with the classical Taylor (1921) diffusion result for an exponential autocorrelation function as shown by Hanna (1979). A method for analyzing a finite size, finite duration source is presented in a companion paper, Lee and Stone (1983).

Since the Eulerian and Lagrangian statistical properties of the turbulent field contain the same information, particle trajectories can also be calculated using the Eulerian statistics. In the first part of our analysis we use an Eulerian reference frame which moves with the mean wind speed $\bar{u}$. This will be referred to as the convective reference frame and will be denoted by the subscript C. To calculate the particle trajectories in this reference frame, Eq. (2) is replaced by the relation

$$v(t + \delta t) = v(t)\, R_C(\delta y, \delta t) + v' \qquad (4)$$

where R_C is the Eulerian space-time velocity autocorrelation function in the convective reference frame. It depends only on the spatial separation ζ and the time separation τ, $R_C(\zeta,\tau) = \overline{v(y,t)v(y + \zeta, t + \tau)}/\overline{v^2}$. In Eq. (4) $R_C(\delta y, \delta t)$ is coupled to $v(t)$ since $\delta y = v(t)\delta t$ from Eq. (1).

A relation between $R_L(\delta t)$ and $R_C(\delta y,\delta t)$ can be obtained by multiplying Eqs. (2) and (4) by $v(t)$, taking the ensemble average, and equating the resulting right hand sides of the equations. This relation, which is valid only for a time step $\delta t << t_L$, can be written as

$$R_L(\delta t) = \overline{v^2(t) R_C(\delta y = v(t)\delta t, \delta t)}/\overline{v^2} \qquad (5)$$

The ensemble average in Eq. (5) can be evaluated if the probability density function for v and the functional form of $R_C(\zeta,\tau)$ are known. We assume that v is a normally distributed random variable with a zero mean and a standard deviation of $\sigma_v = (\overline{v^2})^{1/2}$. In our analysis it is convenient to let $v = \sigma_v u$ where u is a random variable with $\bar{u} = 0$, $\overline{u^2} = 1$, and a probability density function $P(u) = (2\pi)^{-1/2} \exp(-u^2/2)$. Since the use of Eq. (2) produces an exponential for $R_L(\tau)$ it seems likely that Eq. (4) will produce an exponential for $R_C(\zeta,\tau)$. We have verified this by numerical Monte Carlo experiments. Our results show that the Eulerian approach converges to a solution that is independent of the step size δt only if R_C is of the form $R_C(\zeta,\tau) = \exp(-|\zeta|/L)\exp(-\tau/t_E)$ where L and t_C are the Eulerian integral length and time scales in the convective reference frame. Using these expressions for v and R_C, Eq. (5) can be written as an integral relation

$$R_L(\delta t) = (2/\pi)^{1/2} \exp(-\delta t/t_C) \int_0^\infty u^2 e^{-au} e^{-u^2/2}\, du \qquad (6)$$

where the parameter a is defined by $a = \sigma_v \delta t/L$.

The integral in Eq. (6) depends only on the parameter a. It can be evaluated to obtain R_L as a function of δt, σ_v, L, and t_C for $\delta t << t_L$. However, a more general and useful result can be obtained by noting that, for an exponential autocorrelation function, t_L can be obtained from the relation, Gifford (1982),

$$1/t_L = \lim_{\delta t \to 0} [(1 - R_L(\delta t))/\delta t] \qquad (7)$$

The limiting value of R_L as $\delta t \to 0$ can be obtained by expanding the exponentials $\exp(-\delta t/t_C)$ and $\exp(-au)$ in Eq. (6) for small values of δt. This gives a series of integrals which can be evaluated analytically. Substituting the resulting expression into Eq. (7) provides the desired relation between the Lagrangian and convective integral scales

$$1/t_L = (1/t_C) + (8/\pi)^{1/2}\, \sigma_v/L \qquad (8)$$

It is useful to express Eq. (8) in terms of the Eulerian parameter $\alpha = \sigma_v t_C/L$ since this parameter has been used in previous studies of Eulerian-Lagrangian relations, e.g., Philip (1967) and Baldwin and Johnson (1972). The result is

$$t_L/t_C = 1/(1 + (8/\pi)^{1/2}\, \alpha) \qquad (9)$$

A priori α is expected to be of order unity, and for $\alpha = 1$, $t_L/t_C = 0.39$.

The statistical properties of turbulence are normally measured in a fixed-frame Eulerian coordinate system which we will denote by the subscript E. Since t_C cannot be easily measured, it is useful to relate t_C to t_E. This can be done by noting that the structure of homogeneous isotropic turbulence is invariant under a uniform translation of the coordinate system. Therefore, the three-dimensional Eulerian autocorrelation functions R_E and R_C are related by the transformation

$$R_E(\delta x, \delta y, \delta z, \delta t) = R_C(\delta X = \delta x - \bar{u}\delta t, \delta y, \delta z, \delta t) \qquad (10)$$

where $\bar{u}$ is the mean wind speed and x and X are the mean-wind coordinates in the fixed and convective reference frames, respectively. We assume that R_C varies exponentially in δX for consistency with the exponential variation in δy in the above analysis, i.e.

$$R_C(\delta X, \delta y, 0, \delta t) = \exp(-(|\delta X| + |\delta y|)/L)\exp(-\delta t/t_E) \qquad (11)$$

Using Eqs. (10) and (11), the temporal variation of R_E can be expressed as $R_E(0,0,0,\delta t) = \exp(-\bar{u}\delta t/L)\exp(-\delta t/t_C)$. The temporal variation of R_E can also be expressed as $R_E(0,0,0,\delta t) = \exp(-\delta t/t_E)$. Equating these two expressions leads to

$$1/t_E = (1/t_C) + (\bar{u}/L) \qquad (12)$$

Eq. (12) can also be expressed in terms of the parameter α

$$t_C/t_E = 1 + (\alpha/i) \qquad (13)$$

where i is the turbulence intensity, $i = \sigma_v/\bar{u}$. For low turbulence intensity, $i \approx 0.1$, t_C is an order of magnitude larger than t_E.

The assumption that R_C varies exponentially in δX and δy with a single length scale L violates the Karman and Howarth (1938) relation for the spatial variation of the autocorrelation function in three-dimensional homogeneous isotropic turbulence. However, Eqs. (9) and (13) agree very closely with more exact calculations which use the Karman and Howarth relation as will be discussed in Section 3.

An equation for $\beta = t_L/t_E$ can be obtained by eliminating t_C from Eqs. (8) and (12) resulting in

$$\beta = [1 - (\bar{u}t_E/L)(1 - (8/\pi)^{1/2}\, i)]^{-1} \qquad (14)$$

Since the length scale L is the same in the fixed and the convective reference frames, Eq. (14) provides a relation for calculating t_L if the Eulerian parameters t_E, L, and i are known. This result can be expressed in terms of α by multiplying Eq. (9) by Eq. (13)

$$\beta = [1 + (\alpha/i)]/[1 + (8/\pi)^{1/2}\alpha] \qquad (15)$$

For $\alpha \approx 1$ and $i << 1$ Eq. (15) reduces to $\beta \approx C/i$ where the constant $C = \alpha/(1 + (8/\pi)^{1/2}\alpha)$. For $\alpha = 1$, $C = 0.39$ which is within the range of theoretical estimates summarized by Pasquill (1974) in which the "constant" C ranges from 0.15 to 0.8.

The direct measurement of L is not easy since it requires an array of anemometers along a line that has a fixed orientation relative to the mean wind. Therefore, the Taylor or frozen turbulence hypothesis is frequently used to determine L. In this approximation it is assumed that the structure of the turbulence in the convective reference frame is frozen in time and is convected with the mean wind speed $\bar{u}$. This leads to $L = \bar{u}t_E$ and permits L to be estimated from a single fixed-point Eulerian measurement of t_E. Substitution of this approximation into Eq. (12) leads to $t_C = \infty$ and, therefore, the convective autocorrelation function R_C is independent of δt. Setting $L = \bar{u}t_E$ in Eq. (14) results in $\beta = 0.61/i$, which is also within the range of theoretical results summarized by Pasquill (1974).

Additional insight into the Taylor hypothesis can be obtained by expressing $L/\bar{u}t_E$ in terms of the parameters α and i. Using Eq. (11) and the definitions of α and i we obtain

$$L/\bar{u}t_E = 1 + (1/\alpha) \qquad (16)$$

It is seen that $1/\alpha << 1$ is a necessary condition for assuming $L \approx \bar{u}t_E$. Using $\alpha \approx 1$ in Eq. (16) may provide a better way of estimating L if t_E and i are known, but this is not certain! Although α is of order unity, it may vary significantly for different flow fields.

3. COMPARISONS TO MONTE CARLO SIMULATIONS AND OTHER THEORIES

The analytic results presented in Section 2 were derived from the hypothesis that valid Monte Carlo simulations of turbulent diffusion can be formulated in either the Lagrangian or the Eulerian reference frame. More specifically, we have assumed that either Eq. (2) or Eq. (4) can be used in these simulations. In order to verify this hypothesis and the analytic results we have conducted extensive Monte Carlo simulations using both the Lagrangian and the Eulerian approach. Typical results are presented here.

In both approaches the variance of the random velocity v' must be related to $R_L(\delta t)$ as shown in Eq. (3). Therefore, in the Eulerian approach $R_L(\delta t)$ must be calculated at each time step for the specified values of t_C, L, and σ_v. This can be done using Eq. (5) by numerically calculating the ensemble average at each time step. It can be done more easily using the relation $R_L(\delta t) = \exp(-\delta t/t_L)$ where t_L is related to t_C, L, and σ_v by Eq. (8). As a consistency check we performed the calculations both ways, and the results were the same.

The standard deviation of the particle displacements, $\sigma_y = (\overline{y^2})^{1/2}$, is shown in Fig. 2. The solid curve was obtained from the Taylor (1921) integral equation using an exponential Lagrangian autocorrelation function, $R_L = \exp(-t/t_L)$. This result can be expressed as

$$\sigma_y/(2^{1/2}\sigma_v t_L) = [(t/t_L) - 1 + \exp(-t/t_L)]^{1/2} \qquad (17)$$

The symbols are numerical results that were calculated in the convective reference frame as a function of t for specified values of t_E, L, and σ_v. Ensemble averages were obtained by averaging over 10,000 particle trajectories. The Lagrangian integral time scale t_L was calculated

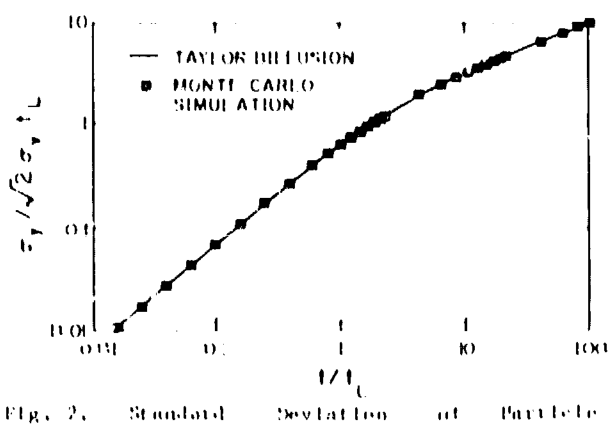

Fig. 2. Standard Deviation of Particle Displacements

numerically using the velocities along these trajectories. This value of t_L was used to normalize t and σ_y for direct comparison to Eq. (17). It is seen that the numerical results reproduce the Taylor diffusion curve very well. Since the Taylor curve is an exact solution in the Lagrangian reference frame, this comparison demonstrates the validity of the Eulerian Monte Carlo approach.

A comparison of analytic and Monte Carlo results for the autocorrelation function is presented in Fig. 3. An exponential autocorrelation function was used as input in the Monte Carlo calculations, $R_C(\zeta,\tau) = \exp(-|\zeta|/L)\exp(-\tau/t_C)$, and the solid curve shows the temporal variation of this function for $\zeta = 0$. The values used for the input parameters t_C, L, and σ_v result in a value of $\alpha = 0.91$. The square symbols are calculated values of R_L in which 10,000 particle trajectories were used to evaluate the ensemble averages. The dashed curve is the analytic solution for R_L which, using Eq. (9), can be written as $R_L = \exp(-\tau/t_L) = \exp[(-\tau/t_C)(1 + (8/\pi)^{1/2}\alpha)]$. This can also be expressed as $R_L = R_C(\zeta = (8/\pi)^{1/2}\sigma_v\tau,\tau)$ which shows that R_L drops off more rapidly in time than R_C because the "average" value of the particle displacement is $\zeta = (8/\pi)^{1/2}\sigma_v\tau$. The analytic and numerical results are almost identical. Equally good agreement was obtained over a large range of values of α, $0.1 < \alpha < 6.4$, by varying the input values of t_C, L, and σ_v.

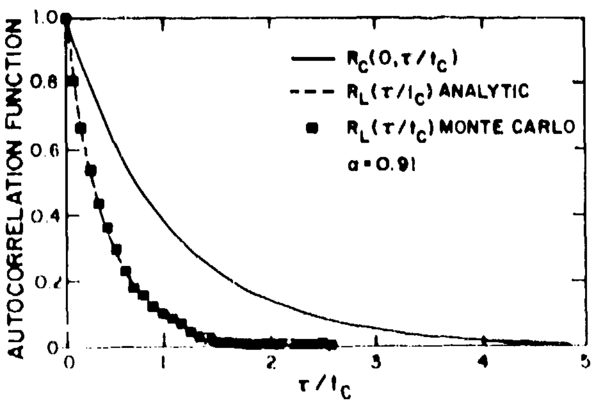

Fig. 3. Autocorrelation Functions

A comparison of the ratio of the Lagrangian to the convective integral time scales is shown in Fig. 4 as a function of the Eulerian parameter α. The solid curve is the analytic result from Eq. (9), and the square symbols are the Monte Carlo results. The dashed curve will be discussed later. The close agreement of the results in Figs. 3 and 4 demonstrate consistency between the analytic results in Section 2 and the numerical Monte Carlo simulations using Eq. (6).

There is a large body of literature on Eulerian Lagrangian relationships. Summaries of this work can be found, for example, in Pasquill (1974), and the general mathematical nature of the problem is discussed by Lumley (1962). It seems to be generally accepted that there is no exact theoretical relationship between the Lagrangian and Eulerian statistics. However, there are a large number of approximate and semi

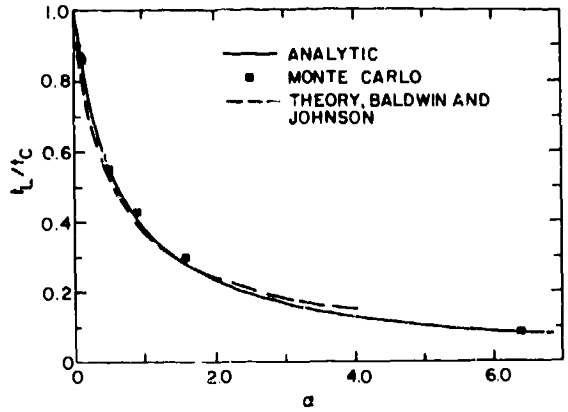

Fig. 4. Ratio of Lagrangian to Convective Time Scales

empirical relations for first order statistical properties such as the velocity autocorrelation function and the corresponding integral scales. One of the more useful theoretical approaches is the independence hypothesis suggested by Corrsin (1959) in which the Lagrangian autocorrelation function is related to the Eulerian convective space-time autocorrelation function by properly weighting the latter to account for the spatial distribution of diffusing particles. This general approach was used by Philip (1967) and Saffman (1963) to relate $R_L(\tau)$ to $R_C(\zeta,\tau)$. Philip's analysis has been extended and improved by Baldwin and Johnson (1972) who also provide an excellent survey and evaluation of existing theories and data. It seems appropriate to evaluate our analytic solutions by comparison to the theory of Baldwin and Johnson since their results represent the most detailed and complete application of Corrsin's independence hypothesis. Their results are also in general agreement with many other theories and experiments. Experimental studies are being conducted by Li and Meroney (1982) to further verify Baldwin and Johnson's theory, and their initial data are in close agreement with the theory.

Baldwin and Johnson's results for t_L/t_C are compared to our analytic results in Fig. 4. A comparison of t_L/t_E is shown as a function of the parameter α/β in Fig. 5. The parameter $\beta = t_L/t_E$ is compared in Fig. 6 as a function of β for a range of values of α. The very close agreement between these two theories is remarkable, especially since Baldwin and Johnson use the exact form of the Karman and Howarth (1938) relation for the three-dimensional spatial variation of R_C. They also use the best available experimental data to specify the temporal variation of R_C. This agreement may be partially fortuitous, but it also illustrates the value of the Eulerian Monte Carlo approach to turbulent diffusion. This approach is equivalent to the Lagrangian Monte Carlo approach and to the random force theory used by Gifford (1982) and by Lee and Stone (1983). Therefore, the close agreement with the theory of Baldwin and Johnson further establishes the usefulness of the random force theory.

4. CONCLUSIONS

The results of this study show that Monte Carlo simulations of diffusion in homogeneous turbulence can be formulated in terms of the Eulerian space-time velocity autocorrelation function. Numerical results obtained using this approach agree with results obtained by Taylor (1921) using the Lagrangian autocorrelation function. We have used the equivalence of the Lagrangian and Eulerian Monte Carlo approaches to derive analytic relations between the Lagrangian integral time scale and the Eulerian integral space and time scales. These analytic results have been verified by comparison to Monte Carlo simulations and to other theoretical results. They are in general agreement with many existing theories and semi-empirical relations.

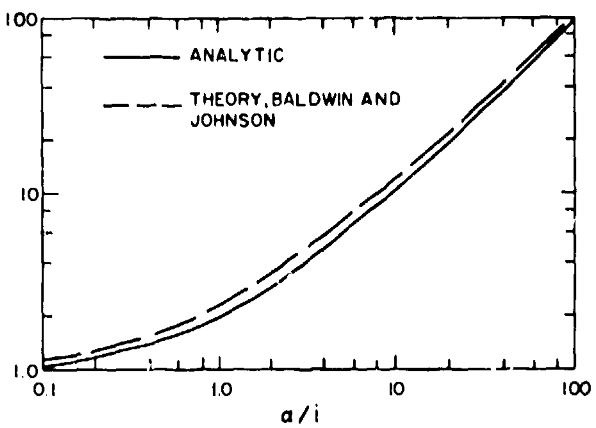

Fig. 5. Ratio of Convective to Fixed-Frame Eulerian Time Scales

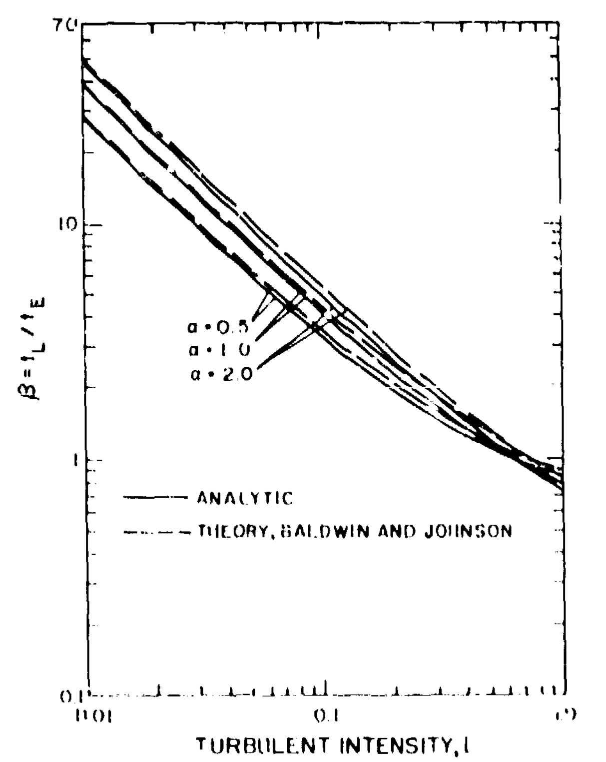

Fig. 6. Ratio of Lagrangian to Fixed-Frame Eulerian Time Scales

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