LA-UR -82-3034

Conf-830307--4



LA-UR--82-3034

DE83 003479

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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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THE USE OF EULERIAN INITIAL CONDITIONS IN A LAGRANGIAN MODEL OF TURBULENT DIFFUSION*

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## 1. INTRODUCTION

Gifford (1982a,b) has shown that the random-force theory of turbulent diffusion describes many features of horizontal diffusion in the atmosphere. In this theory Langevin's equation is used to calculate trajectories of tracer particles through a field of homogeneous turbulence. The statistics of a large number of these particles are used to describe the diffusion of puffs and plumes. Gifford analyzed single-particle diffusion from a point source. He accounted for relative diffusion by using conditioned initial velocities for the particles, and his final results contain the effective source velocity as a free parameter.

In this paper we extend Gifford's analysis to clusters of particles from finite-size, finite-duration sources. We use the Eulerian space-time velocity autocorrelation function to describe the statistics of the particle initial velocities. Gifford's effective source velocity is replaced by two new parameters: the ratio of the source size to the Eulerian integral length scale and the ratio of the release time or sampling time to the Eulerian integral time scale.

## 2. THEORETICAL ANALYSIS

We consider diffusion in one space dimension y and time t. This is a reasonable approximation to horizontal diffusion in the atmosphere where t is the travel time downwind of the source. In our analysis y is the cross-wind coordinate and v is the cross-wind component of the turbulent velocity. Smith (1968) proposed that the turbulent velocity could be written as the sum of correlated and random components, $v(t + \tau) = v(t)R_L(\tau) + v'$, where $R_L$ is the Lagrangian autocorrelation function which depends only on the time separation $\tau$, $R_L(\tau) = \overline{v(t)v(t + \tau)}/\overline{v^2}$, and $v'$ is a random velocity. Overbars denote ensemble averages. Gifford (1982a) used this relation to derive a form of Langevin's equation

$$\frac{dv}{dt} + \beta v = \eta(t) \tag{1}$$

where $\eta(t)$ is the random acceleration. Gifford (1982b) showed that the Lagrangian autocorrelation function consistent with Eq. (1) is an exponential, $R_L = \exp(-\tau/t_L)$, for arbitrary values of the initial velocity $v_o$. The Lagrangian integral time scale is $t_L$ and $\beta = 1/t_L$. A general discussion of the application of Eq. (1) to turbulent diffusion can be found in Gifford's papers and the references therein. Smith's linear velocity relation has also been used in Monte Carlo simulations of turbulent diffusion. This numerical approach is equivalent to the use of Eq. (1).

In this study we consider the diffusion of particles released as one-dimensional clusters. These clusters can be used to construct a plume from a finite-size, finite-duration source as shown schematically in Fig. 1. The width of the source is d and the release time is $t_R$. This is a one-dimensional version of the familiar spreading-disk plume model in which the clusters contain material that is released sequentially from the source during small time increments, and axial diffusion is neglected. Each cluster is divided into an arbitrary number N of tracer particles or tagged elements of fluid. Each particle represents a fraction 1/N of the mass in one cluster.

The trajectory of each particle after its release is assumed to be governed by Eq. (1). The particle displacement y(t) can be found in the literature on Brownian motion, e.g. Uhlenbeck and Ornstein (1930), and is given by

$$y(t) = y_o + (v_o/\beta)(1-e^{-\beta t}) - \beta^{-1}e^{-\beta t}\int_o^t e^{\beta\xi}\eta(\xi)d\xi + \beta^{-1}\int_o^t \eta(\xi)d\xi \tag{2}$$

where $y_o$ and $v_o$ are the initial position and velocity of the particle, respectively. Expected values of the meandering of the plume centroid and the relative diffusion of particles about the plume centroid can be obtained by using Eq. (2) and averaging over an ensemble of plumes. The plume in Fig. 1 is one particular realization or trial in the ensemble. Each trial consists of M clusters containing N particles each, where M is a large number for all finite values of $t_R$ and $2 \le N \le \infty$. For a particular trial, averages at a fixed observation point $t = x/\bar{U}$ are obtained by averaging over the N particles in each cluster and over the M clusters in each trial as the

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

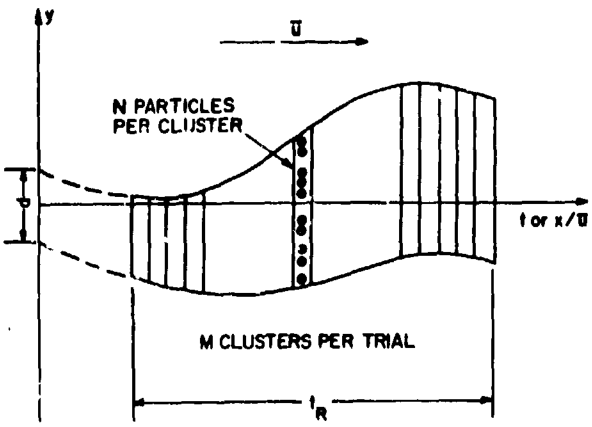


Fig. 1. Plume from a Finite-Size, Finite-Duration Source

clusters pass the observation point. Expected values are then obtained by averaging over the large number of trials which make up the ensemble. Solutions for the instantaneous release of a single puff, $t_R \to 0$, can be obtained by using only one cluster per trial, $M = 1$.

The most important aspect of this study is the treatment of the particle initial velocities $v_o$ in calculating the ensemble averages from Eq. (2). Since each particle is a tracer, its velocity is equal to the local value of the turbulent field velocity $v(y,t)$ during its entire trajectory. Therefore, we set $v_o$ equal to the turbulent field velocity at the source, i.e. $v_o = v(y_o, t_o)$ where $y_o$ is the initial spatial coordinate of the particle within a cluster and $t_o$ is the time at which the cluster is released from the source. The initial velocities in each cluster are spatially correlated over the source width d and the velocities from cluster to cluster are temporally correlated over the release time $t_R$. In our model this correlation of velocities is accomplished by use of the Eulerian space-time velocity autocorrelation function which depends only on the space separation $\zeta$ and the time separation $\tau$, $R_E(\zeta, \tau) = \overline{v(y,t)v(y+\zeta, t+\tau)}/\overline{v^2}$. The ensemble statistics of the initial velocities can be calculated for given values of d and $t_R$ if $R_E$ is known. We assume that $R_E$ can be represented by exponentials, $R_E = \exp(-|\zeta|/L)\exp(-\tau/t_E)$, where L and $t_E$ are the Eulerian integral length and time scales, respectively. The calculated values of the initial velocity statistics depend upon d/L and $t_R/t_E$.

This approximation for the particle initial velocities neglects many real source effects such as bouyancy and momentum of the source material and the aerodynamic interaction between the source and the ambient flow. We assume there is a transition region immediately downwind of the source within which the effluent comes into equilibrium with the turbulence in the atmosphere. The results of this theory apply downwind of the transition region, and the source size d should be regarded as the width of the plume at the end of the transition region.

In calculating ensemble averages as described above we assume that the random particle accelerations $\eta(t)$ are statistically independent for each particle trajectory. We account for inter-particle velocity correlations when we assign the particle initial velocities $v_o$, but we do not explicitly account for these inter-particle correlations when calculating the particle trajectories. This is quite different from the classical approach of Batchelor (1950) and Brier (1950), in which relative diffusion is described in terms of the two-particle Lagrangian velocity correlation function $R_{2L}(t,\tau) = \overline{v_1(t)v_2(t-\tau)}/\overline{v^2}$ where $v_1$ and $v_2$ are the velocities of two different particles and $0 \le \tau \le t$. Batchelor derived a kinematic relation for the mean-square separation of a pair of particles in terms of $R_L$ and $R_{2L}$. This relation is exact, but it is very difficult to apply since $R_{2L}$ is an unknown nonstationary function of t and $\tau$, even for stationary homogeneous turbulence. In two recent articles, Sawford (1982a, b) has used this approach to obtain numerical solutions for the relative diffusion of pairs and clusters of particles. His results are dependent upon the assumed form of $R_{2L}$. It is easily shown that our model produces a two-particle correlation function of the form $R_{2L}(t,\tau) = R_E(\delta y_o, 0)\exp(-t/t_L)\exp(-(t-\tau)/t_L)$ where $\delta y_o$ is the initial particle separation. This form was suggested by Brier (1950) and was dismissed by Sawford (1982a) as being physically unrealistic. However, as we will show in this paper, it leads to reasonable results that are in agreement with many of the known characteristics of relative diffusion.

Mathematical details of the averaging process described above and general solutions for $2 \le N \le \infty$ are presented in Lee and Stone (1983b). The classical two-particle diffusion results can be obtained by setting $N = 2$ in the general solutions. Here we present the solutions for the limiting case of $N \to \infty$ which is the appropriate limit for application to plumes and puffs in the atmosphere.

The displacement statistics which we will consider in this paper are the relative diffusion, the meandering, and the total diffusion. The relative diffusion $\sigma_R$ is defined as the expected value of the standard deviation of the displacements of the particles in a cluster relative to the centroid of the cluster. This is equivalent to the expected value of the standard deviation of the instantaneous concentration distribution. The meandering $\sigma_C$ is defined as the expected value of the standard deviation of the displacements of the cluster centroid positions relative to the average centroid position, where the "average" centroid position refers to a particular trial of M clusters. This is equivalent to the expected value of the "half-width" of the envelope of plume centroid positions that would be observed during an experiment. The total dispersion $\sigma_T$ is defined by the usual relation for the summation of variances, $\sigma_T^2 = \sigma_R^2 + \sigma_C^2$. This definition of $\sigma_T$ is equivalent to the expected value of the standard deviation of the time-averaged concentration distribution that would be measured by a fixed array of samplers during an experiment. Both $\sigma_C$ and $\sigma_T$ depend upon the averaging time which, for a particular experiment, is equal to the sampling time $t_S$ or the release time $t_R$. If $t_R > t_S$ only the material released during a period of time equal to the sampling period $t_S$ will be observed. If $t_S > t_R$ the samplers will collect material only during a period of time equal to the release time $t_R$. Therefore, the shorter of these two times is the appropriate averaging time and will determine the values of $\sigma_C$ and $\sigma_T$. In the remainder of this paper $t_R$ and $t_S$ will be used interchangeably.

The theoretical results are presented in terms of the dimensionless variance and time defined by $\Sigma^2 = \sigma^2/2\overline{v^2}t_L^2$ and $T = t/t_L$ where $\overline{v^2}$ is the variance of the velocity in the turbulent field and $t_L$ is the Lagrangian integral time scale. The theoretical plume solutions are given by

$$\Sigma_R^2 = \Sigma_o^2 + T - (1-e^{-T}) - (\overline{S}/2)(1-e^{-T})^2 \qquad (3)$$

$$\Sigma_C^2 = \qquad (1-\overline{R})(\overline{S}/2)(1-e^{-T})^2 \qquad (4)$$

$$\Sigma_T^2 = \Sigma_o^2 + T - (1-e^{-T}) - (\overline{R}\overline{S}/2)(1-e^{-T})^2 \qquad (5)$$

We have assumed that the initial spatial distribution of particles is uniform over the source width corresponding to a "top-hat" concentration profile. Therefore, the dimensionless standard deviation of the plume at the source is given by $\Sigma_o^2 = D^2/12$ where D is the dimensionless source width, $D = d/(2\overline{v^2})^{1/2}t_L$. The dimensionless parameters $\overline{S}$ and $\overline{R}$ result from the spatial and temporal averaging, respectively, of the particle initial velocities. In general, they are functions of N, d/L, $t_R/t_E$, and the functional form of the Eulerian space-time autocorrelation function. For $N \to \infty$ and an exponential space-time autocorrelation function, they are given by the relations $\overline{S} = F(d/L)$ and $\overline{R} = F(t_R/t_E)$ where the function F is given by the relation

$$F(\zeta) = (2/\zeta^2)(\zeta - 1 + e^{-\zeta}) \qquad (6)$$

The function $F(\zeta)$ is plotted in Fig. 2. Note that $F(\zeta)$ is unity at $\zeta = 0$ and approaches zero like $1/\zeta$ as $\zeta$ approaches infinity.

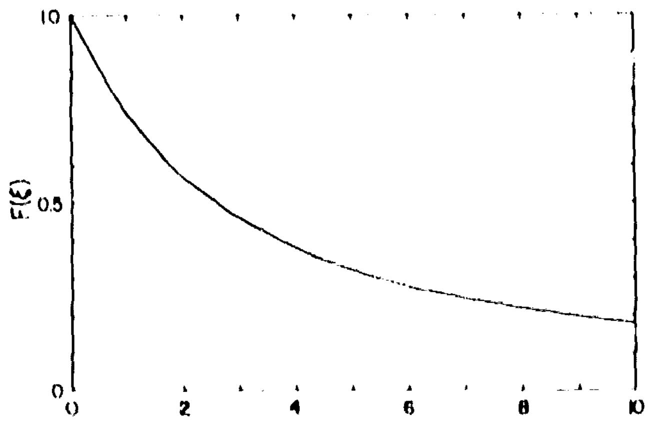


Fig. 2. Source Correlation Function

Equations (3)-(6) illustrate some interesting properties of atmospheric diffusion. The total diffusion $\Sigma_T$ depends upon the spatial extent of the source d/L and the temporal extent of the source $t_R/t_E$ in a symmetric manner through the parameters $\overline{S}$ and $\overline{R}$. If $d/L \to \infty$ ($\overline{S} = 0$) or if $t_R/t_E$ and $t_S/t_E \to \infty$ ($\overline{R} = 0$) the last term in Eq. (5) drops out and $\Sigma_T$ becomes equal to the classical Taylor diffusion result for an exponential Lagrangian autocorrelation function. For a finite value of either d/L, $t_R/t_E$, or $t_S/t_E$, the total diffusion $\Sigma_T$ is less than Taylor diffusion.

The relative diffusion $\Sigma_R$ depends only upon the spatial extent of the source, d/L, through the parameter $\overline{S}$. For $d/L \to \infty$ ($\overline{S} = 0$) the initial velocities are not spatially correlated and $\Sigma_R$ is equal to Taylor diffusion. For $d/L \to 0$ ($\overline{S} = 1$) the initial velocities are perfectly correlated in space and $\Sigma_R$ is less than Taylor diffusion. The parameter d/L will be very small for most concentrated sources in the atmosphere, but it may be of order unity for area sources.

The meandering $\Sigma_C$ vanishes when $d/L \to \infty$ ($\overline{S} = 0$) since we then have Taylor type diffusion. It also vanishes when $t_S/t_E \to 0$ ($\overline{R} = 1$). This latter result arises from our definition of $\Sigma_C$ as the meandering of the plume centroid about its average position for a particular trial or experiment. In terms of a sampling array, this simply means that the measured plume width $\Sigma_T$ is equal to the actual plume width $\Sigma_R$ if $t_S \to 0$.

The instantaneous release of puffs corresponds to $t_R/t_E \to 0$ ($\overline{R} = 1$). However, because of the way $\Sigma_C$ is defined, Eqs. (3)-(5) do not reduce to a useful form in this limit. For puffs it is more useful to define the meandering of the centroid relative to the axis of the mean wind, y = 0. With this modification, the solutions for instantaneously released puffs may be written as

$$\Sigma_R^2 = \Sigma_o^2 + T - (1-e^{-T}) - (\overline{S}/2)(1-e^{-T})^2 \qquad (7)$$

$$\Sigma_C^2 = \qquad (\overline{S}/2)(1-e^{-T})^2 \qquad (8)$$

$$\Sigma_T^2 = \Sigma_o^2 + T - (1-e^{-T}) \qquad (9)$$

Equations (7)-(9) are ensemble average values that would be obtained by releasing a very large number of puffs under "identical" conditions and averaging the results. Note that Eqs. (3)-(5) with $t_R/t_E$ and $t_S/t_E \to \infty$ ($\overline{R} = 0$) are identical to Eqs. (7)-(9). Thus, the particle displacement statistics for a continuous plume with a large sampling time are the same as for a large ensemble of instantaneously released puffs. This equivalence is further illustrated by the fact that the relative diffusion $\Sigma_R$ does not depend upon the release time and is the same for plumes and puffs, Eqs. (3) and (7).

The analytic results presented above, Eqs. (3)-(9), can also be obtained using a numerical Monte Carlo approach. This approach, which can be formulated in either a Lagrangian or Eulerian reference frame, is discussed in detail by Lee and Stone (1983a). We have done extensive Monte Carlo calculations and have found very close agreement between the numerical and analytic results. Details of the numerical method and comparisons to analytic resutls are presented in Lee and Stone (1983a).

## 3. RESULTS

The solutions for instantaneously released puffs or for a continuous plume with a large sampling time, $t_S/t_E \to \infty$, are shown in Fig. 3. We have plotted the growth of the standard deviation $\Sigma$ relative to the initial value $\Sigma_o$ as a function of time after release T. The upper curve is the total or Taylor diffusion $\Sigma_T$ from Eq. (9). The lower three curves are the relative diffusion $\Sigma_R$ from Eq. (7) for a range of source sizes indicated by the parameter $\xi = d/L$. Reference lines with slopes of 1/2, 1, and 3/2 are shown for comparison. The total diffusion increases like T for $T < 0.5$ and like $T^{1/2}$ for $T > 3$ with a transition region between. The relative diffusion curves show regions of accelerated growth in which $\Sigma_R$ increases more rapidly than T. For a point source, $d/L \to 0$, this accelerated growth region is of the form $\Sigma_R \propto T^{3/2}$ for $0 < T < 0.5$. For $d/L > 0$ the initial growth is linear in T followed by an accelerated growth region out to $T \approx 1.0$. The region of accelerated growth becomes smaller as d/L increases and virtually disappears for $d/L > 1$. These results are in general agreement with Bachelor's (1950) similarity theory for two-particle relative diffusion in the inertial subrange.

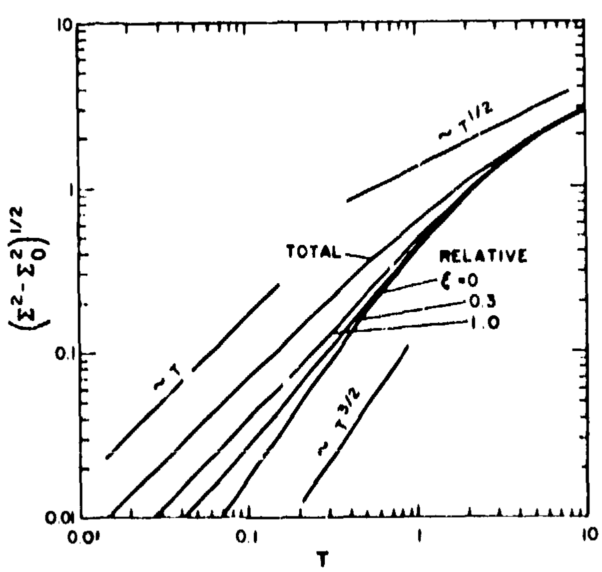


Fig. 3. Diffusion of Puffs and Plumes

The nature and extent of the accelerated growth region can be seen more clearly in Fig. 4 where we have plotted the relative diffusion divided by the total diffusion. For $d/L = 0$ the accelerated growth region in which $\Sigma_R \propto T^{3/2}$ has a slope of 1/2 in this figure. It is seen that the accelerated growth rate is generally less than $T^{3/2}$ for $d/L > 0$.

The effect of sampling time on the measured plume width $\Sigma_T$ for a continuous point source is

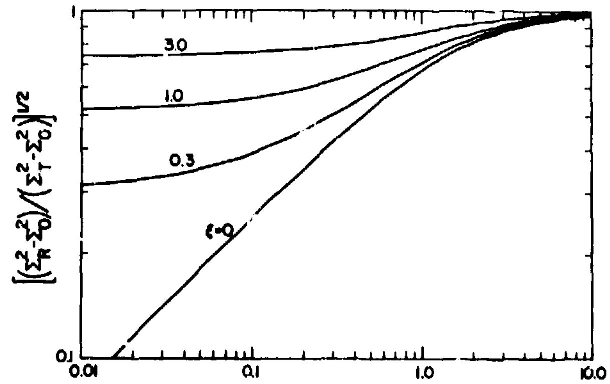


Fig. 4. Ratio of Relative to Total Diffusion

also represented by the curves in Fig. 3. This can be seen by letting $d/L \to 0$ ($\bar{S} = 1$) in Eq. (5) and comparing to Eq. (7). The lower three curves in Fig. 3 give the total diffusion $\Sigma_T$ from Eq. (5) for a range of sampling times by setting $t_S/t_E = \xi$. The upper curve is the limiting value for $t_S/t_E \to \infty$ ($\bar{R} = 0$). The apparent accelerated growth of $\Sigma_T$ reflects the increasing contribution of $\Sigma_R$ to $\Sigma_T$ as the sampling time decreases; i.e. Eq. (5) becomes more like Eq. (3) as $\bar{R} \to 1$.

Figure 5 is a linear plot of the total diffusion, relative diffusion, and meandering for puffs and for a continuous source with a large sampling time, Eqs. (7)-(9), for $d/L = 0$. It is seen that $\Sigma_C > \Sigma_R$ for $T < 1$. For $T > 3$, the meandering becomes small compared to the relative diffusion and approaches a constant. The relative diffusion is, effectively, just displaced below the total diffusion for $T > 1$. The accelerated growth of the relative diffusion which is obvious in Figs. 3 and 4 is difficult to see on this linear plot.

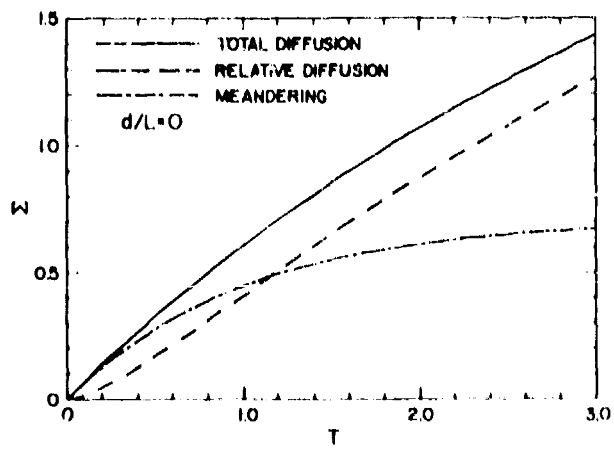


Fig. 5. Solutions for a Point Source

These solutions can be applied to the problem of fluctuating concentration. For example, in Gifford's (1959) fluctuating plume model the ratio of the peak instantaneous concentration to the peak mean concentration, $C_{PI}/C_{PM}$, is equal to the ratio of the variances $\Sigma_T^2/\Sigma_R^2$. From Eqs. (3) and (5) we see that this ratio depends upon the source size and the sampling time. This ratio is plotted in Fig. 6 for a continuous point source ($\bar{S} = 1$) for a range of sampling times $t_S/t_E$. One implication of Fig. 6 is that a sampling time of $t_S \approx 3\ t_E$ is required to measure a $C_{PM}$ value that is within a factor of two of the long time averaged Taylor value.

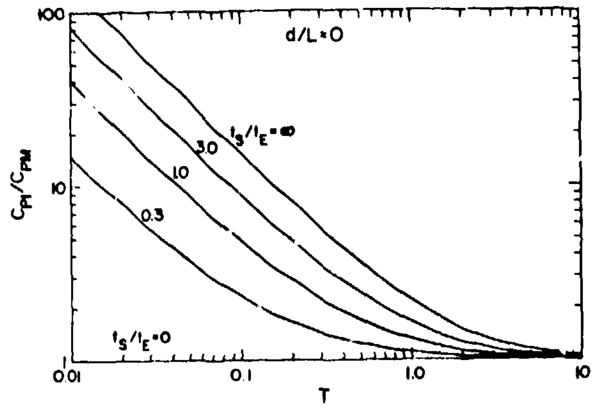


Fig. 6. Instantaneous-to-Mean Concentration Ratio

## 4. CONCLUSIONS

We have obtained simple analytic solutions for relative diffusion and meandering of puffs and plumes based upon the random-force theory of turbulent diffusion. These solutions assume that the initial velocities of the tracer particles are identical to the turbulent field velocities at the source location. The spatial and temporal correlation of these velocities are, therefore, determined by the Eulerian space-time autocorrelation function, and the appropriate ensemble averages can be calculated if this correlation function is known. These solutions exhibit many of the known features of relative diffusion and are in general agreement with similarity theory for the inertial subrange.

Our solutions are presented in dimensionless form and are applicable to turbulent diffusion on any scale. To apply these results to actual experiments, the magnitude of the Eulerian integral length scale L and the Eulerian and Lagrangian integral time scales $t_E$ and $t_L$ must be known. These can be determined only from experimental data. In a companion paper, Lee and Stone (1983a), we present a method for relating $t_L$ to $t_E$ and L. Gifford's (1982a, b) analysis of long and short range data suggests that, for horizontal diffusion in the atmosphere, $t_L$ is of the order of $10^4$ sec. This is much larger than the generally accepted value of $t_L$ and has led Gifford to suggest that very large scales of motion should be treated as turbulence in modeling horizontal atmospheric diffusion. However, this leaves unanswered the important practical question of how to make a separation between the mean wind and turbulence in modeling transport and diffusion.

## REFERENCES


Batchelor, G. K., 1950: The application of the similarity theory of turbulence to atmospheric diffusion. Quart. J. R. Met. Soc., 76, p. 133-146.

Brier, G. W., 1950: The statistical theory of turbulence and the problem of diffusion in the atmosphere. J. Met., 7, p. 283-290.

Gifford, F. A., 1959: Statistical properties of a fluctuating plume dispersion model. Adv. In Geophysics, 6, p. 117-137.

Gifford, F. A., 1982a: Horizontal diffusion in the atmosphere: a Lagrangian-dynamical theory. Atmos. Env., 16, 3, p. 505-512.

Gifford, F. A., 1982b: The random-force method applied to calculating short-range atmospheric diffusion. LA-9583-MS, Los Alamos National Laboratory.

Lee, J. T. and G. L. Stone, 1983a: Eulerian-Lagrangian relationships in Monte-Carlo simulations of turbulent diffusion, Sixth Symposium on Turbulence and Diffusion. American. Met. Soc., Boston, MA.

Lee, J. T. and G. L. Stone, 1983b: Effects of Eulerian spatial and temporal velocity correlations at the source on turbulent diffusion in the atmosphere: theoretical results. LA-MS, Los Alamos National Laboratory (to be published).

Sawford, B. L., 1982a: Comparison of some different approximations in the statistical theory of relative diffusion. Quart. J. R. Met. Soc., 108, pp. 191-206.

Sawford, B. L., 1982b: Lagrangian Monte Carlo simulation of the turbulent motion of a pair of particles. Quart. J. R. Met. Soc., 108, p. 207-213.

Smith, F. B., 1968: Conditioned particle motion in a homogeneous turbulent field. Atmos. Env., 2, p. 491-508.

Uhlenbeck, G. E. and L. S. Ornstein, 1930: On the Theory of the Brownian Motion. Phys. Rev., 36, p. 823-841.