A Monte Carlo study of turbulent diffusion

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A MONTE CARLO STUDY OF TURBULENT DIFFUSION

by

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The prediction of heat and mass transfer rates is of vital importance in many industrial fluid flow processes. In order that an adequate design may be accomplished for a particular operation, a knowledge of the condition of flow and how it affects the transfer process is necessary.

Since the dispersion of heat, mass, and momentum is greatly enhanced when the fluid is in turbulent flow, the prediction of the phenomenon of turbulent diffusion becomes important. Although considerable effort has been made in the experimental study of turbulent transport, little has been accomplished in expanding the understanding of the basic mechanism involved.

The dispersion caused by the eddies of a turbulent fluid can be compared with the intermixing due to the kinetic motion of molecules in molecular diffusion. Although the concept is useful in gaining a general picture of the mechanism involved in turbulent diffusion, the quantitative use of this analogy can lead to conflicting conclusions. The paths of molecules are random in nature according to the theory of kinetic motion and have been adequately described by statistical models. The Brownian
motion descriptions of molecular diffusion have also been experimentally verified.

The eddies of a turbulent fluid can similarly be depicted by stochastic processes. The difficulty of applying the Brownian process to the description of turbulent diffusion is that the scale of the observation is often the same order of magnitude as the eddy size or mixing distance in a turbulent fluid, whereas in molecular diffusion, the scale of observation is always much greater than the mean free path of the molecules. Also, the Brownian motion model is based on the concept of collisions of discrete particles with molecules while the turbulent fluid is considered as a continuum.

The purpose of the present research has been two-fold. The first objective was to develop an adequate stochastic model to describe the turbulent diffusion process. The second objective was to study turbulent diffusion by simulating the process and analyzing the results for various conditions.

The stochastic process presented describes the movements of the fluid as a random walk procedure. Each motion of an element of fluid is the solution of a stochastic differential equation. And, the distribution of the velocity and velocity time derivatives is determined
according to the motion of the element at the end of the preceding step.

On the basis of the stochastic model developed, the turbulent diffusion process has been simulated by Monte Carlo techniques. Both steady state and transient turbulent diffusion from a continuous point source in a pipe were simulated.

Since the motion of a single element of fluid is followed in the random walk, the local diffusate velocity is also predicted. Thus, the local flux could be calculated from the generated local concentrations and velocities. With this information on the local flux of the diffusate, the eddy diffusivity tensor was evaluated directly from its definition rather than having to fit the partial differential equation of diffusion to the concentration profiles.

Several assumptions have commonly been made as to the nature of the eddy diffusivity tensor when the components have been evaluated from the experimental concentration profiles. It was possible to evaluate the components of the diffusivity tensor under each of these assumptions from the simulated flux and concentration profiles. From these evaluations, the region of flow for which the assumptions are most likely to be valid
were studied using a variance ratio. Also, the transport ratio was used as a means of studying the importance of each of the diffusivity tensor components.
REVIEW OF LITERATURE

Studies of Turbulence

The effects of turbulence in many chemical engineering applications must be taken into account to be able to complete an adequate analysis of any process under study. Of interest are not only the effects on the transport of fluids, but also the heat and mass dispersion caused within the fluid.

Introductory discussions of turbulence and the associated chemical engineering considerations are given by Treybal (133), Perry (98), and Foust et al. (47). One of the most extensive coverages of the theories of turbulence is given by Hinze (58) who gives an excellent review on the theories of turbulence covering measurement techniques, isotropic and nonisotropic turbulence, wall turbulence and transport processes. Batchelor (11) presents a treatment of homogeneous turbulence. The subject of boundary layers is given special emphasis in a book by Schlichting (114). Pai (96) discusses turbulent flow in his survey of viscous flows. Spectral functions and correlation coefficients used to statistically characterize turbulence are examined by Frenkiel (50). Agostini and Bass (1) discuss theories of statistical mediums in relation
to turbulent flow. Cooper and Tulin (25) review the status of turbulence measurements and the significant experimental investigations utilizing the techniques of hot-wire anemometry. Bird et al. (16) and Knudsen and Katz (68) relate many of the theories of turbulence to chemical engineering studies of transport phenomena.

Structure of turbulence

As a first consideration of the problem of turbulent diffusion, an analysis can be made as to the nature and structure of turbulence. At low flow rates, a fluid motion known as laminar flow is said to exist. As the flow rate is increased, a condition known as turbulence develops. To demonstrate the difference between these two flow conditions, Reynolds (103) made his classical experiment consisting of the injection of a dye into a glass tube of flowing water. The laminar flow was characterized by a smoothness of motion in which the dye injected traces out a slender streakline without lateral mixing. For turbulent flow, there was a rapid lateral mixing motion of the fluid elements in addition to the basic motion of the flow. The dye injected was resolved into distinct curls indicating rapidly changing eddies having a circular motion when an electric spark was used to view the turbulent flow. A more precise description of turbulence has been given recently
Turbulent fluid motion is an irregular condition of flow in which the various quantities show a random variation with time and space coordinates, so that statistically distinct values can be discerned.

Realizing that a knowledge of the statistical properties of the velocity fluctuation would lead to a greater understanding of turbulence, Reynolds (104) modified the Navier-Stokes equations. Using the concept that the velocity is composed of a mean value and a fluctuation from the mean, he developed a set of equations differing from the Navier-Stokes equations only in that they contained additional terms known as the eddy stresses or Reynolds stresses.

Another approach to the study of turbulence was introduced by Taylor's application of the concept of isotropic turbulence to the problem of decay of turbulence in a wind-stream (124, 125). Although this type of turbulence is quite restricted by definition, its simplicity has allowed a further examination of turbulence. Also, experimental conditions such as the center core of an air duct, behind a grid in a wind tunnel, and the upper atmosphere offer opportunities for testing the theories developed for isotropic turbulence (26, 54, 79).

According to the definition of isotropic turbulence, the mean values of any function of the fluctuations at a
point must be invariant under any rotation or reflection of the axes of reference. A reduction of unknowns in the Reynolds equations follows from this definition. Considering this, Von Karman and Howarth (137) developed a relationship for the correlation of any component of the fluctuation at a given point with any component of the velocity fluctuation at another point.

Taylor (123) also applied another important tool to the examination of turbulence. As a more detailed description of turbulence he considered the distribution of energy among eddies of different sizes. Thus by analyzing the electric current produced by a hot-wire anemometer subjected to velocity fluctuations, he was able to separate the energy into a spectrum according to frequency. As such, the mean value of $u^2$ may be regarded as the sum of the contributions from all frequencies. And, if $u^2 f_\omega(\omega)$ is the contribution from frequencies between $\omega$ and $\omega + d\omega$, then

$$\int_0^\infty f_\omega(\omega)d\omega = 1$$

The relation between the correlation function and the energy spectrum was also studied by Taylor (123). He found that the energy spectrum and the correlation function can be developed from each other by using a Fourier transform. For the turbulent velocities at a fixed point in space, the correlation at the fixed point and the energy
spectrum are related by the expressions

\[ f_w(w) = \frac{2}{\pi} \int_0^\infty \cos(\omega s_1) R(s_1) ds_1 \]  \hspace{1cm} (2)

\[ R(s) = \int_0^\infty \cos(ss_1) f_w(s_1) ds_1 \]  \hspace{1cm} (3)

Extensive work has been done in studying the energy spectrum developed under various turbulent conditions (6, 7, 24, 50, 75, 112, 113). Of particular interest are those studies from which information on time and space correlations can be obtained (41, 42, 43, 73, 74, 111).

Among the first statistical properties of turbulence investigated was the velocity profile of flowing fluids (14, 33, 73, 74, 106). Correlations have been proposed (32, 55, 95, 108) to interpolate and extrapolate the experimental results. Smoothed velocity profiles from a number of investigators were tabulated by Tichacek et al. (127) in conjunction with a study of axial mixing in pipes.

One of the most complete studies of the structure of turbulence in fully developed pipe flow of air was made by Laufer (74). Measurements, principally with a hot-wire anemometer, were made in a 10-inch pipe at speeds of approximately 10 and 100 feet per second which correspond respectively to Reynolds numbers of 50,000 and 500,000. The results include relevant mean and statistical quantities such as the radial, angular and axial turbulence intensities, shearing stresses, turbulent dissipations, and energy spectra.
Similar measurements were made in a 4-inch tube for Reynolds numbers 50,000, 100,000, 200,000, and 300,000 by Sandborn (111). Excellent agreement was obtained with the measurements of turbulence by Laufer (74) for the Reynolds number of 50,000.

An experimental and analytical study of adiabatic turbulence was conducted by Deissler (32) on air flow in tubes. Deissler and Taylor (33) generalized and applied previous work on flow in tubes to non-circular passages of equilateral triangular and square cross-section. Velocity distributions, wall shear-stress distributions and friction factors were also calculated.

Barbin and Jones (5) report measurements of mean velocities, turbulence intensities, and Reynolds stresses for the first 40 pipe diameters in the inlet region of a smooth pipe. Fully developed flow was not obtained in this pipe length for a Reynolds number of 388,000.

Measurement of the statistical properties of flowing fluids other than gases is difficult. By using probe wires 5 to 10 times thicker than those utilized in standard hot-wire anemometry studies of air, Sparks and Hoelscher (118) had partial success in overcoming some of the problems associated with liquid phase measurements.

Cermak and Baldwin (22) measured some of the statistical properties of turbulence in water for a variety of flow
fields. The relative intensities of the turbulent velocity fluctuations were inferred from the fluctuating electrokinetic potential difference between two small, closely spaced electrodes. Among the data reported were the intensity and shear stress profiles and one-dimensional spectra in fully developed pipe flow. The assumption of a direct proportionality between the electrokinetic-probe output and the velocity fluctuation is implicit in the application of this method. There is no reason to believe that the turbulent intensity in the core of a fully developed pipe flow depends on the fluid. And, the relatively good agreement of these electrokinetic-potential surveys with the hot-wire anemometer results of air (74, 111) seem to support this assertion.

The significance of the number of zeros of the fluctuating velocity components and examples of measurements for determination of the microscale of turbulence from zero counts was presented by Liepmann et al. (79). Later, Liepmann and Robinson (80) studied the methods of measuring the probability distributions and mean values of random functions as encountered in turbulence research. Applications to the measurement of the probability distribution of the axial fluctuation $u(t)$ and its derivative, $du/dt$, in isotropic turbulence were shown in this study. The assumption of independent probability distributions of
u(t) and du/dt was investigated and the results indicate that the assumption is satisfied within a few percent.

**Turbulent transport phenomena**

As was noted in the foregoing literature survey, much of the research emphasis has been placed on the study of the causes of turbulence and its effects on the mean velocity profiles. However, of more importance to most chemical engineering problems is the effects of turbulence on the heat, momentum, and mass transfer processes. The literature which describes the various investigations of turbulent transfer of these properties is immense.

The studies of mass transfer have been generally concerned with four system types.

1. Packed and fluidized beds
2. Wetted-wall columns
3. Free jets
4. Co-axial fluid streams

It is the last of these system types which was simulated in this study. Only papers considered pertinent to the present investigation are presented in the following literature review.

Opfell and Sage (93) have prepared an extensive survey of turbulent transfer. Seagrave and Fahien (117) include a review of various papers on mass, heat, and momentum transfer
which provide information on the mechanism of the turbulent diffusion process. A similar review of literature on the transport of heat and momentum in turbulent liquids is available in a study by Beckwith and Fahien (14).

One of the first turbulent diffusion experiments on gas streams was conducted by Towle and Sherwood (129). Carbon dioxide and hydrogen were introduced at the center of the duct, and concentration traverses over the central third of the duct diameter were obtained at points downstream. The values of diffusivity obtained were approximately 100 times the molecular diffusivity and were independent of the tracer gas used. The eddy diffusivity was found to increase with higher Reynolds numbers.

Flint et al. (45) conducted similar investigations of turbulent diffusion from a small source located at the center of a 3-inch pipe. Hydrogen and carbon dioxide were mixed in air, and potassium chloride solution was mixed with water. The mean square displacement data was given for air flow over a Reynolds number range of 9,700 to 87,000.

An investigation of turbulent motion and mixing in a pipe was made by Lee and Brodkey (77). A dye solution was injected at the center of a 3-inch pipe and studied by means of a light probe developed for the measurement of concentration fluctuations. The mean velocity and intensity profiles of the turbulent water flow were measured
with a pitot-static tube and a hot-film probe for the Reynolds number of 50,000.

Studies of turbulent diffusion downstream from a line source of heat are presented by Baldwin and Walsh (4). Hot-wire anemometer surveys showed that the turbulence axial core was nearly homogeneous and isotropic. The Lagrangian correlation coefficients, as inferred by G. I. Taylor's theory of diffusion by continuous movements (121) from the concentration data, had shapes similar to the Eulerian correlations over most of the range of time and space investigated.

Mickelsen (88) made an experimental comparison between the Lagrangian and Eulerian correlation coefficients in the central core of a turbulent pipe flow. The Lagrangian correlation coefficient was characterized by measurements of the turbulent diffusion of helium from a point source. The turbulence intensity and Eulerian correlation coefficients were measured by hot-wire anemometry. The resulting Lagrangian and Eulerian correlation coefficients had similar shapes related by a linear proportionality between their space and time coordinates.

The composition and point velocity were determined as functions of radial position and distance from the point of mixing of coaxial streams of air and natural gas by Schlinger and Sage (115). The eddy diffusivity was assumed
independent of radial position and calculated from the material balance and equation of continuity.

Lynn et al. (81) made an experimental study of the mixing of natural gas and air at Reynolds numbers of 44,000 and 79,000 under turbulent velocity conditions in a 6-inch tube. Total diffusivities of the natural gas were found near the center of the tube as functions of position.

Klinkenburg et al. (67) present a mathematical discussion of turbulent diffusion in a fluid moving at a uniform velocity in a tube. They assumed the radial and axial diffusivities to be constant but not equal. That is, the flow field assumed was homogeneous and nonisotropic. A numerical analysis of a similar steady state diffusion process was presented by Hiby and Schummer (57). Tensor notation was used to represent the nonisotropic diffusion equation with the nondiagonal elements of the diffusivity matrix being assumed zero.

The diffusion equation was solved explicitly by Lauwerier (76) for a two dimensional flow field having a linear velocity gradient. Axial diffusion was neglected and the lateral diffusivity was assumed constant.

Equations were developed by Taylor (120, 121) for the eddy diffusivities of a material diffusing from a point source. These equations were utilized by Kalinske and Pien (64) to determine the eddy diffusivities in a turbulent water stream.
For short diffusion times, Townsend (130) demonstrated how the turbulence may rotate and strain the diffusing wake to increase the contribution of molecular diffusion to the total dispersion. Mickelsen (89) measured the lateral dispersion of helium and carbon dioxide in air from a continuous point source in a wind tunnel. The results of using these two gases, which have widely different diffusivities, indicated that the accelerated molecular diffusion was negligible for long diffusion times. In a later study, Saffman (110) found that the interaction between the molecular diffusion and the turbulent motion reduces the dispersion from the value it would have if the processes of molecular and turbulent diffusion were independent and additive.

The solution of the diffusion equation for steady state mass transfer allowing both the effective radial diffusivity and velocity to vary with radial position was first presented by Fahlen and Smith (40). Later Dorweiler and Fahlen (37) modified this semi-numerical method and extended the mass transfer data for packed beds to very low flow rates.

Frandolig and Fahlen (48) conducted experimental studies of mixing of coaxial streams of carbon dioxide and air in a vertical 4-inch pipe. Total diffusivities of the carbon dioxide in air for the entire radius of the pipe were com-
puted by the semi-numerical method of Dorweiler and Fahien (37). The work was continued by Roley and Fahien (106) for the same system. As in the previous study of Frandolig and Fahien (48) the concentration profiles were determined at several axial positions and Reynolds numbers. From these data, mass transfer Peclet number, and eddy viscosity were determined for the diffusion of carbon dioxide in air.

Seagrave and Fahien (117) studied a system of fluorescein dye injected at the center of a turbulent water stream in a 4-inch tube. Two methods of solving for the diffusivities as a function of position were applied. The non-diagonal elements of the diffusivity tensor were assumed zero while the diagonal elements were assumed to be functions only of radial position. By placing the injection point at the center of the tube the system had angular symmetry and only the values of the axial and radial diffusivities were computed. The radial component of the mass diffusivity tensor varied with radial position reaching a maximum away from the center of the tube.

Konopik (70) determined the terms of the nonisotropic tensor for a nonsymmetrical flow system. Experimental data were obtained in a 4-inch copper tube with two salt injection tubes placed diametrically at the wall of the tube. The salt concentrations were obtained at various Reynolds
numbers as functions of the angular, radial, and longitudinal position by an electrical conductivity method.

Stochastic Models

Statistical vs. deterministic models

With any physical phenomenon there are an infinite set of other events which in some way influence the particular process under study. Thus a problem of analyzing any physical process is that of deciding what effects are important and subsequently finding their influence. The theory or model developed will not apply completely to the original physical phenomenon but to some simplified hypothetical situation. Any true test of the model will be to determine how well it compares with the physical situation and all of its complexities.

There are available solutions to many problems for which the subsequent behavior of the system is completely determined when given a set of definite external forces and an initial state. Examples are solutions of a differential equation for the flow of heat in a semi-infinite bar or for the potential force between two rigid bodies. Any solution of this type, which completely determines the result from a given set of causes, can be called a dynamic solution.
Another approach to the solution of many physical problems is the use of a statistical model. This concept finds wide application where the process is primarily determined by a great number of causes of nearly equal effect. A classical example of the statistical approach is the kinetic theory of gases. While a dynamic model could be developed to describe the motion of each of the molecules in some container, it would be impossible to solve for the entire behavior of such a complex system even with the high speed computers presently available. Further, any solution of the motion of each of the many molecules in this system would be of little value and no general conclusions would be available. Of primary interest are the macro-features such as pressure, temperature, and density. Although the process is composed of a large number of individual molecules, it is their joint characteristics which are of interest.

A characterization of the properties of the molecules can be made in statistical terms. That is, probability distributions may be assumed for the velocity and the initial positions of the molecules. Also the collisions between molecules and their type of motion can be specified. With these considerations, a statistical evaluation of the model has led to the development of statistical laws explaining the physical observations of gas behavior.
In general if the phenomenon being investigated is uniquely determined by a few boundary conditions and external forces then it is best studied by means of a dynamic model. However, if the phenomenon is determined by a large number of nearly equivalent effects then a statistical model may be best applied.

Quite often a phenomenon is to be studied over time. If the model used is statistical and thus is controlled by probabilistic laws, then the system under study is known as a stochastic process (36, p. 2; 97, p. 1).

**Brownian motion**

One of the first applications of the theory of stochastic processes was that of describing the ceaseless irregular motions of a microscopic particle immersed in a fluid. The above phenomenon was discovered by the English biologist, Brown, in 1826 and is named after him.

**Einstein explanation** On the assumption that the particle is being continually bombarded by the molecules of the surrounding medium, Einstein (39) gave an explanation of the Brownian motion and developed a fundamental basis for treating the process statistically. By considering the displacement $X(t)$ of the particle at time $t$ as a chance variable, Einstein found the distribution of $X(t) - X(0)$ to be normal with a zero mean and variance $\sigma^2 t$. If
the impacts on the Brownian particles are very frequent and irregular and if $s$ is large compared to the average time between impacts, the displacement $X(t + s) - X(t)$ may be considered to be the sum of a large number of small displacements caused by the collisions. Further, there are assumed to be negligible connections between the particle and the surrounding medium except on impact.

**Wiener process** Wiener was the first to discuss this stochastic process rigorously. As a mathematical statement of the above physical conditions, he considered the random displacements $X(t + s) - X(t)$ of the particle during non-overlapping time intervals to be independent. Under these assumptions, the Brownian motion can be represented by the Wiener process which is defined by the following:

1. The process $X(t)$ ($t > 0$) has stationary independent increments.
2. For every $t > 0$, $X(t) - X(0)$ is normally distributed.
3. For all $t > 0$, $E[X(t)] = 0$
4. $X(0) = 0$.

With these axioms, Wiener was able to show that the stochastic process $X(t)$ is continuous. However, the process may not be expected to represent the Brownian motion at short times; and even if it did, mathematically the process is non-differentiable (97, p. 84) as well as being of un-
bounded variation. Thus as Doob (34) points out, the path curves of the Wiener process have infinite length.

**Ornstein-Uhlenbeck process** More realistic models of Brownian motion have been developed such as the Ornstein-Uhlenbeck stochastic process (135, 139). The transition probability of the velocity of the particle from the velocity $u(t)$ at time $t$ to a velocity $u(t+s)$ at time $t+s$ is considered normal with

$$E[u(t+s)] = u(t)\exp(-|s/\theta|) \quad (4)$$
$$\text{Var}[u(t+s)] = \sigma^2(1 - \exp(-2|s/\theta|)) \quad (5)$$

Under this model, the distribution of the displacement, $X(t+s) - X(t)$ during time $s$ is again normal with

$$E[X(t+s) - X(t)] = 0 \quad (6)$$
$$\text{Var}[X(t+s) - X(t)] = \sigma^2 \theta \left( \exp(-|s/\theta|) - 1 + |s/\theta| \right) \quad (7)$$

Doob (35) analyzed the Ornstein-Uhlenbeck process and came to a generalization concerning the type of process. Suppose $u(t)$ ($-\infty < t < +\infty$) is a one-parameter family of random variables determining a stochastic process which is a strictly stationary Markovian normal process. Then, as Doob (34) has shown, there is a constant $\theta$ such that for $t_1 < t_2 < \ldots < t_n$ the $u(t_1), u(t_2), \ldots, u(t_n)$ have a $n$-variate normal distribution with common mean $\mu$ and variance $\sigma^2$ and correlation coefficients determined by

$$\text{Cov}[u(t), u(t+s)] = \sigma^2 \exp(-|s/\theta|) \quad (8)$$
And, thus the velocity correlation defined by
\[ R(s) = \frac{\text{Cov}[u(t), u(t + s)]}{\text{Var}[u(t)] \text{Var}[u(t + s)]} \] (9)
will be
\[ R(s) = \exp\left(-\frac{|s|}{\theta}\right) \] (10)

The velocity in the Ornstein-Uhlenbeck process is thus a continuous, non-differentiable process and, as Doob (35) further proves, can be expressed in terms of the Wiener process.

Another sophistication of the study of Brownian motion has been advanced recently by Rubin (109). And, a more general survey of the development of the Brownian motion theory is available in Wax (143).

**Turbulent diffusion descriptions**

Before a stochastic model of turbulent diffusion can be developed, one must be able to predict the random macroscopic movements of the fluid. The velocity can be expressed as the average velocity plus a fluctuation
\[ U = \overline{U} + u \] (11)

A first approximation of the velocity could be to assume the fluctuation to have only two possible values
\[ u = \pm |\text{const.}| \] (12)

The velocity would be constant over an interval of time at the end of which, the velocity fluctuation for the next time interval is chosen from the two possible values.
This is essentially the model of turbulent motion which has been applied in the descriptions of turbulent diffusion given by Taylor (121), Goldstein (51), Gupta (52), Davies et al. (30) and Bourret (18). Kirmse (66) found this model to be inadequate and has considered the velocity to be described stepwise by a truncated Taylor's series.

**Taylor description**  
G. I. Taylor (121) in his 1921 paper on diffusion by continuous movements, laid the groundwork for a statistical study of turbulent diffusion. By advancing the concept of the Lagrangian correlation coefficient, he was able to develop a statistical theory for turbulent diffusion in terms of the paths of the fluid elements.

An insight into the theoretical basis for a statistical model of turbulent diffusion can be had by following Taylor's original development. The general considerations are important in that they relate the eddy diffusivity to the Lagrangian correlation function.

Consider a fluid flowing in the z direction where the turbulence is homogeneous and isotropic. At a point in the stream where \( z = 0 \), a dye is injected. As the fluid moves in the z direction, the dye will diffuse in all directions.

Now consider the transport of the dye perpendicular to the flow, that is along the x-axis. This lateral diffusion is caused by the random motions of the fluid elements,
and after some period of time, the total displacement, $X_n$, of a fluid element will be the sum of several individual displacements of length $x_i$ or

$$X_n = \sum_{i=1}^{n} x_i$$  \hspace{1cm} (13)

The mean displacement of the fluid would be

$$\overline{X} = \frac{1}{N} \sum_{n=1}^{N} X_n$$  \hspace{1cm} (14)

where the average is taken over $N$ fluid paths. The mean square displacement

$$\overline{X^2} = \frac{1}{N} \sum_{n=1}^{N} X_n^2$$  \hspace{1cm} (15)

however would not be zero and would be a measure of the variance or net diffusion of the dye.

If one considers a plane perpendicular to the x-axis through which the dye is diffusing, the flux can be written as

$$J_x = -D_t (\frac{\partial \overline{C}}{\partial x})$$  \hspace{1cm} (16)

where $\overline{C}$ is the time averaged concentration and $D_t$ is the eddy diffusivity defined by the above equation. Taylor assumes that the concentration gradient is constant over a region of width $X$ and that the mass diffuses across the plane with velocity $u$. Then, the flux can also be written

$$J_x = Xu (\frac{\partial \overline{C}}{\partial x})$$  \hspace{1cm} (17)
for all paths. Therefore, the diffusivity will be

$$D_t = \overline{Xu} \quad (18)$$

However, $$u = \frac{dX}{dt}$$ so it follows that

$$D_t = \overline{(XuX/dt)} = \frac{1}{2} \overline{dX^2/dt} \quad (19)$$

Therefore, the eddy diffusivity can be obtained from a knowledge of the mean square displacement $$\overline{X^2}$$. And, in terms of the Lagrangian velocity correlation function,

$$R(s) = \overline{u(t)u(t + s)} / u^2 \quad (20)$$

$$\overline{X(t)^2} = (\int_0^t u(t)dt)^2 \quad (21)$$

$$= 2 \int_0^t \int_0^{s_1} u(s_1)u(s_1 - s_2)ds_2ds_1 \quad (22)$$

$$= 2u^2 \int_0^t \int_0^{s_1} R(s)dsds_1 \quad (23)$$

Relationships for $$\overline{X^2}$$ as a function of time can be developed by considering models of the velocity and time variations. The simplest model would be represented by an oscillogram in which the velocity and time for each step were constants. For this discontinuous model, Taylor assumed the correlation between individual steps to be given by

$$c^j = x_i x_{i+j}/a^2 \quad (24)$$

where $$x_i = d$$ for $$i, j = 0, 1, 2, ..., n$$

and thus

$$x_{ni}^2 = nd^2 + 2n^2d^2/(1-c)c(1-c^2)d^2/(1-c^2) \quad (25)$$
By defining \( u = \frac{d}{\tau} = \text{constant} \) and \( t = n\tau \), the limit of the mean square displacement, as \( \tau \) goes to zero and \( c \) goes to one, will be

\[
X(t)^2 = u^2(2At - 2A^2(1-\exp(-t/A)))
\]  

(26)

**Goldstein description**  
A more complete discussion of diffusion by discontinuous movements was later presented by Goldstein (51). In particular, he considered an instantaneous point source of a large number of particles at the origin which move with a constant speed \( u \) along a straight line for a period of time \( \tau \). Initially half of the particles start in each direction but at the end of each time increment they can continue their present direction with a probability \( p \) or reverse their direction with a probability \( q = 1 - p \). Thus, the model of velocity is seen to be the same as Taylor's when it is realized that the correlation of consecutive time increments will be \( c = p - q \) and the partial correlations between non-consecutive intervals is zero. Goldstein then found a difference equation for the fraction of particles at a distance \( y = u\tau j \) from the origin after a time \( t = n\tau \). The limiting form of the difference equation as \( \tau \) goes to zero and \( c \) goes to one for constant \( u \) is the one-dimensional diffusion equation or telegraph equation.

\[
\frac{\partial^2 c}{\partial x^2} - \frac{1}{D_t}(\frac{\partial c}{\partial t}) - \frac{1}{u^2}(\frac{\partial^2 c}{\partial t^2}) = 0
\]  

(27)
where $D_t$ is the diffusivity defined by

$$D_t = \frac{u^2}{2} \lim_{r \to 0} (q/r)$$

(28)

A further investigation of the model was made by Gupta (52) and Davies et al. (30) in terms of the transition probabilities.

**Bourret description** More recently Bourret (18) discusses the one-dimensional Taylor-Goldstein model and later derives the two and three-dimensional diffusion equations (19). The procedure is essentially as before in that the particles are imagined to hop from site to site on a two or three-dimensional lattice according to some stochastic rule. Again the description of this process can be formulated in a set of finite difference equations which reduce to partial differential equations by making the lattice infinitely fine grained. For the two-dimensional case, the diffusion equation is of fourth order and the three-dimensional case gives a sixth order diffusion equation. These equations are of inconveniently high order and would give results significantly different from a generalization of the simpler one-dimensional equation only when high frequencies and transient conditions are considered. However, the importance of Bourret's discussion is that it shows the form of the diffusion equations which describe the motion of the diffusing particles as simulated by his model of diffusion.
A model of continuous turbulent motion

The marginal distribution of the velocity has been experimentally determined to be approximately a normal distribution (80).

\[ P_u(u) = \frac{1}{(2\pi)^{\frac{3}{2}} \sigma_u} \exp\left(-\frac{1}{2}(u/\sigma_u)^2\right) \]  \hspace{1cm} (29)

where \( \sigma_u^2 = \overline{u^2} \)

This property of the fluid motion could easily be incorporated in the model by randomly choosing the velocity for each step from a normal distribution. However, the modification would add little to the generality of the model. Also, at the scale the fluid motion is being observed, the fluid behaves as a continuum. The discontinuous velocities of the above model do not represent a continuum, but instead represent the changes of velocity due to instantaneous rigid collisions.

To approximate more closely the continuous motion of a fluid element, consider the velocity fluctuation as being described by the following relationship over each time interval

\[ u = u_{i+1} + (t - t_i) u_i' \quad \text{for} \quad t_i < t < t_{i+1} \]  \hspace{1cm} (30)

where \( u_{i+1} \) is the velocity at the end of the last time interval. And, \( u_i' \) is the acceleration during the present step and is randomly chosen at the beginning of the step.
From experimental results, the acceleration is also approximately normally distributed

\[ P_{u'}(u') = \frac{1}{(2\pi)^{\frac{3}{2}} \sigma_{u'}^2} \exp\left(-\frac{1}{2}(u'/\sigma_{u'}^2)^2\right) \] (31)

where \( \sigma_{u'}^2 = \langle u'^2 \rangle \)

If the turbulence has temporal homogeneity, the correlation between the acceleration and velocity is zero (132).

\[ \overline{u^2} = \text{constant} \] (32)

\[ \overline{u'u} = 0 \] (33)

To satisfy the four conditions given by Equations 29, 31, 32, and 33, the acceleration chosen for each step has to be related to the velocity. This may be done by randomly choosing the magnitude of the acceleration from a half-normal distribution, where the sign of the acceleration is determined by the probability of the velocity being greater or less than its value at the beginning of the step. This is, the probability of \( u' \) being greater than zero equals the cumulative distribution of the velocity

\[ P [u'_1 > 0] = P [u > u_1] = \int_{u_1}^{\infty} P_u(u) \, du \] (34)

where \( P_u(u) \) is the probability density function of the velocity.

The changes in acceleration can be considered as being due to the random forces of the turbulent flow. If each
disturbance has no knowledge of when the others occur, then the time between changes of acceleration can be shown to be exponentially distributed \((97, \text{p. 123})\).

\[
p_\gamma(\gamma_i) = \frac{1}{\lambda_t} \exp(-\frac{\gamma_i}{\lambda_t}) \quad \gamma_i > 0 \tag{35}
\]

where
\[
\gamma_i = t_{i+1} - t_i
\]
\[
\lambda_t = \frac{\gamma}{T}
\]

To use this distribution, one needs to know the average step time, \(\bar{\gamma}\), which will be related to the velocity and acceleration. It can be shown \((79)\) that for any motion meeting all four of the above conditions expressed as Equations 29, 31, 32, and 33, the average time between occurrences of the velocity fluctuation equaling zero is given by

\[
\Delta t(u = 0) = \bar{\gamma}((\bar{u}^2 / (\bar{u}^\prime)^2)^{\frac{1}{2}}) \tag{36}
\]

This relationship was used as a cue for assuming the average time between acceleration changes and for a check on the consistency of this assumption. As an assumption, \(\lambda_t\), was set equal to the same ratio as Equation 36.

\[
\lambda_t = K (\bar{u}^2 / (\bar{u}^\prime)^2)^{\frac{1}{2}} \tag{37}
\]

Digital computer programs were written and used to calculate the random walk as described by Equations 30, 31, 34, 35, and 37. All the conditions given by Equations 29, 32, 33, and 36 were found to be satisfied \((66)\) only when \(K = 1\).
The above tests on the model proved the consistency of the assumptions involved. And, as a first test of the model for describing turbulent diffusion, the one dimensional mean square displacement from a continuous point source was predicted. To do this, the position of a fluid element was found by integrating Equation (11).

\[ X(t) = \int_{0}^{t} U(t) \, dt \]  

(38)

The expected mean square displacement as a function of time was estimated by averaging the squares of the displacement for many simulations of the motion of a fluid element. These results were compared to experimental diffusion calculations of the radial mean square displacement from a continuous point source at the center of a duct given by Flint et al. (45). The model prediction fit the experimental data and hence it was felt that this description of turbulent motion could be used in simulating turbulent diffusion.

Evaluation of Stochastic Processes

The Monte Carlo approach

To determine the behavior predicted when a particular model is used to simulate a physical process, it is necessary to evaluate the results under the conditions imposed. Some-
times this may be accomplished directly by analytical means or with additional simplifying assumptions to the model. Another procedure is to solve the equations arising from a mathematical analysis using finite difference methods, if the analytical solution is not possible. Both of these methods involve the reduction of the model to a set of differential equations which in turn must be solved. The restrictions involved in the reduction of the models to a mathematical form and the hypothesis necessary for the solution of these mathematical statements may need to be so stringent that important features of the model cannot be included. Also, in some instances, the calculations involved can be so numerous or intractable that a direct solution is not feasible.

In the case of stochastic models it is often possible to use the model to simulate the process which is controlled by the probabilistic laws included in the model. Having made several simulations with the same initial conditions and external forces, the results of these trials are statistically evaluated from which an estimate of the value desired is calculated. This method of evaluating some property of the process is known as the Monte Carlo method (21, 83, 86, 87, 136) and is defined in more generality by Bauer (13).
The Monte Carlo method consists of formulating a game of chance or a stochastic process which produces a random variable whose expected value is the solution of a certain problem. An approximation to the expected value is then obtained by means of sampling from the resulting distribution. As in almost all numerical processes, only an approximation to the correct answer is obtained. In this case, instead of the primary source of error being due to round-off, the primary source of error is due to the fact that only a finite sample can be taken. It follows of course, that the degree of accuracy depends on the sample size.

Although the use of the sampling techniques was known earlier in history, it was not until the advent of high speed computers that the use of this procedure became feasible. An early application of Monte Carlo methods was that of solving the problems of neutron diffusion through slabs (82, 142). A few examples of the later uses of Monte Carlo have been the simulation of physical systems such as molecular flow rates through cylindrical elbows and pipes (31), equation of state calculations (85), operational analysis of scheduling (69), studies of electric fields (99), the solution of boundary value problems (38, 63), matrix inversion (46), and the solution of integral equations (29).

The great versatility of the Monte Carlo method is indicated by its wide variety of applications. This is because one can include nearly all the known information about the problem in the solution. However, as indicated previously, the error depends on the number of samples taken.
Therefore, if the calculations involved are lengthy, the computation time required even with use of the high speed computers now available can be quite large (128, 138). The reduction of the amount of necessary calculations and the extraction of the largest amount of information from the computations is the primary role of Monte Carlo (62). In fact, the more information for the same amount work, the better the Monte Carlo technique is said to be (53).

Monte Carlo applications as a whole fall into two categories, the first of these being the solution of mathematically difficult statements as for instance the evaluation of high order integrals and integral equations (2, 29), the inversion of large matrices (46), and the solution of simultaneous differential equations (28, 38, 141).

The other general use of Monte Carlo techniques is that of simulating physical processes by analogy (15, 65, 94 126). An analog of the system is first developed by specifying probability distributions for the behavior of an element when involved in any condition allowed by the analog. Using the same boundary and initial conditions, several elements are allowed to move within the analog. The average of the histories of each of the individual elements then is a solution to the behavior of the whole analog.

Involved in the analog type problem is what is known as the random walk procedure (60, 61, 78, 84, 140). That is, an element is allowed to move through a given space.
At the end of each step, the next movement is randomly chosen from a probability distribution which depends on the past history of the motion of the element. The problem is to determine the probability of traversing to another point in the space in a specific number of steps or a certain period of time (44, p. 330).

**Random number generation**

Fundamental to the application of Monte Carlo techniques is the ability to rapidly obtain random values having a given distribution. In theory, a truly random number can be only developed from such proverbial devices as the perfect roulette wheel. Yet, it is possible to produce pseudo-random numbers which satisfy various properties and tests of random numbers (23, 27, 107).

For hand calculations a simple method would be to take the values from published random number tables (100). However, this can be quite time consuming when using high speed computers, particularly if a large number of random values are required. Hence for high speed computers, a more satisfactory manner usually will be to generate the pseudo-random numbers internally.

An important theorem is that any probability density for a continuous variate $s_2$ may be transformed to the
uniform probability density

\[ f(s_1) = \begin{cases} 1, & 0 < s_1 < 1 \\ 0, & \text{otherwise} \end{cases} \quad (39) \]

by letting the \( s_1 = F(s_2) \) where \( F(s_2) \) is the cumulative distribution (91, p. 107).

To obtain a random variable \( s_2 \) having a given cumulative distribution \( F(s_2) \), a uniformly distributed random number \( s_1(0 < s_1 < 1) \) can be generated and the variable \( F^{-1}(s_1) \) will have desired probability density. However in many cases, notably the normal probability density, the inverse function \( F^{-1}(s_1) \) is not easily calculated.

Methods other than the direct calculation of an inverse of the cumulative distribution are also possible for obtaining random numbers having a desired distribution. If the computer memory storage is sufficiently large, the range of the variate can be partitioned into, say, \( k \) increments such that the cumulative value of the probability density over each increment is equal to \( 1/k \). A table consisting of the mean value of the variate for each increment may then be located in the computer memory. And, by selecting the members of the table from a uniform distribution, the values obtained will have the desired distribution.

Also, approximations of some distributions can be generated. The central limit theorem provides the basis for developing an approximation for the normal distribution
That is, by adding several uniformly distributed random numbers together and adjusting the sum by known constants, an approximation of a normally distributed random variable is obtained (59, 62).

As the above discussion would indicate, if there exists a means of generating an uniformly distributed random variable, then other distributions are also possible. Simple fast generators of uniformly distributed pseudo-random numbers are available. One of the more popular of these arithmetic schemes is that of the power residue method which adequately meets several requirements and tests of randomness when certain parameters are used (62, 92, 119). A more recent modification of this multiplicative procedure has been to use the shifting operation of a computer instead of multiplying. This essentially makes the method additive and thus greatly reduces the time of generation of an individual random number (27, 107).
THEORETICAL DEVELOPMENT

Introduction

The ultimate question in any study of the diffusion process is; given the concentrations of a field at a certain time, what will be the concentrations at a later time?

Several approaches to determining the answer to the above question can be taken. The most direct attack on the problem would be to conduct an actual experiment. Samples could be drawn from the flow field at the various times and positions. By smoothing the data, the concentration profiles for the desired conditions could be estimated. The initial conditions and boundary conditions would be determined by the experimental procedure and apparatus used to solve the problem. While this would give the concentrations for specific conditions, the information by itself would lend little to the general knowledge of the diffusion process.

A more fundamental approach is required if any general description of the diffusion mechanism is to be obtained. A partial differential equation can be developed to describe the diffusion process. By fitting the equation to the diffusion data, the unknown terms in the equation can
be found. On the basis of these evaluated coefficients, the diffusivities under the various turbulence conditions can be compared. Also, having a knowledge of the diffusivities one can predict the concentrations under other turbulence conditions by solving the partial differential equation.

Extensive experimentation is required to find the necessary concentration data when the turbulent diffusion mechanism is investigated using the above approach. For a number of conditions, it is difficult to obtain good samples. And, the fitting of the partial differential equation to the data is tedious. To simplify the analysis of the data, various assumptions are commonly made with respect to the diffusivity terms of the diffusion equation. The general application of the coefficients found under these assumptions is often questionable.

Another approach to studying the turbulent diffusion process, other than by actual experimentation, is to simulate the experiment with a stochastic process. Analogous to the development of a partial differential equation, a statistical description is made of the turbulent diffusion mechanism. From this description, a stochastic process is developed which can be used to predict the concentrations in the same sense as the partial differential equation is used to solve for the concentrations.
It is this latter approach of statistical sampling which has been used in this research to investigate the problem of turbulent diffusion. The present chapter is concerned with the development of a stochastic process for simulating the dispersion caused by the turbulent motion of the fluid. Also discussed is the programming of the Monte Carlo technique and the analysis of the generated data.

Essential to the stochastic model of turbulent diffusion is an adequate description of the random motions of the macroscopic fluid elements. The statistical model of the turbulent motion used in the present research was developed in a previous study by this author (66). And, the basic model has been expanded to include a description of three-dimensional motion.

Monte Carlo techniques were used to evaluate the stochastic process describing the turbulent diffusion. As will be noted, the simulation of the experiment generates more information than is available from the actual experiment. By using this additional information, the diffusivities could then be evaluated directly from their definition. And hence the computation was greatly simplified in comparison to the fitting of the partial differential equation to the concentration profiles.
Not only does the simulation of the experiment allow for rapid analysis of concentration data, but it also provides a means of studying turbulence properties which are difficult to observe experimentally.

Diffusion Simulation

An analysis of molecular diffusion

To understand how the random walk procedure can be used to simulate the diffusion due to turbulent flow, first consider the molecular diffusion process.

Concentration determinations Assume that one can follow the diffusion of single molecules from a point \( x_0 \). Consider a molecule released into the flow field at time \( t = t_1 \). At time \( t = t_1 + T \), the location of the molecule can be recorded. Another molecule could be released from \( x_0 \) at time \( t = t_1 \), and its position also recorded at time \( t = t_1 + T \). In fact, a large number of molecules could be released and their locations recorded after a time lapse of \( T \).

The recorded positions represent the distribution at time \( t = t_1 + T \) of the molecules which have diffused from an instantaneous point source at \( x_0 \). The local average molar concentration of the diffusing molecules can be
estimated by dividing the volume of some neighborhood surrounding a point into the number of molecules recorded as being located in that neighborhood.

**Flux determinations** The concentration is not the only property of the diffusion process which can be evaluated if one can follow a molecule. The velocity of the molecule can also be recorded as well as the location after a time \( T \). The average of the velocities recorded in some neighborhood surrounding a point is an estimate of the local average velocity of the diffusing molecules a time \( T \) after their release. And, the product of the local average velocity and molar concentration gives the local molar flux referenced to fixed coordinates for the diffusing molecules.

In summary, if the molecule can be followed as it moves through the flow field, the local average concentration can be found in a similar manner to that done in ordinary physical experiments. That is, the number of molecules per unit volume is established. For the physical experiments, the counting is accomplished by such means as refractive index measurements, densities, and titrations. Also, by following the molecules, one can directly evaluate additional properties of the diffusion process such as the local average velocities and fluxes.
Turbulent diffusion

Of interest is the Lagrangian description of the dispersion of the diffusate caused by the macroscopic motion of the fluid. The fluid element in which the diffusate is thought to be entrained is defined as large in comparison to the molecular scale and small in comparison to the microscale of turbulence. Furthermore, the fluid element will be thought to remain intact during the time interval it is observed. That such a hypothetical definition of a fluid element is possible is discussed in Appendix B.

Instantaneous point sources The diffusion caused by turbulence can be visualized as occurring in an analogous manner to that described above for molecular diffusion. An element of fluid is released at a point \( x_0 \) and moves through the flow field as is described in the section on the random walk of a fluid element. After the element has been in motion for a time \( T \), the location of the element is recorded. This procedure is repeated for a large number of elements. After all the walks are completed, the local average concentrations and velocities for the diffusing elements can be found for all points in the flow field as was described for molecular diffusion. In this case the averaged values are ensemble averages. Since, they represent the expected result of all possible diffusions occurring under the same initial and boundary conditions.
Continuous point sources. A modification of the above procedure can be used to simulate a continuous point source. Here the diffusate is injected at time \( t = 0, \Delta t, 2\Delta t, \ldots, T \) as instantaneous point sources. And, the elements simulating the diffusate injected at time \( t = k\Delta t \) would be allowed to walk a total time \( T - k\Delta t \) and then be recorded.

Sources of varying strength. To simulate a point source of varying strength, the number of elements \( N_k \) injected at time \( t = k\Delta t \) would be made proportional to the strength of the continuous source at the same time.

Multiple point sources. Multiple sources can be simulated by merely considering them to be a set of point sources. And, the number of elements that are started at each point would be proportional to the strength of the member of the multiple source which that point source is simulating.

Finite sources. In this case, the starting location would be determined from a probability distribution covering the area of the source. The probability density would be proportional to the rate of injection across the surface of the injector.
Walk efficiency improvements

Uniform strength sources If the turbulence properties of the flow field have temporal homogeneity, it is possible to improve the Monte Carlo efficiency by obtaining more information from each walk. Instead of recording only the position at the end of the walk, record the position of the element after each increment of time $\Delta t$. How this is possible is explained below.

Let the total time for each walk be $T$. For an element starting at time $t = 0$, there will also be one starting at each of the times $t = \Delta t, 2\Delta t, \ldots, T - \Delta t$. Thus the positions recorded at times $t = \Delta t, 2\Delta t, \ldots, T$ represent positions that could be occupied by the elements starting at times $t = T - \Delta t, T - 2\Delta t, \ldots, \Delta t$ respectively.

Varying strength sources For a source which is varying in strength with time, the recorded information can be weighted. If the recording is made at time $k\Delta t$, then a value which is proportional to the strength of the source at $T - k\Delta t$ can be associated with the information recorded.

Hence, much more information can be obtained from each walk by requiring little more computer time than storing away the additional information.

Steady state simulation

The simulation of steady state behavior is analogous to the establishment of the steady state condition in any
actual experiment. That is, set the total time $T$ after initiating the experiment to be long compared to the time dependent processes involved.

**Equations Describing Diffusion**

To analyze turbulent diffusion, first investigate the equations describing the diffusion process.

**Molar fluxes**

The molar flux of a component is a vector quantity which denotes moles of the component passing through a unit area per unit time (16, p. 500). When the molar flux is referenced to stationary coordinates, it is given by

$$N_C = C U_C$$

(40)

where

\[ C = \text{The local average molar concentration of a given component} \]

\[ U_C = \text{The local average velocity of the component with respect to stationary coordinates} \]

The equation of continuity for the component is then

$$\frac{\partial C}{\partial t} = -(\nabla \cdot N_C)$$

(41)
This is the partial differential equation which describes the diffusion process; and, as such, is the one which must be solved to determine variations of concentration with position and time.

Another description of the diffusion process is to reference the flux relative to the local mass average velocity by

\[ J = C(\nabla C - U) \]  \hspace{1cm} (42)

where

\[ \nabla = \text{The local mass average velocity} \]

**The diffusivity tensor**

The flux relative to the local mass average velocity can be related to the concentration gradient as follows

\[ J = -E \cdot \nabla C \]  \hspace{1cm} (43)

where \( E \) is the total diffusivity tensor and is defined by the above mathematical expression. When this is introduced into the equation of continuity, the relationship becomes

\[ \frac{\partial C}{\partial t} + \nabla (CU) = \nabla \cdot E \cdot \nabla C \]  \hspace{1cm} (44)

Note that in this equation, the values of \( CU \) and \( E \) are in general functions of both position and time.

The above analysis is equally true when the ensemble average properties of the flowing fluid and diffusate are
considered. And, it is these ensemble averaged properties which are available from the actual and simulated experiments.

**Boundary conditions**

The stochastic model can be used to study turbulent diffusion in any flow field provided statistical data is available to describe the turbulence. Both steady state and time dependent diffusion processes can be simulated. The unsteady state case can include several types of time dependency. The turbulence structure may be simulated as changing with time. And, the source may be of varying strength which would include the transient case of starting the experiment.

In the present investigation, the flow field studied is fully developed turbulence in a pipe. The source simulated was chosen so that the angular symmetry of the field is maintained. Thus the generated data was stored as a two dimensional array.

The flow system described above may be more precisely defined by the following list of boundary conditions.

1. No radial diffusion can occur at the confining walls of the pipe.

\[
\frac{\partial C}{\partial r} = 0 \quad (r = R_0, \ z = \ z, \ t = t) \quad (45)
\]
2. Radial symmetry exists about the tube center.
\[ \frac{\partial C}{\partial r} = 0 \quad (r = 0, \ z = z, \ t = t) \quad (46) \]

3. Angular symmetry exists throughout the flow field.
\[ \frac{\partial C}{\partial \theta} = 0 \quad (r = r, \ z = z, \ t = t) \quad (47) \]

4. The diffusate becomes uniformly distributed at an infinite distance from the source.
\[ \frac{\partial C}{\partial r} = 0 \quad (r = r, \ z = \infty, \ t = t) \quad (48) \]

5. The system eventually approaches steady state.
\[ \frac{\partial C}{\partial t} = 0 \quad (r = r, \ z < \infty, \ t = \infty) \quad (49) \]

The statistical properties of the turbulent flow are assumed to be undisturbed by the injected diffusate and that they are functions of radial position only.
\[ U = \bar{U} = (0, 0, \bar{U}_z(r)) \quad (50) \]
\[ U_C = (U_{Cr}(r, z, t), 0, U_{Cz}(r, z, t)) \quad (51) \]
\[ C = C(r, z, t) \quad (52) \]

Assuming that the ergodic theorem applies, boundary condition five means that the ensemble averages will be equivalent to the time averages when the steady state is reached.
Determination of diffusivity tensor terms

For laminar flow, the diffusion equation can be greatly simplified. A good assumption is that $E$ can be represented by a constant isotropic molecular diffusivity. Hence, for laminar flow

$$E = \begin{pmatrix} D & 0 & 0 \\ 0 & D & 0 \\ 0 & 0 & D \end{pmatrix}$$

(53)

where $D$ is the molecular diffusivity defined by Fick's first law of diffusion.

Experimental approach The determination of the nature of the diffusivity tensor for turbulent flow conditions has been the object of much recent research (40, 48, 57, 70, 106, 116, 117). Most of these studies have been concerned with the problems of non-transient diffusion processes. In these cases, the ensemble averages are estimated by the time averaged values obtained from the turbulent flow experiments.

To be able to fit Equation 44 to the experimental data, a number of assumptions have often been made as to the nature of $E$. Common assumptions have been that certain terms of $E$ are either functions of radial position only, that they are constants, or that they are zero. These simplifications have generally been applied by necessity and there has been little opportunity to check their validity.
Random walk approach  Essentially the above approach is to solve the equation of continuity by an experiment. And, having the solution in terms of concentration profiles, a restricted form of the partial differential equation is fitted to the data to obtain values of $E$.

In the present research, both the concentration and velocity ensemble averages of the diffusate are predicted by the random walk. This means that it is not necessary to fit these data to the non-linear, second order, partial differential equation of diffusion to obtain values of $E$. Instead, the molar flux $N_C$ can be calculated directly from Equation 40. And, the terms of the diffusivity tensor can be evaluated from the definition of $E$, Equation 43.

A combination of Equation 42 and 43 gives a relation between the concentration, the mass average velocity, and the diffusate velocity.

$$C(U_C - U) = -E \cdot \nabla C$$  (54)

When angular symmetry is considered, the expansion of the above vector equation in cylindrical coordinates is

$$CU_{Cr} = -E_{rr} \frac{\partial C}{\partial r} - E_{rz} \frac{\partial C}{\partial z}$$  (55)

$$C(U_{Cz} - U_z) = -E_{rz} \frac{\partial C}{\partial r} - E_{zz} \frac{\partial C}{\partial z}$$  (56)

There are two linear equations of the above form for each point in the flow field. It is from these equations that
the four terms of the eddy diffusivity tensor may be calculated.

For the assumption that the terms of $E$ are functions of $r$ only, the equations of all the points having the same radial distance form a set of simultaneous linear equations. And, the diffusivities may be estimated from this set of equations by using least square techniques. A check can also be made for the dependence of $E$ on axial position and time. The data can be partitioned along the axial direction and the estimate of diffusivity terms can be made for each partition. The values of $E$ would then be given relative to the radial and longitudinal position. For the time dependency check, the simulation can be made for total walk times such that the diffusion front has not reached the downstream limit of the sampling lattice. The values of $E$ obtained would then be applicable for that total time after starting the injection.

This method of calculating the diffusivity tensor permits a comparison of assumptions commonly made in solving the diffusion equation because a least square estimate of $E$ can be made under each hypothesis. The validity of the assumption can then be checked by considering the magnitude of the terms estimated and the variance of the regression.

In summary, the additional information of the velocity of the diffusate allows a more direct means of finding $E$. 
than is available when only concentration profiles are obtained. The use of Equations 54 and 55 requires less stringent assumptions on the nature of the diffusivity tensor than are necessary if a feasible fit of Equation 44 is to be made to the data.

Turbulent Motion Simulation

Stochastic models of fluid motion

Consider a small element of fluid which will remain intact during the time it is observed. As the element moves through the turbulent field, its velocity will fluctuate in an apparently random manner. The development of models describing such motion was the subject of previous research by this author (66) and is discussed in the Review of Literature.

For the present work, the relationship describing the position of the element will include the velocity and acceleration. Hence, during each step, the position of the element is given by

\[ X(t) = x_i + (t-t_i)u_i + \frac{1}{2}(t-t_i)^2 u_i' \quad t_i < t < t_{i+1} \]  

(57)

where the velocity and acceleration are determined as in Equations 29 through 37.
When more than one dimension is considered, there will be a set of truncated Taylor's series for each direction. And, the distribution of the velocity, acceleration and time for each direction will be related.

For pipe flow, Sandborn (111) found that the stress tensor is of the form

\[
\begin{pmatrix}
\overline{u^2} & \overline{uv} & 0 \\
\overline{vu} & \overline{v^2} & 0 \\
0 & 0 & \overline{w^2}
\end{pmatrix}
\]

Thus, for the present research, the only directional correlation considered is that between the longitudinal and lateral velocity fluctuations, \( \overline{uv} \). This correlation represents the turbulence shear stress and can be numerically evaluated from the mean longitudinal velocity profile (74, 111). The analytical expression relating the \( \overline{uv} \) to \( \overline{U} \) for turbulent pipe flow has been developed by Pia (95) and Laufer (74) to be

\[
\overline{uv} = \frac{d\overline{U}}{dr} + r \frac{U_y^2}{R_o}
\]

(58)

where \( U_y^2 \) is the friction velocity

\[
U_y^2 = - \gamma \left( \frac{d\overline{U}}{dr} \right)_{r = R_o}
\]

(59)
This correlation is included in the turbulent motion simulation through the Lagrangian acceleration which is discussed in a later section. How this correlation arises can be seen from the following phenomenological discussion.

For pipe flow, the mean longitudinal velocity is a monotonically decreasing function of the radius. Whenever an element moves toward the wall, it will have a positive radial velocity. And, since it is moving from a region of higher to lower mean longitudinal velocity, it would more likely have a positive deviation from the mean longitudinal velocity of the region it is entering. The product of these two deviations would be positive. When the element moves toward the center, the radial velocity is negative and the mean longitudinal velocity is greater. Therefore the longitudinal velocity deviation is more likely to be negative and the product of the deviations would be positive. Thus a positive value of $\overline{uv}$ would be expected to result from the radial fluctuations. The result of these radial fluctuations is the transfer of momentum in addition to the molecular momentum flux.

**Symmetry and non-homogeneity of the turbulence**

For pipe flow, the turbulence is not homogeneous but the turbulence properties do have angular symmetry. To simulate the non-homogeneous condition and take advantage of
the symmetry, the cross section of the pipe can be divided into concentric annuli about the center. The average turbulence properties of each annulus are the correlations used to determine the distributions of the velocity, acceleration, and step time of the element while it is in that annular region.

If the statistical properties of the turbulence are not temporally homogeneous, the time could also be divided into equal increments $\Delta t$. And, a different set of statistical properties could be used to represent the turbulence for each time increment.

The model as developed applies for diffusion being described in a rectangular coordinate system. A transformation of the joint probability distribution of the velocities and accelerations to cylindrical coordinates is required. Following such a transformation the conditional probability density of the radial acceleration is

$$p_{v'}(v' \mid v, w) = \begin{cases} p_v(v') \int_{-\infty}^{v} p_v(h) dh \ (v' - w^2/R) < 0 \\ p_v(v') \int_{v}^{\infty} p_v(h) dh \ (v' - w^2/R) > 0 \end{cases} \tag{60}$$

where

$$p_v(v) = \frac{1}{(2 \pi)^{\frac{1}{2}} \sigma_v} \exp\left(-\frac{1}{2} \left(\frac{v}{\sigma_v}\right)^2\right) \tag{61}$$
The longitudinal acceleration is still described in the same manner as is expressed by Equation 34. The joint marginal density function of the velocity components will remain the same under the transformation and is the product of their separate marginal distributions, each of which is a normal distribution similar to that given by Equation 61.

Since the system has angular symmetry, the radial and longitudinal positions need only be known. This eliminates having to follow the angular motion to find the angular positions as a function of time. However an angular velocity fluctuation is required for the distribution of the radial acceleration. Without the angular fluctuation there would be no angular turbulent diffusion and the system would act the same as a flow between two parallel walls since the diffusion could occur only along radians from the center. Thus the angular velocity need only be known whenever a new radial acceleration is to be chosen. An average value of $w^2$ was used in this research. As such, it represents a mean radial acceleration as a function of radial position.

**Recording Data**

One way to record the location of the fluid element is to form a matrix representing the field. The flow field
can be partitioned into small units where each unit of the field is then represented by a term of the matrix. To illustrate this, consider the following example for a two-dimensional flow field, which will be represented by a matrix \([a_{ij}]\).

The diffusate will be assumed to be released at \(x = 0, y = 0\). The field can be partitioned by a lattice having vertical lines at \(x = k_1^i\) and horizontal lines at \(y = k_2^j\) where \(k_1\) and \(k_2\) are scale factors. The area unit bounded by \(x = k_1^i, x = k_1^{i+1}, y = k_2^j, \) and \(y = k_2^{j+1}\) would then be represented as the matrix term \(a_{ij}\).

Initially the flow field is assumed void of any diffusate. Hence, the matrix terms are all set to zero before the first walk is started. To record the location of a fluid element, it is only necessary to increment the matrix term representing the field unit in which the element is located. Should the element go outside the lattice, the location will have to be recorded by other means.

Special considerations

For the study of non-transient behavior, only those regions of the flow field where the diffusion has established a steady state condition would be of interest. And, the lattice partitioning the flow field need only cover the steady state region. Elements located outside this region need not be recorded.
In line with this, special consideration can be given to the case of a flow field having a mean velocity as might occur for flows between two parallel walls or in a tube. The walks which reach positions downstream of the lattice can be discontinued when it is certain that they can not return to the lattice. It is not necessary to waste computing time on a walk which will yield no further information.

Analysis of Generated Data

Once the experiment has been simulated, it is necessary to analyze the generated data as would be done for the results of an actual experiment. The basis of this analysis is the diffusion equation. The use of this equation has been discussed in a previous section. The method of evaluating for the terms of the eddy diffusivity tensor under each of the assumptions considered and the comparison of these results in the subject of the present section.

Evaluation of terms of the eddy diffusivity tensor

The evaluation of the terms of the eddy diffusivity tensor was accomplished using least square techniques. At each point of the flow field investigated, there is a longitudinal flux and a radial flux. Each of these can be repre-
sented in terms of the local concentration gradient and diffusivity by Equations 55 and 56. The assumption is made that the diffusivity is approximately independent of longitudinal position within a given longitudinal partition. This means that the flux at a given radial distance from the center forms a set of samples represented by linear equations have constant coefficients.

To investigate and compare the common assumptions made as to the nature of the diffusivity tensor requires an explanation of the equations used in describing the models. As was noted above, there are two samples of flux taken at each point. Although they are not independent, they do represent two different quantities. The statistical model of these for a given radial position can be stated as

$$J_{ij} = -E_{rr} \frac{\partial C}{\partial r} \delta_{ir} -E_{rz} \frac{\partial C}{\partial z} \delta_{ir}$$
$$-E_{rz} \frac{\partial C}{\partial r} \delta_{iz} -E_{zz} \frac{\partial C}{\partial z} \delta_{iz} + \epsilon_{ij} \quad (63)$$

where

$$J_{ij} = \text{the flux in direction } i \text{ at longitudinal level } j$$
$$i = \text{the direction of flux}$$
$$= r, z$$
$$j = \text{the longitudinal level}$$
$$= n_1, n_1 + 1, n_2 + 2, \ldots, n_2$$
$$\delta_{ir}, \delta_{iz} = \text{the kronecker delta function}$$
\[ e_{ij} = \text{deviation of predicted flux from the observed flux} \]

\[ n_1, n_2 = \text{the range of levels over which the least square fit is made} \]

\[ E_{r2} = \text{the diffusivity terms relating the radial flux to the concentration gradient in the longitudinal direction. The other diffusivity terms are similarly defined.} \]

Common assumptions as to the nature of the eddy diffusivity tensor are that certain terms are either distinct, zero, equal to another term, or constants independent of radial position. Equation 63 can be used to represent any combination of these assumptions. If a diffusivity tensor component is to be equated with another component of the tensor, it needs only to be replaced by its equivalent in Equation 63. If a term is to be assumed zero, the term and its driving force need only to be removed from the statistical model. The result of these three possible assumptions as to the nature of each of the four diffusivity terms gives rise to 51 distinct combinations of diffusivity terms.

For the assumption that the diffusivity terms are constants independent of radial position, the set of diffusivities used in the least square fit includes those found for all radial positions within the longitudinal partition considered.
Analysis of the models

A means of systematically comparing the various models as well as determining the relative importance of the terms within a given model is required. Several methods of making such comparisons based on statistical tests and transport ratios have been employed.

Comparison of models The most general of the possible models is the one in which the four terms have been assumed to be individually distinct. In studying the models, this general model was used as the basis of comparison.

An F test can be used to test the null hypothesis specified under each model against the alternate hypothesis specified by the general model. Specifically what the test checks is the significance of the sums of squares of the deviations removed due to the additional generality of the alternate hypothesis over the null hypothesis

$$F = \frac{(SSH_o - SSH)/df_1}{SSH/df_2}$$

(64)

where

$$SSH_o = \text{sum of squares of deviations under the null hypothesis}$$

$$SSH = \text{sum of squares of deviations under the alternate hypothesis}$$

$$df_1 = p - q$$

$$df_2 = n - p$$
p = number of distinct terms in the general model
q = number of distinct terms in the null hypothesis
n = number of samples of flux used in the least square fit

The assumption is made that the conditions specified under the Gauss-Markoff theorem are adequately satisfied in applying the least square fit of Equation 63 for each model.

For the assumption of all terms in a particular model being independent of radial position, another basis of comparison was used. In this case, the alternate hypothesis was formed from the general model for each of the radial positions included. Thus the sum of squares for the alternate hypothesis was the sum of the SSH found for each radial position. And, the number of distinct terms in the alternate hypothesis was four times the number of radial positions included in the test.

The importance of terms within models

Several means of checking the relative importance of each term in a given model were used.

The t test

The t test (91, p. 304) was used to check the significance of each diffusivity term evaluated within a given model relative to the assumption that it is zero.

\[ t = \frac{(E_i - E_i^*)}{\left[ (a_i^i)(SSH_0)/(n-q) \right]^{\frac{1}{2}}} \]  \hspace{1cm} (65)
where

\[ E_i = \text{the estimate of a given diffusivity tensor component } i \text{ as found by the least square fit} \]

\[ E_i = \text{the unknown diffusivity tensor component which is set equal to zero for the test} \]

\[ a_{ii} = \text{the } i, i \text{ term of the variance-covariance matrix} \]

**Confidence interval** A confidence interval based on the t distribution was found for each diffusivity term. For this work, a 90% confidence interval was chosen. This is

\[ P \left[ E_i + CI > E_i > E_i - CI \right] = .90 \quad (66) \]

The value of the minimum half width of the confidence interval is given by

\[ CI = t_{.10} \left[ \frac{(a_{ii})(SSH_o)}{(n - q)} \right]^{\frac{1}{2}} \quad (67) \]

where

\[ P \left[ -t_{.10} < t < t_{.10} \right] = 0.90 \quad (68) \]

and the variable t has the "Student's t" distribution with n-q degrees of freedom.

**Transport ratio** To check the relative importance of the flux given by the product of a diffusivity tensor component and its associated concentration gradient, a transport ratio was used. The average flux predicted by
a particular term in the diffusion equation is compared to
the magnitude of the average observed flux vector component
in the same direction.

\[ \text{TR}_{ij} = \frac{\hat{E}_{ij} \sum \frac{\partial C}{\partial j}}{|\sum J_i|} \quad (69) \]

where

\[ \sum \frac{\partial C}{\partial j} = \text{the sum of the concentration gradients observed in the } j \text{ direction at the points used in the regression} \]

\[ \sum J_i = \text{the sum of the observed flux in the } i \text{ direction at the points used in the regression} \]

\[ i = r, z \]

\[ j = r, z \]

Also, a comparison of the magnitude of the average predicted
flux vector to the magnitude of the average flux vector ob-
served was calculated at each radial position. This check
was made in the form of a transport ratio between the two
quantities

\[ \text{TTR} = \left[ \left( \hat{E}_{rr} \sum \frac{\partial C}{\partial r} + \hat{E}_{rz} \sum \frac{\partial C}{\partial z} \right)^2 \right]^{\frac{1}{2}} / \left[ (\sum J_r)^2 + (\sum J_z)^2 \right]^{\frac{1}{2}} \quad (70) \]

\[ + \left( \hat{E}_{zr} \sum \frac{\partial C}{\partial r} + \hat{E}_{zz} \sum \frac{\partial C}{\partial z} \right)^2 \]
Eulerian to Lagrangian Data Transformation

Statistical properties describing the structure of turbulence are needed to be able to simulate the random motion of a fluid element. Three coefficients are required for the stochastic model used in this research. The statistical values needed are the mean velocity, the variance of the velocity, and the variance of the velocity time derivative. As will be shown, these values can be obtained from correlations commonly used to characterize turbulence.

Most studies of the statistical properties of turbulence are made in the Eulerian system. This is because the turbulence intensity and correlation coefficients can be measured by such means as fixed point hot-wire anemometry. However, for turbulent diffusion problems, the dispersion can be more easily represented in terms of the Lagrangian system. The primary example of the use of the Lagrangian correlation coefficient to explain turbulent mixing is Taylor's theory of diffusion by continuous movements (121) as was described in the Review of Literature. Thus to use the available statistical turbulence data in the present model requires that it be transformed from the Eulerian system to the Lagrangian system.
Velocity transformations

For the present description of diffusion, the model assumes that the diffusate is being dispersed by the local motion of the fluid. That is, the velocity of the diffusate is the same as the local moving medium. The substantial derivative can be used to transform the local Eulerian properties observed by the diffusate following the fluid

\[
\frac{DS}{Dt} = \frac{\partial S}{\partial t} + (\mathbf{U} \cdot \nabla)S
\]

(71)

where \( S \) is some property of the fluid. As an example, consider the property of position \( X \). The Lagrangian rate of change of position is thus

\[
\frac{DX}{Dt} = \mathbf{U}
\]

(72)

Hence, the velocity which the element experiences is the same as the velocities of the points it passes through. Similarly, the variance of the velocity will be the same as the local velocity variance.

Acceleration transformations

A requirement of the motion of a fluid element is that it must satisfy the equation of motion. For a general discussion of this equation, the reader is advised to study
Bird (16, p. 76). Pai (95) and Laufer (74) have applied the equation of continuity to the equation of motion under the assumption of an incompressible turbulent flow. It follows directly from the analysis made by these last two authors that the mean value of the Lagrangian acceleration is

$$\frac{\bar{V}}{\text{Dt}} = \frac{1}{r} \frac{d}{dr} (r \bar{u} \bar{v})$$ (73)

$$= - \frac{1}{\rho} \frac{\partial F}{\partial z} + \gamma \left( \frac{d \bar{U}}{dr} + \frac{1}{r} \frac{d \bar{U}}{dr} \right)$$ (74)

$$\frac{\bar{V}}{\text{Dt}} = \frac{1}{r} \frac{d}{dr} (r \bar{v}^2) - \frac{w^2}{r} - \frac{1}{\rho} \frac{\partial F}{\partial z}$$ (75)

$$\frac{\bar{W}}{\text{Dt}} = 0$$ (76)

What these terms represent is the mean rate of change of momentum due to the pressure drop. The pressure distribution data is not available, but the Reynolds stresses are given by Laufer (74) and Sandborn (111). Thus, the expressions given by Equations 73 and 75 can be used to find the mean Lagrangian accelerations as a function of radial position.
Expressions relating the Eulerian correlations to the variance of the Lagrangian acceleration can also be found from the equation of motion. However, terms arise in the relationship for which there are no physical data available. To find the variances of the Lagrangian accelerations, the following empirical approach was taken.

As may be noted, finding the variance of the Lagrangian acceleration is related to the general problem of making the transformation of correlations from the Eulerian to the Lagrangian system. Among the first to discuss the problem was Brier (20). Later considerations have been made by Frenkiel (49), Mickelsen (88), and Baldwin and Walsh (4). The approach of Mickelsen and Baldwin was to experimentally compare the Lagrangian and Eulerian correlation coefficients. The turbulent intensity and the Eulerian correlation coefficient were measured by hot-wire anemometry. The Lagrangian correlation was characterized by turbulent diffusion of helium and by turbulent heat transfer. Cross plots of the turbulent spreading showed a linear relation between the shapes of the Lagrangian and Eulerian correlation coefficients.

The following is a summary of the basis of Mickelsen's (88) analysis. A Lagrangian scale of turbulence can be defined as
\[ L_L = \sigma_u \int_0^\infty R_{tL}(t) \, dt \quad (78) \]

where

\[ R_{tL}(t) = \frac{u(X(0))u(X(t))}{\sigma_u^2} \quad (79) \]

In an analogous manner, an Eulerian scale can be defined as

\[ L_E = \int_0^\infty R_{xE}(x) \, dx \quad (80) \]

where

\[ R_{xE}(x) = \frac{u(x_0)u(x)}{\sigma_u^2} \quad (81) \]

For a homogeneous field of turbulence, the Lagrangian and Eulerian scales are proportional

\[ L_E = BL_L \quad (82) \]

If the Lagrangian and Eulerian correlation coefficients have the same functional form, then they can be compared according to the following expression

\[ R_{xE}(x) = R_{tL}(x/B \sigma_u) \quad (83) \]

From this comparison Mickelsen (88) found the relation between the time and space coordinates of the Lagrangian and Eulerian correlation coefficients to be a linear proportionality.
This relationship can be readily applied with the model of turbulent motion used in the present research. The velocity can be represented by the model in both the Lagrangian and Eulerian system. Consider the values of the velocity as observed by an element following the fluid

\[ u(X(t_1), t_1) = u(X(t_o), t_o) + \int_{t_o}^{t_1} u'(X(t), t) dt \quad (84) \]

where \( X(t) \) is the position of the element as a function of time and \( u'_t \) is the acceleration of the element. The ensemble average of the product of the velocities at two times gives the Lagrangian correlation coefficient expressed by Equation 79. The correlation coefficients developed by the random walk model were found in a previous study (66) to be linearly related. That is, by scaling the time variable, a single correlation coefficient is developed.

\[ R_{t_t}(t) = R^* \left( t/\left( \sigma_u/ \sigma_u' t \right) \right) \quad (85) \]

Consider now the values of the velocity over space for a given instant of time \( t_o \).

\[ u(x_1, t_o) = u(x_o, t_o) + \int_{x_o}^{x_1} u'(x, t_o) dx \quad (86) \]

The random walk model can also be used to develop a random variable simulating this Eulerian velocity. Instead
of traversing over a time scale, the path traversed is over space at a given instant of time. The Eulerian correlation coefficient expressed by Equation 81 is obtained by time averaging the products of the velocities at two points in the space. In this case, the correlation coefficients developed by the model are related by scaling the space dimension. The necessary scale factor is the ratio of the standard deviation of the velocity to the standard deviation of the rate of change of velocity with distance.

\[ R_{XE}(x) = R^*(x/(\frac{\sigma_u}{\sigma_{u_x}})) \]  

Thus the functional forms of the correlation coefficients developed by the model for the Eulerian and Lagrangian systems are the same. By substituting Equations 85 and 87 into Equations 78 and 80

\[ L_L = (\frac{\sigma_u^2}{\sigma_{u_t}}) \int_0^\infty R^*(s)ds \]  

\[ L_E = (\frac{\sigma_u}{\sigma_{u_x}}) \int_0^\infty R^*(s)ds \]  

From Mickelsen's results, these two scales are related by a linear proportionality as is given by Equation 82

\[ \sigma_{u_t} = B \sigma_u \sigma_{u_x} \]  

This gives a means of empirically transforming the available Eulerian spacial derivative variance data found from hot-wire
Random Walk Calculation Procedure

To improve the efficiency of the random variable generation and the sampling of the resulting distributions is a primary goal of the Monte Carlo method. The generation of random variables has been discussed in the Review of Literature. Sampling efficiency can be improved by using information which is known about the process as was discussed in the sections on source simulations and the recording of walk data. Improvements of the computational efficiency can also be obtained by considering the computer operations.

Reformulation of the random walk

The time duration of each step of the walk is exponentially distributed for each direction. Hence, the time duration of the steps in each direction will in general be different. When a new acceleration term is chosen for the longitudinal direction, the radial position will have to be calculated for the equivalent time of the radial direction to determine which annular set of velocity correlations apply.
The multiplication and division times of the computer used are approximately five times greater than the addition time. As may be seen from above, several multiplications and divisions are required for each step of the walk. Furthermore, to take advantage of the time homogeneity as was described in the source simulation discussion requires that the location and velocity of the fluid element be known after equal increments of time \(\Delta t\). A substantial reduction in computing time can be realized if the computational procedure is expressed as additive operations.

To accomplish these improvements in efficiency, the time duration between disturbances for the longitudinal and radial directions were chosen as integral multiples of a constant time increment \(\Delta t\). The equivalent form of Equations 30 and 57 for these integerized steps would be

\[
\begin{align*}
    u_{k+1} &= u_k + u_{k+1} \Delta t \\
    x_{k+1} &= x_k + \frac{1}{2}(u_k + u_{k+1}) \Delta t
\end{align*}
\]

By scaling the velocity and acceleration, the multiplication by the constant increment of time \(\Delta t\) can be avoided. The new parameters chosen were

\[
x_k^* = x_k / L_x
\]

\[(94)\]
\[
U^* = \frac{U_C}{\Delta x} / (2L_x) \\
U_k^t = \frac{(\Delta t)^2}{2L_x} (96)
\]

where \( L_x \) is the distance scale in the x direction.

Equations 91, 92, and 93 become

\[
U_k^* = U^t_k + U^t_{k+1} \]

\[
U_k^* = U_{k+1}^* + U_k^* \]

\[
x_k^* + x_{k+1}^* + u_k^* \]

Thus, the velocity and locus are generated for each
direction by a series of incremental additions. The only
restriction on \( \Delta t \) is that it must be small compared to the
expected step time between disturbances \( \lambda_t \).

**Calculation of cumulative distributions**

The generation of the random variables having the de-
sired distributions is described in a previous section. The
method applied in this work is to generate a uniformly dis-
tributed random number and find the inverse of the cumula-
tive distribution in a table stored in the computer memory.

To determine the sign of the acceleration for either
the radial or longitudinal direction requires evaluating
the cumulative distribution of the velocity in that direction.
This integral can easily be made a function of a single variable

\[ P \left[u'_i > 0\right] = G(h) \]  \hspace{1cm} (100)

by the linear transformation

\[ h = (u'_i - \bar{U}) \left(1/ \sigma_u\right) \]  \hspace{1cm} (101)

where \( G(h) \) is the cumulative normal distribution.

Thus the cumulative distributions could also be tabulated in terms of the value of the transformed variable.
And, the normalizing factors can be found from values tabled according to the annular region in which the element is located. Instead of having to integrate for the conditional cumulative distribution at the end of each step, the integral could be evaluated from stored tables.

**Boundary conditions**

**At the wall** The boundary condition imposed on the model at the wall is that the element is reflected whenever it hits the wall. The opposite assumption would be to consider the energy to be totally dissipated when the element hits the wall.

In conjunction with the preliminary checks of the program, both of these assumptions were considered. For the elastic collision case the element was reflected by the
amount it was calculated to be outside the tube and the signs of velocity and acceleration were both made minus. The inelastic collision case was simulated by relocating the element just inside the tube, setting the velocity equal to zero, and the sign of acceleration negative.

A response to the different boundary conditions was noted in the results. For the inelastic case, the concentration at the wall became larger than the concentrations in the intermediate annular regions. The assumption of an elastic collision with the wall did not display this peculiarity. It is also felt that the assumption of conservation of energy is more correct because any generation or dissipation of energy is considered by the mean Lagrangian acceleration.

At the center Radial symmetry was assumed at the center of the tube. To simulate this boundary condition, the motion of the element was set to its mirror image when the radial distance of the element was found to be negative after an incremental change of position.

Radial position determination

As was mentioned previously, the properties of pipe turbulence can be tabulated with respect to annular regions. And to exploit this simplification, one must be able to easily determine the annular region in which the fluid element is located.
The model developed for simulating turbulent motion is described in terms of rectangular coordinates. The radial position based on motion in a rectangular system is

\[ r = (x_0 + \int x'\,dt)^2 + (y_0 + \int y'\,dt)^2)^{\frac{3}{2}} \] (102)

Similarly the radial velocity is

\[ v = ((x_0 + \int x'\,dt)x' + (y_0 + \int y'\,dt)y')/r \] (103)

To simplify the calculation and to avoid the multiplication and square root procedures required by Equations 102 and 103 the following consideration was made.

When the distributions are transformed to cylindrical coordinates as is represented by Equations 60 through 63, the velocity marginal distributions transform directly. But, the acceleration distributions involve functions of the radial and angular velocities. If the coordinate systems are initially aligned so that the x-direction parallels the radial direction, the radial acceleration is

\[ v' = x'' + \frac{w^2}{r} \] (104)

In this relationship the radial acceleration is the lateral acceleration plus an acceleration represented by the angular velocity term. Since the angular position is not required, one approximation would be to use some mean
value of \( w^2 \). As may be noted, the term becomes undefined at \( r = 0 \). To overcome this difficulty, the walk was considered to be stepwise transformed. That is, after each step of the walk the coordinate systems are realigned. To do this, a mean lateral acceleration \( x'' \) was sought such that Equations 102 and 103 would be approximately satisfied at the end of each step.

When the coordinate systems are initially aligned

\[
\begin{align*}
  x_0 &= r_0 \quad y_0 = 0 \\
  x' &= v \quad y' = w
\end{align*}
\]

An average value of \( x'' \) is required such that

\[
r = x_0 + \int x'dt + \int\int x''dt \, dt
\]

To evaluate \( x'' \), Equations 102 and 106 were equated and average lateral and tangential velocities were assumed.

\[
x'' = \left( (x_o \pm \sigma_v \lambda_t)^2 + (\sigma_w \lambda_t)^2 \right)^{\frac{3}{2}} - (x_o \pm \sigma_v \lambda_t)/ \lambda_t^2
\]

The mean value of the lateral acceleration used was dependent on the sign of the radial velocity.

**Programming the random walk**

The calculation of the random walk is greatly simplified when the above procedures are applied. The walk as
reformulated is reduced to a series of additions, normalizations, tabled data retrievals, data storages, and logic decisions.

The program for calculating the random walk was written for the IBM 7074 digital computer. The input, output, table computations, and evaluations are written in the IBM FORTRAN language. To be able to make the most efficient use of the machine operations, the random walk is written as a subroutine in the IBM AUTOCODER language.

The order of the computational procedure is given as follows:

1. Input operation codes defining the flow field and analysis procedures.
2. Input all statistical properties of the turbulent flow field.
3. Calculate and table the distributions required for the random walk.
4. Simulate the diffusion process by the random walk procedure.
5. Output concentration profiles and velocity profiles in tabled form.
6. Analyze and output the generated data in terms of diffusivities.

The programs written for this simulation and analysis of diffusion from a point source in turbulent pipe flow are
presented in Appendix E. A general picture of the simulation procedure can be gained from the basic flow sheet in Figures 1 and 2.
Begin Simulation

NW := No. of walks
N := 0
KT := Total time

Begin New Walk

k := 0
k_r := 0
k_z := 0
r := 0
z := 0
I := 0
J := 0

Generate RN
K := RN
v_k := (v_o)_K

Generate RN
K := RN
u_k := (u_o)_K

New Axial Step

Generate RN
K := RN
k_z := k_z + ((\gamma_z)_I)_k

Generate RN
K := RN
|u^t| := ((u^t)_I)_K

Generate RN
K := RN
v^t := ((v^t)_I)_K

New Radial Step

Generate RN
K := RN
k_r := k_r + ((\gamma_r)_I)_K

Generate RN
K := RN
|v^t| := ((v^t)_I)_K

Generate RN
K := RN
v^t := ((v^t)_I)_K

Increment Step

u^t := +|u^t|

v^t := +|v^t|

Figure 1. Flow diagram I of the random walk
Figure 2. Flow diagram II of the random walk
The purpose of the present research has been to demonstrate the applicability of Monte Carlo techniques to studying chemical engineering problems and turbulent diffusion in particular. The Monte Carlo procedure has been used to simulate the turbulent diffusion from a continuous point source at the steady state condition and several transient times. The results of these simulations have been used to investigate several of the assumptions commonly made in describing the turbulent diffusion process.

The primary type of Monte Carlo application is the comparison of proposed processes. For instance, the question investigated in neutron diffusion studies is often which materials and construction designs give the best shielding. Or, for inventory control, the problem may be to determine which purchase policies give the greatest profit.

In many of these studies, the absolute numbers may be unrealistic but the relative values between cases are meaningful. From the results of the simulations made for each of the cases, statistical inferences can be made as to the significance of the differences between the various proposals.

For studies such as the investigation of neutron diffusion, the flux through particular shield designs can be experimentally determined. Also, the experiments can be
simulated and the generated data compared with the physical data. The effectiveness of other shield designs can also be predicted by simulating the experiment for testing the shield. And if absolute values of the flux are desired, the previously made comparison between the simulated and experimental flux can be applied.

The degree of accuracy associated with the Monte Carlo simulation depends on the sample size. Thus, the magnitude of the differences one should expect to be able to discern is limited because only a finite number of samples will be taken in any particular simulation.

With the above conditions in mind, the following types of Monte Carlo simulations were made of turbulent diffusion.

1. A steady state continuous point source turbulent diffusion experiment was simulated for a Reynolds number of 50,000. This was compared with the available steady state concentration profiles to determine the Eulerian to Lagrangian transformation factor.

2. Time dependent simulations were made of turbulent diffusion from a continuous point source for given times after the injection was started. Instead of the concentrations going to a uniform profile with distance from the source as in the case of steady state diffusion, large concentrations gradients were realized both radially and longitudinally.
Figure 3. Steady state longitudinal concentration profile for $r/R_o = 0.45$
The turbulence structure data used in these simulations is presented in Appendix A.

Discussion of Simulation Procedure

Sample fluctuations

The values sampled for the concentration and velocities are the average value of the contributions made by the elements passing through the cell. For large gradients the error introduced by the fluctuations due to the finite sample size is relatively small. When small differences are to be examined such as those occurring in the region of a uniform concentration profile, the effect of the fluctuations is appreciable. As an example of this, the steady state longitudinal concentration profile is plotted in Figure 3 for a radial distance of \( r/R_0 = 0.45 \). These fluctuations are quite severe since a first derivative of this curve is required to evaluate the eddy diffusivity tensor components.

The effect of these sample fluctuations is observed in the calculated confidence interval. For the downstream half of the lattice considered in the steady state case, Figure 34, it is noted that the 90 per cent confidence half interval is of the order of magnitude of the estimated eddy diffusivity tensor components.
The fluctuations of the samples can be reduced by doing more random walks in each simulation. In this study a substantial reduction of the fluctuations was observed in the 1000 walk simulation presented over the preliminary 100 walk trials used in checking the program. The 1000 walk simulation and analysis made of the steady state case required approximately nine minutes on the IBM 7074 digital computer. Of this time, roughly six minutes were used to simulate the diffusion process. Any substantial increase in the number of walks made to reduce the fluctuations may not be worth the additional computer time required.

As an alternate approach the data could be smoothed as is commonly done for experimental diffusion data before an analysis is made. A possible smoothing procedure is discussed in Appendix C. For the present analysis, a form of local smoothing was done by taking the average values of four cells to represent the conditions at the corner point common to the four cells.

The low concentration predicted for the cell containing the source is due to an error in the initial count procedure. The time increment was adjusted so that the element would make approximately 10 contributions per longitudinal partition it passes through. No contribution was made until the end of the first increment. If a contribution had also been made at the beginning of the first increment after release,
the concentration would be approximately ten per cent
greater.

**The Eulerian to Lagrangian transformation factor**

The empirical Eulerian to Lagrangian transformation procedure discussed in a previous section was used to find the Lagrangian acceleration variances. The value of 2 used for B in the simulations presented in Appendices D and F was determined by trial and error during the time the program was being checked. How well the simulated results compare in the steady state case is illustrated by Figure 4.

In a sense, the transformation factor has been used to fit the model to the physical process. For the purposes of comparing the turbulent diffusion process at different times after the initial injection, the factor was believed to be adequate.

**Problems associated with the tube geometry**

The center represents a pole due to the transformation from rectangular to cylindrical coordinates. Having the diffusate injected at the center as a point source seemed to impose a severe strain on the approximation used to make the stepwise transformation. As a first approach \( \bar{w}^2/r \) was used as the mean radial acceleration due to the geometric transformation. This approach was found to have a strong inter-
Figure 4. Comparison of simulated and experimental steady state concentration profiles
action with the value of the Eulerian to Lagrangian transformation coefficient applied. For small values of \( B \), the center concentration would drop to zero and then fluctuate between 3 and 5 at large distances from the source. When large values of \( B \) were used, the effect of \( \frac{w^2}{r} \) was negligible.

As may be noted for the stepwise transformation approximation used in this work, a uniform profile was not reached at large distances from the source in the steady state experiment. This represents an inadequacy of the approximation. The method was first tested by not considering the direction of the radial velocity. In this case, the center concentration approached a value of 6 instead of the value of 3 found when the radial velocity direction was considered. A better approximation would be to consider the magnitude as well as the direction of the radial velocity for obtaining the mean radial acceleration.

The cylindrical geometry also poses problems as to the relative smoothness of the results. As an example, consider a pipe divided into 10 annular regions. Any contribution by an element has a weight of 1 in the center annulus but has a weight of only 1/19 in the outer annulus.
Discussion of Turbulent Diffusion Predictions

As was indicated earlier, the steady state concentration profiles were matched with the available experimental concentration profiles. On the basis of this comparison other properties of turbulent diffusion were investigated. The smoothed transient concentration profiles predicted are illustrated in Figures 5 through 8.

The prediction of transient concentration profiles was only a part of the purpose of simulating the turbulent diffusion experiment. A more general purpose has been to study the nature of the eddy diffusivity tensor and to investigate the conditions for which the commonly made assumptions apply. Specifically, the simulations chosen were intended to allow the following studies.

1. To estimate the eddy diffusivity tensor components for the general model as well as for a number of the commonly assumed tensor forms.

2. To study the importance of each of the components of the eddy diffusivity tensor.

3. To compare the restricted forms of the eddy diffusivity tensor to the general model.

4. To investigate the longitudinal position dependency of the eddy diffusivity tensor.
Figure 5. Smoothed longitudinal concentration profiles for $r/R_o = 0.05$
Figure 6. Smoothed longitudinal concentration profiles for $r/R_o = 0.15$
Figure 7. Smoothed longitudinal concentration profiles for \( r/R_o = 0.45 \)
Figure 8. Smoothed longitudinal concentration profiles for $r/R_0 = 0.75$
5. To investigate the time dependency of the eddy diffusivity tensor.

The regression procedure used to estimate and analyze the simulation data has been described in a previous section. The results of a number of these analyses are shown in Appendix F.

The importance of a given component of the eddy diffusivity tensor cannot be judged solely on its magnitude. However, it is profitable to look at the values of the tensor components in relation to each other in studying the nature of the eddy diffusivity tensor.

Two observations were made from the analysis of the simulations given in Figures 33 through 38. As a whole, the components of the tensor associated with the longitudinal gradient tended to be as much as an order of magnitude larger than the components associated with the radial gradient. The second observation is that the component $E_{rz}$ tended to be negative while the other components were generally positive. However, the importance of these two observations is tempered by the following discussion of the significance and transport ratio associated with each component.

The significance of a tensor component was studied through the statistic $t$ defined by Equation 65. Also the confidence interval of each term was calculated using Equation 67 on the basis of the "Student's $t$" distribution. It
will be noted that the confidence interval increases quite rapidly as the wall is approached. It is felt that it is due primarily to the random fluctuations of the samples. As was discussed previously, for regions where the relative differences of concentrations and velocities become small between cells, it is difficult to discern small trends.

A large confidence interval was also noted for diffusivity tensor components associated with the longitudinal concentration gradient. This is also felt to be primarily due to the small relative differences in the longitudinal direction. A prime illustration of this is Figure 3 in the region where a uniform concentration is being approached.

The transport ratio proved to be a valuable means of interpreting the importance of the components of the diffusivity tensor. A general observation based on the analysis given in Figures 33 through 38 is that the radial and longitudinal flux associated with the longitudinal gradient is important at the center and then again near the wall. This may be partially explained on the basis of the boundary conditions expressed by Equations 45 and 46. As the wall or center is approached, the radial gradient goes to zero. Thus if there is to be any flux as expressed by Equations 55 and 56, the driving force must be the longitudinal gradient.
It is also interesting to note the importance of the longitudinal and radial components of the flux vector. This may be seen in Figure 41 which represents the evaluation of the eddy diffusivity tensor under the assumption that the flux occurs only in the radial direction. As is noted by the value of the total transport ratio, the flux is essentially radial in the center. However, as the wall is approached the longitudinal flux becomes as important as the radial flux. This is thought to occur from two causes. In the center the longitudinal bulk flow is quite large compared to the longitudinal fluctuations. As the wall is approached, the mean longitudinal velocity decreases and at the same time the longitudinal intensity becomes quite large.

Assumptions are often made as to the nature of the eddy diffusivity tensor to be able to evaluate the tensor components from experimental concentration profiles. As was noted in the foregoing discussion the importance of a particular component depends on the radial position. Analogously, it would be expected that a particular combination of terms will be a better assumption in one region than another.

The values of the components of the eddy diffusivity tensor were evaluated for a number of the plausible assumptions. The analysis presented in Figures 39 through 40 is for the steady state simulation. The models were evaluated also for the transient cases, but no appreciable difference
from the steady state case was noted for the variance ratio of any given model.

To study the various models the variance ratio $P$ defined by Equation 64 was evaluated at each of the radial positions. If one tests the significance, the results indicate that most of the tests are significant at the 90% significance level. However, in the present study the variance ratio has been used to determine for what conditions the given model has a lower significance.

Two single component diffusivity tensors were investigated. The first assumes that all the diffusion occurs in the radial direction due to the radial concentration gradient. This has been analyzed in Figure 46 and is compared to that calculated by Konopic (70) in Figure 9. The model assuming that the only diffusion occurs in the longitudinal direction due to the longitudinal gradient appears to be valid only near the wall. This is in line with what was indicated by the transport ratio and the fact that such a model does not represent any of the radial flux which occurs in the central region. Both of these single component models do not describe the diffusion very well in the intermediate region.

When the two terms $E_{rr}$ and $E_{zz}$ are used together as is given by Figure 45, they still do not represent the intermediate flow region. However, compared to the other two component models, Figures 41, 43, and 44, the two components
Figure 9. Inverse radial peclet numbers
E_{rr} and E_{zz} represent the best combination for describing diffusion for the center and the wall.

Of the two component models studied, the best combination representing the diffusion in the intermediate region was $E_{rr}$ and $E_{zr}$ which is given in Figure 44. This combination was also previously indicated to be a good two parameter description of the turbulent diffusion process by Konopic (70).

To study the time and longitudinal displacement dependency of the eddy diffusivity tensor, the results were divided into two groups according to whether they were in the first or second half of the longitudinal range considered. An analysis was made of each of these groups as well as the combined longitudinal range. In the transient simulation, the range of the longitudinal positions considered was set so that the elements would still be within it when the walks were discontinued. This allowed the range to be more finely partitioned for the time dependent cases and to still be equivalent to the whole range considered in the steady state case since there would not be any contribution made by elements outside this range.

By this partitioning of the results, the terms of the eddy diffusivity tensor could be estimated at a given time for two longitudinal regions. The comparison of these two results gave a check for the longitudinal displacement de-
pendency of the diffusivity tensor. Similarly the evalua-
tion of the diffusivity tensor over the whole longitudinal
range at several times gave a means of checking the time
dependency.

However, no conclusions could be drawn as to the de-
pendency of the diffusion tensor on time and longitudinal
position. Any trends that did appear were also masked by
the large confidence intervals of the prediction.

The results of these tests are influenced by two
sources of error. The first is a result of the sampling
fluctuations which are common to any experiment. The
second is that the stochastic model describing the diffusion
process is not completely correct. That is, certain trends
noted in the analysis of the simulation may be reflections
of some inconsistency of the stochastic model. An analogous
situation arises when an instrument records information other
than what it is believed to be measuring. While these errors
must be considered, the Monte Carlo technique has proven to
be a useful means of simulating and studying turbulent dif-
fusion for many different conditions.
CONCLUSIONS AND RECOMMENDATIONS

1. A stochastic model can be used to adequately simulate the turbulent diffusion process by Monte Carlo techniques. The simulation can in turn be used to study the turbulent diffusion process by an appropriate statistical analysis procedure.

2. The importance of a given component of the eddy diffusivity tensor is dependent on the radial position. This determines which combination of terms gives the best description of the diffusion process in a given region.

3. For the region intermediate to the central core and to the wall, a restricted two component tensor composed of $E_{rr}$ and $E_{zr}$ was demonstrated to be the best combination of those tested. However, for the wall and the tube center, the two components $E_{rr}$ and $E_{zz}$ gave a better fit to the simulated diffusion data.

4. Further investigations of the dependence of the diffusivity tensor components on time and position by simulating the diffusion from other types of injectors such as ring sources and finite sources are suggested. This can be done by starting the random walk at a radial position other than the center.

5. Instead of a cylindrical flow field, the turbulent diffusion between parallel plates should be studied. This
would eliminate the problem encountered with the transformation of coordinates of the probability distributions.

6. The relation between the Eulerian and the Lagrangian systems could be investigated on the basis of the analysis used to estimate the Lagrangian acceleration variance.

7. Some means of experimentally measuring the local flux should be developed. The method used in this study for evaluating the components of the eddy diffusivity depends on a knowledge of the local flux. In the Monte Carlo simulation, this was predicted as a result of the random walk procedure. If one could experimentally determine the local flux, then the same method of calculating the diffusivity tensor components could be used. Thus the components of the diffusivity tensor could be evaluated directly from the diffusivity tensor definition rather than having to fit the second order non-linear partial differential equation of diffusion to the concentration profiles.
NOMENCLATURE

The following nomenclature applies to all preceding sections. In some instances a term has been used with a particular meaning other than that listed in the following nomenclature and is defined as such within the text of the section for which it applies.

Arabic

A Constant in Taylor displacement equation

\( a_{ij} \) A term in the variance-covariance matrix

\( [a_{ij}] \) Matrix representing flow field

B Transformation ratio of Eulerian to Lagrangian scales

C Molar concentration of diffusate

\( \text{Cov}[H] \) Covariance of \( H \)

CI Confidence half interval

c Correlation coefficient of Taylor-Goldstein model

D Molecular diffusivity; substantial derivative operator

\( D_t \) Eddy diffusivity of Taylor diffusion model

d Differential operator; step distance of Taylor-Goldstein model
E General diffusivity tensor component, with double underscore \( (E) \) denotes diffusivity tensor, with double subscript \( (E_{ij}) \) denotes diffusivity tensor component for flux in \( i \) direction caused by a concentration gradient with respect to \( j \) direction

\[ E[H] \] Expected value of \( H \)

\( e_i \) Deviation of estimate \( i \)

\( F \) Statistical ratio defined by Equation 64

\( F(s) \) Probability distribution function

\( f(s) \) Probability density function

\( J_i \) Flux in direction \( i \)

\( J \) Flux vector

\( K \) Proportionality constant

\( k \) Integer valued index

\( L_E \) Eulerian scale of turbulence

\( L_L \) Lagrangian scale of turbulence

\( N_C \) Flux referenced to fixed coordinates

\( P \) Pressure

\[ P[H] \] Probability that \( H \) is true

\( p \) Probability of continuing in the same direction; number of distinct terms in general model

\( p_u(u) \) Probability density function of \( u \)

\( p_v(v) \) Probability density function of \( v \)

\( p_{v'}(v'|v,w) \) Conditional probability density function of \( v' \) given \( v, w \)

\( q \) Probability of reversing directions at the end of a step; number of distinct terms in the null hypothesis
\( R_0 \)  
Pipe radius

\( R_{tL}(t) \)  
Lagrangian correlation coefficient

\( R_{xE}(x) \)  
Eulerian correlation coefficient

\( r \)  
Radial position

\( SSH \)  
Sum of squares of deviations under the alternate hypothesis

\( SSH_0 \)  
Sum of squares of deviations under the null hypothesis

\( s \)  
Time difference; dummy variable of integration

\( s_1, s_2 \)  
Dummy variables

\( T \)  
Total time from beginning of experiment

\( TR \)  
Transport ratio defined by Equations 69 and 70

\( t \)  
Statistical variable defined by Equation 65; time

\( U, V, W \)  
Instantaneous values of the velocities in the \( z, r \) directions respectively

\( U_i \)  
Velocity in direction \( i \)

\( U_C \)  
Local average velocity of diffusate

\( U_f^2 \)  
Friction velocity defined by Equation 59

\( u \)  
Velocity fluctuation

\( u_i \)  
Velocity fluctuation at \( t_i \)

\( u, v, w \)  
Instantaneous values of velocity fluctuations in the \( z, r \) directions respectively

\( \text{Var}[H] \)  
Variance of \( H \)

\( X \)  
Total displacement

\( X \)  
Position vector
\[ X(t) \] Position of Lagrangian element

\[ X_n \] Total displacement in \( n \) steps

\( z \) Longitudinal position

Greek

\( \Delta \) Delta quantity

\( \Delta t \) Time increment

\( \Delta t(0) \) Time interval between zero counts

\( \delta_{ij} \) Kronecker delta function

\( \theta \) Angular position

\( \lambda_t \) Average time per step

\( \pi \) Irrational constant \( 3.14159 \ldots \)

\( \rho \) Density

\( \Sigma \) Summation operator

\( \sigma_u^2 \) Variance of \( u' \)

\( \sigma_u^2 \) Variance of \( u \)

\( \tau \) Time between changes of velocity in Taylor-Goldstein model

\( \tau_i \) Time duration of step \( i \)

\( \nu \) Kinematic viscosity

\( \omega \) Cyclic frequency

Symbols

* Asterisk denotes dimensionless variable

^ Hat denotes estimate or estimator
Prime denotes first derivative

Overbar denotes an average

Underscore denotes vector

Double underscore denotes matrix or tensor

\nabla \quad \text{Del operator}

\cdot \quad \text{Dot product operator}

\int \quad \text{Integration operator}

\partial \quad \text{Partial derivative operator}

\infty \quad \text{Infinity}
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Statistical data describing turbulence

The data used in the random walk procedure simulating turbulent diffusion was that given by Laufer (74) for fully developed turbulent pipe flow. The interpolated dimensionless values as applied are shown in Figures 10 and 11. An explanation of the column headings used as identifiers is given by the following equations:

\[ UU = \frac{\bar{U}}{U_A} \]  
\[ SIGU = \frac{\sigma_u}{U_A} = \frac{(u^2)^{\frac{1}{2}}}{U_A} \]  
\[ SIGV = \frac{\sigma_v}{U_A} = \frac{(v^2)^{\frac{1}{2}}}{U_A} \]  
\[ SIGW = \frac{\sigma_w}{U_A} = \frac{(w^2)^{\frac{1}{2}}}{U_A} \]  
\[ SIGUV = \frac{\sigma_{uv}}{U_A^2} = \frac{\bar{uv}}{U_A^2} \]  
\[ SIGUP = \left( \frac{\partial u}{\partial z} \right)^2 / (U_A / R_0) \]  
\[ SIGVP = \left( \frac{\partial v}{\partial r} \right)^2 / (U_A / R_0) \]

Hot-wire anemometry was used by Laufer to study the statistical properties of turbulent pipe flow. A short discussion of the relationships used to obtain the Eulerian ve-
### Table of Statistical Properties of Turbulence

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**Note:** The table above represents statistical properties of turbulence as determined from experimental data.
locity derivative data and the relationship of the derivative to the microscale of turbulence and energy spectra follows.

The variance of the Eulerian velocity space derivative is related to Taylor's microscale of turbulence, which may be defined as

$$\lambda_{XE}^2 = \overline{u^2} / \overline{\left( \frac{\partial u}{\partial x} \right)^2}$$  \hspace{1cm} (A-8)

The most convenient means of experimentally determining the microscale is to apply the following approximation

$$\lambda_{XE}^2 = \overline{u^2} \overline{\left( \frac{\partial u}{\partial t} \right)^2}$$  \hspace{1cm} (A-9)

By electronically differentiating the hot-wire anemometer signal, \( (\partial u/\partial t)^2 \) may be easily obtained. The assumption of Taylor's hypothesis

$$\left( \frac{\partial u}{\partial t} \right) = \overline{u} \left( \frac{\partial u}{\partial x} \right)$$  \hspace{1cm} (A-10)

provides the relationship to calculate the microscale.

Other methods of determining the microscale are through the energy spectrum and correlation function measurements. As originally defined by Taylor, the microscale is given by

$$\frac{1}{\lambda_{XE}^2} = \lim_{x \to 0} \frac{1-R_x(x)}{x^2}$$  \hspace{1cm} (A-11)
Using the approximation

\[ x \approx \overline{U_t} \]  \hspace{1cm} (A-12)

the Eulerian time correlation of the velocity is related to the Eulerian space correlation

\[ R_{tE}(t) \approx R_{xE}(\overline{U_t}) \]  \hspace{1cm} (A-13)

And the microscale is given by

\[ \frac{1}{\lambda_{xE}^2} = \left( \frac{2}{u^2} \right) \lim_{t \to 0} \frac{1 - R_{tE}(t)}{t^2} \]  \hspace{1cm} (A-14)

If \( R_{tE}(t) \) is symmetric and the turbulence has temporal homogeneity, then it can be shown (121) that

\[ R_{tE}(t) = \frac{1}{u^2} \sum_{n=0}^{\infty} \frac{(-1)^n t^{2n} (u^n)^2}{(2n)!} \]  \hspace{1cm} (A-15)

Hence,

\[ 2 \lim_{t \to 0} \frac{1 - R_{tE}(t)}{t^2} = R_t(0) \]  \hspace{1cm} (A-16)

Thus, the microscale can be represented by the second derivative of the Eulerian time correlation function.

While \( R_{tE}(t) \) cannot be accurately measured in practice, it is possible to evaluate it from the energy spectrum. As was shown by Taylor (123), the correlation function is the Fourier transform of the energy spectrum, Equation 3. Hence
Thus, an integration of the energy spectrum provides another means of finding the Eulerian time microscale of turbulence

$$\lambda_{tE}^2 = -1/R_{tE}^0$$  \hspace{1cm} (A-18)

which in turn can be related to the Eulerian spacial microscale by Taylor's hypothesis.
APPENDIX B

Fluid Element Definition

When observing turbulent fluid motion from the
Lagrangian viewpoint, the successive values of the veloc-
ity as a function of time are those of a single fluid
element. For molecular motion, the element being followed
is readily defined as being a molecule. Or, similarly in
Brownian motion, the tagged element is the Brownian parti-
cle. However, in turbulent fluid motion, the choice of a
fluid element is not as apparent since the moving medium
is considered to act as a continuum.

The fluid element defined in the statistical model of
this research will be one which does not lose its entity
for a time interval sufficiently long compared to the pe-
riod of observation. Thus, such a fluid particle must have
dimensions much smaller than the smallest eddy. And at
the same time, it must be sufficiently large compared to
the molecular scale.

Since the minimum scale of eddy size is limited by
viscosity, such an element can exist as is illustrated by
Hinze (58, p. 7). He notes that the relevant turbulent
fluctuations are between 1 and 1,000 cm/sec. While for air,
the mean velocity of molecules is in the order of 50,000 cm/sec. Further, the turbulence frequencies vary, between 1 and 10,000 sec\(^{-1}\). Whereas, the molecular collision frequencies of air are about 5 \times 10^9 \text{ sec}^{-1}. If this condition exists for air, then the definition will also be applicable for more dense materials such as liquids.

Hence, it will be considered possible to define a small volume of homogeneous, continuous mass which will act as a single particle following the fluid motion. The velocity of the element will then be the local velocity of the fluid along the locus of the path of the element.
APPENDIX C

Data Smoothing

For such problems as fitting the general diffusion equation to the generated data, a more elaborate smoothing procedure is required. Such a procedure for smoothing the concentration and flux data is considered below for the case of steady state diffusion data. The concentration smoothing procedure can be used as a general method, but the material balance smoothing procedure applies only when steady state conditions have been reached.

Concentration data

Longitudinal smoothing The concentration data can be smoothed in two directions, first longitudinally and then radially. For the longitudinal direction, the concentration does not vary appreciably from cell to cell for a given radial distance from the center. Hence, a quadratic curve is adequate to represent the data longitudinally in the neighborhood of a given cell. The average concentration of particles in a cell and the two cells above and below it can be subjected to a least square fit to find the quadratic equation representing the average concentrations in the z direction. The equation can then be solved for the average concentration.
$C^+(i, z)$ of an annular region $i$ across the center of the cell.

**Radial smoothing** To find the concentration profiles as a function of the radius, a series of cosine functions can be used. The general form of a possible series would be

$$C(r^*, z) = \sum_{j=0}^{k} A_j(z)\cos\left((r^*)^j\eta\right) + \sum_{j=1}^{k} B_j(z)\cos\left((r^*)^{1/j}\eta\right) \quad (C-1)$$

where

$$r^* = r/R_0 \quad (C-2)$$

It may be noted that this functional form satisfies the boundary conditions given by Equations 45 and 46.

The simulated concentration data for the annular regions is related to the concentration profile by the following relation

$$C^+(i, z) = \frac{\int_{r_i}^{r_{i+1}} rC(r, z)dr}{\int_{r_i}^{r_{i+1}} r\,dr} \quad (C-3)$$

Thus, the integrated form of Equation C-1 is used to find the values of the coefficients $A_j(z)$ and $B_j(z)$. This
is done by making a least square fit to the z direction smoothed concentration data for the radial direction. The number of terms which may be included in the series is limited by the number of annular regions the equation is to fit. If the exact number of terms are included as there are annular regions, no smoothing along the radius occurs. With fewer terms, a smoothing occurs and the least square fit will give information as to the confidence limits of the smoothed results.

Material balance corrections

Molar flux calculations The molar fluxes can be smoothed by applying material balances. First, the average velocity of the diffusate across each surface of a cell is found. This is done by interpolating between the average velocities perpendicular to the surface of the two cells having the surface in common. The average velocity perpendicular to the surface times the integral of the smoothed concentrations over the surface gives an estimate of the molar flux across the surface.

Two-dimensional representation From the symmetry, the flow field can be represented as two-dimensional. And, any closed line integral of the product of $2\pi r$ and the flux equals the negative of the sum of the strengths of the sources enclosed by the curve.
The flux can be calculated for each surface of each cell in the manner described in the previous paragraph. On the two-dimensional representation, each of these surfaces is represented by a line segment. And, the value of the line integral along that line segment equals the total flux across the surface it represents. Hence, for any combination of these line segments which form a closed curve, the sum of the fluxes of the surfaces the line segments represent will equal the negative of the total strength of the sources enclosed. This is illustrated in Figure 12.

For lines CD and EF, the sum of the fluxes is zero. This is true since the flux across the wall and the radius are zero, and thus the line segments along the wall and radius making the curves closed have a value of zero. Line AB has a value of \(-C_0\). This follows because the concentration is zero at \(z = -\infty\). A line connecting the wall and center at \(z = -\infty\) and lines along the wall and center can be used to close the curve. The flux sum of these lines closing the curve is zero. And, in this case, the closed curve includes the source \(C_0\).

Least square correction of fluxes The material balance may also be expressed mathematically as the following summation

\[-(\sum C_0)_j = \sum_i B_{ij} A_{ij} + e_j\] (C-4)
Figure 12. Two-dimensional representation of flux surfaces
where

\[ i = \text{the } i\text{-th line segment of the closed curve} \]

\[ j = \text{the } j\text{-th combination of line segments forming a closed curve} \]

\[ (\sum C_o)_j = \text{the sum of the sources enclosed by the } j\text{-th closed curve} \]

\[ A_{ij} = \text{the sum of the fluxes across the line segment } i \text{ of the } j\text{-th closed curve} \]

\[ e_j = \text{the error in the material balance for the } j\text{-th closed curve} \]

When the estimations of the fluxes are in perfect material balance, the coefficient \( B_{ij} \) associated with the flux of the \( i\)-th line segment is unity. If all the error terms are not zero, then a least square fit can be made for the \( B_{ij} \). That is, the linear unbiased estimate \( \hat{B}_{ij} \) of the linear coefficient \( B_{ij} \) will be a correction factor for the flux across the \( i\)-th line segment.

The number of distinct equations which would be included in such a least square fit would be the same as the number of possible closed curves which would be formed over the lattice covering the field. The number of normal equations of the regression would then be equal to the number of line segments in the lattice. For the present study, the number of normal equations would be too large to solve in a reasonable time. Hence, a statistical sampling approach could have been used.
Statistical sampling to apply least square Instead of making a least square fit of all the line segments in the lattice at once, adjust only those between levels \( z_1 \) and \( z_2 \). The right hand side of Equation C-4 would include only those line segments between these two levels. The remaining line segments in the closed curves formed would be included as sources on the left hand side of Equation C-4.

Random walks could be made to determine the closed curves forming the linear equations. For each line segment between the levels of \( z_1 \) and \( z_2 \), a random walk is made from each end of the segment. Every step of the walk is along a line segment of the lattice. At the end of each step, the direction of the next step is randomly chosen. Returning over the same line segment for the next step would not extend the curve. So, the choice of the next step is randomly chosen to be one of the three other line segments at the lattice juncture.

The walk is continued until the wall or center is reached. These two walks will always form a closed curve and hence give one equation as was explained for line segment AB of Figure 12. The required number of closed curves to be formed starting from a given line segment is one more than the number of replications desired for that line segment.

Not only does the least square fit give a means of correcting the flux data for material balance, but it also gives
some estimate of the variance of the data. The product of \( \hat{B}_i \) and the flux across the i-th surface will be the best linear unbiased estimate of the flux across that surface. And, the variances of each term from the least square analysis can be used to estimate confidence intervals for each flux value.
APPENDIX D

Diffusate Concentration and Velocity Data

The local values of the dimensionless concentrations and velocities are given in Figures 13 through 21. What these generated values represent are the ensemble averages for the given experiment being simulated. The steady state experiment is given by the simulation in which the total walk time was such that all the walks were discontinued after the elements were downstream from the region of interest. Where the total walk time, $T$, was such that at least some of the walks were discontinued within the recording lattice, the simulation represents the ensemble average of an experiment where the diffusate injection was started a time $T$ before the samples were taken.

The local average velocities are represented as the ratios of the local velocities to the area average longitudinal velocity $U_A$, where $U_A$ is defined as

$$ U_A = \frac{\int_0^{R_o} \bar{U} \, dr}{\int_0^{R_o} r \, dr} $$ \hspace{1cm} \text{(D-1)}

The local average velocities were found as was described in the section on recording data. During the simulation of
the experiment, the velocities of the element are added after equal increments of time to the member of the matrix representing the area in which the element is then located. After the simulation is completed, the local average longitudinal and radial flux velocity is found by dividing the sums in each member of the matrix by the number of recordings which were made in that cell.

The concentrations were found from the number of recordings made for each cell of the lattice covering the region of interest. This relationship can be expressed in the following manner.

\[
C_{ij} = \frac{\int_{V_{ij}} C \, dV}{\int_{V_{ij}} dV} = \frac{M_A N_{ij}}{\int_{V_{ij}} dV}
\]

\[\text{(D-2)}\]

where

- \(C_{ij}\) = the average molar concentration for cell \((i,j)\)
- \(C\) = the point molar concentration
- \(N_{ij}\) = the number of recordings made in cell \((i,j)\)
- \(M_A\) = the number of moles of diffusate each element recorded represents
- \(V_{ij}\) = the volume of cell \((i,j)\)

The concentration is presented in the following dimensionless form
where $C_A$ is the average concentration developed in the steady state experiment at a large distance downstream from the source. This value is related to the injection rate and consequently to the number of walks made in the following manner. The total flux across any surface perpendicular to the axis of the tube downstream from the source in the steady state experiment is given by

$$\int_S C U_C dS = C_A U_A S \quad (D-4)$$

where $U_C$ is the longitudinal velocity of the diffusate and $S$ is the area of the surface perpendicular to the flow. This flux is equal to the injection rate.

$$SC_A U_A = M_A N_w / \Delta t \quad (D-5)$$

where

$N_w =$ the number of walks made in the simulation

$\Delta t =$ the time between recordings of the position of the element

A combination of Equation D-3, D-4, and D-5 gives the dimensionless local concentration which was recorded

$$C_{ij}^* = \frac{C_{ij}}{C_A} \quad (D-6)$$
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<th>RADIAL POSITION (r/R0)</th>
<th>LOCAL AVERAGE CONCENTRATION, IC/CA</th>
<th>LOCAL AVERAGE CONCENTRATION, IC/CA</th>
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Figure 13. Steady state concentration
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**Figure 14. Transient concentration**
Figure 15. Transient concentration
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**LOCAL AVERAGE DIFFUSATE RADIAL VELOCITY, (VC/UA)**

**Figure 16. Steady state radial velocity**
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<tr>
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<tr>
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<td>0.000</td>
</tr>
<tr>
<td>12:00</td>
<td>0.000</td>
</tr>
</tbody>
</table>

*Figure 49: Transient Failure Rate After Repair (Cycle)*
Longitudinal position, (Z/Ro) & Radial position, (R/Ro) & Local average diffuse radial velocity, (VC/UA) & Key numbers: Number of walks = 50000. Number of walks = 2000 Z/Ro = 0.00 Z/Ro = -0.00 DZ/Ro = 0.00 DZ/Ro = 0.00 Time/UA/Ro = 10.00

<table>
<thead>
<tr>
<th>Longitudinal Position</th>
<th>Radial Position</th>
<th>Local Average Diffuse Radial Velocity, (VC/UA)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.15</td>
<td>0.0393671</td>
<td>-0.0000000</td>
</tr>
<tr>
<td>0.25</td>
<td>0.0442903</td>
<td>-0.0000000</td>
</tr>
<tr>
<td>0.35</td>
<td>0.0439229</td>
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<tr>
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<td>0.0498269</td>
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</tr>
<tr>
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<td>0.0421082</td>
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</tr>
<tr>
<td>0.75</td>
<td>0.0369477</td>
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<td>0.0327274</td>
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<tr>
<td>0.95</td>
<td>0.0294978</td>
<td>-0.0000000</td>
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<tr>
<td>1.00</td>
<td>0.0252506</td>
<td>-0.0000000</td>
</tr>
<tr>
<td>1.10</td>
<td>0.0215170</td>
<td>-0.0000000</td>
</tr>
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<td>1.20</td>
<td>0.0183397</td>
<td>-0.0000000</td>
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<tr>
<td>1.30</td>
<td>0.0150529</td>
<td>-0.0000000</td>
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<tr>
<td>1.40</td>
<td>0.0111647</td>
<td>-0.0000000</td>
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<tr>
<td>1.50</td>
<td>0.0091091</td>
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<td>1.60</td>
<td>0.0051243</td>
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<td>0.0016448</td>
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<td>1.80</td>
<td>0.0005287</td>
<td>-0.0000000</td>
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<tr>
<td>1.90</td>
<td>0.0000779</td>
<td>-0.0000000</td>
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<td>0.0000276</td>
<td>-0.0000000</td>
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<td>0.0000021</td>
<td>-0.0000000</td>
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<td>-0.0000000</td>
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<td>-0.0000000</td>
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<tr>
<td>3.00</td>
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<td>-0.0000000</td>
</tr>
</tbody>
</table>

Figure 18. Transient radial velocity.
### Local Average Diffusate Longitudinal Velocity (\(\langle U - U \rangle/U \rangle\))

<table>
<thead>
<tr>
<th>Longitudinal Position, ((L/R))</th>
<th>0.05</th>
<th>0.15</th>
<th>0.25</th>
<th>0.35</th>
<th>0.45</th>
<th>0.55</th>
<th>0.65</th>
<th>0.75</th>
<th>0.85</th>
<th>0.95</th>
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</thead>
<tbody>
<tr>
<td>0.50</td>
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<td>-0.021505</td>
<td>-0.000000</td>
<td>-0.000000</td>
<td>-0.000000</td>
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<td>0.03107777</td>
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<td>-0.000000</td>
<td>-0.000000</td>
<td>-0.000000</td>
<td>-0.000000</td>
<td>-0.000000</td>
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<td>0.0154061</td>
<td>0.0193733</td>
<td>0.0610953</td>
<td>0.0712757</td>
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<td>5.00</td>
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<td>0.0920920</td>
<td>0.0920920</td>
<td>0.0920920</td>
<td>0.1190476</td>
<td>0.1293537</td>
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<td>0.8080808</td>
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</tr>
</tbody>
</table>

**Figure 19.** Steady state longitudinal velocity
### LOCAL AVERAGE DIFFUSATE LONGITUDINAL VELOCITY, \((\text{LUC}-\text{UI/UAL})\)

<table>
<thead>
<tr>
<th>LONGITUDINAL POSITION, ((Z/RO))</th>
<th>0.05</th>
<th>0.15</th>
<th>0.25</th>
<th>0.35</th>
<th>0.45</th>
<th>0.55</th>
<th>0.65</th>
<th>0.75</th>
<th>0.85</th>
<th>0.95</th>
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</thead>
<tbody>
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<td>0.15</td>
<td>-0.0036572</td>
<td>-0.0000000</td>
<td>-0.0000000</td>
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<td>-0.0000000</td>
<td>-0.0000000</td>
<td>-0.0000000</td>
<td>-0.0000000</td>
<td>-0.0000000</td>
<td>-0.0000000</td>
</tr>
<tr>
<td>0.25</td>
<td>0.0021164</td>
<td>-0.0000000</td>
<td>-0.0000000</td>
<td>-0.0000000</td>
<td>-0.0000000</td>
<td>-0.0000000</td>
<td>-0.0000000</td>
<td>-0.0000000</td>
<td>-0.0000000</td>
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</tr>
<tr>
<td>0.35</td>
<td>-0.0015291</td>
<td>-0.0000000</td>
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<td>-0.0000000</td>
<td>-0.0000000</td>
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<td>-0.0000000</td>
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<td>-0.0000000</td>
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<td>-0.0000000</td>
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<tr>
<td>0.65</td>
<td>-0.0001600</td>
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<td>-0.0000000</td>
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<td>-0.0000000</td>
</tr>
</tbody>
</table>

**Figure 21.** Transient longitudinal velocity
APPENDIX E

Computer Programs

The programs for simulating and analyzing the turbulent diffusion experiment were written for the IBM 7074 digital computer. Input, output, table computation, and analysis procedures were written in the IBM FORTRAN language. The random walk simulation procedure was written in the IBM AUTOCODER language as a subroutine. These programs are given in Figures 22 through 32. The programing nomenclature is listed following the programs.
Figure 22. Turbulent diffusion simulation program
Figure 23. Turbulent diffusion simulation program
C COMPUTE STATISTICAL AVERAGES
C INPUT SECTIONS OF LATTICE TO BE AVERAGED
READ INPUT TAPE IN,309,NDIV,(DIVA(JJ),JJ=1,14)
DO 301 JDUM = 1,NDIV
DIVA(JJ) = DIVA(JJ+1)
301 CONTINUE
C COMPUTES BASIC ELEMENTS OF VARIANCE-COVARIANCE MATRIX
DO 94 IR-1,10
C IF AT R=0, A SPECIAL CASE
94 CONTINUE
CALL ANALIR,SSIJJ,IR,RE,NW,ZZA,ZZB,TIME)
STOP 69
END

Figure 24. Turbulent diffusion simulation program
SUBROUTINE ANAL(RRA,55,RE,NW,ZIA,ZIB,OZI,TIME)
C SUBROUTINE ANAL CALCULATES THE DIFFUSIVITY TERMS
C UNDER EACH MODEL AND COMPARES THE MODEL
C TO THE GENERAL MODEL
C D. W. KIRKE
C JULY 4, 1964
DIMENSION JBBU),JA(4),JBU),JCH(3),SSS(5),SS(15,5),TRAT(5)
DIMENSION SS(15,11),FLUX(11),FFORM(11),I(4),J(4),SSVA(11)
DIMENSION JATN(4),JBTN(4),FLUXR(11),FLUXZ(11)
IN = 1
IOUT = 2
C INPUT MODEL SPECIFICATIONS
READ INPUT TAPE IN',180,NC
180 FORMAT(I10)
181 FORMAT(3X,A10)
READ INPUT TAPE IN',190
190 FORMAT(A40,F20.12)
C WRITE OUTPUT TAPE OUT',170,FORM
170 FORMAT/1X,A10,F10.8
READ INPUT TAPE IN',199,FORM
195 FORMAT(I12)
WRITE OUTPUT TAPE OUT',173,FORM
173 FORMAT(/3X,A10,F10.8)
C SET LOCATIONS OF DISTINCT TERMS
220 I = 1,4
JATN(I) = JA(I)
JBTN(I) = JB(I)
IF(JCH(I))= 1,221,223
221 JA(I) = 1
JB(I) = 1
196 R = R * .1
IR = IR * 1.
OJ = J
OF = SS(15,IR) - OJ
UFl = 4-J
OFl = SS(15,IR) - 2.
GO TO 190
229 DO 230 I = 1,4
JATN(I) = JA(I)
JBTN(I) = JB(I)
ASSIGN 229 TO JKKK
227 J = 0
DO 229 I = 1,5
IF(JATN(I))= 115,115,115,115,110
110 J=J+1
115 CONTINUE
K1 = JBB(1)
K2 = JBB(2)
K3 = JBB(3)
GO TO JKKK,228,186
186 R = R * .1
IR = I
OJ = J
DF = SS(15,IR) - 0.J
UFl = 4-J
OFl = SS(15,IR) - 2.
IF(10-1R)194,190,190
194 CONTINUE
WRITE OUTPUT TAPE OUT',187
187 FORMAT(A40,F10.8)
READ INPUT TAPE IN',194,FORM
190 CONTINUE
DO 126 K = 1,5
SS(J,K) = 0.
126 CONTINUE
Figure 25. Turbulent diffusion simulation program
159

127 DICC(K1,K2) = 0.
126 TAT(K1) = 0.
100 IF(0) GO TO 101
101 GO TO 102
IF(IF155,155,155,732)
732 CONTINUE
T10 = 1.045 +1.7789*(DF=(1-1.0274))

C COMPUTE ELEMENTS OF NORMAL MATRIX

SSS(1,1) = SSS(I,I)
SSS(1,2) = SSS(I,J)
SSS(1,3) = SSS(I,K)
SSS(1,4) = SSS(I,L)
SSS(2,1) = SSS(J,I)
SSS(2,2) = SSS(J,J)
SSS(2,3) = SSS(J,K)
SSS(2,4) = SSS(J,L)
SSS(3,1) = SSS(K,I)
SSS(3,2) = SSS(K,J)
SSS(3,3) = SSS(K,K)
SSS(3,4) = SSS(K,L)
SSS(4,1) = SSS(L,I)
SSS(4,2) = SSS(L,J)
SSS(4,3) = SSS(L,K)
SSS(4,4) = SSS(L,L)

DO 111 K = 1,4
111 SSS(K,K) = SSS(K,K)
CHEK155,155,732

C ARRANGE MATRIX ACCORDING TO MODEL
SUM EQUAL TERM NORMAL FACTORS

DO 120 K = 1,5
120 K = K + 1
121 SSS(K,K) = SSS(K,K)
CHEK155,155,732
125 CONTINUE

C INVERT MATRIX, J = NO. INDOP TERMS

DO 144 J = 1,4
144 DET = SSS(I,I)*SSS(J,J) - SSS(I,J)*SSS(J,I)
145 DICC(J,J) = 1./SSS(J,J)
146 DICC(J,I) = -SSS(J,I)/DET
147 DICC(I,I) = SSS(I,I)/DET
148 DICC(K,L) = DICC(K,L)
150 CONTINUE

C INVERSE MATRIX, J = NO. INDOP TERMS

DO 164 L = 1,4
164 E(L) = E(L)
165 SSS = SSS - E(L)*E(L)
160 CONTINUE

C DIFFUSIVITIES

SS = SSS(1,1) + SSS(1,2) + SSS(1,3) + SSS(1,4) + SSS(2,1) + SSS(2,2) + SSS(2,3) + SSS(2,4) + SSS(3,1) + SSS(3,2) + SSS(3,3) + SSS(3,4) + SSS(4,1) + SSS(4,2) + SSS(4,3) + SSS(4,4)

DO 166 L = 1,4
166 E(L) = E(L)
167 CONTINUE

C CONFIDENCE INTERVAL, 90 PERCENT

DO 170 I = 1,4
170 E(I) = E(I)
171 CONTINUE

Figure 26. Turbulent diffusion simulation program
SUBROUTINE RNWIK SIMULATES THE TURBULENT DIFFUSION EXPERIMENT BY A RANDOM WALK PROCEDURE

DALE W. KIRMSE
JULY 6, 1964

ORIGIN CNTRL 1000
01 EXECUTE CNTRL 7
02 NAME OF SUBPROGRAM

10 DC GRNWIK A
11 +0000000000 NUMBER OF DATA L
12 +0000000000 NUMBER OF LOC AT
13 +0000000000
14 +0000000000
15 ORIGIN CNTRL 1000
16 IX X
17 SIMULATE XIA 08.0081
18 AS 99 IN STORAGE
19 BLK 99.0008
20 XU 94 SAVEXIT
21 BV1 +1
22 BV2 +1
23 ZAI IX1(2,5)+5
24 STOL CSV(4,9)
25 ZAI IX1(2,5)+6
26 STOL CSV(4,9)
27 ZAI IX1(2,5)+7
28 STOL CSV(4,9)
29 ZAI IX1(2,5)+8
30 STOL CSV(4,9)
31 ZAI IX1(2,5)+9
32 STOL CSV(4,9)
33 ZAI IX1(2,5)+10
34 STOL CSV(4,9)

Figure 27. Turbulent diffusion simulation program
Figure 28. Turbulent diffusion simulation program
Figure 29. Turbulent diffusion simulation program
Figure 30. Turbulent diffusion simulation program
Figure 31. Turbulent diffusion simulation program
Figure 32. Turbulent diffusion simulation program
APPENDIX F

The method of analyzing the various models is discussed earlier in the text. The values calculated for the components of the diffusivities and the analysis of each model is given in Figures 32 through 48.

A short explanation of the Alphamerics used to identify the various terms is given below.

\[
\begin{align*}
\text{ERR}/(2*B_0*UA) &= E_{rr}/(2R_0 UA) \\
\text{ERZ}/(2*B_0*UA) &= E_{rz}/(2R_0 UA) \\
\text{EZR}/(2*B_0*UA) &= E_{zr}/(2R_0 UA) \\
\text{EZZ}/(2*B_0*UA) &= E_{zz}/(2R_0 UA)
\end{align*}
\]

\( F = \) the value of \( F \) given by Equation 66 to test the significance of the given diffusivity term

\( T = \) the value of \( t \) given by Equation 65 to test the significance of the given diffusivity term

\( TDF = \) the degrees of freedom for the \( t \) test

\( FDF_1 = \) the degrees of freedom in the numerator of \( F \)

\( FDF_2 = \) the degrees of freedom in the denominator of \( F \)

\( 90\% \text{ CI} = \) plus and minus this quantity gives the 90\% confidence interval as expressed by Equation 67
TRANSPORT RATIO = the average transport ratio over the longitudinal interval of interest as evaluated by Equation 69

TOTAL TRANSPORT RATIO = the ratio of the magnitude of the average predicted flux vector to the magnitude of the average observed flux vector which is calculated according to Equation 70

SS OF DEVIATIONS = the sum of squares of the deviations of given model at the particular radial position from the data

It may be noted that the values of the diffusivity tensor components are presented as inverse Peclet numbers.

For the center, R/RO = 0, a modification of the general calculation procedure was made. Since the radial concentration gradient is zero, a number of the models are indeterminate, notable the general model. To be able to make a comparison, the particular model was modified if it was indeterminate. Unless a diffusivity term associated with a radial gradient was equated to another term, it was set to zero.

At the bottom of each figure is the evaluation of the diffusivity terms assuming that they are independent of radial position.

The values used represent the conditions at the corners of the cells. That is, the partial derivatives were taken in such manner as to represent the concentration gradient at the common corner of the four cells involved.
The concentration and velocities at the corner were taken to be the averages of the four cells.

For the center of the tube, the procedure was modified. The radial gradient was set to zero, and the longitudinal gradient was the average gradient between the two adjacent cells in the longitudinal direction.
### Diffusivity Terms as Calculated for Model - ERR, EER, EER, EEE, General Model - All Terms Distinct

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<tr>
<th>R/D</th>
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<th>ERR/(2-RO+UA)</th>
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Average Values Independent of Radial Position:

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Reynolds Number = 50000. Number of Walks = 1030 ZZA/RD = 1.00 ZZA/RD = 2.50 DZZ/RD = 1.00 Time UA/RD = 999.00

Figure 33. General model diffusivities
### DIFFUSIVITY TERMS AS CALCULATED FOR MODEL - ERR, ERZ, EZR, EZZ

#### GENERAL MODEL - ALL TERMS DISTINCT

<table>
<thead>
<tr>
<th>R/RO</th>
<th>ERR/(2<em>R0</em>UA)</th>
<th>ERZ/(2<em>R0</em>UA)</th>
<th>EZR/(2<em>R0</em>UA)</th>
<th>EZZ/(2<em>R0</em>UA)</th>
<th>SS OF DEVIATIONS</th>
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<td>TRANSPORT RATIO</td>
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**AVERAGE VALUES INDEPENDENT OF RADIAL POSITION**

-0.00 0.18353E+01 0.15582E+01 0.12700E+01 0.12700E+01 0.17352E+01 0.38944E+01 0.19131E+01 0.23525E+01 0.19131E+01 0.23525E+01 0.19131E+01

**REYNOLDS NUMBER = 50000. NUMBER OF WALKS = 1000**

-0.00 0.15582E+01 0.12700E+01 0.12700E+01 0.17352E+01 0.38944E+01 0.19131E+01 0.23525E+01 0.19131E+01 0.23525E+01 0.19131E+01

**Figure 34. General model diffusivities**
### Diffusivity Terms as Calculated for Model - ERR, ERZ, EZR, EZZ

#### General Model - All Terms Distinct

<table>
<thead>
<tr>
<th>R/RO</th>
<th>ERR/(2<em>R0</em>UA)</th>
<th>ERZ/(2<em>R0</em>UA)</th>
<th>EZZ/(2<em>R0</em>UA)</th>
<th>SS of Deviations</th>
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#### Transport Ratio

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#### Average Values Independent of Radial Position

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#### Reynolds Number = 50000. Number of Walks = 1000. ZIA/RO = 0.50. ZIB/RO = 12.50. DIZ/RO = 0.50. Time*UA/R0 = 16.00

Figure 35: General model diffusivities
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AVERAGE VALUES INDEPENDENT OF RADIAL POSITION

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|      | 0.93934E-01   | 0.42759E-01   | 0.18532E-02   | 0.42759E-01   |
|      | 0.53915E-00   | 0.19365E-02   | 0.52714E-00   | 0.19365E-02   |

REYNOLDS NUMBER = 50000. NUMBER OF WALKS = 1000 ZIA/RO = 12.50 ZIB/RO = 24.50 DIZ/RO = 0.50 TIME=UA/RO = 16.00

Figure 36. General model diffusivities.
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<th>I2/E</th>
<th>ERR/(2<em>R0</em>U)</th>
<th>I2/E</th>
<th>ERR/(2<em>R0</em>U)</th>
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AVERAGE VALUES INDEPENDENT OF RADIAL POSITION

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<th>I2/E</th>
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Figure 37. General model diffusivities
## Diffusivity Terms as Calculated for Model - ERR, ERZ, E2R, E2Z, General Model - All Terms Distinct

### R/R0 ERR/(2*R0*UA)  ERZ/(2*R0*UA)  E2R/(2*R0*UA)  E2Z/(2*R0*UA)  SS of Deviations

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### Average Values Independent of Radial Position

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### Reynolds Number = 50000, Number of Walks = 2000, ZZA/R0 = 7.50, ZZB/R0 = 14.70, DZZ/R0 = 0.30, Time*UA/R0 = 10.00

Figure 38. General model diffusivities
### Diffusivity Terms as Calculated for Model - Err, Ez, Ez, Ez = 0

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<th>ERR/(2*RO+UA)</th>
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**Average Values Independent of Radial Position**

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|      | 0.605907E-04 | 0.280999E-02 | 0.330700E-04 | 0.399138E 02 |
|      | 0.047697E 02 | 0.314633E 01 | 0.177978E 01 | 0.427033E 01 |
|      | 0.047697E 02 | 0.346803E 01 | 0.364961E 01 | 0.729402E 00 |

**Key: Reynolds Number = 50000. Number of Walks = 1000.**

Figure 39. Restricted model diffusivities
### Diffusivity Terms as Calculated for Model - ERR, ERz, EZR, O, EZZ

<table>
<thead>
<tr>
<th>R/RO</th>
<th>ERR/(2•R0•Ua)</th>
<th>ERz/(2•R0•Ua)</th>
<th>EZR/(2•R0•Ua)</th>
<th>EZZ/(2•R0•Ua)</th>
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**Average Values Independent of Radial Position**

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**Reynolds Number = 50000. Number of Walks = 1000 ZZA/R0 = 1.00 ZIB/R0 = 25.00 DIZ/R0 = 1.00 TIME/UA/R0 = 9999.00**

*Figure 40. Restricted model diffusivities*
### Diffusivity Terms as Calculated for Model - ERR, ERZ, EZR, O, EZ = O

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<th>ERZ/(L2+RO=UA)</th>
<th>EZR/(L2+RO=UA)</th>
<th>OZ/(L2+RO=UA)</th>
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**Average Values Independent of Radial Position**

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-0.37284E-02 0.23807E-02 0.000000E 00 0.000000E 00 0.420E 00
-0.81039E-06 0.24408E-02 0.000000E 00 0.000000E 00 0.7018E 00

**Reynolds Number = 50000. Number of Walks = 10000. Z1A/RU = 1.00. Z1B/RD = 25.00. OZ/RD = 1.00. Time = UA/RD = 9999.00.**

Figure 41. Restricted model diffusivities.
### Diffusivity Terms as Calculated for Model - ERR, ERZ, EZR

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<th>R/RO</th>
<th>ERR/(2<em>R0</em>UA)</th>
<th>ERZ/(2<em>R0</em>UA)</th>
<th>EZR/(2<em>R0</em>UA)</th>
<th>EZZ/(2<em>R0</em>UA)</th>
<th>SS of Deviations</th>
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**Average Values Independent of Radial Position**

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<td>0.244418E-03</td>
<td>0.138898E-01</td>
</tr>
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</table>

### Reynolds Number = 50000. Number of Walks = 1000. ZZB/RO = 1.00. ZZB/RO = 25.00. D3Z/RO = 1.00. Time-UA/RO = 999.00

Figure 42. Restricted model diffusivities
<table>
<thead>
<tr>
<th>R/RO</th>
<th>ERR/(2*RO+UA)</th>
<th>ERRZ/(2*RO+UA)</th>
<th>EZZ/(2*RO+UA)</th>
<th>SS OF DEVIATIONS</th>
</tr>
</thead>
<tbody>
<tr>
<td>T</td>
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<td>T</td>
<td>T</td>
<td>Transport Ratio</td>
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<tr>
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<td>0.323978E-02</td>
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</tbody>
</table>

**AVERAGE VALUES INDEPENDENT OF RADIAL POSITION**

| -0.00 | 0.127837E-02 | 0.361371E-03 | 0.361371E-03 | 0.714548E+00    |
|       | 0.337008E-04 | 0.337008E-04 | 0.337008E-04 |                 |
|       | 0.176770E-02 | 0.176770E-02 | 0.176770E-02 |                 |
|       | 0.367681E-02 | 0.367681E-02 | 0.367681E-02 |                 |

**REYNOLDS NUMBER = 50000. NUMBER OF WALKS = 1000. ZZA/RO = 1.00. ZZB/RO = 25.00. DIZ/RO = 1.00. TIME+UA/RO = 9999.00.**

Figure 43. Restricted model diffusivities
<table>
<thead>
<tr>
<th>R/RO</th>
<th>ERR/(2*(R0*UA))</th>
<th>ERZ/(2*(R0*UA))</th>
<th>EZZ/(2*(R0*UA))</th>
<th>SS DF DEVIATIONS</th>
</tr>
</thead>
<tbody>
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<td>0.000000E+00</td>
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<tr>
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<td>0.000000E+00</td>
</tr>
<tr>
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<td>0.000000E+00</td>
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<td>0.000000E+00</td>
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<tr>
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<td>0.000000E+00</td>
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<td>0.215208E-02</td>
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<td>0.000000E+00</td>
<td>0.000000E+00</td>
</tr>
</tbody>
</table>

AVERAGE VALUES INDEPENDENT OF RADIAL POSITION

| -0.00 | 0.128177E-02  | 0.000000E+00  | 0.346666E-03  | 0.000000E+00  |
| 0.00 | 0.337530E-04  | 0.000000E+00  | 0.337530E-04  | 0.000000E+00  |
| 0.20 | 0.136282E-02  | 0.000000E+00  | 0.366961E-00  | 0.000000E+00  |

Figure 44. Restricted model diffusivities
<table>
<thead>
<tr>
<th>R/RO</th>
<th>ERR/(2*RO+UA)</th>
<th>ERZ/(2*RO+UA)</th>
<th>EZZ/(2*RO+UA)</th>
<th>SS OF DEVIATIONS</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.00</td>
<td>-0.000000E 00</td>
<td>-0.000000E 00</td>
<td>-0.000000E 00</td>
<td>0.168464E-01</td>
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<tr>
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<td>-0.000000E 00</td>
<td>0.184442E-02</td>
</tr>
<tr>
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<td>0.000000E 00</td>
<td>0.018165E-01</td>
</tr>
<tr>
<td>0.30</td>
<td>0.230781E-02</td>
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<td>0.000000E 00</td>
</tr>
<tr>
<td>0.40</td>
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<td>0.000000E 00</td>
<td>0.000000E 00</td>
</tr>
<tr>
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<td>0.000000E 00</td>
<td>0.000000E 00</td>
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<tr>
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<td>0.000000E 00</td>
</tr>
<tr>
<td>0.70</td>
<td>0.26134E-02</td>
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<td>0.000000E 00</td>
<td>0.000000E 00</td>
</tr>
<tr>
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<td>0.000000E 00</td>
<td>0.000000E 00</td>
</tr>
<tr>
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<td>0.000000E 00</td>
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</table>

Values for transport ratio in the table are as follows:

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<th>TRANSPORT RATIO</th>
<th>TRANSPORT RATIO</th>
<th>TRANSPORT RATIO</th>
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<td>0.000000E 00</td>
<td>0.000000E 00</td>
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<tr>
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<td>0.000000E 00</td>
</tr>
<tr>
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<td>0.000000E 00</td>
<td>0.000000E 00</td>
<td>0.000000E 00</td>
</tr>
<tr>
<td>0.70</td>
<td>0.000000E 00</td>
<td>0.000000E 00</td>
<td>0.000000E 00</td>
</tr>
<tr>
<td>0.80</td>
<td>0.000000E 00</td>
<td>0.000000E 00</td>
<td>0.000000E 00</td>
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<tr>
<td>0.90</td>
<td>0.000000E 00</td>
<td>0.000000E 00</td>
<td>0.000000E 00</td>
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</tbody>
</table>

Average values independent of radial position:

<table>
<thead>
<tr>
<th>R/RO</th>
<th>ERR/(2*RO+UA)</th>
<th>ERZ/(2*RO+UA)</th>
<th>EZZ/(2*RO+UA)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.00</td>
<td>-0.000000E 00</td>
<td>-0.000000E 00</td>
<td>-0.000000E 00</td>
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<tr>
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<td>0.000000E 00</td>
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</tbody>
</table>

**Figure 45.** Restricted model diffusivities
### Diffusivity Terms Calculated for Model

<table>
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<tr>
<th>R/RO</th>
<th>ERR/(2R0+UA)</th>
<th>ERZ/(2R0+UA)</th>
<th>EZZ/(2R0+UA)</th>
<th>SS of Deviations</th>
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<td>90 PC Cl</td>
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</tbody>
</table>

<table>
<thead>
<tr>
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<th>ERR/(2R0+UA)</th>
<th>ERZ/(2R0+UA)</th>
<th>EZZ/(2R0+UA)</th>
<th>SS of Deviations</th>
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Total Transport Ratio

![Figure 47](https://via.placeholder.com/500x500)

**Figure 47.** Restricted model diffusivities
<table>
<thead>
<tr>
<th>R/RO</th>
<th>ERR/(2<em>RO</em>UA)</th>
<th>ERRZ/(2<em>RO</em>UA)</th>
<th>EZR/(2<em>RO</em>UA)</th>
<th>EZZ/(2<em>RO</em>UA)</th>
<th>SS OF DEVIATIONS</th>
</tr>
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<tbody>
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<td>0.030199E-00</td>
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</tr>
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<td>0.347678E-03</td>
</tr>
<tr>
<td>AVERAGE VALUES INDEPENDENT OF RADIAL POSITION</td>
<td>0.000000E+00</td>
<td>0.000000E+00</td>
<td>0.000000E+00</td>
<td>0.000000E+00</td>
<td>0.000000E+00</td>
</tr>
</tbody>
</table>

**Figure 48. General model diffusivities**
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