A Stochastic Model for Turbulent Diffusion of Particles or Drops

A stochastic model is presented for turbulent diffusion of particles or drops in a turbulent field. The model is free of arbitrary adjustable constants and is applicable to realistic situations where the flow is nonhomogeneous such as in boundary layers or in pipe flow. New experimental data is presented for dispersion of glass beads in the boundary layer of the University of Houston Environmental Wind Tunnel. Good agreement with the theoretical model is demonstrated.

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SCOPE

Predicting the rate of diffusion of particles or drops in a turbulent field is still an unsolved problem despite its importance to the design of many industrial processes and to the calculation of dispersion of particulates in the atmospheric boundary layer. Plans for increased use of coal for power generation and the expected increase in emission of particulates from stacks makes this problem of immediate concern; but the ability to predict diffusion of a dispersed phase is also important in the design of gas-liquid pipeline contactors and reactors, emergency core cooling systems for nuclear reactors, spray columns, dispersed phase chemical reactors, condensers, film evaporators, separators and a wide variety of other process equipment.

Much remains to be understood about diffusion in single phase systems. Thus, it is to be expected that the diffusion of a particulate phase would be less well understood. One approach has been to assume that the gradient type diffusion equations are valid with a variety of expressions proposed for the eddy diffusivity of the particles. For small particulate sizes in turbulent pipe flow this diffusivity has been assumed equal to that of the continuous phase (Friedlander, 1957) and for larger sizes methods for estimating the difference have been proposed (Hutchinson et al., 1971). Similar approaches have been explored by Householder (1969) for particles in free jets and by Godson (1958) and Smith (1962) for diffusion in the atmosphere. None of these methods which are based on the use of an eddy diffusivity is satisfactory on theoretical grounds and all require experimental diffusion data to establish the coefficients.

A second general approach, which has been applied primarily to diffusion in the atmosphere, is semistatistical in nature in that it assumes the concentration distribution down wind is Gaussian. This method used by Godson (1958) and Csanady (1963) does not describe the physical nature of the process and requires experimental data on the concentration variance in order to be useable.

A third method is to attempt to solve the equations of motion for the particles written in Lagrangian form in order to track the particle motion. The extensive literature on this approach as reviewed by Hinze (1975) shows that the instances where solutions are possible do not correspond with most cases of practical interest, especially for larger particles.

In this paper a new method is presented based on the properties of a stochastic differential equation which describes this process. A technique for simulating the diffusion of solid particles or droplets using this equation is developed based on the unique capability of a modern hybrid computer to repeatedly solve a stochastic equation very rapidly. New experimental data on particle diffusion in a wind tunnel boundary layer is reported and shown to be in good agreement with predictions from the simulation method.

CONCLUSIONS AND SIGNIFICANCE

The Lagrangian time history of the fluctuating velocity for a particle can be described by an equation of the Langevin type:

$$\frac{dv'_p}{dt} + \beta v'_p = n(t)$$

where β is a constant and $n(t)$ is a stochastic forcing function having the characteristics of band limited white noise. This paper shows how the value of β and the statistics of the forcing function can be specified from a knowledge of the Eulerian characteristics of the turbulence of the continuous phase. Once β and $n(t)$ are known, the equation can be repeatedly and rapidly solved using the analog components of a modern hybrid computer at rates up to 100,000 times a second. For each solution the position of the particle can be found

$$x_p = \int_o^t (u_p + v'_p)dt$$

With a hybrid computer the position of the particle in each realization of this stochastic process can be digitally stored. After enough solutions to give statistical reliability, average concentrations at all locations in time and space can be calculated. Thus, the solution of the particle diffusion problem is obtained yielding concentration distributions of the dispersion from a knowledge of the turbulence characteristics of the continuous phase. In this way the need for diffusion data to find the coefficients as empirical constants for the diffusion process is avoided.

Concentration distributions were obtained for dispersion of 58 and 69 micron glass beads in the boundary layer of the

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University of Houston Environmental Wind Tunnel. A comparison of these data with theoretical predictions using this methodology shows very good agreement as indicated in Figures 7-12.

Because the basic equation is so simple to solve on an analog machine, this process of solution is extremely economical in the use of computer time even with multiple sources and sinks in the system.

THE MODEL

Lee and Dukler (1978) proposed a stochastic model for single phase turbulent diffusion in the presence of velocity gradients and shear. Given the Eulerian statistics of the turbulent field (spacial distribution of the mean velocity, turbulent shear stress, turbulent intensity and spectral density of the velocity), this model predicts the mean square displacement or mean concentration distribution of the diffusing component downstream from sources of arbitrary number, location and configurations. Because the model for turbulent diffusion of particles discussed in this paper follows the concepts presented earlier for single phase flow, the underlying ideas are outlined below.

If, as suggested by many investigators (Kalinske and Pien, 1944; Hinze, 1975), the Eulerian correlation coefficient of the fluctuating field can be expressed as an exponential

$$R_E(\tau) = \frac{\overline{u(t)u(t+\tau)}}{\overline{u^2_{Rms}}} = e^{-\beta'\tau} \tag{1}$$

and if the Lagrangian correlation coefficient decays with time in a manner similar to the Eulerian coefficient but with a different time scale as suggested by Hay and Pasquill (1959):

$$R_L(\gamma\tau_E) = R_E(\tau_E) \tag{2}$$

or

$$F_v(f) = \gamma F_u(\gamma f) \tag{3}$$

then, using linear systems analysis applied to stochastic processes, Lee and Dukler (1978) showed that the process which characterizes the diffusion is:

$$\frac{dv}{dt} + \beta v = n(t) \tag{4}$$

where $\beta = \beta'/\gamma$ and $n(t)$ is a Gaussian stochastic process. This equation is recognized as the Langevin equation if $n(t)$ is true white noise of infinite band width and when the cross correlation between $n(t)$ and $v(t)$ is zero. This is the case when β' is small. Then the equation characterizes the Markoff process of Brownian motion. However, if β' is of the magnitude necessary to characterize the correlation in Eq. 1 and if $n(t)$ is band limited, then the cross correlation between n and v is non zero and the process characterized by Eq. 4 is an excellent representation of turbulence; that is, the process is non Markovian and the spectral density of $v(t)$ has the essential features of a Lagrangian turbulent velocity.

Now the simulation of diffusion can proceed as follows:

1. Find β and $n(t)$ from the Eulerian statistics as functions of position. (See below.)
2. Make repeated solutions of the stochastic Eq. 4. Each realization follows a packet of fluid containing a specified amount of diffusate from its source. As the process proceeds, the position of the packet is calculated from

$$x(t) = \int_0^t [\overline{u}(\vec{x}) + v(t)]dt \tag{5}$$

The flow field is divided into cells and the position of the packet is located after each realization and stored. The mass of diffusate in each packet is set so as to meet the source release rate.

3. After a large number of realizations the concentration distribution can be obtained easily by dividing the mass by the cell volume.

This simulation can be carried out readily by the use of a hybrid computer. Multidimensional problems are executed by the simultaneous solution of 2 or 3 equations such as Eq. 4. Furthermore, forcing functions n_1, n_2 for two directions can be generated in such a way that they are correlated to any degree and this results in correlation between the velocities v_1 and v_2 (Lee and Dukler, 1976). Thus, the effect of turbulent shear can be incorporated.

Lee and Dukler showed that β and $n(t)$ could be specified from the Eulerian properties of the field through

$$F_u(f) = \frac{4\beta'}{\beta'^2 + (2\pi f)^2}\, u^2_{RMS} \tag{6}$$

and

$$u^2_{RMS} = \frac{\gamma F_n(0)}{4\beta'} \tag{7}$$

where $F_n(0)$ is the zero frequency noise spectrum. β' can be found for each position from a curve fit to the Eulerian spectrum through Eq. 6. Since γ has been shown to depend only on the mean Eulerian velocity and u_{RMS} (for example, Wandel et al., 1962), $F_n(0)$ can be calculated from equation (7) and the amplitude of a Gaussian noise generator can then be specified.

Particle Motion

The method of simulation for particle diffusion proceeds in a manner parallel to that for single phase flow presented above. However, here it will be necessary to involve some speculations, their validity to be tested by comparing the simulation results against data.

Assume that the autocorrelation of the Lagrangian fluctuating velocity for the particle, v_p, is of exponential form

$$R_{v_p}(\tau) = e^{-\beta_p \tau} \tag{8}$$

where β_p is the constant which characterizes the diffusion process and v_p is Gaussian. There is strong evidence that the correlation should be expressed in an exponential-cosine functional form (Snyder and Lumley, 1971; Nir and Pismen, 1979). But, Calabrese and Middleman (1979) have recently shown Eq. 8 to be an excellent practical approximation to R_{v_p}. Then, in a manner entirely analogous to single phase flow the stochastic equation for the fluctuating velocity must be

$$\frac{dv_p}{dt} + \beta_p v_p = n(t) \tag{9}$$

where $n(t)$ is band limited white noise. The trajectory of the particle can be calculated from

$$x_p = \int_0^t (u_p + v_p)dt \tag{10}$$

where u_p is the average velocity of the particle which incorporates the effect on the particle of gravity. Applying linear system analysis (Lee and Dukler, 1978) to Eq. 9 gives the relationship between the spectrum of the noise $F_n(f)$ and the velocity $F_{v_p}(f)$.

$$F_{v_p}(f) = \frac{F_n(f)}{\beta_p^2 + (2\pi f)^2} \tag{11}$$

If it is assumed that over the range of low frequencies which control the diffusion the spectrum is essentially constant at $F_n(0)$, then

$$F_{v_p}(f) = \frac{F_n(0)}{\beta_p^2 + (2\pi f)^2} \tag{12}$$

If the particle velocity spectrum is known, both $F_n(0)$ and β_p can be found from a curve fit using Eq. 12. Then the particle motion can be simulated by repeated solution of Eq. 9 in a manner identical to that described above for a single phase system. Thus, the problem comes down to finding this spectral density, $F_{v_p}(f)$. Of course, the problem can be simulated in multiple dimensions.

Estimating the Particle Lagrangian Velocity Spectrum

Figure 1 shows two concepts for estimating F_{v_p}. Path 1 requires that the Lagrangian spectrum of the fluid, F_v, be related to its Eulerian representation, F_u (path 1A). A method for doing this has already been discussed through the Hay-Pasquill hypotheses which leads to Eq 3. Next the particle velocity Lagrangian spectrum, F_{v_p} must be related to F_v (path 1B). Equations of motion have been formulated which characterize v_p (Tchen, 1947; Hinze, 1975). Once these equations have been linearized they can be used to generate the required relation between F_v and F_{v_p} (Chao, 1964). However, the step of linearization requires many assumptions, the most serious of which is that each particle remain surrounded by the same fluid element or eddy along its entire trajectory. This restriction is clearly unacceptable for large particles which do not follow the turbulence as a result of inertia and/or whose trajectory is influenced by gravity.

In an effort to eliminate this restriction, the possibility of arriving at F_{v_p} through path 2 is considered. The time variation of the Eulerian velocity of a fluid at a fixed point results from the instantaneous velocity of successive fluid eddies or packets which sweep across that point. In a similar way, a pseudo-Eulerian particle velocity is visualized as being continuous; although it is, of course, actually intermittent. At each instant at the fixed point the Eulerian particle and fluid velocities can be related through the equation of motion. For a Stokes type resistance law this becomes:

$$\frac{du_p}{dt} = \theta_1 \frac{du}{dt} - \theta_2\theta_1(u_p - u) - \theta_i\left(\frac{3\theta_2}{\pi}\right)^{1/2} \int_{t_0}^{t} \frac{\frac{d}{d\tau}(u_p - u)}{\sqrt{t-\tau}}\, d\tau + \theta_3 \tag{13}$$

where θ_3 results from the gravity force.

$$\theta_1 = \frac{3\rho}{2\rho_p + \rho} \qquad \theta_3 = \frac{2}{2\rho_p + \rho}(\rho_p - \rho)g$$

$$\theta_2 = \frac{3\nu}{a^2}$$

Since this equation describes the motion of particles at local positions in space, it no longer requires that the particle remain surrounded by the same eddy in the course of its path. Furthermore, Eq. 13 is linear since the Eulerian velocity of the fluid is a simple function of the spacial coordinates and the statistics of the fluctuating Eulerian turbulent field. This linearity makes it possible to relate F_{u_p} to F_u using Fourier transforms as was done by Chao (1964).

$$\frac{F_{u_p}(f)}{F_u(f)} = \frac{4\pi^2\left(\frac{f}{\theta_2}\right)^2 + 4\sqrt{3\pi^3}\left(\frac{f}{\theta_2}\right)^{3/2} + 6\pi\frac{f}{\theta_2} + 2\sqrt{3\pi}\left(\frac{f}{\theta_2}\right)^{1/2} + 1}{\frac{4\pi^2}{\theta_i^2}\left(\frac{f}{\theta_2}\right)^2 + \frac{4\sqrt{3\pi^3}}{\theta_1}\left(\frac{f}{\theta_2}\right)^{3/2} + 6\pi\frac{f}{\theta_2} + 2\sqrt{3\pi}\left(\frac{f}{\theta_2}\right)^{1/2} + 1} \tag{14}$$

Thus, given the Eulerian spectrum of the fluid, F_u, the particle size and the fluid and particle properties, the Eulerian spectrum of the particle velocity, F_{u_p}, can be calculated from

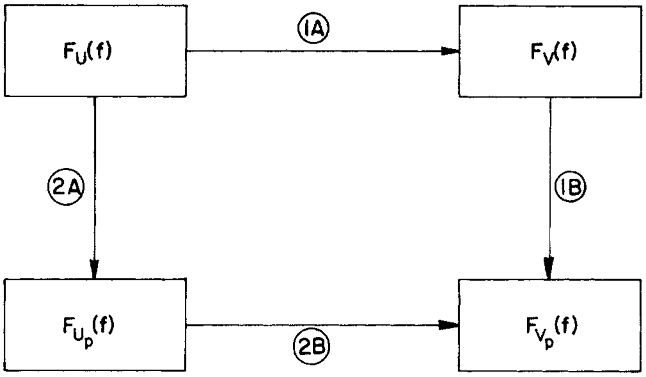

Figure 1. Two paths for estimating the Lagrangian spectrum of particle velocity.

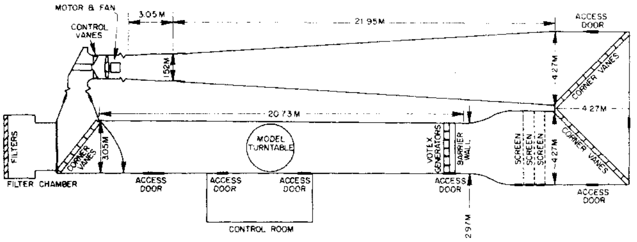

Figure 2. Environmental wind tunnel.

Eq. 14. The particle Lagrangian spectrum, F_{v_p}, is then calculated from its Eulerian value by assuming that the Hay-Pasquill hypotheses applies equally to the particle field. A curve fit of Eq. 12 can then provide $F_n(0)$, the zero frequency of the random noise, $n(t)$ and β_p, the coefficient of v_p in the controlling stochastic Eq. 9.

In order to test these speculations experiments were carried out in a large wind tunnel in order to compare measured particle concentration distribution values predicted from simulations using this concept.

Some recently published results are of interest in connection with the work reported here. Pismen and Nir (1978) and Nir and Pismen (1979) obtained particle correlation from Eulerian fluid correlation for two special cases: a particle in an isotropic homogeneous field without body force and an anisotropic field with body force dominant in comparison to turbulent force. These special conditions permit certain linearizations and the results are promising. The treatment presented here is not restricted in the same way.

EXPERIMENTAL EQUIPMENT AND OPERATING CONDITIONS

The Wind Tunnel

The University of Houston Environmental Wind Tunnel was used to measure the concentration distribution of particles released at a known rate from a point source located in a thick boundary layer. The working section of the wind tunnel is a rectangular channel 20.7 m long having a cross section at the sampling location of 3.05 m laterally by 1.4 m vertically. The tunnel circuit is shown in Figure 2.

Thick boundary layers were generated by conditioning the upstream flow with vortex generators and a barrier followed a rough surface on the floor of the tunnel. The mean velocity distribution was measured using a single wire hot film anemometer which was calibrated in a smooth channel using a precision pitot tube and micromanometer. Turbulence proper-

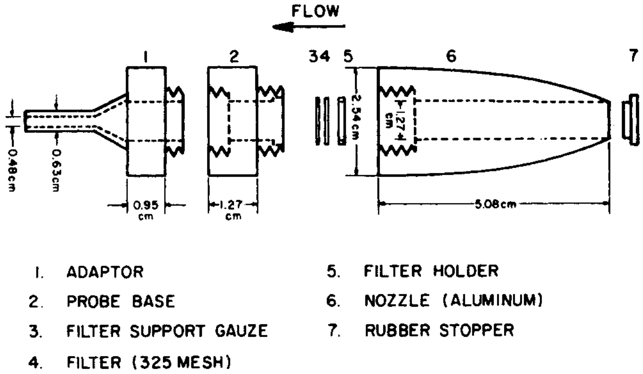

Figure 3. Isokinetic sampler.

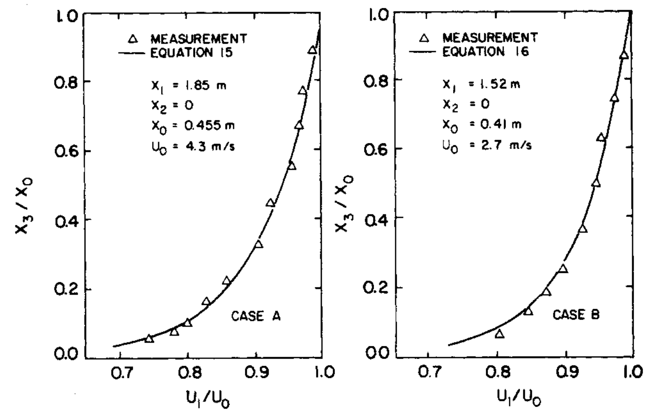

Figure 4. Mean velocity distribution.

ties were taken with a calibrated crossed film sensor (x configuration). Each sensor was composed of two identical cylinders of quartz coated with tungsten with diameter and length of 0.005 and 0.10 cm, respectively. Data were generated through two Thermo Systems Inc. Model 1010 constant temperature anemometers. Bridge voltage outputs were recorded on a Hewlett-Packard 3960 multichannel instrumentation recorder. Recorded voltage signals were processed through digitizers to an IBM 360/44 where the hot film and the voltages were related to the velocities through the calibrations. Turbulence quantities were calculated by averaging and the power spectra were extracted using fast Fourier transforms. Automatic positioning devices in the wind tunnel made it possible to obtain traverses both in the vertical and lateral directions as well as for various distances along the length of the tunnel.

Particles and Feed System

Microspheres obtained from the supplier were screened to provide samples of two narrow particle size ranges: 53-63 microns (58 μ mean) and 63-74 microns 69 μ mean). The density of the spheres was 2.6 gm/cc and microphotographs demonstrated that essentially all of the solid was in the form of true spheres with negligible broken pieces.

The glass beads were injected through a 1.25 cm diameter tube which penetrated the floor of the wind tunnel and released particles 25.5 cm above the floor. The beads were fluidized with air in a vessel designed to give uniform particle distribution, as well as particle and air rates which met the needs of the experiment. Input quantities were determined by weighing the entire fluidizer before, after and during the course of the experiment. A uniform feed rate of 50 g/15 min was used for all runs.

Sampling

Particles were sampled isokinetically. This type of measurement was recently reviewed by Fuchs (1975). The collector was designed to retain the solids, the amount trapped being the difference between the total and tare weights of the collector. An exploded view of this device is shown in Figure 3. Five collectors were mounted in either a horizontal or vertical array facing into the flow. The rubber stoppers were removed and air drawn through each device using separate rotary vacuum pumps so that the velocity of air through the 1.27 cm diameter entry would match that of the approaching stream. Air flow rates were measured with rotameters. At completion of the experiment the stoppers were carefully inserted and the collectors weighed on a Mettler H 18 balance having a sensitivity of 0.1 mg. The entry nozzle was streamlined to minimize the streamline distortion upstream of the collector.

Measured Properties of the Flow Field

Mean Velocity. Distribution of the mean velocity was measured along the vertical (x_3) direction at a series of lateral (x_2) and longitudinal (x_1) positions. The velocity was a single valued function of x_3 over the entire diffusion distance x_1 and to within several centimeters of the side walls. Thus, a single valued

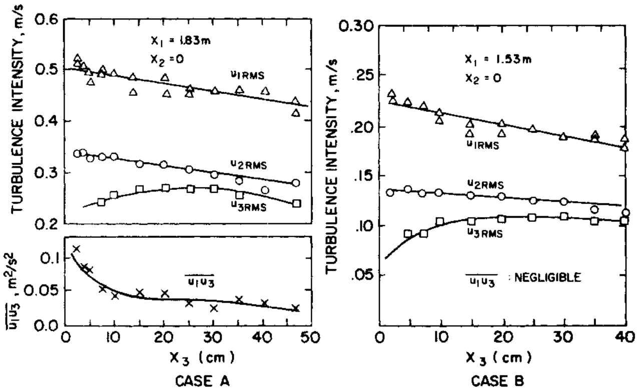

Figure 5. Distribution of turbulence intensities.

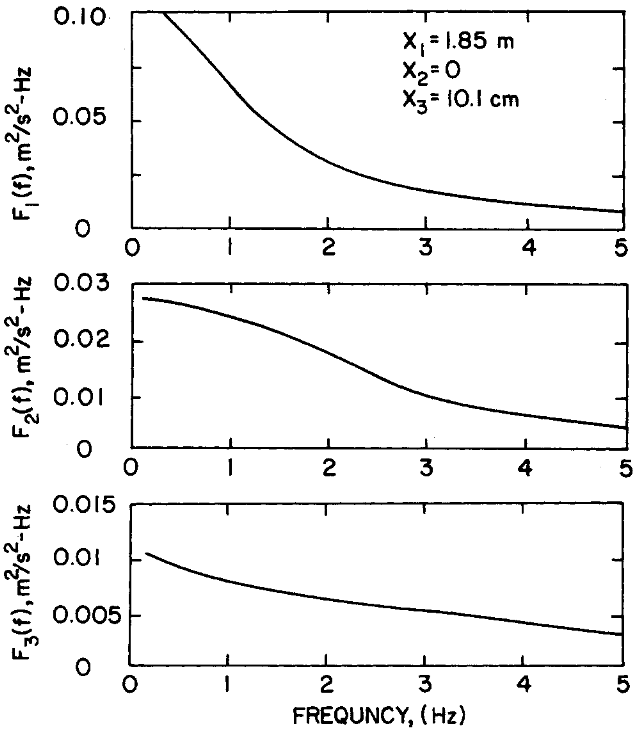

Figure 6. Spectral density of velocity fluctuation X_1 = 1.85 m; x_2 = 0; x_3 = 10.1 cm; u_o = 4.3 m/s.

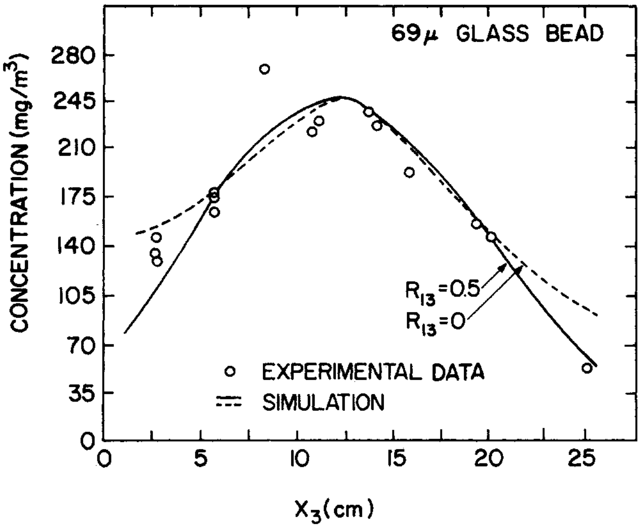

Figure 7. Comparison of theory and experiment variation of concentration with vertical position x_1 = 1.22 m; H_2 = 0; u_o = 4.3 m/s.

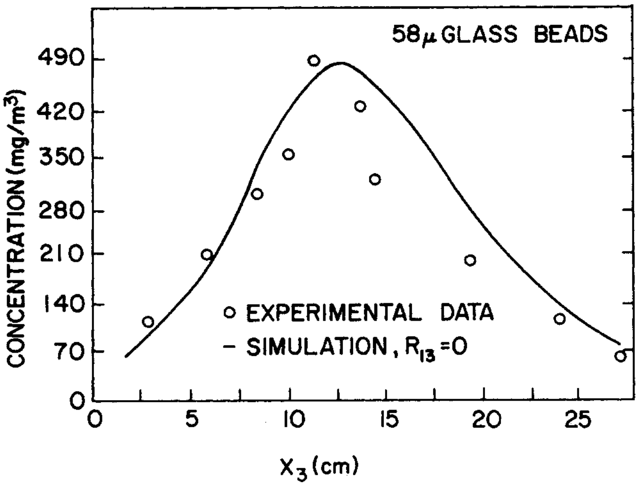

Figure 9. Comparison of theory and experiment: variation of concentration with vertical position x_1 = 0.91m; x_2 = 0; u_o = 2.7 m/s.

velocity profile could be used to describe the mean field. The wind tunnel blower was operable at two speeds and the resulting velocity profiles are shown in Figure 4. The solid lines represent these equations:

Case A: Free stream velocity, $u_0 \simeq 4.3$ m/s

$$\bar{u}_1 = 0.380 \ln x_3 + 4.57 \tag{15}$$

Case B: Free stream velocity, $u_0 \simeq 2.7$ m/s

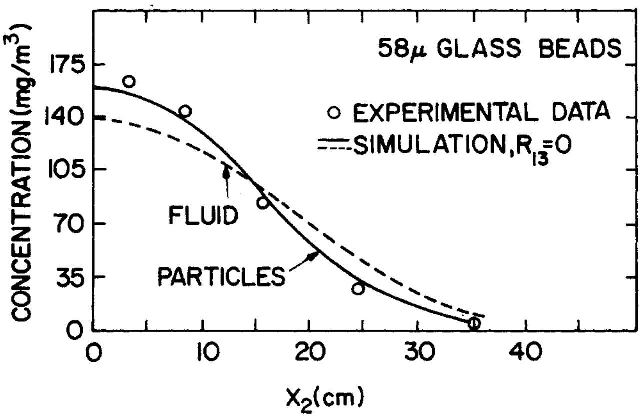

Figure 11. Comparison of theory and experiment: variation of concentration with lateral position x_1 = 1.52m; x_3 = 0.14m; u_o = 4.3 m/s.

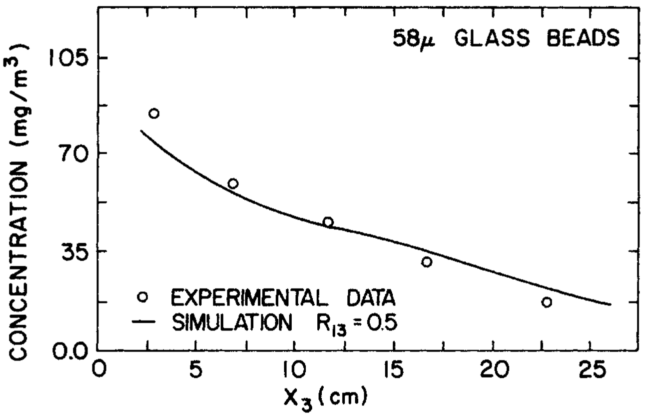

Figure 8. Comparison of theory and experiment: variation of concentration with vertical position x_1 = 3.05m; x_2 = 0; u_o = 4.3 m/s.

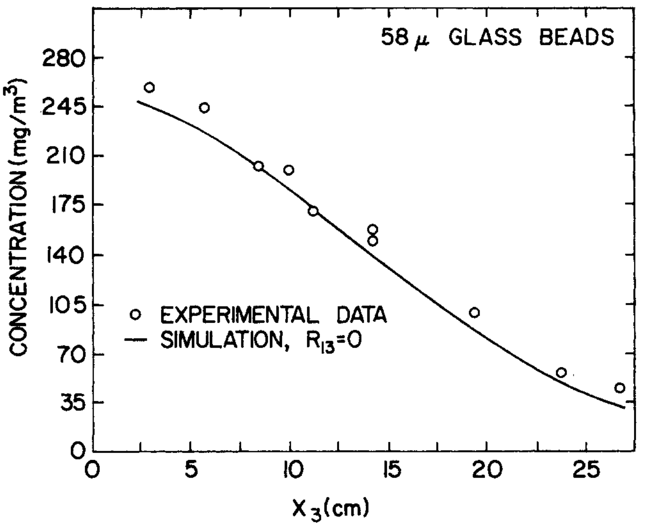

Figure 10. Comparison of theory and experiment: variation of concentration with vertical position x_1 = 1.52m; x_2 = 0; u_o = 2.7 m/s.

$$\bar{u}_1 = 0.207 \ln x_3 + 2.87 \tag{16}$$

which were used in the simulation. In these equations x_3 is in meters and $\bar{u}_1$ in m/s.

Turbulence. The turbulence intensities and the shear related correlation, $\overline{u_1 u_3}$ were calculated from the hot film anemometer signals. Experimental results are shown in Figure 5 for the two air speeds. The solid curves represent the following equations which were used to describe the field in the simulation

Case A: Free stream velocity, $u_0 \simeq 4.3$ m/s

$$u_{1rms} = 0.509 - 0.171\, x_3 \tag{17a}$$

$$u_{2rms} = 0.350 - 0.171\, x_3 \tag{17a}$$

$$u_{3rms} = 0.216 + 0.455\, x_3 - 0.850\, x_3^2 \tag{17c}$$

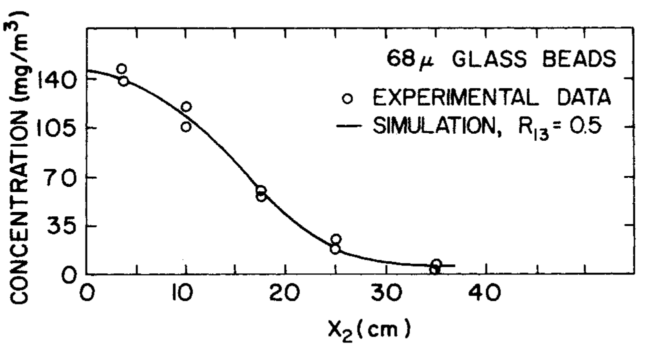

Figure 12. Comparison of theory and experiment: variation of concentration with lateral position x_1 = 1.52m; x_3 = 0.09m; u_o = 4.3 m/s.

Case B: Free Stream velocity, $u_0 \simeq 2.7$ m/s

$$u_{1rms} = 0.226 - 0.140\, x_3 \quad (18a)$$

$$u_{2rms} = 0.134 - 0.40\, x_3 \quad (18b)$$

$$u_{3rms} = 0.061 + 0.40\, x_3 - 0.787\, x_3^2 \quad (18c)$$

Turbulence data were digitized and spectral densities obtained using a fast Fourier transform. Sample spectral densities for case A are shown in Figure 6.

METHOD OF SIMULATION

The method of simulation is similar to that used by Lee and Dukler (1978) modified for the effect of gravity on the particle velocity. Eqs. 9 and 10 were programmed for repeated solution on an analog computer where the digital computer is used for control of the analog and for bookkeeping. A large number of particles, each of known mass, is allowed to diffuse through the field, each such realization representing one solution of Eqs. 9 and 10. The continuous solution for particle position is digitized along the path to obtain maximum information.

Details of the analog circuitry are given by Lee (1976). These are dependent on the configuration of the particular computer which is used. The effect of gravity was accounted for by recognizing that the equation of motion is linear in v_p. A separate circuit was used to solve the equation:

$$\frac{dv_{pg}}{dt} + \frac{9}{2a^2\rho_p} v_{pg} = g \quad (19)$$

and the resulting velocity component due to gravity v_{pg}, is added to that obtained from the solution of Eq. 9 before the position is found through the integration of Eq. 10.

The boundary condition at the floor ($x_3 = 0$) was taken to be totally absorbent.

EXPERIMENT RESULTS AND COMPARISON WITH THEORY

A comparison of experimentally measured profiles with the simulations appears in Figures 7-12. These comparisons are typical of many such results which appear in more complete detail in the thesis by Lee (1976). Figures 7-10 show typical concentration profiles in the vertical direction at various locations downstream of the source. The curves marked $R_{13} = 0$ represent the simulations where the noise in the 1 and 3 directions were generated so that they were uncorrelated. $R_{13} = 0.5$ represents a correlation coefficient between these two velocities of 0.5 generated by the method discussed by Lee and Dukler (1976).

Figures 11 and 12 compare measured lateral concentration distributions with values obtained from the simulation. In all cases the measured concentration profiles are in satisfactory agreement with the profiles predicted from the simulation. It should be noted that the simulation predicts a wider dispersion for the fluid than the particles (Figure 11). No arbitrarily adjustable constants were used to fit the data, the only input to the simulation being the known source rate, the fluid and particle properties and the measured turbulence properties of the fluid field. The result appears to justify the premise, the validity of the stochastic differential equation used to describe the process and the proposed method for determining the coefficient, β_p, and the stochastic driving function, $n(t)$.

NOMENCLATURE

a	= particle radius
g	= acceleration of gravity
f	= frequency
$F_u(f)$	= Eulerian power spectral density for the fluid
$F_v(f)$	= Lagrangian power spectral density for the fluid
$F_{u_p}(f)$	= Eulerian power spectral density of the particles
$F_{v_p}(f)$	= Lagrangian power spectral density of the particles
$F_n(f)$	= power spectral density of the stochastic forcing function
R_E	= Eulerian correlation coefficient for the fluid
R_v	= Lagrangian correlation coefficient for the fluid
R_{v_p}	= Lagrangian correlation coefficient for the particles
t	= time
u	= Eulerian velocity of the fluid
u_o	= free stream velocity
u_p	= Eulerian velocity of the particles
u_{rms}	= turbulence intensity
v	= Lagrangian velocity of the fluid
v_p	= Lagrangian velocity of the particles
v_{pg}	= Lagrangian velocity component due to gravity
x	= position of the fluid packet
x_p	= position of the particle
x_1	= longitudinal distance along wind tunnel
x_2	= lateral distance from wind tunnel centerline
x_3	= vertical distance from floor of wind tunnel

Greek Symbols

β'	= coefficient in exponential description for the Eulerian correlation coefficient for the fluid (Eq. 1)
β	= ratio of β' to the time scale ratio γ
β_p	= coefficient in the exponential description of the Lagrangian correlation coefficient for the particle (Eq. 8)
γ	= time scale ratio
μ	= fluid viscosity
ν	= fluid kinematic viscosity
ρ	= fluid density
ρ_p	= particle density
τ	= delay time

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