LA-UR -85-2745

RECEIVED BY OSTI AUG 07 1985

CONF-851177--1

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LA-UR--85-2745

DE85 015727

SUBMITTED TO: AMS Seventh Symposium on Turbulence and Diffusion
Nov. 12-15, 1985
Boulder, CO

MASTER

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1. INTRODUCTION

Monte Carlo techniques have been used extensively to simulate absolute or total diffusion in a turbulent flow field. Less effort has been devoted to simulating relative diffusion in spite of its importance in analyzing the statistics of plume meandering, instantaneous plume widths and concentration fluctuations. Since most models of relative diffusion are based on the statistics of pairs of tracer particles, calculating the trajectories of particle-pairs is a key problem in Monte Carlo simulations.

An approximate method for the analysis of relative diffusion has been discussed in several recent publications. In this approach the trajectories of particles released as pairs or in clusters are assumed to be statistically independent, but the initial particle velocities are "conditioned" to account for the effects of interparticle velocity correlations. Due to the independence of the trajectories, this approach is referred to as a one-particle model. It was recently applied to atmospheric diffusion from a continuous point source by Gifford (1982) and to diffusion from a finite-size finite-duration source by Lee and Stone (1983a), hereafter referred to as LSa. It was critised by Smith (1983), defended by Gifford (1983) and reviewed by Sawford (1984), but its validity has not been resolved in a definitive manner. There is an obvious inconsistency in the model since it accounts for interparticle velocity correlations at the source but ignores them in the particle trajectory calculations downwind of the source.

In this study we modify the one-particle Monte Carlo simulations of relative diffusion in LSa to account for interparticle velocity correlations both at the source and along the particle trajectories. The interparticle correlations are calculated directly from the Eulerian space-time velocity autocorrelation function. Since the particle trajectories are coupled, this is referred to as a two-particle model. Results from these two-particle simulations are compared to our previous one-particle results to determine the importance of the interparticle correlations downwind of the source. The models are evaluated by comparison with new wind-tunnel data on the absolute diffusion and meandering of a plume in a field of grid-generated turbulence.

2. THEORETICAL ANALYSIS

We consider the one-dimensional motion of a pair of tracer particles in a field of stationary homogeneous turbulence as illustrated schematically in Fig. 1. Here t is the time after release of the particles, U is the mean wind velocity, y is the cross-wind coordinate, v is the cross-wind component of the turbulent velocity and ℓ is the particle separation. The velocity of each tracer particle is equal to the local value of the turbulent field velocity v(y,t) along its trajectory. Therefore, the particle velocities can be simulated using the Eulerian space-time velocity autocorrelation function for the turbulent field, R_E. However, it is more convenient to use the Eulerian autocorrelation function R_C in the convective reference frame which moves with the mean wind velocity U. We assume that R_C is an exponential function of separation in space ζ and time τ, i.e. $R_C(\zeta,\tau) = \exp(-|\zeta|/L)\exp(-\tau/t_C)$ where t_C is the Eulerian integral time scale in the convective reference frame and L is the Eulerian integral length scale. Exponential autocorrelations are physically unrealistic in some ways, but they are consistent with many of the well known properties of absolute and relative diffusion as discussed by Tennekes (1979) and Sawford (1984). They also permit the time scale t_C and the Lagrangian integral time scale t_L to be simply related to the fixed-frame Eulerian scales t_E and L as derived by Lee and Stone (1983b), hereafter referred to as LSb.

The displacements of the particles from time t to $t + \delta t$ are assumed to be linear, i.e. $y_2 = y_1 + v_1 \delta t$ and $y_4 = y_3 + v_3 \delta t$ where $\delta t << t_L$. We also assume that the velocities at time $t + \delta t$ are the sum of correlated and random parts and that the correlated parts can be related to the velocities at time t in a linear manner as follows:

$$v_2 = av_1 + bv_3 + cv_4 + v_2' \quad (1)$$

$$v_4 = dv_3 + ev_1 + fv_2 + v_4' \quad (2)$$

where v_2' and v_4' are uncorrelated random velocities. The coefficients in these equations and the variances of the random velocities v_2' and v_4' are determined by taking moments and ensemble averages in which the relative positions of points 1, 2, 3, and 4 are held fixed, i.e. Eulerian ensemble averages. The velocity correlations in the resulting equations are set equal to the value dictated by R_C. For example, the term $[v_2 v_3]/[v^2]$ is set equal to $R_C(\zeta = y_2 - y_3, \tau = t_2 - t_3)$ where [ ] denote Eulerian ensemble averages. Thus the coefficients have different numerical values at each time step and for each particle-pair trajectory in the Lagrangian ensemble. Details of the evaluation of these coefficients are presented in Lee, et al. (1985).

Use of the Eulerian autocorrelation function R_C introduces the parameter $\alpha = \sigma_v t_C / L$ into the problem. This parameter appears in studies of Eulerian-Lagrangian relationships in homogeneous turbulence, e.g. Baldwin and Johnson (1972) and LSb. Based upon their theoretical studies and analysis of wind tunnel data, Baldwin and Johnson suggest that α is of order unity and will probably be limited to the range of values $0.3 < \alpha < 5$. In this study we considered the range $0.3 < \alpha < \infty$ since the $\alpha = \infty$ limit corresponds to the frequently used Taylor hypothesis of frozen turbulence in which $L = Ut_E$ (LSb). As a practical matter, the numerical solutions are very near the frozen turbulence limit for $\alpha > 5$.

The relative diffusion σ_R and the meandering σ_C are defined respectively as the standard deviation of the particle displacements relative to the centroid of the particle-pair and the standard deviation of the centroid displacements relative to the mean wind. The absolute or total dispersion σ_T is the standard deviation of the particle displacements relative to the mean wind, and $\sigma_T^2 = \sigma_R^2 + \sigma_C^2$. They are presented in the dimensionless form of $\Sigma^2 = \sigma^2/2[v^2]t_L^2$ as a function of $T = t/t_L$. A comparison of one-particle and two-particle results is presented in Fig. 2 for an initial particle separation of $\ell_o/L = 0.01$ and $\alpha = 1$. Both solutions have an initial region in which Σ_R increases as T followed by an accelerated growth region in which Σ_R increases approximately as $T^{3/2}$ in agreement with the inertial range scaling law of Batchelor (1950). All of the curves approach an asymptotic growth rate of $T^{1/2}$ with $\Sigma_R = \Sigma_C = \Sigma_T/(2)^{1/2}$ as T approaches infinity which is also in agreement with Batchelor's theory. The effect of the interparticle correlation terms in the two-particle model is to delay the onset of the accelerated growth region. The one-particle Σ_R values are, at most, a factor of about 3 larger than the two-particle values. The effect of the parameter α on the solutions is presented in Lee, et al. (1985).

3. EXPERIMENTAL STUDIES

The theoretical results presented in Section 2 were evaluated using grid-generated turbulence in the Meteorological Wind Tunnel at the EPA Fluid Modeling Facility which is described by Snyder (1979). A schematic of the experimental arrangement is shown in Fig. 3. The standard grid was modified by the addition of a checkerboard pattern of 20-cm-square Masonite squares with a 40 cm horizontal and vertical spacing between squares in order to produce more meandering of the plume. The mean axial velocity, the turbulence intensities in the axial and vertical directions, and the temporal and spatial correlations of the axial and vertical velocities were measured using hot-wire and hot-film X-array sensors.

The turbulence intensity was nearly uniform in the plane normal to the flow. It decayed slowly in the downwind direction from a value of 0.076 at the source location, $x = 0$, to 0.04 at the downstream end of the experimental region, $x = 6$ m. The mean velocity U was nearly uniform throughout the experimental region with a value of 3.1 ±0.1 m/s. Data on the autocorrelation of the vertical velocity w as a function of the time delay at a fixed point in space were fit with exponential curves to determine the integral time scale t_E. Data on the autocorrelation of the axial velocity u and the vertical velocity w as a function of the vertical separation z between two probes were also fit with exponentials to determine the respective integral length scales L_{uz} and L_{wz}. These quantities are tabulated in Table 1 for three axial locations downwind of the source. Values of Ut_E/L_{uz} are also tabulated in Table 1. These ratios are very close to unity which indicates frozen turbulence with α approaching infinity.

x	σ_w	t_E	L_{wz}	L_{uz}	Ut_E/L_{uz}
m	m/s	s	m	m	
0.5	0.207	0.0224	0.109	0.0712	0.960
3.0	0.159	0.0282	0.133	0.0858	1.002
6.0	0.130	0.0321	0.144	0.0995	0.984

Table 1 Eulerian integral length and time scales along the axis of the wind tunnel ($y = 0$, $z = 0$).

The absolute or total diffusion σ_T was determined by injecting ethylene (C_2H_4) continuously and isokinetically into the flow field through a small diameter tube as shown schematically in Fig. 3. Plume samples were withdrawn through a sampling rake of four 1.6 mm diameter tubes, each tube being routed to a separate flame ionization detector. The rake was traversed across the plume vertically at various axial positions downstream of the source. The measured concentration profiles were fit to the Gaussian plume equation to determine the mean and the standard deviation σ_T of the distributions. We assumed that $\sigma_y = \sigma_z = \sigma_T$, and this was verified by measuring both vertical and lateral profiles at a few axial locations.

The meandering of the plume centroid σ_C was determined by taking instantaneous photographs of a smoke plume which was injected isokinetically into the tunnel through a small tube as shown schematically in Fig. 3. The plume was photographed at one second intervals using a shutter speed of 1/500 s. Negatives of the exposures were digitized using a scanning microdensitometer to obtain vertical profiles of optical density, and the z-coordinate of the plume centroid was obtained by taking the first moment of these profiles. A typical photograph, optical density profiles and centroid locations are shown in Fig. 4

for $0 < x < 3$ m. Values of σ_C for an ensemble of 70 photographs are shown in Fig. 5 along with the σ_T values discussed above.

Results of the Monte Carlo simulations for the wind tunnel conditions are also shown in Fig. 5. Values of σ_w and L_{wz} measured as a function of distance downwind of the source were used in these simulations, and the turbulence was assumed to be frozen with α and t_C infinitely large. Thus there were no free parameters to adjust in the model. The agreement between the experimental results and the two-particle simulations is very good, but the one-particle model underestimates σ_C significantly. It is therefore concluded that the two-particle model provides a more accurate description of plume meandering and relative diffusion. This experimental evaluation is limited, however, since it consists of only one set of flow conditions which produced frozen turbulence.

ACKNOWLEDGMENTS

The participation of Los Alamos personnel in this project was supported by the U.S. Army Atmospheric Sciences Laboratory and the U.S. Dept. of Energy. We gratefully acknowledge the contributions of William Ohmstede, Donald Hoard, Carmen Nappo, Brian Templeman, William Snyder, and Roger Thompson.

REFERENCES

Baldwin, L. V. and Johnson, G. R. (1972) The estimation of turbulent diffusivities from anemometer measurements - I. Fluid particles. Colorado State University, CEP71-72LVB-GRJ42.

Batchelor, G. K. (1950) The application of the similarity theory of turbulence to atmospheric diffusion. Q.Jl R. met. Soc. 76, 133-146.

Gifford, F. A. (1982) Horizontal diffusion in the atmosphere: a Lagrangian-dynamical theory. Atmospheric Environment 16, 505-512.

Gifford, F. A. (1983) Discussion of "Horizontal diffusion in the atmosphere: a Lagrangian-dynamical theory." Atmospheric Environment 17, 196-197.

Lee, J. T., Stone, G. L., Lawson, R. E. and Shipman, M. (1985) Monte Carlo simultion of two-particle relative diffusion using Eulerian statistics. Los Alamos National Laboratory, LA-UR-85-2008, Los Alamos, NM 87545.

Lee, J. T. and Stone, G. L. (1983a) The use of Eulerian initial conditions in a Lagrangian model of turbulent diffusion. Atmospheric Environment 17, 2477-2481.

Lee, J. T. and Stone, G. L. (1983b) Eulerian-Langrangian relationships in Monte-Carlo simulations of turbulent diffusion. Atmospheric Environment 17, 2483-2487.

Sawford, B. L. (1984) The basis for, and some limitations of, the Langevin equation in atmospheric relative dispersion modeling. Atmospheric Environment 18, 2405-2411.

Smith, F. B. (1983) Discussion of "Horizontal diffusion in the atmosphere: A Langrangian-dynamical theory." Atmospheric Environment 17, 194-196.

Snyder, W. H. (1979) The EPA meteorological wind tunnel: its design, construction and operating characteristics. U.S. Environmental Protection Agency, EPA-600/4-79-051. Nat. Tech. Info. Service, Springfield, VA 22161.

Tennekes, H. (1979) The exponential Lagrangian correlation function and turbulent diffusion in the inertial sub-range. Atmospheric Environment 13, 1565-1567.

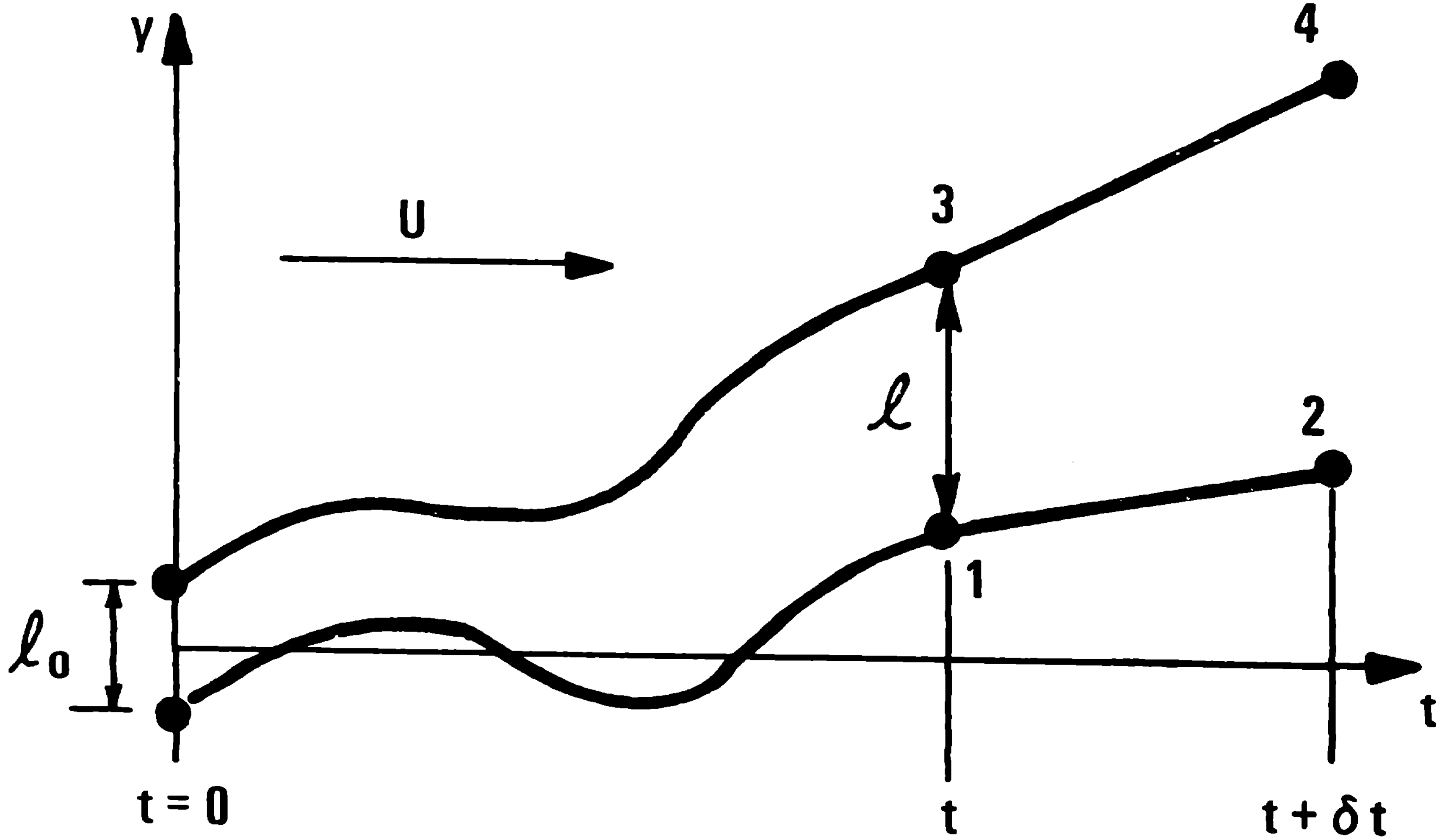

Fig. 1 Schematic of a typical particle-pair trajectory.

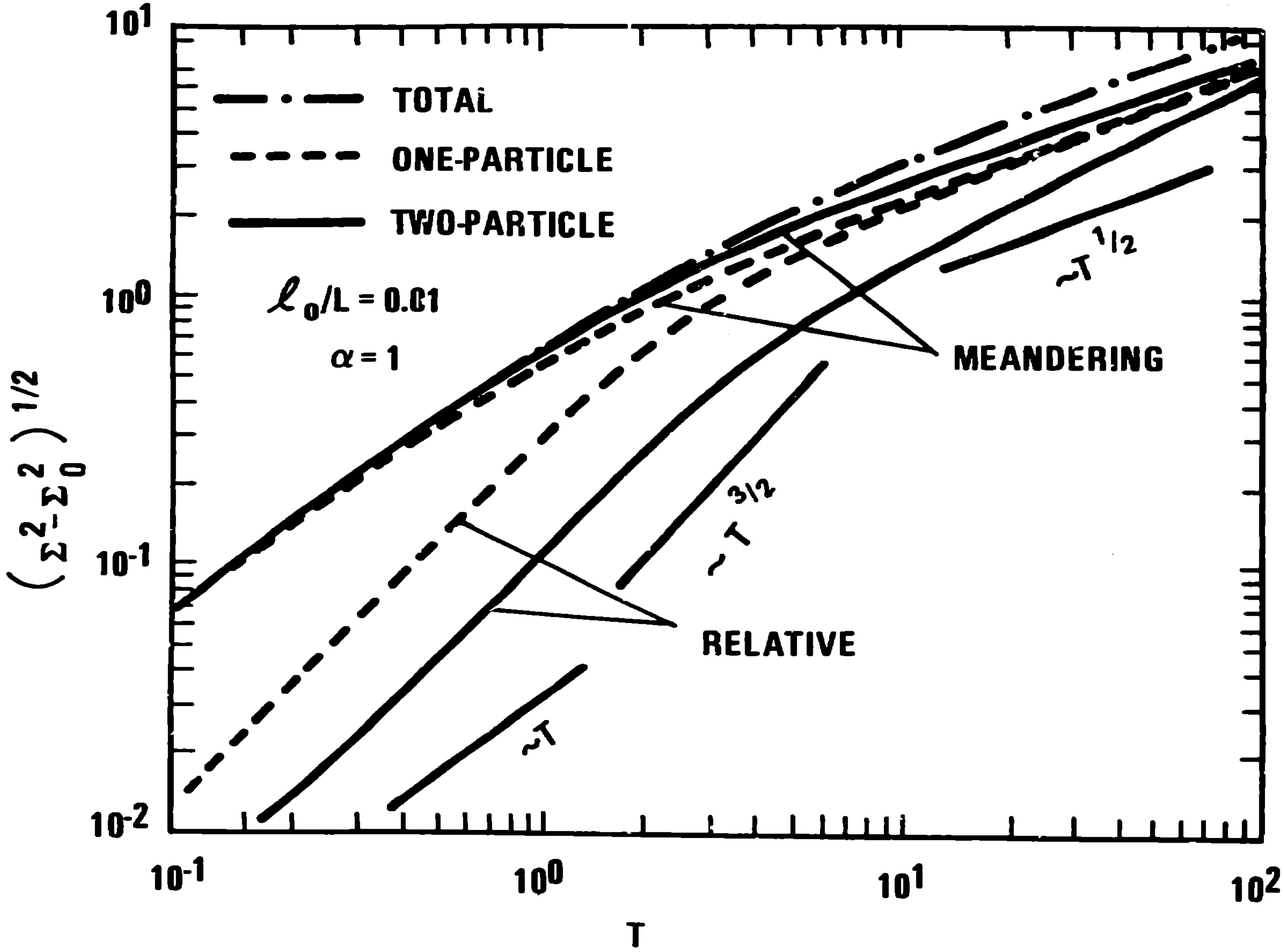

Fig. 2 Comparison of one-particle and two-particle models of meandering and relative diffusion.

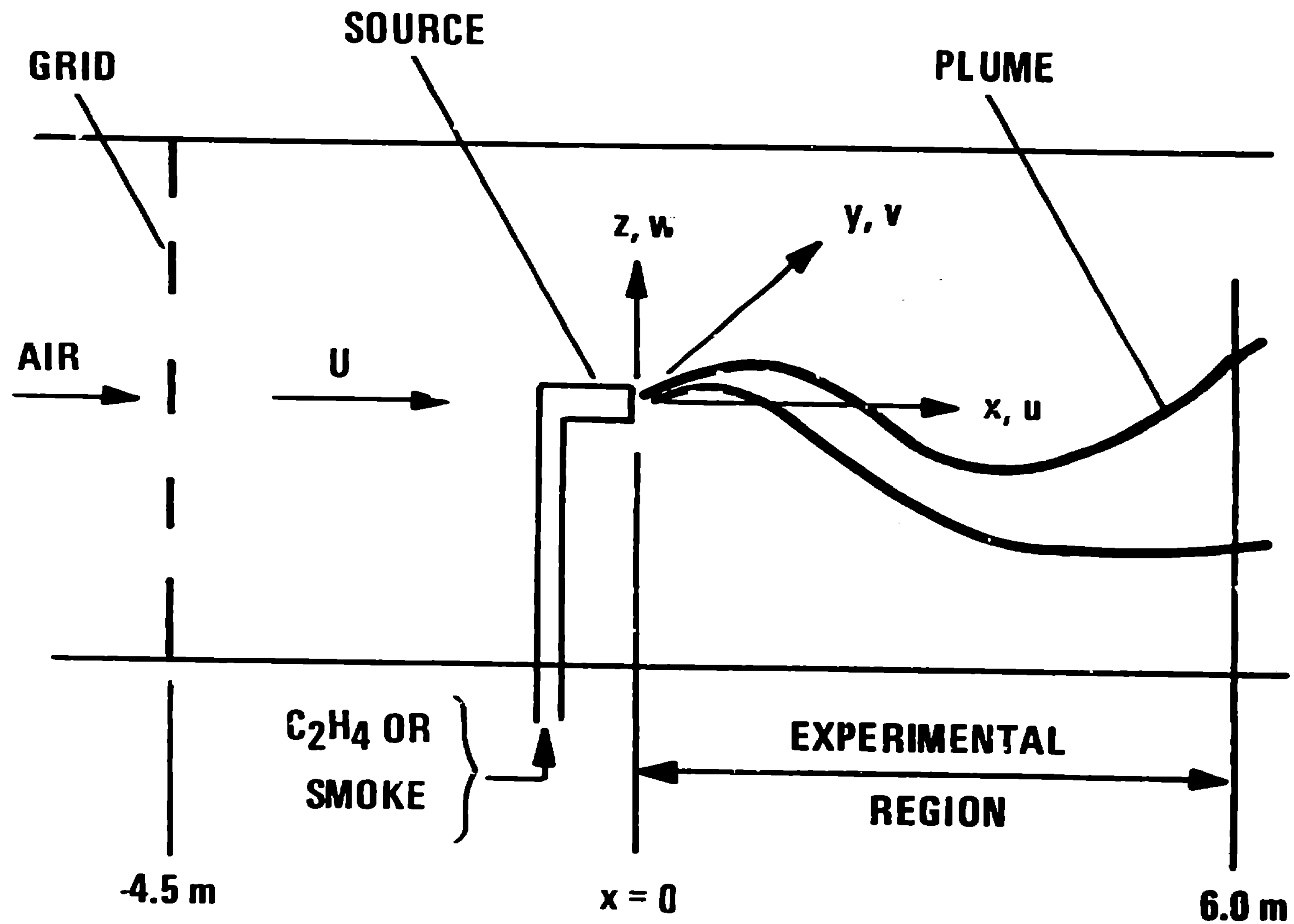

Fig. 3 Schematic of experimental arrangement, side view.

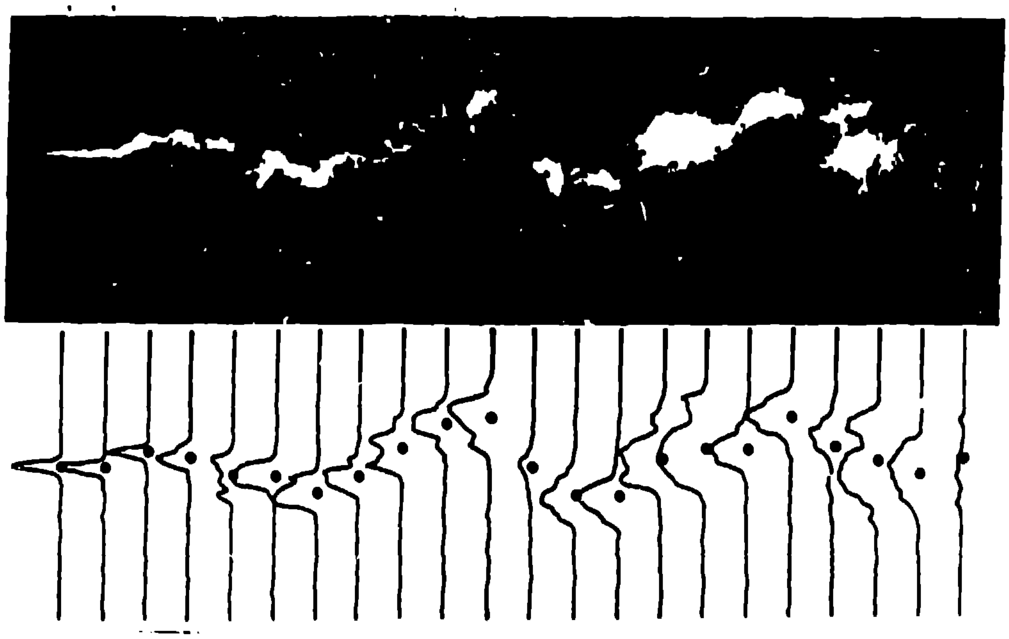

Fig. 4 Instantaneous [redacted] photographs of the smoke plume with vertical profiles of the optical density and centroid positions over the region 0 < x < 3 m.

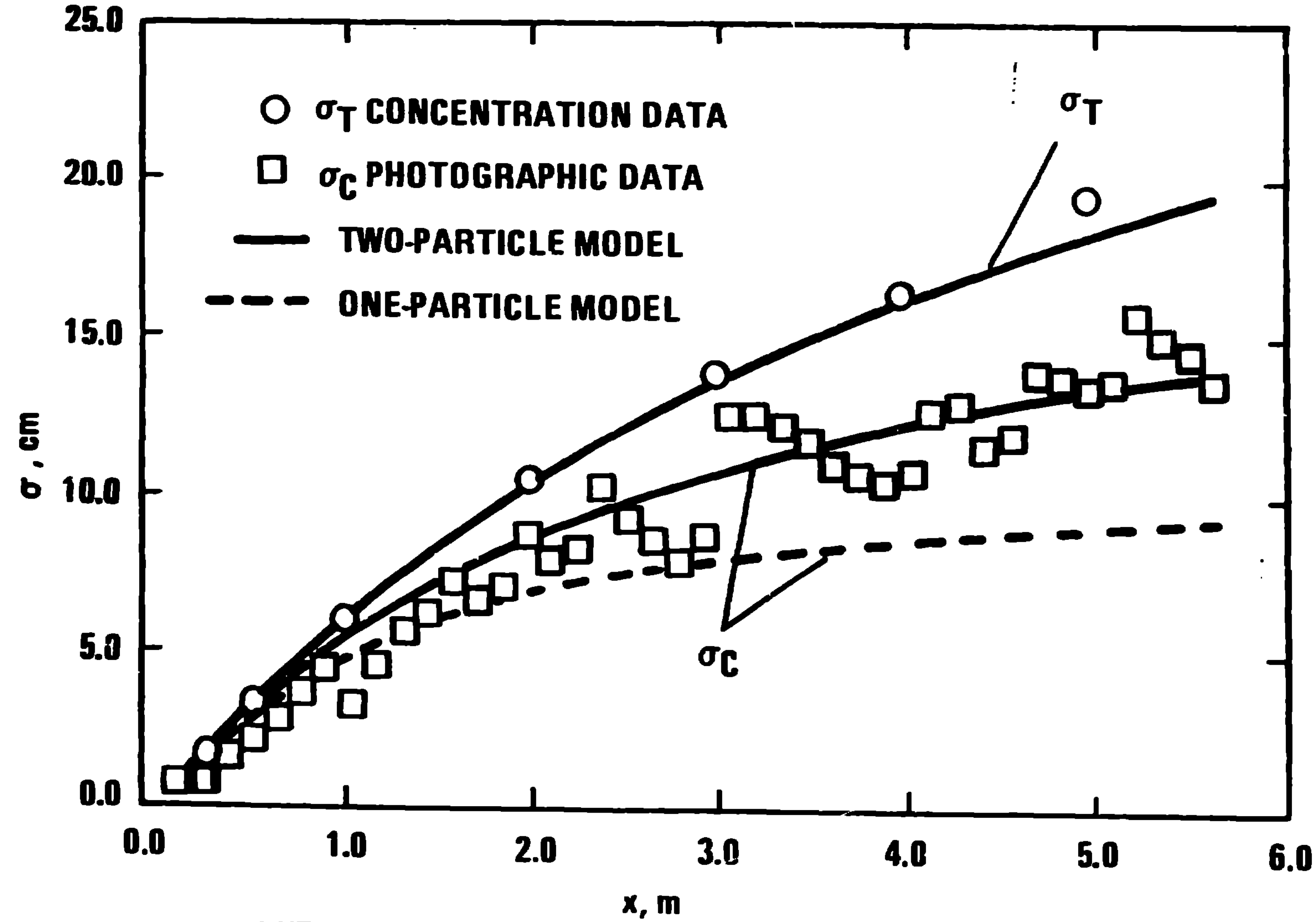

Fig. ~~16~~ 5 Comparison of concentration and photographic data to one-particle and two-particle Monte Carlo simulations.