VIth World Congress on
Air Quality (IUAPPA),
Paris, May 16-20, 1983

NUMERICAL SIMULATIONS OF LAGRANGIAN PARTICLE DIFFUSION BY MONTE-CARLO TECHNIQUES

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INTRODUCTION AND SUMMARY

Particle modeling is the most recent and powerful computational tool for the numerical discretization of a physical system. It has been particularly successful in a wide spectrum of applications (Hockney and Eastwood, 1981), which range from the atomic scale (electron flow in semiconductors, molecular dynamics), to the astronomical scale (galaxy dynamics), with other important applications to plasma and turbulent fluid dynamics.

Transport terms, whose correct numerical treatment is very difficult with Eulerian (grid) models, are handled in a straightforward manner, by particle models. Particles, in fact, have a Lagrangian nature, since they simply move following the main flow. For this reason, they are often called Lagrangian particles.

Particle models can be purely deterministic or possess statistical (random) characteristics. In the first case, particle motion is generated by forces originate from particle interactions and/or potential fields. These simulations are fully deterministic and particle trajectories are uniquely calculated. In the second case, semi-random pseudo-velocities are generated using Monte-Carlo computer techniques. In this case, the trajectory of a single particle does not contain any important information, since it represents just a realization from an infinite set of possible solutions. Important considerations, however, can be inferred from the computation of average particle ensemble properties, which are not affected by the randomness of the pseudo-velocities if a sufficient resolution (i.e., enough particles) is used for the numerical discretization of the phenomenon.

Monte-Carlo methods are particularly important since, in several applications, they allow every particle to move independently from the others. Therefore, they provide a computational algorithm which is generally faster than the corresponding deterministic computations, where interactions between neighbouring particles, need t be computed.

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This paper deals with the application of the above Monte-Carlo technique for the simulation of turbulent atmospheric transport processes in the boundary layer. The next section presents a brief review of previous applications of particle methods to air quality simulations, with some emphasis on recent developments and findings. Then, in the following section, atmospheric diffusion simulations, for both elevated and ground level releases, are presented and discussed. Computer plots of time-dependent particle dynamics are used to evidentiate the advantages and the great potential of such method. Conclusive remarks and considerations are finally presented in the last section.

ATMOSPHERIC DISPERSION SIMULATION BY PARTICLE METHODS

Even though a fully satisfactory theoretical treatment of turbulent diffusion has not yet been achieved, Lagrangian particle numerical methods seem particularly suitable to simulate the diffusion of a substance released into a turbulent flow. In the atmospheric boundary layer, for example, emitted gaseous material can be described by a suitable number of particles moving, at each time step, according to pseudo-velocities. These pseudo-velocities simulate the effects of the three basic dispersion components: 1) the transport due to the mean fuid velocity (average wind), 2) the (seemingly) random turbulent fluctuations of wind components (both horizontal and vertical), and 3) the molecular diffusion (if not negligible). Only several thousands particles can be handled by present computers. Therefore the pseudo-velocities cannot simulate a single molecule's motion, but just define an algorithm for the computation of the particle density distribution on a particle ensemble basis.

Pseudo-velocities computation is the most important (and difficult) task in particle modeling. Due to their Lagrangian nature, particle displacement should be computed using suitable Lagrangian measurements of the flow. Unfortunately Lagrangian properties are difficult to measure and, therefore, must be inferred from Eulerian measurements. Different methods have been proposed for relating Eulerian and Lagrangian statistics, but none of them has been found totally satisfactory. Among many studies in this field, an acceptable statistical estimator, at least for ocean currents, has been presented by Davis (1982), while Hanna (1979a; 1981a) has evaluated and tested semi-empirical relations for the atmospheric boundary layer.

Pseudo-velocity vectors $\underset{\sim}{u}_e$ for each particle have been frequently approximated by

$$\underset{\sim}{u}_e = \bar{\underset{\sim}{u}}_e + \underset{\sim}{u}'_e \qquad (1)$$

where $\bar{\underset{\sim}{u}}_e$ is the best estimate of the average (Eulerian wind field at the particle location) and $\underset{\sim}{u}'_e$ is a "diffusivity" velocity. Moreover, some properties known to be valid for Eulerian measurements have been assumed to be an acceptable approximation for $\underset{\sim}{u}'_e$. For example, starting from Smith (1968), $\underset{\sim}{u}'_e$ components have been frequently assumed to be independent stationary first-order autoregressive (Markov) processes

$$u'_e(t+\Delta t) = R_e(\Delta t)\; u'_e(t) + u''(t+\Delta t) \qquad (2)$$

where u" is a zero-mean normally distributed random component (white noise). Eulerian measurements of wind fluctuations σ_u have been generally used to evaluate $\sigma_{u'_e}$, while semi-empirical formulations have been proposed to evaluate R_e from the autocorrelation structure of Eulerian measurements (e.g., Hanna, 1981b).

In addition to the general reservation about the above extention of Eulerian statistics to Lagrangian parameters, major problems have been found regarding:

1) the treatment of the negative cross-correlation between along wind and vertical wind fluctuations

2) the conditions for zero correlation between the two horizontal components of wind fluctuations

3) the skewed distribution of the vertical wind fluctuation

4) the treatment of vertical variation of turbulent fluctuation intensities, i.e., $\sigma = \sigma(z)$.

The first problem derives from the fact that Eulerian measurements have shown a non-zero (negative) correlation ($\overline{u'w'} < 0$) between the along wind and vertical wind fluctuations. Therefore, it is highly probable that a correct computation of $\underset{\sim}{u}'_e$ must incorporate this effect. A numerical scheme has been proposed (Zannetti, 1981 and 198 to properly treat this phenomenon. If $\underset{\sim}{u}'_e = (u', v', w')$ and $\underset{\sim}{u}'' = (u'', v'', w'')$ such scheme can be written

$$u'(t+\Delta t) = \phi_1 u'(t) + u''(t+\Delta t) \tag{3}$$

$$v'(t+\Delta t) = \phi_2 v'(t) + v''(t+\Delta t) \tag{4}$$

$$w'(t+\Delta t) = \phi_3 w'(t) + \phi_4 u'(t+\Delta t) + w''(t+\Delta t) \tag{5}$$

where ϕ_1, ϕ_2, ϕ_3, ϕ_4, $\sigma_{u''}$, $\sigma_{v''}$, $\sigma_{w''}$ can be computed from algebrical manipulation of known input parameters (intensities and correlation parameters of $\underset{\sim}{u}'_e$ fluctuations).

Regarding the second problem, Eulerian measurements show that the two horizontal wind fluctuations are uncorrelated ($\overline{u'v'} = 0$) if an horizontal axis (generally the x-axis) is chosen to coincide with the main wind direction. But the main wind direction generally varies with the altitude (Ekman Spiral) and with time. For these non-homogeneous non-stationary simulations a Special Reference (SR) system has been proposed (Zannetti, 1982) where the x axis, for each specified altitude z and each tim step (e.g., 10 minutes), is allowed to vary in order to coincide with the main horizor tal wind direction at that altitude and that time. In this SR system it is assumed that $\overline{u'v'} = 0$. Special formulas are also given (Zannetti, 1982) to calculate the $\underset{\sim}{u}'_e$ horizontal intensity fluctuations (σ) in this SR system, using a suitable meteorologic instrumentation (e.g., a meteorological tower or a Doppler Acoustic Sounder) which provides data in a fixed reference system (e.g., East-North).

The third problem has been recently a subject of great interest and investigatior Eulerian observations (e.g., Lenschow, 1970) show that the vertical fluctuation w' has a typical daytime (convective) behaviour in which upward air motion ($w'>0$) is less frequent (e.g., 40%) but more intense (e.g., one and a half) than downward motion ($w'<0$). Hanna (1981c) has reviewed this problem concluding that a correct particle simulation must take into account of this skewness of w', even though good field estimates of such parameter are not yet available. Wilson et al. (1981) provide a formal demonstration of the need of a bias in the Lagrangian vertical velocity w' in the presence of a vertical gradient in $\sigma_{w'}$ (see next point). A similar argument is supported by the work of Diehl et al. (1982) in which particle random-walk simulations are used to represent gradient-transfer (K-theory) conditions in the surface layer. Their computations show that, if particle displacements are allowed to be space-dependent (e.g., greater displacements at higher altitudes in the surface layer) then the particle flux may contain an additional term which is proportional to the concentration itself, instead of its gradient.

The fourth problem is related to the previous one. The atmospheric stratificatic generates a strong vertical variation of the horizontal and (especially) vertical diffusion rates (e.g., very low vertical diffusion inside an inversion layer). This phenomenon can be simulated, for example, by allowing σ_w to vary with the altitude, even though it has been reported (Hall, 1975) that such variation can cause unrealist: particle motion and an excess build-up of concentration in the regions with low σ_w.

NUMERICAL SIMULATIONS

A few three-dimensional computer simulations have been performed according to Eqs. 3-5, following the dispersion pattern of a puff of 2000 particles during differe meteorological conditions. The particles were instantaneously released at the same location, with initial wind fluctuations u', v', and w' equal to zero. Stationary meteorological input was assumed throughout each simulation.

Figs. 1-3 in this section show three different diffusion stages of the same puff, at different times after release (18 Δt, 36 Δt, and 54 Δt, respectively). All units are in the MKS system. The time step Δt is 10 in Figs. 1-2 and 15 in Fig. 3. A black circle locates the emission point in the figures.

Fig. 1 presents a horizontal a) and three vertical b), c), d), sections of the puff evolution. Particles are initially released in (0,500,500), and the meteorological input for a) and b) is $\bar{u}_e = (3,0,0)$, $R_e = 0.7$ for all three components, $\overline{u'w'} = 0$, $\sigma_{u'} = \sigma_{v'} = 0.4$, and $\sigma_{w'} = 0.2$. A vertical shear is added in c) in which the wind speed u (along x), $\sigma_{u'}$, $\sigma_{v'}$ and $\sigma_{w'}$ are a linear function of the altitude z. The additional term $\overline{u'w'} = -0.3$ is added in d). It must be noted, from c) and d), that negative $\overline{u'w'}$ and wind shear (increase with height) work against each other. At the beginning when the puff is small the first prevails, while, when the vertical size of the puff is large enough, the second overcomes.

Fig. 2 presents the vertical section of a simulation of a partial fumigation. Particles are again released at (0,500,500) with $R_e = 0.7$ and $\overline{u'w'} = 0$. The wind speed u (along x) has a linear vertical increase from 1 at the ground to 3 at 500, remaining constant above that altitude. An inversion layer is simulated between 600 and 700 by assuming the following values for σ_w: linear increase from 0.5 at the ground to 1.5 at 600, 0.15 between 600 and 700, 0.5 above 700. Part of the puff is fumigated to the ground, much is trapped inside the inversion layer and only few particles are able to perforate the inversion.

Fig. 3 shows the vertical, a), b), c), and horizontal, d), e), f), sections of a puff released at ground level in (0,500,0). In this case $R_e = 0.7$ and $\overline{u'w'} = 0$ as before, but the wind speed u (along x) is 1.15 for the altitude z between 0 and 1, a power law $4(z/500)^{0.2}$ for $1 < z < 500$, and 4 for $z > 500$. Turbulence intensities are a function of the wind speed u: $\sigma_{u'} = u/4$, $\sigma_{v'} = 2\,\sigma_{u'}/3$, $\sigma_{w'} = \sigma_{v'}$. Perfect particle reflection has been assumed at the ground surface and Δt is 15.

Finally, Fig. 4 a) presents the standard deviation σ_z of the vertical distribution of the particles in Fig. 1 b), as a function of the downwind distance x. Stars represent σ_z values while the continuous circle gives the best power law fitting. It can be seen that the fitting curve $\sigma_z = 0.174\ x^{0.727}$ underestimates diffusion close to the source and overestimates it far downwind. Fig. 4 b), c), d), represents the same data with three different power law fitting curves: d) $\sigma_z = 0.0547\ x^{0.967}$ close to the release point; c) $\sigma_z = 0.241\ x^{0.685}$ at intermediate downwind distance; and b) $\sigma_z = 0.632\ x^{0.540}$ far downwind.

The three different diffusion regimes in Fig. 4 can be explained by considering that all particles are released with the same initial $u' = v' = w' = 0$, and therefore, due to the autocorrelation term $R_e = 0.7$, the initial particle diffusion is strongly correlated ($\sigma_z \div x$). Particle initial correlation, however, is dumped after several time steps, when the memory of the initial state is lost ($\sigma_x \div x^{1/2}$). This final state is reached, in Fig. 4 b), after about 30 time steps when the residual autocorrelation of the Markov process of Eq. 2 (Box and Jenkins, 1976) is $R_e^{30} = 2.25.10^{-5}$ with respect to the initial state.

The above results agree with the statistical theory of diffusion (Taylor, 1921) and with similar numerical experiments (e.g., Hanna, 1979b).

CONCLUSION

We have presented a discussion on Monte-Carlo modeling application to the simulation of turbulent diffusion in the atmospheric boundary layer. Diffusion experiments have been displayed in which particle dynamics can take full account of complex meteorological conditions (e.g., shear effects and an elevated inversion layer). Future work on this field will deal with non-stationary plume simulations, particle deposition and simulation of tracer experiments.

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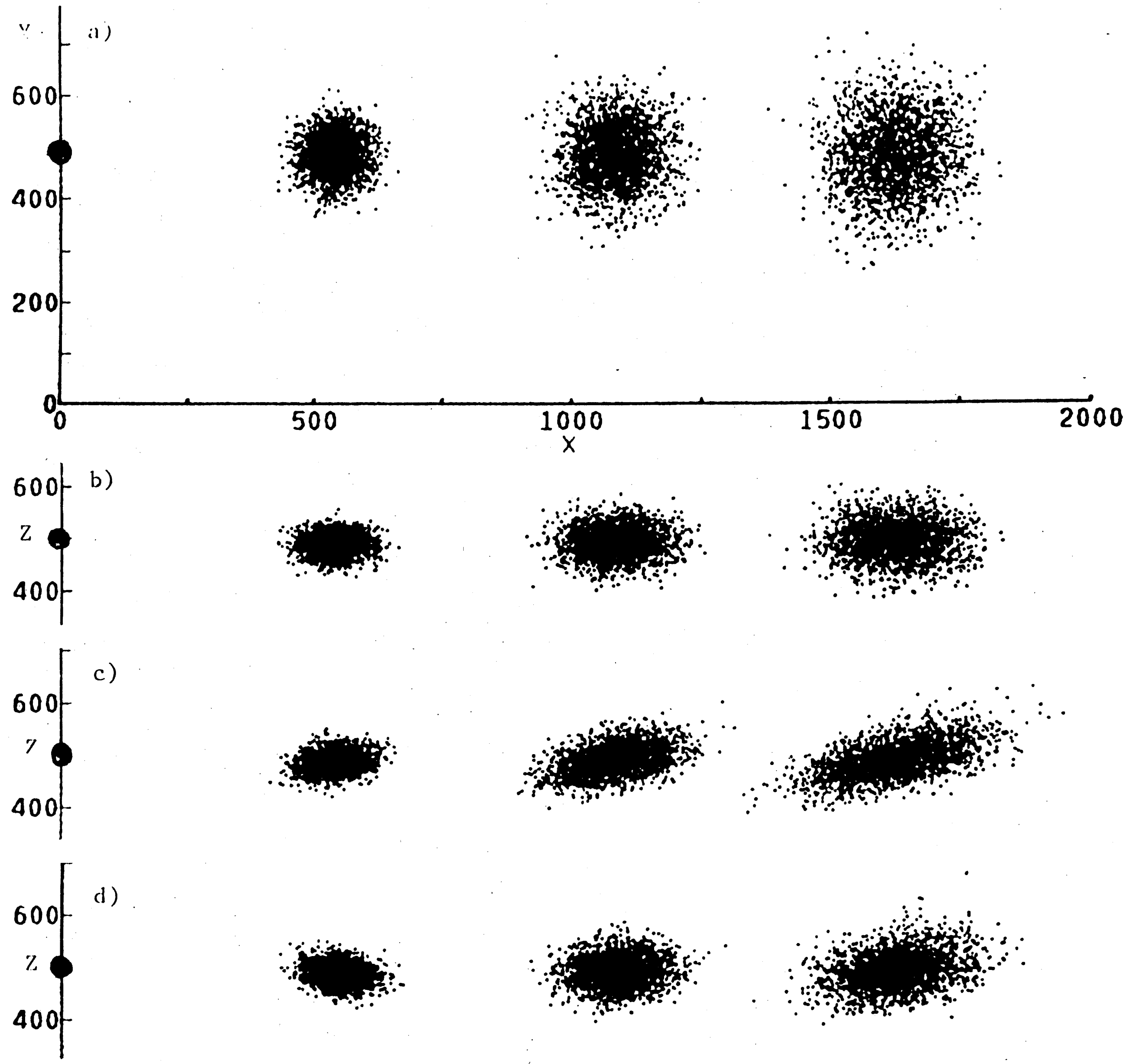


Figure 1 - (See text for explanation of this figure and the following ones)

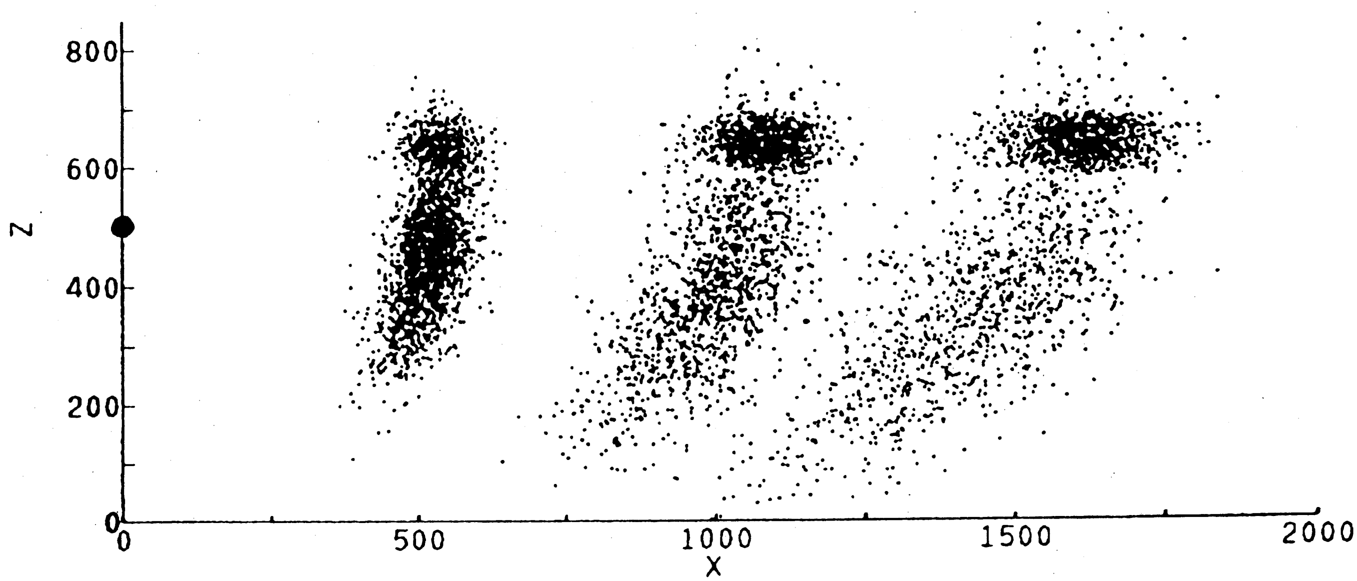


Figure 2

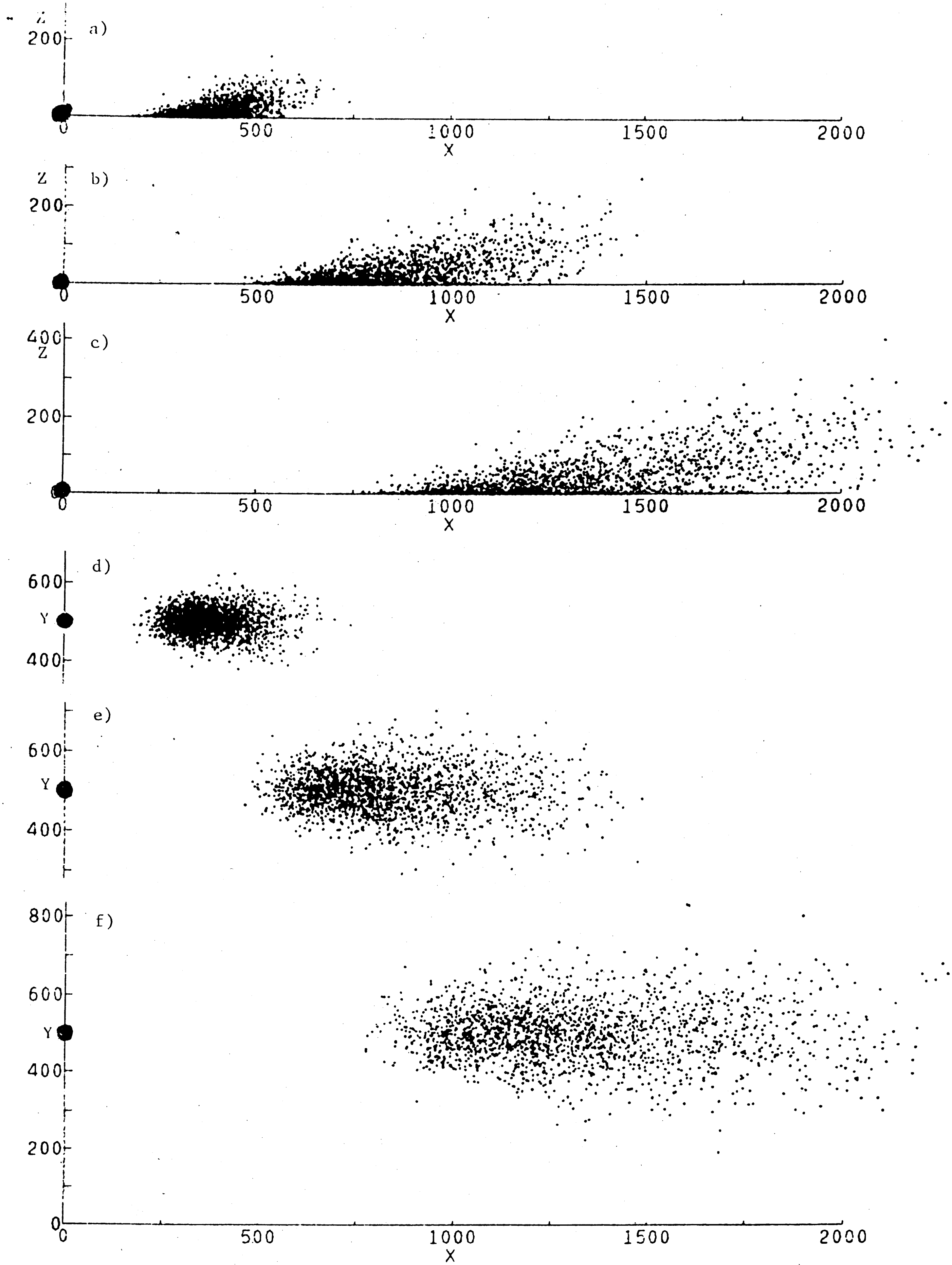
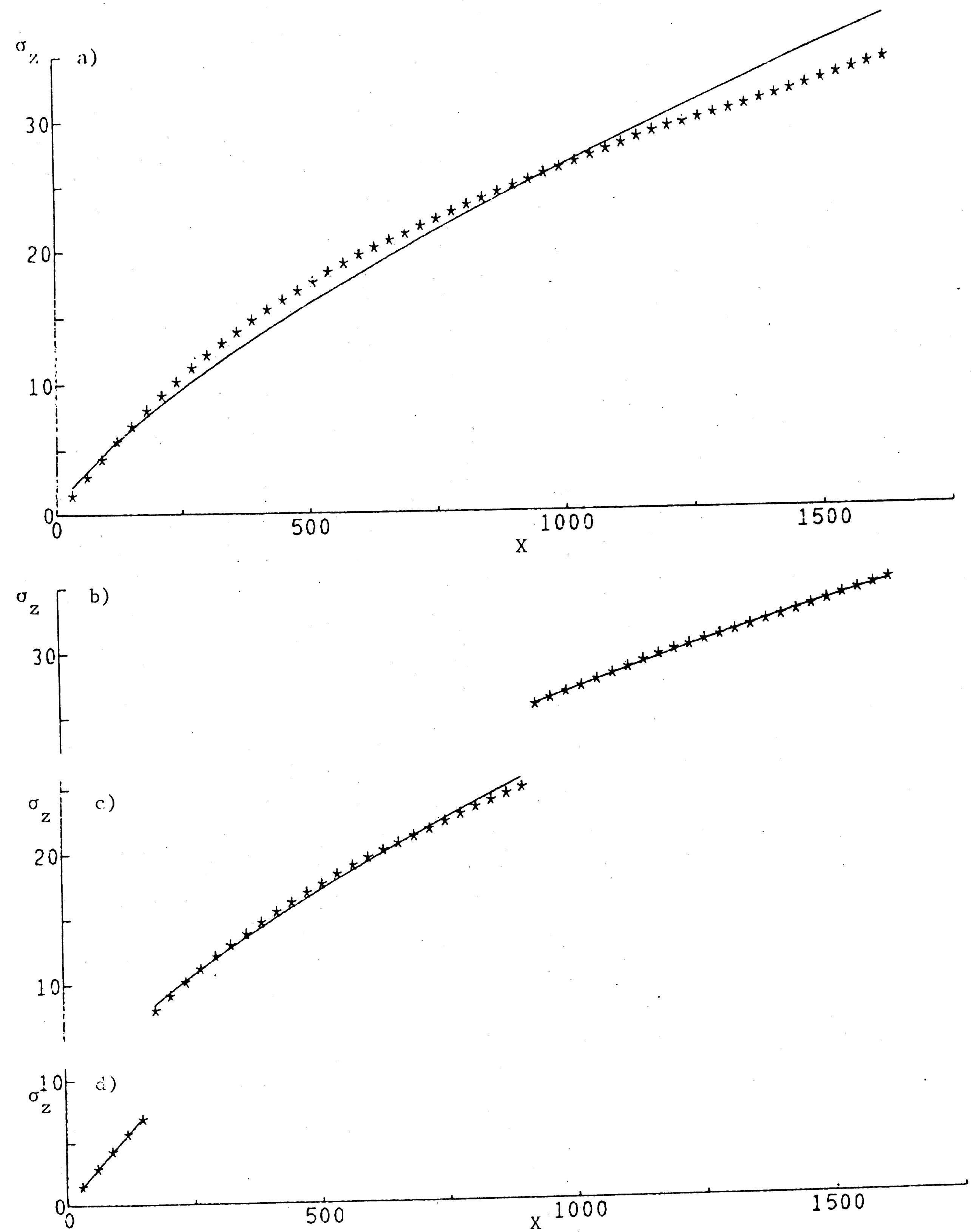


Figure 3



σ_z
a)
30
20
10
0
0
500
1000
1500
X
σ_z
b)
30
σ_z
c)
20
10
σ_z
10
d)
0
0
500
X
1000
1500

Figure 4