P-36

89-43.1

CAN WE CONTINUE TO APPLY DISPERSION MODELS WITHOUT A PROPER LINKAGE WITH METEOROLOGICAL MODELS

PAOLO ZANNETTI

AEOVIRONMENT, INC.
MONROVIA, CALIFORNIA

AIR & WASTE MANAGEMENT
ASSOCIATION
SINCE 1907

For Presentation at the
82nd Annual Meeting & Exhibition
Anaheim, California
June 25–30, 1989

1. INTRODUCTION

Intensive worldwide research in air pollution modeling has been developed in the last three decades. While in the rest of the world this research has remained mostly a scientific exploration, in the U.S. the EPA has elevated[1] air quality models to a high decision-making level, to assess both present impacts and those of future emission scenarios. Consequently, in the U.S., models are major tools in multimillion dollar decisions involving the possible installation of costly emission control devices. This situation has triggered the development of a new science, "regulatory modeling," often, but not always, related to the development of air quality models as pure research tools.

This modeling dichotomy has generated positive and negative consequences. On the positive side, EPA's regulatory goals have provided the incentive for the definition of unambiguous methodologies, mostly based on simple engineering assumptions, that make use of available input data and are relatively easy to apply. Any "subjectivity" in the application of these models is eliminated or minimized, aiming at the development of well-structured, objective techniques that could guarantee an unequivocal, general use for all regulatory applications. The international scientific community must praise the EPA for this effort and, especially, for the EPA-supported research that, particularly in the last decade, has aimed at developing new, improved modeling techniques. Incidentally, many centers around the world have benefited from the EPA's activities by acquiring, for a nominal price, the famous UNAMAP tape, which contains most of the models the EPA recommends.

On the negative side, regulatory models possess "an original sin" that, in spite of some recent efforts, influences today's and tomorrow's applications and developments. This sin is that almost all the EPA's recommended models are based on a very simple (too simple!) approach: the Gaussian steady-state equation for the simulation of atmospheric transport and diffusion. Certainly, there was a good reason, ten years ago, for this choice: it provided a relatively simple, numerically stable, easy-to-use, easy-to-understand (but also easy-to-criticize) approach. But the EPA, under constant pressure the last few years to develop and adopt "better" techniques, chose to devote its efforts to improving the Gaussian model for highly sophisticated applications, instead of moving toward more advanced techniques. The result is that the simple Gaussian approach, which should have been limited to initial screening applications, has become the backbone of the entire regulatory modeling arena and has been forced much beyond its limits of applicability.

Another unpleasant consequence is that a separation has been created between most of the research community, which no longer uses the steady-state Gaussian model, and the regulatory community, which does. What we face today is the emergence of "specialized" Gaussian dispersion models, designed to work under certain emission, meteorological or terrain scenarios, such as coastal diffusion, rough terrain, or toxic gas dispersion. This trend is risky. Atmospheric diffusion is atmospheric diffusion, independently of other considerations. We should be able to simulate it correctly and not just bend or calibrate simple techniques to provide a reasonable fit to experimental data. In other words, we do not want the models just to appear to work well, we want them to work well for the right reason, i.e., because they simulate and reflect an understanding of the complex, three-dimensional dispersion patterns.

Two important changes have affected the development of air quality modeling techniques: 1) the increased availability of three-dimensional meteorological information, and 2) the revolutionary development of faster and cheaper computer hardware. Fifteen years ago the common objection against advanced simulation methods was that the meteorological input was not available and, at any rate, these techniques were too expensive to run. This led to very general parameterizations of the planetary boundary layer (PBL) and to the use of models, such as the Gaussian steady-state equation, in which meteorological parameters (i.e., wind speed, wind direction, turbulence intensities, etc.) are considered homogeneous throughout the entire PBL.

Today, the meteorological information is much more complete and, as outlined in Figure 1, much progress has been made in characterizing the different layers in the PBL and parameterizing their properties. The use of Doppler acoustic sounder instruments is not unusual in atmospheric diffusion studies, and meteorological models (of diagnostic or prognostic type) are often used to provide a time-dependent three-dimensional characterization of the main meteorological parameters. We cannot claim that this three-dimensional meteorological information is error-free. Actually, large uncertainties persist in these calculations. But the data, though approximate, are indeed available, and some use should be made of them. Only advanced diffusion methods, however, can use a three-dimensional meteorological input.

This paper emphasizes the need for a proper linkage between meteorological models and advanced dispersion models. The lack of appropriate linkage is blamed for part of the poor performance that dispersion models have shown when applied in a hands-off manner (i.e., without ad-hoc adjustments or calibrations). Section 2 presents considerations about the unsatisfactory performance of models, while Section 3 discusses dispersion simulation techniques.Section 4 addresses an optimal linkage between meteorological and diffusion models. Section 5 presents conclusions.

2. PERFORMANCE EVALUATION OF DISPERSION MODELS AND ITS IMPLICATIONS

Turbulent phenomena remain the greatest unsolved problems of classical physics. All current air pollution simulation techniques use simplifications and parameterizations based on empirical, experimental data. Consequently, when models are used with data sets different from those originally used for model "tuning," their performance deteriorates.

Several methodologies are available to simulate atmospheric dispersion phenomena. They range from simple techniques, such as the steady-state Gaussian plume models, to advanced methods, such as higher-order closure formulations[2] and particle models.[3] (Particle models are computer methods for the numerical simulation of the dynamics of physical systems. In air quality studies, they can be used to simulate the dispersion of both gases and particulate matter.) Unfortunately, the most complex and promising methodologies, which provide a more rigorous and theoretically acceptable description of the real world, are difficult to apply successfully, mainly for the following reasons:

1. The theories of some advanced models are based on parameterizations whose validity is not completely clear (e.g., the simulation of dispersion under unstable conditions using K-theory models is theoretically questionable).

2. The input requirements of virtually all advanced models are complex and often impossible to satisfy, except during short, intensive atmospheric monitoring experiments.

3. The computer implementation of virtually all advanced models consists of complex research codes, not fully documented and often continually improved and modified by their developers. Therefore, in most cases, these computer codes can properly be used only by their developers and require suitable, and often subjective, adjustments of key model parameters.

As a consequence of these reasons, complex atmospheric dispersion models have not provided satisfactory simulation results when used for short-term (e.g., hourly) dispersion simulations.[4,5,6] Moreover, the conclusions of several studies (e.g., those presented at the DOE Model Validation Workshop, October 23-26, 1984, Charleston, South Carolina) indicate that the more advanced numerical techniques, when applied in a hands-off fashion, do not perform better than simpler numerical approaches and, therefore, have not yet justified their computational cost in terms of simulation performance.

The fact that both simple and complex methods show a similar (unsatisfactory) degree of performance should not lead us to conclude that they are equivalent for practical purposes. If we analyze the reasons that cause the unsatisfactory performance of models when compared with tracer experiments, we find that the principal reason is the insufficient resolution of the meteorological input. In fact, if, for example, a tracer experiment is conducted with ground-level receptors at a distance of, say, 200 m from each other, this requires, for a potentially successful numerical simulation, a meteorological input able to incorporate fluctuations over a spatial scale not greater than 200 m and a temporal scale not greater than 200/u s, where u is the average wind speed. But at least one major meteorological parameter, wind direction, is not known with such an accuracy. Consequently, wind shear does play a major role and, for example, can cause an elevated plume to travel 20-40 degrees away from the direction where the model would forecast the actual ground-level impact.

Actually, specific model performance evaluation methods have been proposed[7,8] to minimize the effects of the uncertainties in wind direction, but the problem still remains for the other meteorological parameters. The major point is that air quality modeling performance evaluation has often been performed, in the past, in a "blind" way by simply assuming that tracer experiments represent the real world and models should just replicate them. This is not true for several reasons. First, measurement errors should fully be included in the evaluation procedures. Models should be allowed to modify their inputs within the corresponding error bounds and should provide outputs that, if within the tracer measurement errors, should be considered fully satisfactory. Second, it should always be remembered that measurements represent a realization of a stochastic process and, as such, will always be somehow different from model outputs, which represent "expectations" or theoretical means. This is often called the intrinsic, unremovable uncertainty of simulation models. Third, and most important, models should not be applied during conditions that are clearly in contradiction with their theoretical foundations. For example, a steady-state Gaussian model should not be applied in calm conditions or when wind direction changes drastically, thus giving a bimodal concentration distribution with two separate peaks, instead of a "bell-shaped" distribution. Modelers should have been, and should be, more active in demanding proper performance evaluations of their models, according to the points discussed above.

In the context of this paper, however, the main conclusion is that models can be divided into two groups: those that cannot handle a complex meteorological input and those that can. The first group should be used only for screening analysis and, with time, they should fade away from both the scientific and the regulatory arenas. The second group comprises models that can, and will, perform better if an appropriate meteorological input is provided. The latter group is discussed in the next section.

3. MODELING TOOLS

Two types of modeling approaches possess a sufficient spatial and time resolution to make full use of the information provided by a three-dimensional meteorological model: "large eddy" models and particle models.

3.1 Large Eddy Simulation Models

As described by Nieuwstadt and de Valk,[9] a large eddy model such as those developed by Deardorff[10] and Nieuwstadt et al.,[11] calculates the large-scale turbulent motions by directly solving a set of modified Navier-Stokes equations. These equations are

- a "filtered" momentum equation with extra subgrid terms (where by "filtering" we mean the elimination of the small-scale motions that are smaller than the numerical grid)
- a "filtered" temperature equation with extra subgrid terms
- a Poisson equation for the pressure
- gradient transfer equations for the closure of all the extra terms describing the subgrid motions
- an equation for the subgrid energy

These equations are solved (typically using finite-difference methods) with grids of about 50 to 100 m and time steps of about 5 s.

A first effort at linking advanced meteorological and diffusion models was made by Lamb,[12] who, using the output of the Deardorff[10] model, successfully simulated the statistics of nonbuoyant particles in convective conditions. Nieuwstadt and de Valk,[9] instead, used a conservation equation for the contaminant, which is solved concurrently with the large eddy model. This second approach was able to replicate well the laboratory experiments by Willis and Deardorff,[13] who reproduced the behavior of a nonbuoyant contaminant in convective conditions. This good agreement, however, was not recreated using a *buoyant* plume simulation and comparing it with the experiments of Willis and Deardorff,[14] who provided one of the few laboratory data sets for buoyant plumes in convective conditions.

3.2 Particle Models

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

Particle models use a certain number of computational (fictitious) particles to simulate the dynamics of a selected physical parameter (e.g., mass, heat, electrical charge density, etc.). Particle motion can be produced by either deterministic velocities (e.g., Lange[16]) or semirandom pseudovelocities generated using Monte-Carlo techniques (e.g., Zannetti and Al-Madani[17]). In this latter case, the trajectory of a single particle simply represents a realization from an infinite set of possible numerical solutions. Important characteristics of the diffusion process can be inferred, however, from the computation of average particle ensemble properties, which are not affected by the randomness of the pseudovelocities, if enough particles are used.

The major advantages of particle models are their ability to handle directly (i.e., without parameterizations) the fundamental processes of turbulent diffusion and their straightforward treatment of nonhomogeneous, nonstationary conditions.

4. THE PROPER LINKAGE BETWEEN METEOROLOGICAL AND DISPERSION MODELS

Linkage between a large eddy model and a meteorological model is straightforward, since both approaches are Eulerian. Linkage with particle models is, however, much more interesting, since they are Lagrangian. Also, in our opinion, particle models, due to their grid-free features and the direct handling of stochastic fluctuations, are the most promising and cost-effective tool for simulating atmospheric diffusion. Therefore, in this section we will focus on the linkage of (Lagrangian) particle models with (Eulerian) meteorological models.

A few authors made an effort to provide a preliminary linking of a meteorological model with a particle model. For example, Rodriguez et al.[18] have developed a well-documented package that links the MATHEW meteorological model (a diagnostic mass-consistent model) with the particle-in-cell model ADPIC. Also, Yamada and Bunker[19] linked the HOTMAC model (a higher order turbulence meteorological model) with RAPTAD (a Monte-Carlo particle model).

In spite of these efforts, the definition of a theoretically acceptable Eulerian-Lagrangian translation remains a critical issue for a correct linking of the two models. In fact, meteorological models provide average values of meteorological variables over a grid of cells, typically 1-10 km in the horizontal and 10-100 m in the vertical. But if the output of a meteorological model is used to simulate atmospheric dynamics with a particle model, the turbulence terms of the particle model must not simulate the entire turbulence spectrum, but only the fraction of it that is not included in the average wind provided as a meteorological input. This is an important clarification, whose theoretical and numerical implications must be fully evaluated and included. In other words, turbulence intensities and characteristics, as simulated by semirandom particle velocities, may change as a function of the accuracy of the meteorological model output. For example, the better the meteorological model and the higher the spatial and temporal resolution of the average wind it provides, the lower the turbulence intensities to be simulated in the particle model.

More specifically, turbulence simulation by the particle model must include all subgrid components as, for example, performed by Lamb,[12] who used the mean subgrid scale kinetic energy generated by the Deardorff[10] model to generate random subgrid particle velocities. Particles' pseudovelocities must also include larger components (e.g., large convective eddies) that may not be explicitly provided by the meteorological model. This turbulence distinction, between the fraction included in the meteorological model and the remaining fraction that needs to be added by Monte-Carlo techniques, is a key issue. Little work has been done on this topic, since almost all particle model studies have been performed without a meteorological model and, therefore, required the Monte-Carlo generation of the entire turbulence spectrum.

5. CONCLUSIONS

Based on the discussion presented in the previous sections, we believe that the answer to the title of this paper "Can we continue to apply dispersion models without a proper linkage with meteorological models?" is "No, we cannot." It seems clear that only through the proper use of accurate three-dimensional meteorological information, will diffusion models be able to improve their credibility and establish themselves as unchallenged simulation tools for both scientific and regulatory purposes.

There are models, such as the steady-state Gaussian plume equation (the backbone of current EPA regulatory models), that cannot incorporate more meteorological information than that currently provided under simple homogeneous and stationary assumptions. These models cannot benefit from current and future improvements, and their further application should be discouraged. On the other side, there are models, such as Monte-Carlo particle models, with unique resolution capabilities, that are able to reproduce, with a proper meteorological input, those effects (such as wind shear effects, convective updrafts and downdrafts, fumigation phenomena, accumulation during stagnant conditions, uncoupling of atmospheric layers, etc.) that are frequently identified during tracer experiments, but often constitute an insurmountable barrier for simple numerical tools that were never designed to simulate such dispersion complexities.

Wind shear effects are probably the easiest to visualize. It is common, today, to measure vertical profiles of wind speed and direction, through tethersonde, radiosonde, meteorological towers or Doppler acoustic sounder instrumentation. These data, especially during low wind speed conditions (which are often most important in air quality studies), frequently show large variations of wind speed and/or direction with height. The time and length scales of these changes are very small and, sometimes, lengths of the order of ten meters separate layers with totally different behavior. Steady-state plume models cannot be applied in these cases. Puff models are theoretically acceptable and, as long as the puffs remain small, can provide successful simulations. However, when puffs become too large, they cover multiple layers associated to different wind vectors, and transport simulation is incorrect. Grid models could be successful, but only if the grid size is smaller than the length scale – often a prohibitive condition for computational reasons. Particle models, however, in their grid-free, Monte-Carlo version, do provide convincing simulations of wind shear, since each particle is moved by a velocity that is interpolated, at each particle current location, using the measured wind profile. Figure 2 shows an example of wind shear effects simulated by a Monte-Carlo particle model for an elevated release, and Figure 3 for a ground-level release. Similar considerations could be applied to other phenomena, besides wind shear, that strongly affect dispersion and require high space and time resolution for their correct numerical description.

We conclude that particle models are uniquely suitable to provide a proper linkage with meteorological models and take fully into account advanced, high-resolution meteorological measurements and model outputs.

REFERENCES

1. U.S. Environmental Protection Agency, "Guideline on air quality models," EPA-450/2-78-025, OAPS No. 1.280," (1978).

2. W.S. Lewellen and M.E. Teske, "Second-order closure modeling of diffusion in the atmospheric boundary layer," Boundary Layer Meteor., 10: 69-90 (1976).

3. P. Zannetti, "Some aspects of Monte-Carlo type modeling of atmospheric turbulent diffusion," 7th Conference on Probability and Statistics in Atmospheric Sciences, American Meteorological Society, Monterey, California (November 1981).

4. W.S. Lewellen, R.I. Sykes, A.K. Varma and S.F. Parker, "Second-order closure model exercise for the Kincaid power plant plume," Electric Power Research Institute Report (EPRI) Report EA-3079 prepared by Aeronautical Research Associates of Princeton, Inc., Princeton, New Jersey for the EPRI, Palo Alto, California (1983).

5. M.K. Liu and G.E. Moore, "Diagnostic validation of plume models at a plains site," Electric Power Research Institute final report EA-3077, Palo Alto, California (1984).

6. S.D. Reynolds, R.E. Morris, T.C. Myers and M.K. Liu, "Evaluation of three first-order closure models -- Plains site," EPRI Report EA-3078, prepared by Systems Applications, Inc., San Rafael, California, for EPRI, Palo Alto, California (1984).

7. D.G. Fox, "Judging air quality model performance," Bull. Amer. Meteor. Soc., 62: 599-609 (1981).

8. D.G. Fox, "Judging air quality model performance," Bull. Amer. Meteor. Soc., 65: 27-36 (1984).

9. F.T.M. Nieuwstadt and J.P.J.M.M. de Valk, "A large eddy simulation of buoyant and nonbuoyant plume dispersion in the atmospheric boundary layer," Atmos. Environ., 21 (12): 2573-2587 (1987).

10. J.W. Deardorff, "Three dimensional numerical study of turbulence in an entraining mixed layer," Boundary Layer Meteor., 7: 199-226 (1974).

11. F.T.M. Nieuwstadt, R.A. Brost and T.L. van Stijn, "Decay of convective turbulence, a large eddy simulation," Proceedings, 199 Euromechn meeting on Direct and Large Eddy Simulation of Turbulence, Munchen, 1985, Friedr. Vieweg & Sohn Braunschweig/Weisbaden (1986).

12. R.G. Lamb, "A numerical simulation of dispersion from an elevated point source in the convective planetary boundary layer," Atmos. Environ., 12: 1297-1304 (1978).

13. G.E. Willis and J.W. Deardorff, "A laboratory study of dispersion from a source in the middle of the convectively mixed layer," Atmos. Environ., 15: 109-117 (1981).

14. G.E. Willis and J.W. Deardorff, "On plume rise within a convective boundary," Atmos. Environ., 17: 2935-2447 (1983).

15. R.W. Hockney and J.W. Eastwood, Computer Simulations Using Particles, McGraw-Hill, New York (1981).

16. R. Lange, "ADPIC -- a three-dimensional particle-in-cell model for the dispersal of atmospheric pollutants and its comparison to regional tracer studies," J. Appl. Meteor., 17: 320 (1978).

17. P. Zannetti and N. Al-Madani, "Numerical simulations of Lagrangian particle diffusion by Monte-Carlo techniques," Presented at the VIth World Congress on Air Quality (IUAPPA), Paris, France, 16-20 May (1983).

18. D.J. Rodriguez, G.D. Greenly, P.M. Gresho, R. Lange, B.S. Lawver, L.A. Lawson and H. Walker, "User's guide to the MATHEW/ADPIC models," USAG 82-16. Lawrence Livermore National Laboratory, University of California Atmospheric and Geophysical Sciences Division, Livermore, California, (1982).

19. T. Yamada, and S. Bunker, "Development of a nested grid, second moment turbulence closure model and application to the 1982 ASCOT Brush Creek data simulation," J. Appl. Met., 27: 562-578 (1988).

20. S.E. Gryning, A.A.M. Holtslag, J.S. Irwin, and B. Sivertsen, "Applied dispersion modelling based on meteorological scaling parameters," Atmos. Environ. 21(1): 79-89 (1987).

21. A.A. Holtslag and F.T.M. Nieuwstadt, "Scaling the atmospheric boundary layer," Boundary Layer Met. 36: 201-209 (1986).

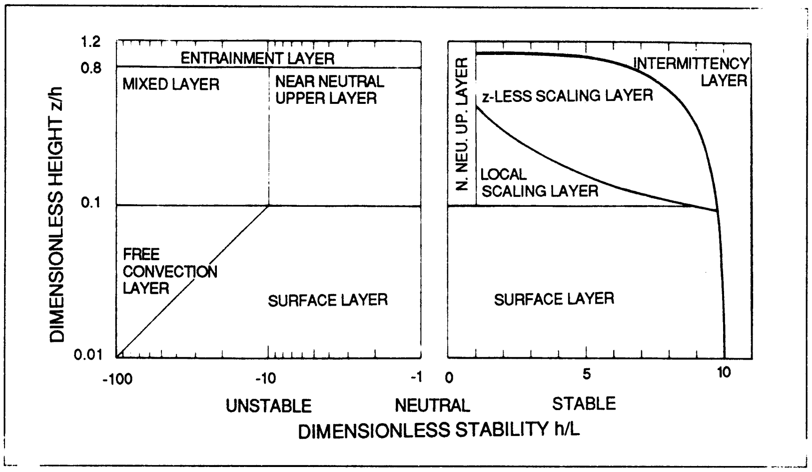

FIGURE 1. The scaling regions of the atmospheric boundary layer, shown as function of the dimensionless height z/h and the stability parameter h/L. When used to determine dispersion regions, the dimensionless height is replaced by z_s/h where z_s is the source height (from Gryning et al.,[20] adapted from Holtslag and Nieuwstadt[21]).

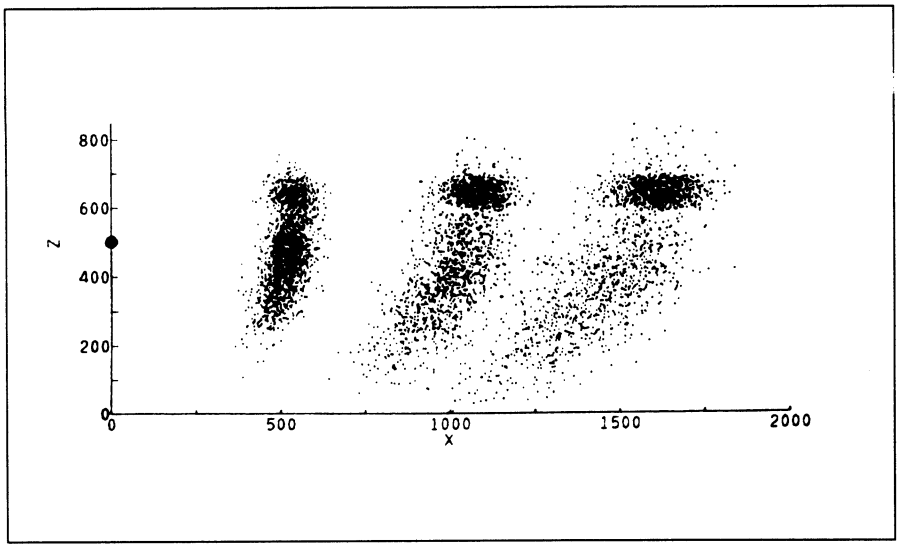

FIGURE 2. Particle simulation of the time evolution of a elevated release of a puff affected by an elevated inversion (between 600 and 700m) and wind shear below the inversion. Horixontal crosswind view. (from Zannetti and Al-Madani,[17]).

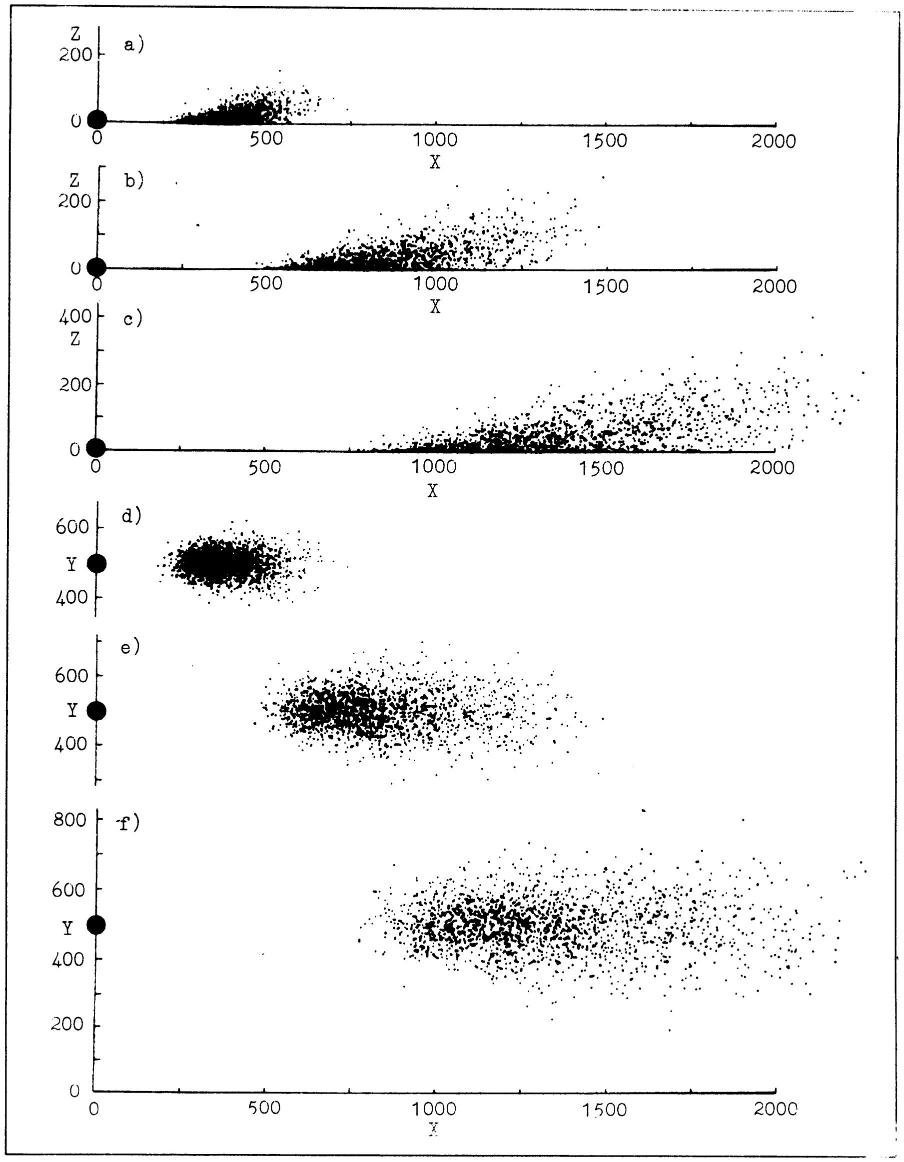

FIGURE 3. Particle simulation of the time evolution of a ground release of a single puff affected by wind shear. Horizontal crosswind view (a,b,c) and top view (d,e,f). (from Zannetti and Al-Madani,[17]).