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# APPLICATION OF AN ATMOSPHERIC DISPERSION MODEL TO SIMULATED POLLUTANT RELEASES IN THE COLORADO FRONT RANGE

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## INTRODUCTION

The 1991 ASCOT (Atmospheric Studies in Complex Terrain) field study in the vicinity of the Department of Energy's Rocky Flats Plant, Colorado, was conducted to study the local and regional circulations and their interactions with synoptic flows over the complex terrain of the Rocky Mountains Colorado Front range. The study was combined with the Rocky Flats Winter validation Study (WVS) which had similar objectives.

Tracer plumes were released as part of this field campaign over the period of February 3–19, 1991 from the Rocky Flats Plant. Twelve intensive experiments, centered around eleven-hour long surface releases of sulfur hexafloride $(SF_6)$ tracer material, were conducted by teams from a number of national laboratories, government agencies and private contractors. One-hourly averaged tracer concentrations were collected from approximately 170 surface samplers deployed along two concentric circles at a radius of 8 km and 16 km from the release location.

The concentration patterns resulting from the transport and turbulent diffusion of the $SF_6$ traces plumes within the atmospheric boundary layer during two night-time, one morning transition, and one day-time period were simulated for this paper. The scenarios selected represent the first choice of all twelve experiments to be addressed, based on the quality and completeness of the collected data base and the presence of the desired meteorological conditions. The model used for these simulations was the Lawrence Livermore National Laboratory (LLNL) three-dimensional (3-D), diagnostic MATHEW/ADPIC atmospheric dispersion model for complex terrain and flow conditions.

In order to model the dispersal of atmospheric pollutants in the planetary boundary layer, the various approaches differ greatly in sophistication and complexity. The Gaussian formula is based on statistical theory and empirical observation of the horizontal and vertical standard deviation of the wind speed $\sigma_y$ and $\sigma_z$. K-theory assumes a gradient transport parameterization and postulates a turbulent diffusivity parameter-K, which must be provided empirically. The stochastic Markov chain (Monte Carlo) method employs generally the Langevin equation to model dispersion with the use of very many particles. The approach needs the empirical prescription of the wind velocity variance $(\sigma_v)^2$ and the Lagrangian integral time scales $T_L$. All three methods have two things in common: they rely on some mathematical scheme and they need empirically derived diffusion parameters.

In these MATHEW/ADPIC simulations of the Rocky Flats experiment the stochastic Langevin method and the flux-gradient K-theory method are compared. Both methods are used in the study of atmospheric diffusion under complex conditions, with the Langevin approach gaining in popularity because of its more direct application of basic turbulence parameters. It also has no need of a computational grid to calculate flux gradients thus avoiding errors due to poor grid cell resolution.

## THE MATHEW/ADPIC MODEL

This model is a combination of the MATHEW diagnostic wind field model and the ADPIC turbulent diffusion model which uses the MATHEW output as the mean wind input about which the turbulence fluctuates.

The MATHEW model[1] generates a mass conservative 3-D gridded mean wind field, including terrain from available interpolated meteorological data and topography by variational methods. The input for the model consists of a digitized topographical surface, spatially interpolated surface winds, vertical wind profiles, and a stability parameter.

ADPIC[2,3,4] is a 3-D, numerical diffusion and transport model capable of simulating the time and space varying dispersal of atmospheric pollutants under complex conditions. It is a particle-in-cell model in which Lagrangian "mass" particles are transported inside a fixed grid. This hybrid property allows ADPIC to be used as a gradient (K-theory) model or as a stochastic Langevin model.

For the gradient method, the model solves the 3-D diffusion-advection equation in flux conservative form,

$$\frac{\partial \chi}{\partial t} + \nabla.(\chi \bar{U}_P) = 0 \quad . \tag{1}$$

Here $\chi$ is the pollutant concentration and $\bar{U}_P$ is a pseudovelocity which is defined as the sum of the mean wind $\bar{U}_A$ and a diffusive velocity $\bar{U}_D$,

$$\bar{U}_P = \bar{U}_A + \bar{U}_D \;;\quad \bar{U}_D = -K \cdot (\nabla \chi) / \chi \quad . \tag{2}$$

and $K$ is the diffusivity parameter in the $x$, $y$, and $z$, directions. The mean wind $\bar{U}_A$ is supplied by the MATHEW model.

ADPIC computes a horizontal and a vertical diffusivity $K_h$ and $K_z$. The horizontal diffusivity, $K_h$, is based on the semi-empirical expression[5]

$$\sigma = \sigma_\theta \bar{U} t \left(1 + \frac{t}{\tau}\right)^{-1/2} \quad . \tag{3}$$

combined with the analytical relationship

$$K_h = \sigma_y d\sigma_y / dt \quad . \tag{4}$$

where $\sigma_y$ is the horizontal standard deviation of the plume, $\sigma_\theta$ the standard deviation of the fluctuation of the wind direction, $\bar{U}$ the local mean wind speed, $t$ is time, and $\tau$ is an empirical time constant.

For the atmospheric boundary layer $K_z$ is of the form[6]

$$K_z = \frac{k u_* z}{\phi(z/L)} e^{-|V_g/u_*| z/h} \quad . \tag{5}$$

where $k$ is the Von Karman constant, $u_*$ is the friction velocity, $z$ is the height above terrain, $\phi(z/L)$ is an atmospheric stability function based on $z$ and the Monin-Obukhov scale length $L$, $V_g$ is the geostrophic wind and $h$ the height of the mixing layer.

The Langevin model consists of a pair of stochastic differential equations that describe the trajectories of "marked" particles. In the vertical dimension these are:

$$dw = \left[ -\left(\frac{C_o \varepsilon}{2\sigma_w^2}\right) w + \frac{1}{2}\left(1 + \frac{w^2}{\sigma_w^2}\right) \frac{\partial \sigma_w^2}{\partial z} \right] dt + (C_o \varepsilon)^{\frac{1}{2}} dW(t) \tag{6a}$$

and

$$dz = w dt \quad . \tag{6b}$$

Here $w$ is the vertical Lagrangian velocity, $\sigma_w^2$ is the variance of $w$, $\varepsilon$ is the mean rate of dissipation of turbulence kinetic energy, $C_o$ is a universal constant, and $dW(t)$ is a Gaussian distributed random numbers with mean of zero and variance $(dt)^{1/2}$.[7] $dz$ is the distance a particle will travel in the time increment $dt$. The $dt$ term in Eq. (6a) is deterministic and the $dW(t)$ term is stochastic. The deterministic term has two components. The first is a "fading memory" component whose meaning become more clear if we introduce the relation

$$T_L = 2\sigma_w^2 / C_o \varepsilon \tag{7}$$

Here $T_L$ is the Lagrangian integral time scale. The value of $C_o$ was chosen as 5.7.[8] The second component of the deterministic term is a "drift correction" which accounts for the vertical inhomogeneity of turbulence. Equations similar to eqn. (6) provide the horizontal components of particle motion with $x$, $y$; $\sigma_u$, $\sigma_v$, and $u$, $v$ replacing $z$; $\sigma_w$ and $w$ respectively.

The turbulence input parameters chosen for this study are

$$\sigma_w^2 = u_*^2 \left\{ 1.6(1 - z/h)^{3/2} + F(z/L) \right\} \tag{8a}$$

$$\sigma_u^2 = \sigma_v^2 = (\bar{U}\sigma_\theta)^2 \tag{8b}$$

$$\varepsilon = \frac{u_*^3}{kz} \left\{ (1 + 3.7\, z/L)(1 - .85\, z/h)^{3/2} + G(z/L) \right\} \tag{9}$$

where $F(z/L)$, $G(z/L)$ are atmospheric stability functions.

## THE MODELED EXPERIMENTS

The combined Rocky Flats ASCOT/WVS campaign fielded a large variety of meteorological instrumentation. A network of meteorological towers, tethersondes, airsondes, radiosondes, minisodar, upper-air profilers, lidar, and a large array of surface stations provided data. Of the twelve tracer experiments, six characterized nighttime downslope flow, four daytime flow, and two transition periods. From these, four representative scenarios were chosen for this study: the two nighttime drainage flow experiments numbers 2 and 3, of February 4/5 and February 6/7, the morning transition experiment number 8 of February 14 and the daytime experiment number 9 of February 15. The respective $SF_6$ source rates were 3.78, 3.78, 6.30, and 6.30 g/s.

Experiment 2 and 3, 2000 to 0700 MST represented a classical drainage flow case with downslope flows emanating from the valleys and canyons of the Front Range.

Experiment 8, 0100 to 1200 MST was the only morning transition release with strong synoptic westerly winds with a weak easterly return flow near the surface.

Experiment 9, 0700 to 1800 MST was one of the daytime releases with the same flow patterns developing over the foothills as during the previous experiment 8.

The boundary layer input parameters chosen for the M/A simulations of the four experiments are shown in Table 1. The wind direction fluctuation $\sigma_\theta$ was based on measurements from towers and vertical soundings; the boundary layer height $h$ was based on temperature profiles; and the Monin-Obukhov length $L$ was based on bulk Richardson numbers. A surface roughness height of $z_o = 0.5m$ was used.

Table 1. MATHEW/ADPIC Boundary layer input parameters.

| Test No. | time (MST) | $\sigma_\theta$ (deg) z = 0 | $\sigma_\theta$ (deg) z = h | h(m) | L(m) |
|---|---|---|---|---|---|
| 2 | 2000-0700 | 18 | 12 | 300 | 10 |
| 3 | 2000-0700 | 18 | 12 | 300 | 10 |
| 8 | 0100-0600 | 25 | 12 | 500 | 50 |
| | 0600-1200 | 20 | 12 | 700 | $\infty$ |
| 9 | 0700-1200 | 25 | 12 | 500 | 50 |
| | 1200-1800 | 30 | 15 | 900 | ~10 |

No sampling was done during the first two hours of the eleven hour releases. This provided nine, hourly averaged $SF_6$ surface air concentrations per sampler at each of the two sampling arcs for each experiment. Of the 172 surface samplers deployed, roughly half of them recorded any concentrations during a given experiment, yielding about 800 samples per experiment to be compared with M/A simulations.

Given hourly averaged winds, M/A was used to predict hourly averaged $SF_6$ air concentrations to be compared with observed values along the 8 km and 16 km sampler arcs. The domain of the M/A model is shown in Figure 1 together with partial sections of the two sampling arcs an the $SF_6$ plume as simulated by ADPIC particles valid at 0400 MST, February 5, experiment 2. Figs. 2 and 3 show the observed and predicted $SF_6$ surface air sampler concentrations in $\mu g / m^3$ as a function of angle in degrees from true north along the 8 km and 16 km arcs, respectively, for the same plume as shown in Figure 1. The figures give a typical example of the performed simulations for both, the Langevin and the gradient method.

The study of the individual, hourly averaged concentrations as illustrated by Figs. 2 and 3 reflect that during the experiments the atmospheric boundary layer of the Front Range showed strong interactions between local and regional flows during the nighttime experiments 2 and 3, and between local, regional and synoptic flows during the morning transition and daytime experiments 8 and 9. The result was a complex dispersion pattern of the $SF_6$ tracer plumes for each experiment. Terrain interactions in the horizontal, strong vertical motions, and speed- and directional wind shears often created rapid shifts and multiple peaks in the observed plume patterns which the M/A simulations were often unable to resolve or duplicate. These errors in plume direction are due to the MATHEW wind field and are common to both the Langevin and gradient method results. The Langevin method consistently shows better agreement with observed peak and small near surface concentrations than the gradient method. The latter effect being due to the absence of grid resolution limitations.

It is difficult to devise a statistical method that in all cases adequately describes a model's performance in complex terrain. The standard correlation coefficient can be overly influenced by a few high concentrations. Thus, another method, which is less biased by a few high concentrations, was selected for comparing the relative accuracy of the Langevin and gradient schemes.

This method involves a band analysis which equally weights the model performance over the entire spatial domain of interest by computing the ratio R of all pairs of observed to predicted concentrations. When the factor R is less than one, then it is replaced by $1/R$ to obtain a series of ratios greater as equal to one. Figure 4 shows a plot of the percentage of all such sample pairs agreeing to within factor R, as a function of R. Shown is the extensive evaluation of the MATHEW/ADPIC gradient diffusion model with a number of experimental data sets ranging over a wide variety of terrain types, tracer release scenarios and meteorological conditions: INEL and SRP [2], TMI, [9] ASCOT[3,4,9], MATS[9], Montalto[9] and PG&E[9]. Also shown are the results of the Langevin method and the gradient method results of this paper's ASCOT-RFP (Rocky Flats Plant) simulations.

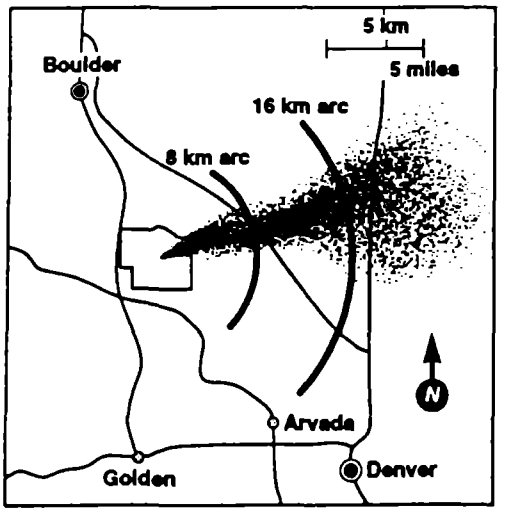


Figure 1. MATHEW/ADPIC model domain and the two sampler arcs at 8 km and 16 km from the source at Rocky Flats. The plume as depicted by ADPIC particles is shown for 0400 MST, February 5, Experiment 2.

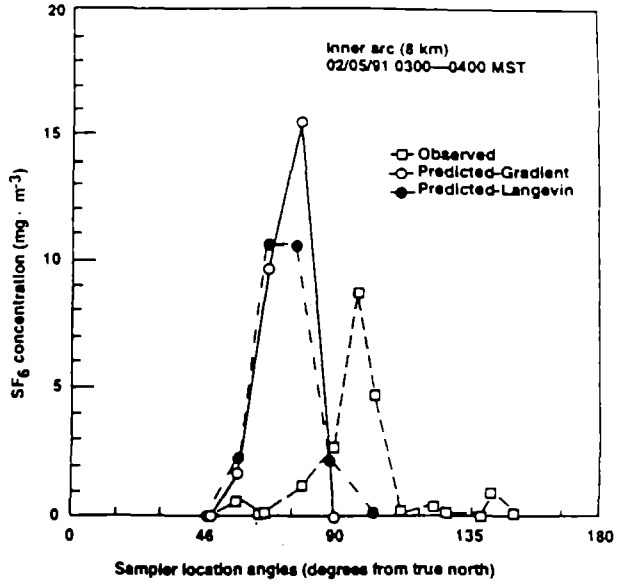


Figure 2. Hourly averaged observed and predicted $SF_6$ surface air concentrations in $\mu g / m^3$ as a function of angle in degrees from true north along the 8 km sampler arc for 0400 MST, February 5, Experiment 2.

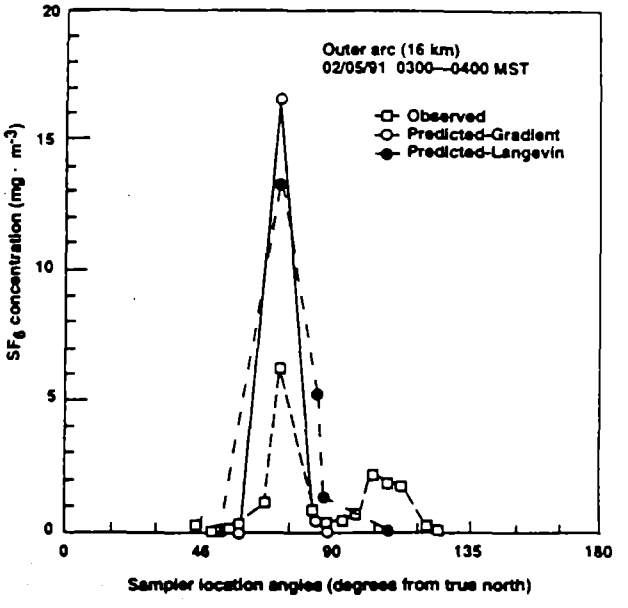


Figure 3. Same as figure 2, except along the 16 km arc.

The figure illustrates the degree of degradation the model suffers in going from simple terrain with simple meteorology of well controlled experiments, to the complex conditions usually encountered in the real world (from 50% of samples within a factor of 2, to a factor of 5). Also visible is the spread of performance over all the experiments.

The only test of the Langevin method in Fig. 4, and the only thorough ADPIC evaluation of it to date, is the ASCOT-RFP 1991 experiment of this paper. Its performance is superior to that of the gradient method also shown in Fig. 4. The reason for this, and the reasonable expectation of more improvement as

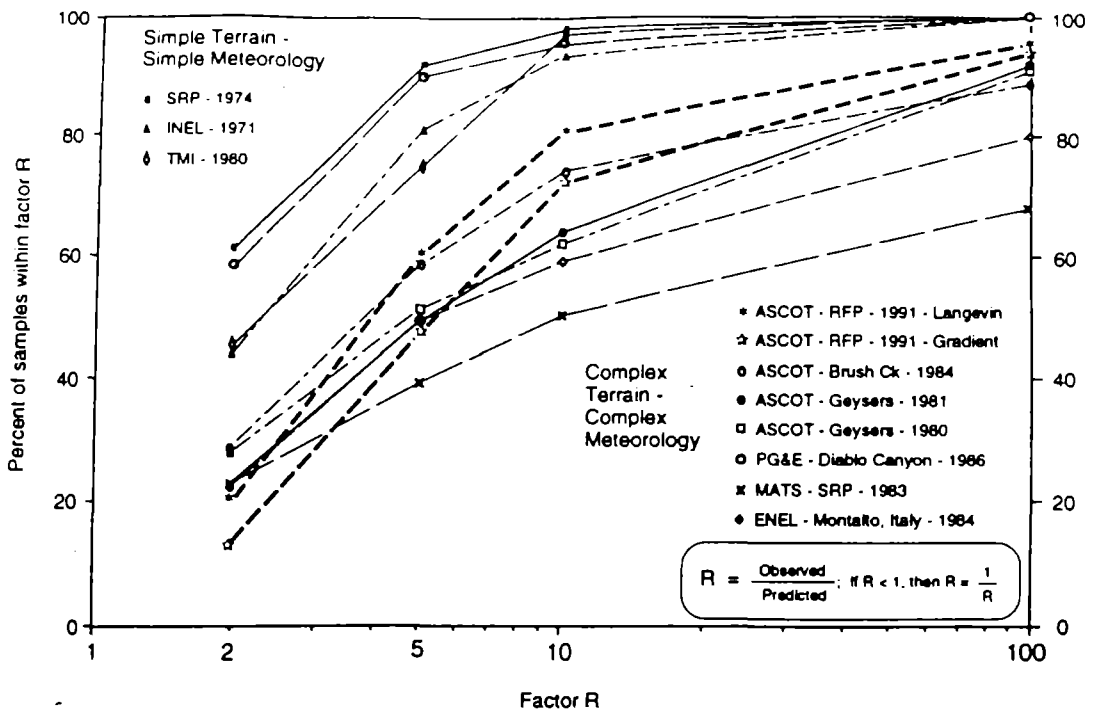


Figure 4. Percentage of observed tracer concentration samples agreeing with those predicted to within a factor R, as a function of R, for a variety of MATHEW/ADPIC model evaluation studies. All studies are for the gradient method except for the bold-dashed lines for ASCOT-RFP 1991 which depict the comparison between the Langevin and the gradient method.

more experience is gained in its use in ADPIC, can be summarized with three points: 1.) The stochastic Langevin model is a more fundamental turbulence model than the gradient K-theory model. It can treat the inhomogeneous turbulence encountered in the real atmospheric boundary layer, and does not suffer from non-realistic negative diffusivities in strongly unstable conditions like the K-theory model. 2.) Because the Lagrangian particles diffuse independently of one another, the method does not depend on a fixed (Eulerian) grid to compute gradients, and consequently does not suffer from resolution, and other grid related problems. 3.) The Langevin equation relies on turbulence input parameters directly related to the Reynold's stress tensor, such as $\sigma_w^2$. While these presently are largely derived semi-empirically, based on u *, z, h, L and various coefficients, future improvement in field measurement technology, especially by remote sensing, should increase the accuracy and availability of these parameters.

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