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The AFTAC Model Integration Project: An Annual Progress Report

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EXECUTIVE SUMMARY

Closure on the development of an operational version of the HADPIC Modeling System (HMS), a multi-faceted application that supports the hemispheric ADPIC (HADPIC) atmospheric dispersion model on a Sun workstation, was achieved toward the end of the fiscal year. The fulfilling tasks over the period encompassed by this report included: 1) the generation of software for calculating average concentrations at arbitrary locations in the model domain and displaying isopleths of concentration and 2) the comprehensive testing of major components of the HMS using IEEE standards. A user's guide was written to provide HMS users with the information necessary to successfully initialize, execute and process the results of the HADPIC model. Copies of the user's guide were mailed to the Air Force Technical Applications Center (AFTAC) several weeks prior to the installation of the HMS at Patrick AFB and the subsequent training of AFTAC personnel in May, 1993.

Scientists from the Lawrence Livermore National Laboratory and the Institute of Experimental Meteorology in Obninsk, Russia, extensively evaluated their respective models (ADPIC/U.S and EXPRESS/Russia) using perfluorocarbon tracer data from the Across North America Tracer Experiment (ANATEX). The results of both models are reported here because of the useful insights they provide regarding limits of performance as a function of model sophistication and the quality of the input meteorology. The criteria for judging model performance were based on protocols devised by the Environmental Protection Agency and on other complementary tests. Most of these measures required the formation and analysis of surface concentration footprints (the surface manifestations of tracer clouds, which were sampled over 24-h intervals), whose dimensions, center-of-mass coordinates and integral characteristics provide a basis for comparing observed and calculated concentration distributions.

MASTER

Generally speaking, the plumes associated with the 20 releases of perfluorocarbon (10 each from sources at Glasgow, MT and St. Cloud, MN) in January, 1987, were poorly resolved by the sampling network when the source-to-receptor distances were less than about 1000 km. Within this undersampled region, both models chronically overpredicted the sampler concentrations. Given this tendency, the computed areas of the surface footprints and their integral concentrations were likewise excessive. When the actual plumes spread out sufficiently for reasonable resolution, the observed (O) and calculated (C) footprint areas were usually within a factor of two of one another, thereby suggesting that the models possess some skill in the prediction of long-range diffusion.

Deviations in the O and C plume trajectories, as measured by the distances of separation between the plume centroids, were on the order of 125 km/day for both models. It appears that the inability of the models to simulate large-scale vertical motions and, more generally, to adequately characterize the meso- and macro-scale flows, mainly as the result of constraints imposed by the temporal and spatial resolution of the rawinsonde network, are major impediments to improved accuracy.

HADPIC MODELING SYSTEM

With the one exception noted below, the Lawrence Livermore National Laboratory (LLNL) has satisfied its current obligations regarding the development of the HADPIC Modeling System (HMS). This system allows the Nuclear Technology Directorate (TNR) at the Air Force Technical Applications Center (AFTAC) to simulate the dispersion of airborne pollutants over continental to hemispheric distances by means of executing the Hemispheric Atmospheric Diffusion Particle-In-Cell (HADPIC) model. The term HMS refers to all components of the application, which include software for: 1) editing and managing the model parameters, 2) accessing the meteorological data, 3) executing the hemispheric model, 4) monitoring the status of the model during its execution, and 5) displaying the model results.

Before elevating the HMS to an operational system, we thoroughly tested its major components. Our test plan involved the creation of test scenarios either to verify that each element of the system satisfied specific requirements or to identify differences between expected and actual results. The test scenarios were grouped into "functional", "exceptional", or "parallel" categories. Functional test scenarios were derived on the basis of expectations concerning the performance of the HMS. Exceptional scenarios, involving extreme or abnormal operating conditions, represented areas of the application that were especially prone to error. Parallel testing refers to the comparison of HADPIC model results on a VAX, the machine on which the model was housed prior to the commencement of this project, and a Sun workstation. In each case, we described the purpose of the test scenario, the anticipated outcome and the testing environment. Whenever an error occurred, the causative factor was identified and corrected. The only components of the HMS that cannot be tested at this time are those related to the retrieval of meteorological data from the WES database and the transference of these data to a Sun workstation.

Testing will resume after problems, which are endemic to the design and implementation of the WES database, are resolved.

A user's manual for the HADPIC Modeling System was written after the completion of the testing phase (Moore and Rodriguez, 1993). Its organization and content consist of the following: 1) the theoretical framework of HADPIC and its input requirements, 2) the graphical user interface through which a user characterizes a release event, executes HADPIC and processes the resulting outputs, 3) the internal control programs (the hidden portion of the application) that request and retrieve meteorological data from the IBM-based database, assemble the various parameters into files whose forms are recognizable to HADPIC, and execute the model, and 4) the administrative functions that manage the application's environment.

After delivering the user's guide and installing the HMS application at AFTAC in May, we trained TNR personnel on the proper usage of the HADPIC Modeling System. This training session was followed by discussions concerning the future course of LLNL's programmatic efforts. Because of recent changes in their mission priorities, AFTAC stressed their desire to obtain a regional-scale modeling capability based on LLNL's MATHEW and ADPIC transport and diffusion models and three subsidiary codes.

The transfer of ARAC's regional atmospheric dispersion models from a VAX to a SUN platform was completed by the end of the fiscal year. This involved developing an approach that replaced VAX-dependent capabilities without sacrificing functionality. The porting process was validated on two of the five models. Qualitative verification through flow visualization will be accomplished using a recently-installed graphics software product called agXToolmaster.

Further enhancements to the HMS will be made after the verification process has been completed. They include: 1) developing a color postscript capability, 2) changing the current Metdata Daemon task to a user-initiated function rather than a background daemon process, 3) allowing the user to save execution parameters without performing a

model execution, 4) implementing a new format to read spatially-varying mixing heights generated by ENSCO for its GAMUT model, and 5) recasting the hemispheric models into newly restructured forms. The term "restructured" refers to recent changes to ARAC's core models which give the models more flexibility in adapting to changes in grid sizes and file definitions.

HADPIC EVALUATIONS

1. Introduction

The generation of tracer databases, which are most often used to evaluate models that simulate the transport and diffusion of pollutants, has become a fairly common practice on the micro- and meso-scales. Comparable experiments over continental distances are much less common due to the cost, complex strategic planning and coordination required to mount such campaigns. There are, of course, events that occur by happenstance, which can provide a wealth of information suitable for model testing. For example, the Chernobyl reactor accident has inspired numerous individual modeling studies of the long-range dispersion and deposition of airborne radioactivity (e.g., ApSimon and Wilson, 1987; de Leeuw *et al.*, 1987; Lange, 1988), and studies involving model intercomparisons (e.g., Klug *et al.*, 1991). Reactor accidents present unique challenges to modelers and other emergency response personnel mainly as the result of uncertainties related to the source term. However, even when handicapped by a lack of source-related information, long-range models can provide a vital service during and after the early stages of a response.

Soon after the Chernobyl accident, a task group, empaneled by the U.S. Department of Energy, was charged with analyzing the health and environmental consequences of the Chernobyl accident (Goldman, 1987). An element of their study involved the use of long-range dispersion models from the United States, the United Kingdom and the Netherlands to: 1) reconstruct the source term through an iterative process, whereby the spatial and temporal distributions resulting from a unit rate release were optimized by means of minimizing the relative errors between measured and predicted concentrations, and 2) use the resulting postulated source term to describe the evolution of the radioisotopic distributions. Obviously, the validity of this approach depends on the accuracy of the model that

makes these assessments under diverse synoptic conditions; in other words, estimates of a source term are susceptible to model bias.

Refinement of the Chernobyl source term over time and the storage of quality-assured measurements in the Radioactivity Environmental Monitoring (REM) data bank at the Joint Research Center (Desiato, 1992) led to the Atmospheric Transport Model Evaluation Study (ATMES, 1991). The challenge to the international participants was to reproduce the Cs-137 and I-131 concentrations at selected times and locations throughout Europe without a foreknowledge of their actual distributions. Releases of PMCH, a perfluorocarbon tracer, during the Cross-Appalachian Tracer Experiment (CAPTEX) also provided opportunities for evaluating long-range dispersion models, but under more controlled circumstances (Ferber *et al.*, 1986). Favorable release periods were forecast to improve the efficiency of tracer collection by a fixed array of surface samplers, which were strategically placed throughout the northeastern U.S. and southeastern Canada. Sampling intervals (typically six hours) were generally short enough to document the arrival and departure of a plume in the absence of lofting.

While these events have obvious value to long-range modelers, we have opted to test our emergency response models using the Across North America Tracer Experiment (ANATEX) database. Our selection was based on several considerations, including: 1) the release heights and release rates of the ANATEX perfluorocarbon tracers are unambiguous; in spite of the diligence of scientists, the source signatures from the Chernobyl release remain somewhat elusive due to their complexity, 2) the use of inert, non-depositing tracers during ANATEX eliminates the uncertainties associated with wet and dry depositions, thereby simplifying our performance analyses and allowing us to focus attention on the advective and diffusive aspects of our models, 3) the air sampling intervals and the initiation of sampling are the same throughout the ground-based sampling network, which forms the basis of our analyses; in contrast, users of the Chernobyl data have frequently manipulated the concentration data from various European countries through integrations

and interpolations for purposes of creating a standard format, and 4) the greater synoptic variability during ANATEX provides enhanced opportunities for exercising the models.

In the following section, we describe those aspects of the Across North America Tracer Experiment that are especially relevant to our study. Section 3 provides a brief description of the EXPRESS (Russia) and ADPIC (U.S.) emergency response models. In Section 4, we discuss our criteria for determining model performance, which have been tailored to or affected by the experimental design of ANATEX. Section 5 describes the results of our applications of these measures, and Section 6 contains our conclusions.

2. ANATEX

2.1 Tracer Releases

Perfluorocarbon tracers—PTCH from Glasgow, MT (GGW), and PDCH from St. Cloud, MN (STC)—were simultaneously released every 2.5 days over 3-h intervals beginning at 0500 UTC or 1700 UTC from 5 January 1987 to 29 March 1987. A third perfluorocarbon (PMCH), released from St. Cloud during the daytime cycle, served as a “control” agent; although not explicitly considered in this study, the subsequent samples of PMCH did provide some information on the natural variability of the atmosphere and on the discrimination of clouds when the PDCH clouds merged during the course of their dispersion. The perfluorocarbons were aerosolized before being vented at a height of about 5 m above ground level. Since they are fully fluorinated hydrocarbons, the tracers are inert, non-depositing and non-toxic (Draxler *et al.*, 1991). Out of all release possibilities, we earmarked the 10 PTCH and 10 PDCH releases occurring in January for our study.

2.2 Sampling

Of the many methods of air sampling—surface, airborne and tower—we have focused our attention on ground-level samples, which were taken at 77 sites. The samplers were

deployed along bands, relative to the source at GW; the approximate source-to-receptor distances of these bands in kilometers are indicated in Fig. 1. Each site had a programmable atmospheric tracer sampler whose lid contained 21 sampling tubes through which 24-h air samples were taken beginning at 1400 UTC on any given day. The release amounts were sufficiently large (40-80 kg) and the tracer backgrounds sufficiently small (about one part in 10^{16} parts of air) to permit the isolation of signals out to distances that often exceeded 3000 km.

2.3 Meteorological Data

A comprehensive set of three-hourly surface observations and rawinsonde observations at 0000 UTC and 1200 UTC over an area that encompassed the sources and the sampling network were archived by the ANATEX organizers. In addition, supplemental upper air soundings at GW and STC and four National Weather Service sites that neighbored one source or the other were taken at 0600 UTC and 1800 UTC and stored in the meteorological database. Also, products from the National Meteorological Center's Nested Grid Model were generated, archived and made available to the modeling community. Since the performance of our models in an early-response mode was of primary interest, we elected to use upper air data as the sole source of model input because of its routine availability and its relative ease of assimilation. Moreover, our decision would appear to be correct given Haagenson *et al's* (1990) finding that the use of surface wind data can degrade the performance of models over continental distances.

3. Model Descriptions

3.1 EXPRESS

The EXPRESS model solves a set of non-stationary, one-dimensional equations derived from semi-empirical equations of turbulent diffusion for the lower moments of the concentration distribution q ,

$$Q_0(t, x_3) = \iint_{-\infty}^{+\infty} q(t, x_1, x_2, x_3) dx_1 dx_2, \quad (1)$$

the mass center coordinates,

$$P_\alpha(t, x_3) = \iint_{-\infty}^{+\infty} x_\alpha q(t, x_1, x_2, x_3) dx_1 dx_2 / Q_0(t, x_3), \quad (2)$$

at $\alpha = 1, 2$ and the variances and covariances,

$$d_{\alpha\beta} = \iint_{-\infty}^{+\infty} (x_\alpha - P_\alpha)(x_\beta - P_\beta) q(t, x_1, x_2, x_3) dx_1 dx_2 / Q_0(t, x_3), \quad (3)$$

at $\alpha, \beta = 1, 2$ (Kostrikov, 1988). In these equations, x_1 and x_2 are the horizontal coordinates, x_3 is the vertical coordinate, t is the time and Q_0 is the integrated concentration. The variance tensor components determine the size and the alignment of a cloud section at any given height. The source is modeled by a widely-known technique that involves the superposition of pollutant plumes released into the atmosphere over successive time intervals.

To reconstruct the three-dimensional concentration field from the six moments described above, we assume that concentrations in the horizontal plane are normally distributed. Profiles of wind velocity components, their horizontal derivatives and the coefficients of horizontal and vertical diffusion at P_α are needed to calculate concentrations on a vertical grid, whose spacing increases over time as a function of plume growth.

The coefficient of horizontal diffusion is described by

$$K_h = 0.2(\epsilon\sigma_y^4)^{\frac{1}{3}} + 10K_z, \quad (4)$$

where $\epsilon = 5810^{-4} \text{ m}^2/\text{s}$ is the tropospheric energy dissipation rate, K_z is the vertical diffusivity, and

$$\sigma_y = \frac{1}{2} \left(d_{11}d_{12} - ((d_{11} - d_{22})_2 + 4d_{12}^2)^{\frac{1}{2}} \right)^{\frac{1}{2}}$$

is the plume-width scale.

The coefficient of vertical diffusion is calculated using Wipperman's (1975) approximation formula,

$$K_z = ku_* \exp \left(-c(\mu) \left(\frac{zf}{ku_*} \right)^{0.764} \right) \quad (5)$$

where

$$c(\mu) = \exp(0.264 + 1.6281^{-2}\mu' + 3.9681^{-4}\mu'),$$

$$\mu' = \mu + 50 \text{ for } -50 < \mu < 50,$$

$$\mu = ku_*/fL \text{ is an intrinsic stratification parameter,}$$

$$u_* \text{ is the friction velocity,}$$

$$L \text{ is the Monin-Obukhov length,}$$

$$k \text{ is the von Karman constant, and}$$

$$f \text{ is the Coriolis parameter.}$$

Meteorological parameters and variables are estimated from rawinsonde observations from the three nearest stations to the plume's center of mass. The model uses a Gaussian weighting function for horizontal interpolations of the data, assuming the variance of this function to be 300^2 km^2 whenever the radius of the plume is less than 300 km and to be equal to the plume variance otherwise. Vertical interpolations of the horizontal wind

components are made by applying a quadratic fit to the three lowest measurements of the sounding and a linear fit to all data at higher levels.

3.2 ADPIC

The Atmospheric Diffusion Particle-In-Cell (ADPIC) model solves a three-dimensional equation of turbulent diffusion with the admixture represented by an ensemble of Lagrangian particles that move within an Eulerian framework by means of "pseudo-velocities" (Lange, 1978). Under the assumption of incompressibility, the standard, non-linear advection-diffusion equation can be rewritten in its flux conservative form,

$$\frac{\partial \chi}{\partial t} + \nabla \cdot \chi \left(\underline{U} - K \frac{\nabla \chi}{\chi} \right) = \frac{\partial \chi}{\partial t} + \nabla \cdot (\chi \underline{U}_p) = 0, \quad (6)$$

where χ is a scalar concentration, K is the diffusion coefficient, $\underline{U}$ is the gridded velocity field, and $\underline{U}_p = \underline{U} - K \frac{\nabla \chi}{\chi}$ is the pseudo-transport velocity.

Turbulent motions are assumed to be isotropic with no distinction being made between the horizontal components of the diffusivity coefficients ($K_{xx} = K_{yy} = K_h$). The horizontal rate of plume diffusion is described by

$$\sigma_y = a(Ut)^b, \quad (7)$$

where σ_y is the cross-wind standard deviation of the plume, U is the speed of a Lagrangian particle and t is its age. In ADPIC, a and b have been defined on the basis of numerous observations of the lateral variance of pollutant plumes out to distances approaching 2000 km (Carras and Williams, 1988). From our interpretation of these data, it appears that $\sigma_y \propto t$ provides the best fit. Assuming its correctness, the coefficient a was derived from a least-squares fit to the dispersion data, yielding a value of 0.056. Obviously, there is no explicit recognition of atmospheric stability in such a derivation.

The horizontal diffusivity is analytically related to σ_y by

$$K_h = \sigma_y \left(\frac{d\sigma_y}{dt} \right). \quad (8)$$

The vertical exchange coefficient is expressed by

$$K_z = k u_* z e^{\frac{-4z}{h}}, \quad (9)$$

where k is the von Karmen constant, u_* is the friction velocity and h is the mixing height (Shir, 1973). Since K_z is dependent on the boundary layer height, local (cell-by-cell) variations in the mixing height can easily be accommodated.

Concentration gradients are ill-defined when the size of the cloud in any dimension is less than two grid cell lengths. For this sub-grid scale situation, particles are diffused according to a Gaussian prescription that utilizes the initial source parameters until such time that the individual standard deviations of the cloud become as large as their respective grid cell sizes. After crossing this threshold, the model switches to gradient diffusion. The grid, whose underlying surface is flat, consists of $41 \times 41 \times 15$ points with a grid point resolution of $100 \text{ km} \times 120 \text{ km} \times 200 \text{ m}$ in the x , y and z directions, respectively.

Inputs to the model are upper-air wind observations and an assemblage of parameters that control the manner in which data are extrapolated in space. Essentially, the winds from individual vertical profiles are linearly interpolated to grid levels before being extrapolated horizontally using a three-point, inverse distance-squared weighting scheme. We assume that vertical shears in wind speed in the surface layer follow a power-law relationship whose exponential value varies in accordance with the atmospheric stability.

4. Performance Criteria

4.1 Treatment of Long-Range Concentration Data

For many statistical analyses, it is assumed that the data approximate a normal distribution, thereby justifying the use of a wide range of statistical techniques. However, if this assumption is not sufficiently satisfied, the use of even a simple statistic, such as a mean, may be misleading. Thus, it is important to substantiate distributional assumptions.

Empirical and hypothetical distributions of the normally distributed and logarithmically transformed peak concentrations obtained from field observations (PTCH and PDCH concentrations from all 20 releases have been combined and then ranked monotonically) are plotted in Fig. 2. The dotted curves represent the integrations of a normal distribution function whose mean and variance are calculated from the samples. The stair-stepped curves, constructed from the observed data, are derived from the application of the Kolmogorov-Smirnov (KS) goodness-of-fit test. If, in the formulation of our null hypothesis, we assume that the empirical data fit the distributions within a significance level of $\alpha = 0.05$, then the maximum absolute difference d between the curves should not exceed the acceptance limit of 0.187 for our sample size. Since the d value is 0.228 (0.093) for an assumed normal (log-normal) distribution, the null hypothesis is rejected (accepted), suggesting that standard statistics, such as untransformed means and variances, be applied to sample populations with circumspection.

If, instead of using peak concentrations to demonstrate the atmosphere's apparent tendency to dilute the tracer material log-normally over time, we consider observed samples that have been grouped according to time, the results of the KS test are less conclusive in regard to the distribution of concentrations. In Table 1, the times refer to the intervals in hours between the start of a PTCH or PDCH release and the midpoint of a sampling period (beyond 81 h, the concentrations are typically within a factor of three of background,

making them unreliable as distributional indicators). The d statistics for the sample populations appear next, followed by the number of samples within each population and the associated level of acceptance. While the d values for the logarithmically-transformed concentrations are lower than their normally-distributed counterparts and universally satisfy the acceptance criteria, the normality assumption is likewise “upheld” in two out of six cases. (It should be noted here that, during the categorization process, the frequent commingling of plumes from different releases of PTCH or PDCH made it difficult, if not impossible at times, to determine their fractional contributions and to ascribe an age to a particular sample.) Given the possibility that the concentrations may, in fact, be normally distributed in space, we have applied an exponential weighting function to interpolate receptor concentrations to regular meshes prior to the application of certain performance measures described below.

4.2 Evaluation Techniques

A surface footprint is defined as a composite of the surface manifestations of all instantaneous puffs within a 24-h sampling period. Within the context of ANATEX, the use of footprint analyses originated with Clark and Cohn (1990), who devised a set of protocols that were customized to the experimental design. Our performance measures are either complementary to, or elaborations of, the Clark and Cohn protocols.

A surface footprint is constructed by fitting a rectangular mesh, whose grid point resolution is $\Delta x = \Delta y = 25$ km, over samples that equal or exceed our chosen threshold of 10 df/l ($= 1.56 \times 10^{-11}$ g/m³). The bounding box extends 250 km beyond the minimum and maximum coordinates of the sampling sites that satisfy the acceptance criterion. A pseudo-concentration of 1 df/l is attached to each side of the box at the point of intersection between the side and a line running perpendicularly through the minimum or maximum sampler coordinate in the four cardinal directions. These four additional values serve to

spatially bound the subsequent, exponentially-weighted interpolations of the observed (O) and calculated (C) concentrations to the mesh centers.

The area A of surface footprint S is computed using the formula

$$A_S = n\Delta x\Delta y, \quad (10)$$

where n is the number of meshes having a concentration q_{ij} equal to or exceeding 10 df/l. A comparison of the O and C footprint areas as the cloud evolves provides some useful information on how well the models simulate the rates of plume diffusion.

The areas of intersection between the O and C footprints,

$$A_{S_O \cap S_C} = n_1\Delta x\Delta y, \quad (11)'$$

normalized by the union of these areas,

$$A_{S_O \cup S_C} = n_2\Delta x\Delta y, \quad (12)$$

allows us to make a statement concerning the ability of our models to match the observed dispersion over time. Here, n_1 refers to the number of meshes for which both the O and C concentrations equal or exceed the threshold and n_2 refers to the number of meshes for which one or the other or both equal or exceed this limit.

In addition to the criteria given above, which mainly indicate errors associated with atmospheric diffusion, it is also important to examine transport errors that reflect inaccuracies in the specification of wind speeds and wind directions. To this end, we have compared the locations of the O and C surface footprints by calculating their center-of-mass coordinates,

$$X_{cm} = \frac{1}{Q}\Delta x\Delta y \sum_i \sum_j x_i q_{ij} \quad (13)$$

and

$$Y_{cm} = \frac{1}{Q} \Delta x \Delta y \sum_i \sum_j y_i q_{ij}, \quad (14)$$

and combining them in various ways. Q , the integral concentration at the 2 m sampling height, is defined by

$$Q = \Delta x \Delta y \sum_i \sum_j q_{ij}. \quad (15)$$

To examine the error contributions due to wind speeds, the ratios L_C/L_O have been formed, where the subscripted L 's refer to the cumulative distances of the trajectory segments of the O and C plumes as measured by their center-of-mass locations. The ratios $\Delta L/L_O$, where ΔL refers to the distance of separation between the O and C plume centroids following each 24 h of sampling, provide information on relative distance errors associated with the miscalculation of plume trajectories. Finally, there is no convenient way to measure the angular discrepancy between the O and C plumes, whose trajectories are intrinsically curvilinear. However, $\Delta L_\perp$, the distance from the calculated plume centroid along a line normal to the most recently observed plume trajectory segment, will be useful in determining whether our calculated plume trajectories exhibit a tendency to veer or back from actual plume trajectories.

5. Results

With the release of perfluorocarbons every 2.5 days, the experimental designers had a reasonable expectation that the PTCH or PDCH clouds would remain segregated over the course of their travels. Merging did, however, occur at times, making it impossible to attribute samples or fractions of samples to particular releases with any certainty. Fortunately, many of the protocols for assessing model performance allowed us to consider combinations of footprint patterns and thus retain a substantial amount of the sample

data for our analyses. The schedule for PTCH and PDCH releases in January, 1987, is presented in Table 2; releases which have been merged for analytic purposes are noted.

The layout of the ANATEX sampling network affected our ability to evaluate the models. Similar to aliasing in sampling theory, which refers to the impossibility of resolving high frequencies whose wavelengths are less than twice the spacing between sample points, tracer clouds in the near-source regions around GGW and STC were incapable of being properly resolved whenever the plume width was less than $2\Delta x$. In our case a plume width was determined by the bounding limits of the plume (10 df/l) and on the average separation between sampling sites ($\Delta x = 250$ km). If we extrapolate this reasoning to areal considerations, then we can argue that the O and C comparisons will have little or no validity whenever the observed footprint area is less than $(2\Delta x)^2$; that is, plumes whose estimated areas are less than $(2\Delta x)^2$ are likely to be an artifact of the assumptions contained in the interpolating procedure. For areas beyond this threshold, plumes will generally reflect several measurements and, thus, be less sensitive to the choice of technique. In the upcoming discussion, the entire body of data will generally be examined; however, data in the undersampled region will occasionally be removed for purposes of illustration.

As previously mentioned, the 77 primary, surface sampling sites were arrayed in bands relative to the source at Glasgow with the greatest density occurring along the 1000 km and 1600 km arcs to improve the spatial resolution of the transient tracer clouds at these distances (see Fig. 1). In general, we can expect the model results to be better for GGW than for STC for the following reasons: 1) the orientation of the samplers favors the more rapid resolution of tracer plumes released from GGW; in contrast, clouds released from STC can travel relatively greater distances before spreading out sufficiently to be resolved; 2) being situated outside and to the west of the sampling network, flows that carry the PTCH releases from GGW into the network are, generally speaking, more organized and thus more easily modeled; in contrast, the (observable) dispersion of PDCH from STC is affected by a greater range of synoptic meteorologies and, given that the source is embedded

within the network, the material has a greater chance of being detected below the spatially resolvable limit, and 3) given their release points, PDCH plumes will, on average, travel a shorter distance than the PTCH plumes before exiting the sampling network.

Figure 3 gives an indication of the undersampling problem at St. Cloud. In this figure, the ratios $\Delta L/L_O$ for all observed and calculated plume trajectories are plotted in a cumulative frequency format. As an illustration of how to read this figure, the spatial deviation between the observed and calculated plume centroids is less than 20% of the total observed trajectory distance 50% of the time for LLNL's 10 simulations of PTCH releases from Glasgow. The EXPRESS and ADPIC models appear to perform equally well, but their performance depends on the source of emissions. The results of both models are significantly degraded when the source is STC for the reasons cited above.

The mid-range, loosely defined here as distances that range from about 1000 km to 2500 km from either source, provides the most fruitful region for model evaluations. Generally speaking, a plume remains coherent within this range and impinges on a sufficient number of samplers within 24 hours for a footprint to be resolved. (Exceptions to this rule have occurred whenever large-scale vertical motions, which neither model can simulate, lofted the tracer out of the planetary boundary layer.) Beyond this limit, the tracer cloud is prone toward deformation, mainly as the result of large-scale eddy effects, with its surface manifestations often appearing as a set of disconnected patches. Obviously, this latter occurrence can undermine the value of a center-of-mass performance measure since a centroid may be located outside the footprint boundaries.

A scatter plot of the observed and calculated footprint areas for both sources is shown in Fig. 4. This figure excludes the undersampled population (those O and C pairs for which the observed area is less than $250 \times 10^3 \text{ km}^2$), which constitutes 48% of the total population. For the 30 data pairs that fall within this region, randomness would suggest that over- or under-predictions of the footprint areas by an unbiased model should be about equal. Instead, the areas computed by EXPRESS (ADPIC) exceed their observed

counterparts 87% (97%) of the time. Moreover, the medians of the ratios of O and C footprint areas—5.4 for EXPRESS and 3.0 for ADPIC—suggest that both models have a bias towards greatly over-estimating diffusion in the near-source region (the complementary effect of generating concentrations that are often excessive in this region will be examined shortly).

The solid line in Fig. 4 represents a one-to-one correspondence between the O and C distributions; the dotted lines represent factor of two differences. A circle within a circle has been added to this figure as a schematic reminder of what a factor of two difference in area means when the plume footprints have a circular aspect. The boxed symbols are those observed data whose footprints have a peak concentration less than a factor of five of our chosen threshold of 10 df/l. They have been recorded at the far range of the sampled tracer, where typically shear and turbulent effects have so deformed the plume that its definition is inexact. While the relationship between the observed and calculated areas is not impressive (correlations of the data in the mid-range of sampling are not significant), the high percentage of calculated plume areas within a factor of two of the observed areas does suggest that the models possess some skill in the prediction of diffusion.

Box plots of the O and C footprint areas of intersection, normalized by their combined areas, are presented in Fig. 5. They possess the usual characteristics: the extrema indicate the range of the distribution, data between the 25th and 75th percentiles occupy the box, and the thin central band denotes the median. There is a diminishment of dispersion over time. The range of the medians over the times considered is quite narrow (0.06 to 0.33 for EXPRESS and 0.09 to 0.27 for ADPIC). A comparison of Fig. 4, in which we see the majority of calculated footprint areas being within a factor of two of the observed footprint areas in the mid-range of sampling, and Fig. 5, in which the means of $A_{S_{O \cup S_C}}$ for the EXPRESS and ADPIC models are 0.24 and 0.26, respectively, suggests that the rate of separation between the O and C plume centroids may be much greater than their rate

of horizontal diffusion. The absence of other apparent trends is probably symptomatic of the sample sizes (six to eight values per time period), which lead to unstable "statistics".

Figure 6 shows the averages of the peak concentrations, ordered as a function of time and presented on a logarithmic scale. This figure excludes data from the merged releases since the attribution of times to peak concentrations is problematic. A line representing a linear least squares fit to the observed data has been added to again demonstrate the log-normal behavior of the atmosphere in regard to the dilution of airborne materials (the least squares calculation excluded the first observed value because of its probable randomness). The parenthetical and bracketed values are ratios of the observed and calculated averages, or their inverses whenever the ratios are less than unity, for the ADPIC and EXPRESS models, respectively.

For the ADPIC model, the ratios exceed a factor of two in two out of eight cases. The generation of excessive peak concentrations at early times may be due to inadequate sampling or to the sampling methodology. ADPIC uses a four-level nesting scheme to improve the sampling resolution near the source of emissions. The masses attached to the Lagrangian particles that traverse a pseudo-sampling cell (the most refined Eulerian cell measures $7.8 \text{ km} \times 6.25 \text{ km} \times 200 \text{ m}$, and is centered on a sampler's coordinates) are summed over 24 h and then divided by the sampling volume before averaging. Obviously, the potential for recording the passage of a cloud, and inflating the values of concentration in general, is enhanced as compared to an actual (point) sampler. This is especially true near St. Cloud, where two of the samplers—one to the southwest of STC and the other to the north of STC—are 14 km and 88 km away, respectively. Agreement between the O and C peak concentrations improves at later times (and greater distances) from the source as the result of better plume resolution. In an average sense, Fig. 6 suggests that the EXPRESS model systematically overpredicts the downwind peak concentrations. The computation of excessive peak concentrations in the near-source region would appear to be a major reason for model overpredictions of the surface dimensions of a plume near a source;

i.e., the boundary expands beyond the plume's actual dimensions whenever exponential weightings are applied to over-estimated sampler concentrations.

In exploring other physical factors that may explain these systematic errors, we calculated the zeroeth moment for the surface concentration distributions. Figure 7 shows the relationships between the measured and calculated values of the integral concentrations (zeroeth moments) as a function of model and source. Solid lines representing factor of two differences have, once again, been added as visual aids for appreciating the relative errors. The EXPRESS and ADPIC model results are closely aligned, with both models exhibiting a tendency for overprediction. The scatter and the relative error are seen to increase with decreasing integral concentration. Since the integral concentration will, in general, decrease over time, this finding suggests that both models underestimate vertical turbulent mixing. For those plumes traveling toward southerly latitudes, the atmosphere will, in general, become less stably stratified. Therefore, it is reasonable to suppose that the vertical diffusion coefficients being used by the models are too small when applied in these areas. Haagenson *et al.* (1990) provide another credible explanation for our overprediction of surface tracer concentrations. Their three-dimensional trajectory results have indicated that large-scale upward displacements of trajectory air parcels, which happened with some frequency, were associated with low tracer concentrations at the surface. In their limited case study, Porch *et al.* (1989) were able to correlate the absence of surface concentrations to large-scale stability zones. Since neither model possesses a mechanism for lofting the tracer by kinematic means, it is not surprising that they exhibit a tendency to overpredict the peak and integral surface concentrations.

Turning our attention now to the protocols related to plume transport, it may be that the simulated plumes are preferentially steered to the left or right of the actual plume trajectories. Consequently, we have plotted $\Delta L_{\perp}$, normalized by the cumulative distance (L_o), against the total distance, as shown in Fig. 8. Both models have three points in the near-source region that are out of bounds in the positive direction. As expected, the

figure gives the appearance of a collapsing envelope as a function of time, with the greatest dispersion occurring in the undersampled region. The numbers of points above and below the line of perfect agreement are 28 and 35, respectively, for the EXPRESS model and 37 and 26, respectively, for the ADPIC model. Neither model exhibits a discernable bias at the 95% confidence limit.

A scatter of the cumulative distances traveled by the observed and calculated plumes, as determined by their centroid coordinates after each 24 h of sampling, are shown in Fig. 9. These paired quantities provide a direct measure of how well the models predict the actual plume speed. The agreement is excellent as demonstrated by the computed correlation coefficients (0.865 for EXPRESS and 0.857 for ADPIC). The means of the ratios L_C/L_O (1.05 and 1.06 for the EXPRESS and ADPIC models, respectively) suggest a minor inclination, if any, toward the over-estimation of wind speed. The two extremities to the right of both figures are derivatives of release #5 from GGW. The determination of associated samples after three days of transport is somewhat uncertain because of the apparent lifting of the PTCH tracer over a warm front at about this time.

The ability to accurately model wind speeds has value if, and only if, the directions of the observed plumes can be reproduced with commensurate accuracy. Figure 10 offers a look at the errors resulting from misrepresentations of the wind velocity fields. The points represent distances of separation between observed and calculated plume centroids (ΔL) that have been averaged over common sampling times. The excursions at the tail of the two distributions may, and probably do, reflect the ambiguities associated with the assignments of 24-h samples to given releases at late times. While both sets of model results compare favorably with those of other researchers (e.g., see Haagenson *et al.*, 1990, and Kahl and Samson, 1986), it appears, thus far, that directional errors dominate all other sources of potential error. Whether trajectories are more sensitive to increases in the spatial resolution of the U.S. rawinsonde network as opposed to increases in the temporal resolution (Kahl and Samson, 1988), or whether the obverse is true (Rolph and Draxler, 1990), the

fact remains that the existing network poses a severe constraint to the improvement of modeling accuracy.

To gain a better understanding of the relative errors associated with plume diffusion as opposed to plume transport, we have: 1) calculated the equivalent radii of the observed (r_o) and calculated (r_c) plumes after each 24-h sampling period (admittedly, this calculation tends to favor diffusion over transport since the outline of a footprint may deviate significantly from circularity as the result of being deformed) 2) normalized the average of the absolute differences of these radii ($|r_o - r_c|$) by the average radius of the observed footprints ($\bar{r}_o$), and 3) compared these values against the average distances of separation between the O and C plume centroids ($\overline{\Delta L}$) at corresponding times, which have also been normalized by $\bar{r}_o$. Using the ADPIC results for illustration, the outcomes of these comparisons for a sample population that excludes undersampled data are shown in Fig. 11. They suggest that transport errors greatly exceed the errors resulting from the model definition of diffusion.

6. Conclusions

The EXPRESS and ADPIC models have been designed to assist emergency personnel in their response to radiological accidents. Such decision makers, faced with the task of formulating a credible response, need two essential pieces of information: the areas of contamination above a designated threshold and the distribution of radioactivity within these areas. Protocols for the determination of model performance were adopted or developed with this requirement in mind. However, during the initial, exploratory phase of our study, we discovered that these protocols must be chosen with care. Our analysis of the ensemble of peak concentrations suggested that the surface concentration distribution was log-normal. Consequently, the use of standard statistics, such as zeroeth, first and second order moments whose applications are based on the assumption of normality, would seem

to be inappropriate without the performance of necessary transformations. The analysis of concentration distributions at "fixed" times has led us to a softer conclusion; the use of these various moments may be appropriate for concentrations that define a single surface footprint or a collection of footprints that are grouped according to time.

The effectiveness of our suite of performance measures is predicated on our ability to resolve surface concentration footprints. We found it impossible, however, to take full advantage of the ANATEX surface concentration database because of the undersampling of plumes in the near-source regions. A plume is undersampled when its concentration distribution in the cross-wind direction is defined by fewer than three samples; even at the upper limit, a plume's characteristics can only be described in an average sense. Our extrapolation of this argument to areal considerations led us to conclude that almost half the surface footprints fall within the undersampled category.

Our models were challenged by the complexity of the synoptic meteorology. Although no attempt was made to classify the model results on the basis of synoptic type, it is certainly noteworthy that the tracer clouds interacted with fronts or troughs in nine of the 20 releases under investigation. The associated dynamic effects on the tracer clouds and the effects of large-scale stability zones at other times were apparent; there were many instances of a cloud "skipping over" samplers along its apparent path, disappearing entirely (presumably, because of being lifted out of the PBL), or delivering concentrations to surface samplers that were below normal expectation. The frequency of these occurrences suggest that we need to make the necessary investment to develop and implement a rational scheme that takes these effects into account. Given the temporal and spatial resolution of the U.S. rawinsonde network, it remains to be seen whether an effective strategy can be developed. A comparison of errors associated with the diffusion and transport of a tracer cloud suggests the dominance of the latter source of error.

The inability of EXPRESS and ADPIC to simulate vertical motions had collateral effects on the model results. The diminishment of surface concentrations, mainly as the

result of dynamically-induced lofting of the tracer plume, led to a general overestimation of these quantities by the models. Using the average peak concentrations as an example of this phenomenon (see Fig. 6), the EXPRESS model produced averages that typically exceeded the observed averages by about a factor of two. The ADPIC-generated averages were also excessive by a similar amount over the first two days. This tendency cannot be fully explained by inadequate sampling of the plume since random chance would suggest that the odds of over- or under-prediction of the peak concentration are about equal. In general, higher estimated concentrations translates to higher integrated concentrations and larger surface footprint areas, both of which are apparent in the model results.

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Table 1. *d* values from the application of the Kolmogorov-Smirnov test, assuming normal and log-normal concentration distributions for data grouped according to common sampling times.

Hour	dstat(max)		n	Accep@ $\alpha=0.05$
	Norm	Log-Norm		
33	0.204	0.112	17	0.330
45	0.319	0.187	24	0.278
57	0.217	0.072	40	0.215
69	0.214	0.196	34	0.233
81	0.276	0.157	54	0.185
93	0.277	0.156	31	0.244

Table 2. Tracer releases over one-month study period (1987)

Glasgow, MT (PTCH)

Date	Time (UTC)	
5 January	17-20	]*
8	05-08	
10	17-20	
13	05-08	
15	17-20	
18	05-08	
20	17-20	
23	05-08	]*
25	17-20	
28	05-08	

St. Cloud, MN (PDCH)

Date	Time (UTC)	
5 January	17-20	
8	05-08	]*
10	17-20	
13	05-08	
15	17-20	
18	05-08	]*
20	17-20	
23	05-08	
25	17-20	
28	05-08	

* plumes merge

Fig. 1. ANATEX surface-based sampling network with approximate source-to-receptor distances (km) indicated along bands.

Fig. 2. Normally distributed (a) and logarithmically transformed (b) peak concentrations for all ANATEX field observations in January, 1987.

Fig. 3. Cumulative frequencies of the distances of separation between observed and calculated plume centroids (ΔL) normalized by the corresponding cumulative distances between sources at GGW or STC and observed plume centroids (L_0).

Fig. 4. Comparison of observed and calculated footprint areas with undersampled populations removed.

Fig. 5. Box plots of the observed and calculated footprint areas of intersection normalized by their combined areas.

Fig. 6. Averages of the observed and calculated peak concentrations.

Fig. 7. Observed integral concentrations (Q_O) at the 2 m sampling height vs integral concentrations (Q_C) calculated by (a) ADPIC and (b) EXPRESS.

Fig. 8. Normalized minimum distances ($\Delta L_{\perp}$) between calculated mass centroids and observed plume trajectory segments vs cumulative transport distance (L_0).

Fig. 9. Comparison of observed and calculated source-to-plume centroid distances (km) for (a) ADPIC and (b) EXPRESS.

Fig. 10. Average separation (km) between observed and calculated plume trajectories.

Fig. 11. Relative errors associated with plume advection and plume diffusion.

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