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AN EXAMPLE OF EMERGENCY RESPONSE MODEL
EVALUATION OF STUDIES USING
THE MATHEW/ADPIC MODELS

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**AN EXAMPLE OF EMERGENCY RESPONSE MODEL
EVALUATION STUDIES USING
THE MATHEW/ADPIC MODELS**

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ABSTRACT

This report summarizes model evaluation studies conducted for the MATHEW/ADPIC transport and diffusion models during the past ten years. These models support the U.S. Department of Energy Atmospheric Release Advisory Capability, an emergency response service for atmospheric releases of nuclear material. Field studies involving tracer releases used in these studies cover a broad range of meteorology, terrain and tracer release heights, the three most important aspects of estimating air concentration values resulting from airborne releases of toxic material. Results of these studies show that these models can estimate air concentration values within a factor of 2 20% to 50% of the time and a factor of 5 40% to 80% of the time. As the meteorology and terrain become more complex and the release height of the tracer is increased, the accuracy of the model calculations degrades. This band of uncertainty appears to correctly represent the capability of these models at this time. A method for estimating angular uncertainty in the model calculations is described and used to suggest alternative methods for evaluating emergency response models.

1. INTRODUCTION

The MATHEW/ADPIC (M/A) models are used as the major operational models for the Atmospheric Release Advisory Capability (ARAC), an emergency response service developed by the Lawrence Livermore National Laboratory (LLNL) for the U.S. Departments of Energy (DOE) and Defense (DOD).^{1,2,3} The ARAC service provides guidance to crisis managers and on-scene commanders that deal with potential or actual atmospheric releases of toxic material. Assessment products calculated by the M/A models provide crisis managers and on-scene commanders with estimates of public health and safety effects of an atmospheric release of toxic material.

In addition to the ARAC service, these models are used now by approximately 10 other countries involved in developing or implementing emergency response services. This broad usage of the models implies an importance for maintaining and expanding statistical data bases on model performance. For the past ten years LLNL has evaluated the models against tracer and meteorological data bases for 6 geographical locations for a total of 26 field experiments. These field studies encompass rolling and complex terrain areas under a variety of meteorological conditions. Other countries, e.g. Italy and Japan, have also evaluated the models against data from field campaigns. Other data sets are presently being analyzed by LLNL and other users for future model evaluation studies. This paper summarizes the model evaluation studies completed to date based on particular criteria chosen over 10 years ago, briefly discusses additional data available for model evaluation studies and suggests other criteria, with examples, for judging emergency response model performance.

2. MATHEW/ADPIC MODEL EVALUATION STUDIES

The wide variety of terrain types, tracer release heights and sampler placements and meteorology represented by these model evaluation studies is discussed below. The specific field experiments used to evaluate the M/A models thus far are:

INEL 1971²

ASCOT 1980^{6,7}

EPRI 1980⁴

EPRI 1981⁵

SRP 1974²

ASCOT 1981⁶

MATS 1983⁸

TMI 1980³

Montalto 1984⁹

The initial evaluations were based on meteorological and tracer data acquired by field experiments conducted in rolling terrain at the Idaho National Engineering Laboratory (INEL) in Idaho and at the Savannah River Plant (SRP) in South Carolina in 1974 over relatively flat terrain.² More recently, several additional data bases have become available. The ARAC response to the purge of Kr-85 from the TMI containment over a 12 day period in 1980 provided an opportunity to compare model predictions with field measurements in rolling terrain.³ This was followed in 1980 and 1981 by the field experiments, conducted by the Electric Power Research Institute (EPRI), of the buoyant plumes generated by the Kincaid coal-fired power plant situated in flat terrain in Illinois.^{4,5}

Our participation in the Department of Energy sponsored ASCOT program has resulted in model improvements and evaluations using data from nocturnal drainage flow field experiments conducted in complex mountain valley settings in northern California

during 1980^{6,7} and 1981.⁶ The models have also been evaluated using a series of daytime tracer experiments conducted during 1983 as part of the Mesoscale Atmospheric Transport Studies (MATS) at the SRP.⁸ In addition to these studies, researchers in Italy have evaluated the models against a series of seabreeze experiments conducted at the Montalto nuclear power plant site situated about 100 km northwest of Rome.⁹

These experiments utilized a multitude of tracers including routine emissions of Ar-41 from the SRP nuclear reactors; the controlled venting of Kr-85 from the TMI containment; I-131 releases at INEL; sulfur hexafluoride releases from the SRP, the Montalto, and Kincaid power plant sites; as well as perfluorocarbon and heavy methane releases that were part of the ASCOT experiments. The releases occurred from the 60 m stacks at the SRP and TMI, and from the 160 m stack at the Kincaid power plant. The remaining releases generally occurred near the surface except for one heavy methane tracer that was released at 60 m during the 1980 ASCOT experiments and one perfluorocarbon tracer released in a cooling tower plume during the 1981 ASCOT experiments. The duration of the releases varied from 15 min to several hours. Extensive surface sampling networks were employed in each series of experiments. Maximum distances were typically 80 km for the 1971 SRP and 1974 INEL studies, 40 km for the EPRI and TMI studies, 30 km for the MATS experiments, 10 km for the ASCOT experiments, and approximately 6 km for the studies at Montalto, Italy. The experiments were supported by a variety of surface and upper air meteorological observations. These measurements ranged from adequate meteorological coverage during the TMI purge of Kr-85 to a wide spectrum of measurement systems, including acoustic sounders, tethersondes, rawinsondes, optical anemometers, and towers, that were an integral part of the ASCOT experiments.

3. RESULTS FROM PREVIOUS STUDIES

It is difficult to devise a statistical process that adequately describes a model's performance when compared to tracer field data, particularly when the field data span a broad spectrum of release and sampling times, sampling distances, terrain and meteorology. For example, the standard correlation coefficient is used sometimes; however, one point at the high end of the scale can influence the entire data set. Early on we chose a rigid technique but one we considered a standard for comparisons of tracer measurements to the MATHEW/ADPIC model calculations. A factor R is computed for each pair of measurements (C_m) and model calculations (C_c) which represents the whole - number ratio between the two. For each experiment the percent of comparisons within a factor R are plotted as a function of R . The definition of R is $R = (C_m + B)/(C_c + B)$, and if $R < 1$, $R = 1/R$, and B is background.

Figure 1 shows results of model comparisons using data from the TMI, SRP 1974 and the INEL experiments. The model calculations were within a factor 2 for 50% of the comparisons and a factor of 5 for approximately 80%. These field campaigns were in areas of relatively flat terrain and included distances out to 80 km. Sampling times varied from 10 min for the Ar-41 measurements using instruments mounted in cars and airplanes to

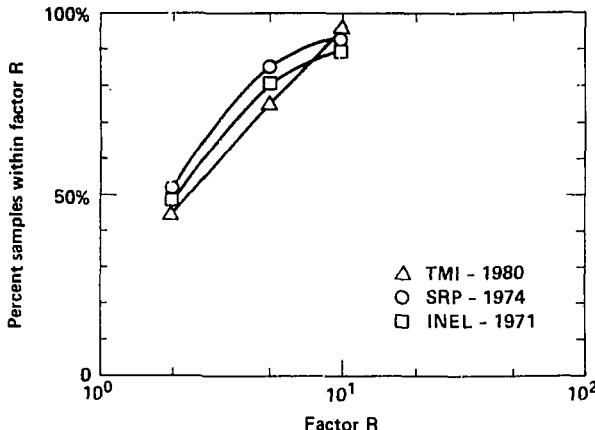


FIGURE 1. Percentage of computed air concentration values within a factor R of measured, for the TMI 1980, SRP 1974 and INEL 1981 tracer experiments.

3 h for the INEL study. Results shown in this figure are the best obtained by the models thus far.

Figure 2 shows results from the 1983 MATS and Montalto studies. In this case we have shown comparisons with no adjustment of the model calculations to those where the model calculations have included a directional change that best matches the measured data. An example of how the unadjusted model calculations compare to measurements is shown in Figure 3. The shape of the two curves is similar, i.e., the diffusion is modeled well; however, the direction in this case is off by 7 degrees. This feature of these comparisons and others we have performed tends to indicate that the calculated concentration patterns are similar to those measured; however, they are displaced by an error in either the wind direction measurements and/or the model adjusted wind fields. In any case, for both the Montalto and the SRP 1983 studies an average directional correction of 5° shifted the comparisons from the lower two curves to the upper two curves, resulting in the adjusted curves being similar to those shown in Figure 2.

Comparisons of model calculated air concentrations with the most complex field studies are shown in Figure 4. The ASCOT 1980 and 1981 surface releases of tracer material show similar results; model calculations are within a factor of 2 about 25% and a factor of 5 about 50% of the time. These field studies were conducted in complex terrain, under stable nighttime conditions, which account for much of the degraded performance of the models. The EPRI study, although conducted in flat terrain, was associated with a power plant plume as the tracer release mechanism. For this study complicating factors were the measurement or modeling of the correct plume rise and the meteorology which varied from stable to unstable during the morning transition and through the daytime hours returning to stable during the evening transition.^{4,5}

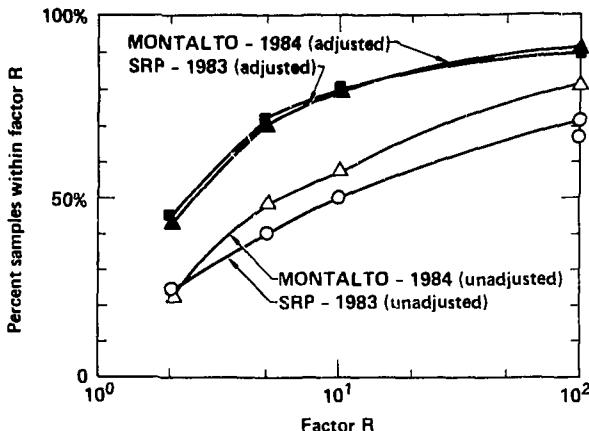


FIGURE 2. Same as Figure 1 for SRP 1983 MATS and Montalto 1984 tracer experiments.

The curves representing the ASCOT 1980 elevated heavy methane and the 1981 cooling tower releases represent complex terrain and elevated releases coupled with stable meteorological conditions.^{6,7} Under these conditions the model results are further degraded by about 10% in the factor of 5 comparisons. Multiple stratification coupled with complex terrain and elevated release heights pose a complex combination of processes that stretch the physical limits of diagnostic models.

Figure 5 depicts a summary bounding the performance of the M/A models thus far. The best simulation of the experimental data is given by the upper curve that is associated with rolling terrain and near-surface tracer releases; while the most difficult simulation is associated with complex terrain and elevated releases. Other situations provide results that are intermediate to these curves. Hence, the best results indicate that the calculated concentrations are within a factor of 2 for 50% of the measured concentrations and within a factor of 5 for 75% of the comparisons. This performance degrades to 20% and 35% for factors of 2 and 5 respectively for the comparisons associated with elevated releases in complex terrain. This degradation of results in complex terrain is due to a variety of factors such as the limited representativeness of measurements in complex terrain, the limited spatial resolution afforded by the models, and the turbulence parameterizations used to derive the eddy diffusivities.

In addition to the studies described above, researchers at the Japan Atomic Energy Research Institute (JAERI) have evaluated models similar to MATHEW/ADPIC, for over 30 data sets during the past 4 years.¹⁰ The two sites used for these studies were a flat coastal area and a mountain region. Meteorological conditions for the experiments were sea-land breeze for the coastal site and complex mountain winds for the complex site. Tracers for these experiments were released from heights that varied from 7 to 150 m and lasted from 30 to 90 min. Surface samplers were located out to 15 km in the horizontal and up to

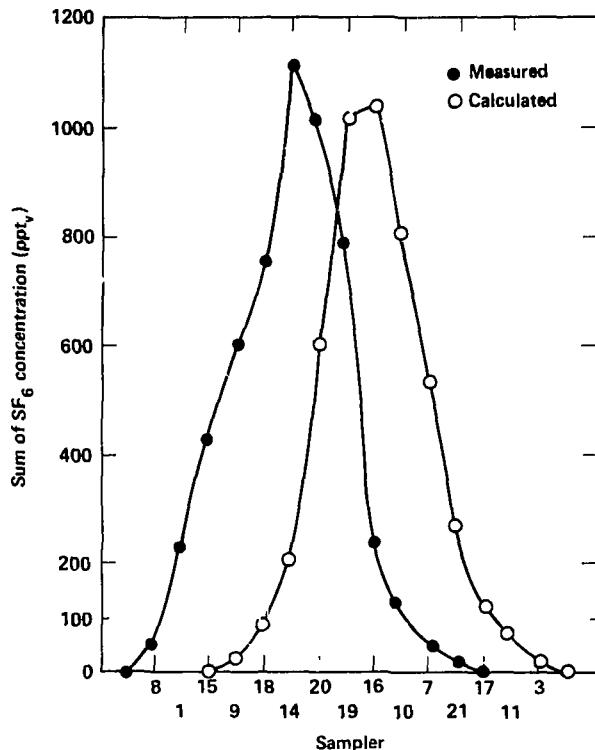


FIGURE 3. Measured and calculated air concentration values for the SRP 1983 MATS tracer experiment number 7.

300 m in the vertical directions. An array of meteorological measurements were made ranging from anemometers on towers to radiosondes and kitoons. Although reports on these studies have not been published in English (JAERI has plans to do so in the future), qualitatively, graphs of comparisons between tracer measurements and model calculations appear to be similar to those discussed above for the SRP MATS and Montalo studies and for the ASCOT studies.

4. ALTERNATIVE METHODS FOR EVALUATING MODELS

As we mentioned in Section 3, the *R* factor analysis provides a rather severe test for the models, particularly when the measurements and model calculations are away from the center-line where the measured and calculated concentration gradients can be steep. In these areas a relatively small deviation in the angle of the wind direction can produce

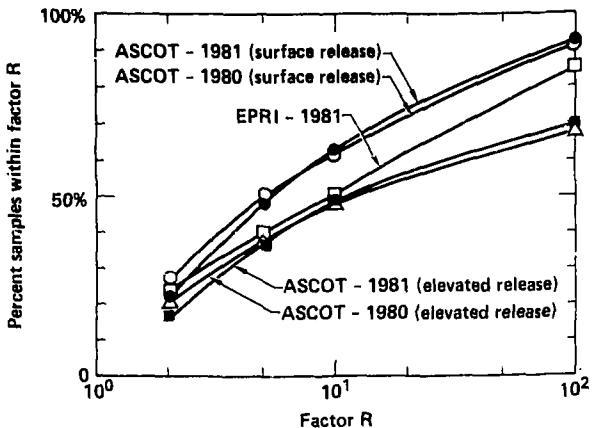


FIGURE 4. Same as Figure 1 for the ASCOT 1980 and 1981 surface and elevated tracer releases and the EPRI 1981 experiment.

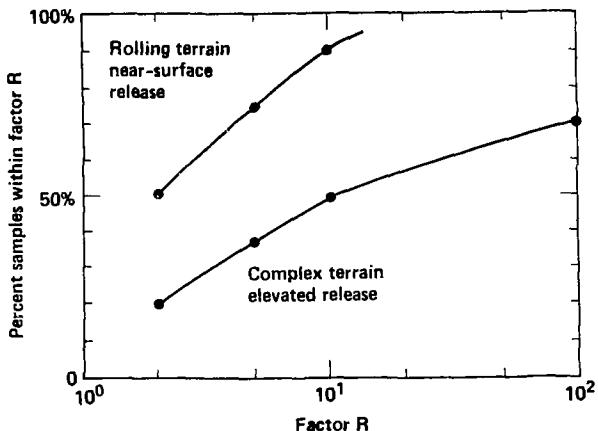


FIGURE 5. Percent of computed air concentrations within a factor R of measured values. The figure provides a measure of the spectrum of model evaluation results that span from near-surface tracer releases in rolling terrain to elevated releases in complex terrain shown in Figures 1-4.

large differences between measured and calculated and concentration values. This feature of the comparisons was shown in figures 2 and 3 where a 7° adjustment in the "modeled"

wind direction produced a dramatic improvement in the model comparisons with a MATS data set. A similar but more general technique was used by Desiato to adjust the model comparisons with the Montalto data set. This technique is described below and is used to adjust model comparisons with a subset of data from the ASCOT 1980 and EPRI field experiments.

In order to provide computed sample concentrations with a range of error bars, an area of uncertainty A is drawn around a sampler location. The size of the area A is defined in terms of an angle of uncertainty $\pm\delta\theta$ as shown in Figure 6. For each sampler, the distance r between the source S and the location of the sampler M is determined, and for a given angular uncertainty $\pm\delta\theta$ the area of computational uncertainty $A=(2r\delta\theta)^2$ is defined. The computed maximum and minimum concentrations C_{c+} and C_{c-} within this area A are determined and are considered the upper and lower extent of an error bar associated with the computed sampler concentration C_c .

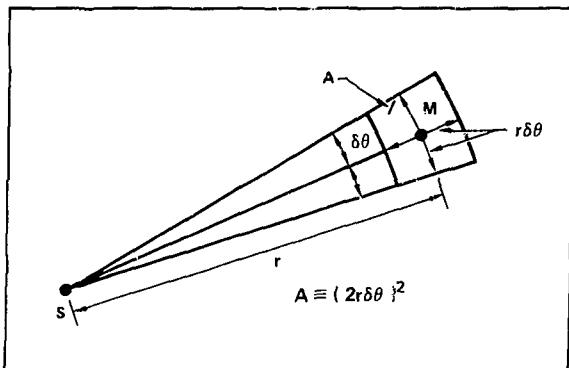


FIGURE 6. Area of uncertainty A defined by the angular uncertainty $\pm\delta\theta$. M is the location of the sampler and r is the distance of the sampler from the source S .

If, for any given sampler, the measured concentration C_m lies within this error bar, i.e. $C_{c+} \geq C_m \geq C_{c-}$, the computed concentration C_c is considered to be the same as measured C_m in the evaluation of the model. For any postulated angular error $\delta\theta$, the R factor analysis can be performed such that,

if $C_m \geq C_{c+}$ then $R = (C_m + B)/(C_{c+} + B)$,

if $C_{c+} \geq C_m \geq C_{c-}$ then $R = 1$,

if $C_m \leq C_{c-}$ then $R = (C_{c-} + B)/(C_m + B)$,

where B is background. In the case of $\delta\theta = 0$ this scheme reduces to the conventional R factor analysis shown in Section 3.

The $\pm\delta\theta$ technique with the R factor analysis is illustrated below using angles of $\delta\theta = 0, 2, 5, 10, 15$ and 20 degrees and subsets of the 1980 ASCOT and EPRI data sets. The drainage flow experiment of Sep. 19/20 1980 was chosen from the complex terrain ASCOT data set with three distinguishable one-hour tracer releases into the surface air (2 Perfluorocarbons and 1 SF6), and about 450 measured samples of average concentrations with averaging times from 10 minutes to 2 hours. Sampling distances ranged from 0 to 8 km. Results of the model comparisons are shown in Figure 7, where the percentage of computed samples agreeing within a factor of R with those measured is plotted against the factor R for the six different angles of uncertainty $\delta\theta$. A similar plot is shown in Figure 8 for the EPRI continuous 187m high stack release of SF6 of May 5 1980 when hourly samples were collected for nine hours at 300 locations out to 50 km distance from the release point.

In comparing figures 7 and 8 attention is drawn to the dramatic improvement in model agreement with increase in the uncertainty angle $\delta\theta$. For the complex terrain ASCOT case (fig. 7) an allowed uncertainty in plume direction of $\delta\theta = \pm 5^\circ$ brings the MATHEW/ADPIC results roughly in line with those for simple releases in flat terrain with $\delta\theta = 0$, (see fig. 1). Although the EPRI release was in flat terrain, the model results were poorer than those for the ASCOT case in complex terrain for $\delta\theta \leq \pm 5^\circ$, indicating that tall stack releases are difficult to model. The larger spread between the EPRI $\delta\theta$ curves (fig. 8) seems to indicate that for a single, well defined EPRI plume with an orderly cross-sectional array of samplers, model results are very sensitive to angular uncertainties in the plume axis. Figure 8 shows that within $\delta\theta = \pm 20^\circ$ (a little less than the standard windrose octant) over 90% of all computed samples match those measured in space and time ($R=1$). The ASCOT simulation (fig. 7) does not quite recover that high an agreement, most likely because the behavior of the three plumes and the sampler deployment were more chaotic. Finally, the number of samples increases with $\delta\theta$ because the number of cases where both measured and computed samples are zero (and are discarded) decreases with increasing $\delta\theta$ (and A).

The property of the R-factor analysis which weighs all samples equally regardless of the magnitude of the concentration is sometimes mentioned as a disadvantage. However, this disadvantage can be overcome by computing the R-factor as a function of concentration. For both the EPRI and the ASCOT data sets the R-factor was computed as a function of the concentration quartiles, i.e. for each sampling period, the sample population with 0 to 25%, 25 to 50%, 50 to 75% and 75 to 100% of maximum concentration was determined, and for each quartile the R-factor analysis was conducted. For this computation the angular uncertainty was fixed at $\delta\theta = \pm 5^\circ$, which corresponds to one cell width for every six downwind cells for the ASCOT and EPRI model grids.

The results, expressed in percentage of computed samples agreeing within a factor of R with those measured for each quartile of concentrations, are plotted vs. the factor R in Figure 9 for the ASCOT and in Figure 10 for the EPRI data sets. The EPRI case (fig. 10) reflects the favoring of lower concentration values by the R-factor analysis, and it also shows that the low concentrations dominated the statistics with 761 sampler in the 0 to 25% quartile and only 24 samples in the 75 to 100% quartile. The favoring of lower concentrations is not so clear in the ASCOT case (fig. 9) where the quartile curves are closer together and show no systematic ordering. This can be attributed once more to the

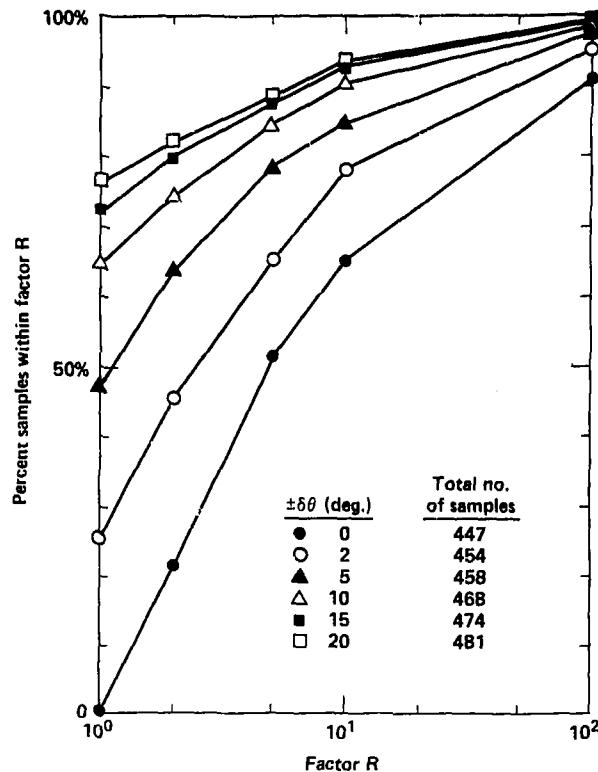


FIGURE 7. Percentage of computed samples agreeing to within a factor of R with those measured for six angles of uncertainty $\pm\delta\theta$. ASCOT data set of Sep. 19/20, 1980.

chaotic plume development and sampler layout in complex terrain as compared to the flat terrain, elevated release of the EPRI experiment.

5. SUMMARY AND RECOMMENDATIONS

Studies described in this paper represent a comprehensive model evaluation program for the M/A models based on field experimental data collected under a variety of topographical, meteorological and tracer release conditions. These studies have shown the M/A models capable of estimating air concentration values, under the conditions described for the various experiments, within a factor of 20% to 50% of the time and within a factor of 40% to 80% of the time. If an angular uncertainty of $\pm 5^\circ$ of the model versus measured

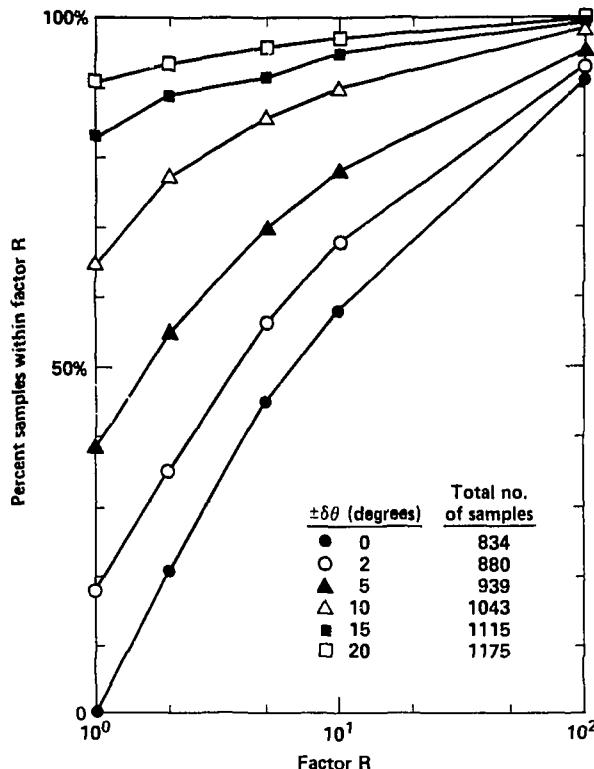


FIGURE 8. Percentage of computed samples agreeing to within a factor R with those measured for six angles of uncertainty $\pm\delta\theta$. EPRI data set of May 5, 1980.

plume direction is accounted for, results for the more complex tracer release conditions improve considerably and closely resemble results for rolling terrain and surface releases.

Using the method for model evaluation that accounts for angular uncertainty between the modeled and measured plumes as an example, expected performance criteria (EPC) need to be developed for emergency response models that can be used to determine quantitatively how well a particular model performs under a given set of calculations as an emergency response model. Hanna¹¹ describes a method for evaluating models based on a set of 5 criteria weighted as to their regulatory significance. For example, emergency response models might be expected to estimate air concentration values within a factor of 5 80% of the time given a $\pm\delta\theta$ of 5° or 10°. In this case, since maximum values are related to dose, the performance criteria relates to how well the model estimates maximum

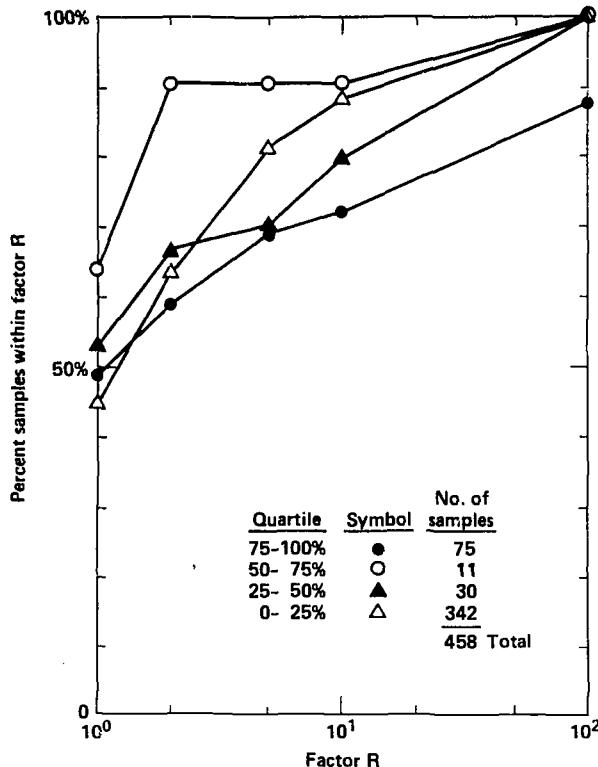


FIGURE 9. Percentage of computed samples agreeing within a factor R with those measured for each quartile of concentrations. ASCOT data set of Sep. 19/20, 1980.

doses in space and time. Another EPC might be a comparison between the top quartile of model calculations and measurements correlated in time but not space. This would provide the user with how well the model estimates maximum concentration values in an absolute sense. Should a model not perform well under this EPC then performance on other more demanding EPC's would be further degraded.

We recommend that the emergency response community work toward establishing EPC's for models that are used as tools in emergency response planning, response and assessment. Data sets are now available that can be used to help provide standardized tests and evaluations of these models and bench mark them against the EPC's once they have been developed.

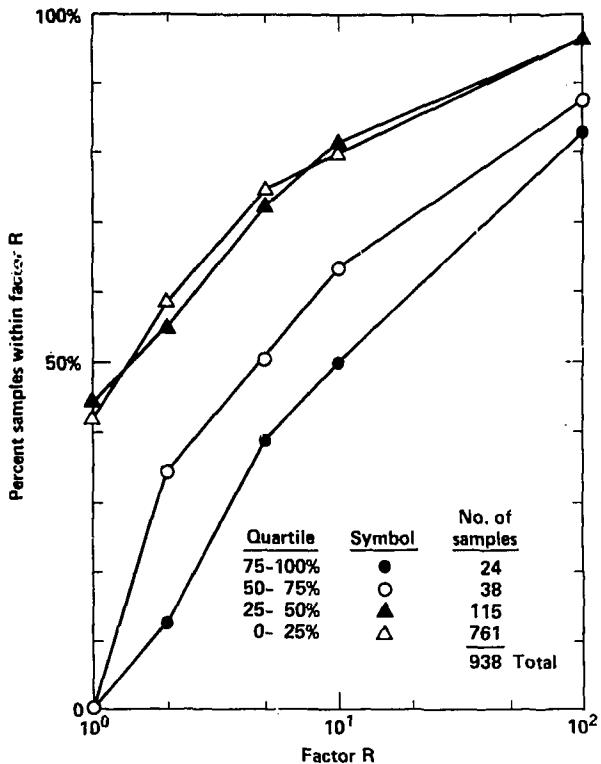


FIGURE 10. Percentage of computed samples agreeing within a factor R with those measured for each quartile of concentrations. EPRI data set of May 5, 1980.

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REFERENCES

1. C. A. Sherman, "A mass-consistent model for wind fields over complex terrain," *J. Appl. Meteor.* 17 (1978) 312-219.
2. 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 (1978) 320-329.
3. M. H. Dickerson, P. H. Gudiksen, T. J. Sullivan, and G. D. Greenly, "ARAC status report: 1985," Lawrence Livermore National Laboratory Report UCRL-53641 (1985).
4. K. R. Peterson and R. Lange, "An evaluation and sensitivity study of the MATHEW /ADPIC models using EPRI plains site data for a tall stack," Lawrence Livermore National Laboratory Report UCRL-91856 (1984).
5. N. E. Bowne and H. S. Bovenstein, "Overview, results and conclusions for the EPRI plume model validation and development project: Plains site," Electric Power Research Institute Report EA-3074 (1983).
6. M. H. Dickerson and P. H. Gudiksen, "Atmospheric studies in complex terrain technical progress report FY-1979 through FY-1983," Lawrence Livermore National Laboratory Report UCID-19851, (ASCOT 84-1) (1984).
7. R. Lange and L. O. Myrup, "Relationship between model complexity and data base quality for complex terrain tracer experiments," Lawrence Livermore National Laboratory UCRL-90747 (1984).
8. D. J. Rodriguez and L. C. Rosen, "An evaluation of a series of SF₆ tracer releases using the MATHEW/ADPIC model," Lawrence Livermore National Laboratory Report UCRL-91854 (1984).
9. F. Desiato and R. Lange, "A sea-breeze tracer study with the MATHEW/ADPIC transport and diffusion model," Proceedings of the *International Symposium on Emergency Planning and Preparedness for Nuclear Facilities*, Rome, Italy Nov. 4-8, 1985, Pages IAEA-SM-280/62
10. M. Chino, Private communication (1985).
11. S. Hanna, "Development and Evaluation of the Offshore and Coastal Model," *JADCA* 35, No 10, 1039-1047 (1985).