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A COMPARISON OF THE WIND SYSTEM ATMOSPHERIC MODELS AND MATS DATA

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1.0 INTRODUCTION

Atmospheric transport and diffusion models have been developed by the Environmental Technology Section (ETS) of the Savannah River Technology Center to calculate the location and concentration of toxic or radioactive materials during an accidental release at the Savannah River Site (SRS). The output from these models has been used to support initial on-site and off-site emergency response activities such as protective action decision making and field monitoring coordination. These atmospheric transport and diffusion models have been incorporated into an automated computer-based system called the WIND (Weather INformation and Display) System and linked to real-time meteorological and radiological monitoring instruments to provide timely information for these emergency response activities (Hunter, 1990).

In an effort to establish more formal quality assurance procedures for the WIND System atmospheric codes, a software evaluation was conducted by the ETS. The evaluation determined the effectiveness of these models in emergency response situations for the SRS. One of the objectives of the software evaluation was to compare the results produced by the WIND System atmospheric models with observational data. The Mesoscale Atmospheric Transport Studies (MATS) tracer experiments were performed at SRS from 1981 - 1985 (Weber et al., 1992) to provide a database for model validation studies. Data from the MATS experiments have already been employed to evaluate a variety of dispersion models (Weber, 1984; Dickerson and Ermak, 1990) that range in complexity from simple straight-line Gaussian to three-dimensional, mass-consistent models.

This study will compare two of the WIND System atmospheric models, PUFF/PLUME and 2DPUF, with a select group of MATS experiments and examine the results in detail to determine the performance of the models. Additional results from this study can be found in Fast et al. (1991).

2.0 DESCRIPTION OF THE MATS EXPERIMENTS

The MATS program consisted of 37 experimental studies over a three year period to investigate the atmospheric dispersion over the gentle rolling terrain in and around the SRS (Weber et al., 1992). The location of the sampling instruments were located at various distances surrounding the SRS as indicated in Fig. 1. Most of the experiments were performed during the day using 15 min releases of sulfur hexaflouride (SF_6). Of the 37 MATS experiments, eight were selected for evaluating PUFF/PLUME and 2DPUFF, namely experiment numbers 8, 12, 14, 24, 27, 31, 32, and 37. Five of the experiments (8, 12, 14, 24, and 31) employed a line of fixed samplers. The remaining three experiments (numbers 27, 32, and 37) employed a mobile sampling vehicle and the numerical results for these experiments are not included in this paper (see Fast et al., 1991).

In choosing the subset of eight MATS experiments, the main criteria used were that they have relatively complete and reliable data sets. The meteorological data were examined to make sure they included upper-air soundings and near-surface observations from the towers throughout the sampling periods. From this group, a subset of cases was selected in which the plume's centerline intersected the sampling arc with a reasonably complete distribution of tracer material on either side. Finally, an effort was made to include experiments representing a variety of wind and stability conditions.

3.0 DESCRIPTION OF THE MODELS

The WIND System atmospheric models PUFF/PLUME and 2DPUF currently run on a VAX 8550 mainframe computer so that they can be easily linked to real-time meteorological and radiological monitoring instruments across the SRS. Both models produce dose or concentration estimates for on-site and off-site locations that are automatically printed out in tabular form and graphically depicted as contours overlaid on SRS background maps. PUFF/PLUME and 2DPUF differ in complexity because each was designed for a different emergency response application; therefore, slightly different dose or concentration estimates may be obtained.

3.1 PUFF/PLUME Code, Version 2.5

The PUFF/PLUME code (Hunter, 1990; Garrett and Murphy, 1981) is a sequential Gaussian model designed to predict plume or puff characteristics and perform dosimetry calculations for the site boundary and beyond due to a release at the site. The code has four options for selecting a wind field based on observations from SRS meteorological towers and Model Output Statistics (MOS) forecasts; however, in each case the wind field does not vary in space but may vary in time. MOS forecasts employ regression equations to link the observed tower data with predictions from the National Weather Service (NWS) Limited Fine Mesh (LFM) model. A single 15 min release duration is used for "puff" calculations, or the user may specify the release duration for "plume" predictions.

3.2 2DPUF Code, Version 3.1

The 2DPUF code (Hunter, 1990; Addis and O'Steen, 1991) is a sequential Gaussian model designed to predict more complex concentration distributions on-site and off-site to obtain accurate dosimetry calculations. The code has three options for the wind field based on observations from SRS meteorological towers, NWS surface and upper-air observations, and MOS forecasts. The wind field may either vary in time but not space for a "local" calculation, or may vary in space and time for "regional" calculation. The total duration of the release is specified by the user. Then, the emission is simulated as a series of "puffs", each with a 15 min release duration.

4.0 PROCEDURE

Both PUFF/PLUME and 2DPUF were executed with the same source term and meteorological data. The models were executed with three different meteorological data sets to determine the model performance. The first data set, M_C, assumed constant meteorological conditions based on an hourly averaged data from the time of the release and a site-area mean (SAM) of the site wind field. The second data set, M_H, consisted of time-dependent meteorological conditions based on hourly averaged data taken from the H-area tower near the release location. The last data set, M_S, also consisted of time-dependent meteorological conditions; however, the hourly averaged data was taken from the SAM wind field. The specific source term and meteorological data used for each MATS experiment can be found in Fast et al. (1991) and Weber et al. (1992).

The model results that incorporated the M_C data set were evaluated to test the validity of constant meteorological conditions near the site. A comparison of the model results for M_H and M_S was made to determine if a site area wind field would characterize transport near the site better. In addition, data from M_H and M_S can be viewed as a "perfect" forecast, since both PUFF/PLUME and 2DPUF can incorporate time-dependent meteorological conditions based on data from NWS forecast models in emergency response situations. MOS forecast data was not available during the MATS experiments; therefore, this capability cannot be evaluated fully at this time.

The depth of the mixed-layer, H, throughout the release period in each of the meteorological data sets was computed by a simple mixed-layer model. The mixed-layer depth in this model was based on the most recent upper-air sounding and hourly values of the surface temperature.

After PUFF/PLUME and 2DPUF was executed with source term and meteorological data, the centerline ground concentration, in parts per trillion (ppt), was extrapolated to the sampler locations using the particular Gaussian method employed by either of the models. A second moment fit technique was used to calculate the half width of the plume (Sigma-y) perpendicular to the sampler network for both the numerical results and the observed values.

5.0 NUMERICAL RESULTS

The numerical results from the models for MATS experiments 8, 12, 14, 24, and 31 were compared to the observed concentrations. The predictions made by the models are subject to errors in (1) source term, and (2) transport and diffusion. In this study, the source term is known with a high degree of accuracy; therefore, most of the differences between the model results and the observations are associated with the transport and diffusion portions of the codes. It is important to remember that the source term is rarely known with such accuracy in emergency response situations, and it is usually the major contribution to model uncertainty. A number of methods for comparing observations to predicted concentrations have been proposed by experts in the field of atmospheric dispersion modeling (Fox, 1980) and employed in this study.

5.1 Temporal -Integration of Concentrations

The SF_6 collected during a sampling period for a particular sampler is defined here as C_i. The sum of the SF_6 concentration all sampling periods, C_t, also referred to here as the total SF_6 concentration is given by:

$$C_t \text{ (sampler)} = \sum_{i=1}^{n} C_i \text{ (sampler)}$$

where n is the total number of sampling periods for a particular MATS experiment. C_t is a useful quantity because it is more comparable to a dose that would be received from a radionuclide release. The width of C_t will give a measure of the horizontal extent of the plume during the entire passage of the plume at the sampler arc. The location of the maximum value of C_t indicates that the centerline of the plume passed over it for a relatively long period of time.

The values of C_t that were observed and computed by 2DPUF at each of the sampler locations for MATS experiments 24 and 31 are depicted in Figs. 2 and 3 (the results from PUFF/PLUME are not shown, but were similar to Figs. 2 and 3). The models performed the "best" for experiment 24 and the "worst" for experiment 31 when compared to the observed concentrations. Neutral stability conditions were observed for both of these experiments; however, the wind direction changed significantly during experiment 31.

For all of the experiments, the ratios of the predicted to the observed C_t listed in Table 1 show that PUFF/PLUME overpredicted C_t as much as a factor of 8.3. PUFF/PLUME underpredicted the value of C_t by no more than a factor of 1.4. Overall, 2DPUF produced values of C_t that were closer to the observations than those computed by PUFF/PLUME. The ratios of the predicted to the observed C_t for 2DPUF listed in Table 1 show that the magnitude of the overprediction was less than a factor of 6.0 and the magnitude of the underprediction was less than a factor of 2.8. The half width of the plume, Sigma-y, produced by

PUFF/PLUME seemed to be in good agreement with the observations as shown in Table 2; however, the model was consistently too narrow. 2DPUF did not predict plume widths that were consistently narrower than the observations, as did PUFF/PLUME.

For MATS experiment 31, the predicted plume path was as much as 15 km from the observed path about 36 km downwind of H-area because of wind direction errors. Nevertheless, the predicted path for most of the MATS experiments was within 5 km of the observed path at the MATS sampler arc.

5.2 Peak concentration

Another measure of the performance of the models is to compare the observed with the predicted maximum concentrations (unpaired in time or space). The ratios of the maximum concentration predicted by PUFF/PLUME to the observed values indicated the magnitude of the overprediction was less than a factor of 13.9 and the magnitude of the underprediction was less than a factor of 1.2. For 2DPUF, the ratios of the maximum concentration to the observed values indicated the magnitude of the overprediction was less than a factor of 13.3 and the magnitude of the underprediction was less than a factor of 2.3. The plume width at the time of the maximum concentration was also well predicted by both models (not shown).

5.3 Timing of transport

The particular time in which the maximum concentration occurs can be used as another measure of the performance of the models to determine the transport errors in the model results. For three MATS experiments (12, 24, and 31), both models predicted the transport speed quite well; however 2DPUF performed better with the M_S data set (not shown). In the other MATS experiments (8 and 14) the models underpredicted the transport speed; in those cases the observed plume arrived before the model predicted it to by as much as an hour. Differences between the observed transport of the plume and predictions by the models are probably due to three factors including (1) wind speed errors, (2) errors in determining the along-wind dispersion parameter, σ_x, or (3) a combination of (1) and (2).

5.4 Paired Concentrations

The ratio method was employed to graphically depict the total SF_6 concentration that was observed predicted by 2DPUF at the sampler locations for all of the MATS experiments examined in this study as shown in Fig. 4 (the results from PUFF/PLUME are not shown, but were similar to Fig. 4). All of the sampler measurements were 25 - 35 km downwind of the source. A R value of 1 indicates that the model results are in perfect agreement with the observations. There is considerable spread about R = 1, but there is no tendency for either model to overpredict or underpredict when individual data points are examined; however there are many cases where the predicted and observed total concentrations differ by more than a factor of 10. PUFF/PLUME tends to overpredict the maximum concentrations, but 2DPUF does not exhibit any bias in these values.

The results from Figs. 4 are summarized in Fig. 5 to show the percentage of the predicted concentrations that are within a factor R of the observations. 59 - 61% is the results from 2DPUF using the M_C and M_S data sets were within a factor of 10 of the observed values; when the wind direction errors are removed, this percentage increased to 88%. 47 - 50% of the results from PUFF/PLUME using the M_C and M_S data sets were within a factor of 10 of the observed values. When the wind direction errors are removed, nearly 80 - 84% of the results from PUFF/PLUME are within a factor of 10 of the observed values. Meteorological conditions from H-area nearly always produced results that were poorer than those obtained from a site-averaged wind field. The local wind behavior at the site did not adequately describe the downwind transport at the sampler network.

5.5 Spatial and Temporal Integration of Concentrations

The total concentrations, C_t, were summed over all of the samplers and the results are presented in Table 3. The results from the MATHEW/ADPIC model (Dickerson and Ermak, 1990) are also presented to demonstrate how the WIND System models perform with other dispersion models. MATHEW/ADPIC is more complex than either PUFF/PLUME or 2DPUF because it can represent a three-dimensional wind field and it uses a particle method to determine pollutant transport. In Dickerson and Ermak (1990), MATHEW/ADPIC was not applied to other MATS experiments (24 and 31) examined in this report.

6.0 CONCLUSION

Considering all of the possible uncertainties associated with dispersion modeling, both PUFF/PLUME and 2DPUF performed reasonably well. The errors in the dispersion forecasts made by PUFF/PLUME and 2DPUF are probably very similar to many other emergency response models based on the Gaussian assumption. It is important to note that the source term was known with a high degree of accuracy in the MATS experiments. In emergency response situations, the source term estimate may be in error by a factor of 10 or more; therefore, the true forecast error produced by these models would be much larger than indicated by this study.

As expected, both models predicted the concentration distribution and location of the plume for MATS experiment 24 particularly well. During the period of the release, the wind speed and direction measured at the SRS meteorological towers was nearly constant in time and space so that the Gaussian assumptions employed by the model were appropriate. The wind direction and speed also must have been spatially invariant; otherwise, the location of the predicted predicted peak concentration would not have agreed so well with the observed one. The meteorological conditions in this case suggest that the Gaussian assumptions employed by the models were satisfied so that excellent forecasts were made. In the cases where the meteorological conditions changed significantly in time (MATS experiments 14 and 31) the models produced results that did not agree as well with the observations.

The results of this study indicate that further research may lead to improvements in the predictions of concentration, plume width, and plume location made by PUFF/PLUME and 2DPUF. The effort required to investigate the improvement of Gaussian-based models such as PUFF/PLUME and 2DPUF must be evaluated against the application of more complex dispersion models at the SRS. The three-dimensional primitive equation model, CSU RAMS, and a companion Lagrangian particle model are currently being examined to test their accuracy and their potential application to emergency response purposes.

7.0 ACKNOWLEDGMENTS

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Table 1. Maximum concentration of the total SF_6 that was observed along the sampler arc and predicted by PUFF/PLUME and 2DPUF where $C_{to}(max)$ is the observed maximum of the total SF_6 concentration (ppt), $C_{tp}(max)$ the predicted maximum of the total SF_6 concentration (ppt), M_C the constant meteorological conditions based on SAM data, M_H the time-dependent meteorological conditions based on H-area data, and M_S the time-dependent meteorological conditions based on SAM data

Exp. #	$C_{to}(max)$	$C_{tp}(max)$ PUFF/PLUME			$C_{tp}(max)$ / $C_{to}(max)$ PUFF/PLUME			$C_{tp}(max)$ 2DPUF			$C_{tp}(max)$ / $C_{to}(max)$ 2DPUF		
		M_C	M_H	M_S	M_C	M_H	M_S	M_C	M_H	M_S	M_C	M_H	M_S
8	809.1	1257.6	* 30.6	578.4	1.55	* 0.04	0.72	795.5	* 5.6	293.0	0.98	* 0.01	0.36
12	745.6	1793.5	563.8	1582.0	2.41	0.76	2.12	886.0	438.9	500.7	1.19	0.59	0.67
14	2221.7	13102.9	5088.8	6145.8	5.90	2.29	2.77	13333.3	2593.1	3097.2	6.00	1.17	1.39
24	521.3	452.4	447.7	423.4	0.87	0.86	0.81	571.0	482.8	535.1	1.10	0.93	1.03
31	329.1	2731.2	* 263.0	1082.5	8.30	* 0.80	3.29	1523.1	* 13.1	851.8	4.63	* 0.04	2.59

asterisk (*) indicates values that may not be meaningful since the predicted plume did not pass directly through the sampler network

Table 2. Plume width of the total SF_6 distribution that was observed along the sampler arc and predicted by PUFF/PLUME and 2DPUF where Sigma-y_{to} is the observed plume width (m) of the total SF_6 distribution, and Sigma-y_{tp} the predicted plume width (m) of the total SF_6 distribution

Exp. #	Sigma-y_{to}	Sigma-y_{tp} PUFF/PLUME			Sigma-y_{tp} / Sigma-y_{to} PUFF/PLUME			Sigma-y_{tp} 2DPUF			Sigma-y_{tp} / Sigma-y_{to} 2DPUF		
		M_C	M_H	M_S	M_C	M_H	M_S	M_C	M_H	M_S	M_C	M_H	M_S
8	2342.7	1781.4	* 830.5	1881.5	0.76	* 0.35	0.80	2028.1	* 661.5	2281.1	0.87	* 0.28	0.97
12	1381.2	1284.7	1307.5	1270.6	0.93	0.95	0.92	1403.3	1566.2	1284.3	1.02	1.13	0.93
14	1691.2	1112.7	1484.7	1182.0	0.66	0.88	0.70	1239.8	1631.8	1338.5	0.73	0.96	0.79
24	1907.2	1486.5	1868.2	1473.5	0.78	0.98	0.77	1625.9	1967.8	1637.1	0.85	1.03	0.86
31	2119.2	1855.4	* 747.6	1826.9	0.88	* 0.35	0.86	2465.9	* 668.5	2217.7	1.16	* 0.32	1.05

Table 3. Integrated SF_6 that was observed at all of the samplers and predicted by PUFF/PLUME, 2DPUF, and MATHEW/ADPIC

Exp. #	ΣC_{to}	ΣC_{tp} PUFF/PLUME			Ratio: $\Sigma C_{tp} / S C_{to}$ PUFF/PLUME			ΣC_{tp} 2DPUF			Ratio: $S C_{tp} / S C_{to}$ 2DPUF		
		M_C	M_H	M_S	M_C	M_H	M_S	M_C	M_H	M_S	M_C	M_H	M_S
8	3717.6	5580.9	* 45.5	3036.3	1.50	* 0.01	0.82	4399.9	* 7.4	1997.3	1.18	* 0.00	0.54
12	1976.2	5076.9	1710.0	4379.5	2.57	0.87	2.22	2839.6	1541.9	1524.9	1.44	0.78	0.77
14	10211.4	32072.6	22946.7	21998.5	3.14	2.24	2.15	33864.0	13017.0	12783.7	4.09	1.27	1.25
24	3360.1	2207.6	2510.3	2143.4	0.66	0.75	0.64	3315.0	2931.5	3089.3	0.99	0.87	0.92
31	1740.6	12665.6	* 355.8	4037.7	7.28	* 0.20	2.32	9629.8	* 16.5	3608.2	5.53	* 0.01	2.07

Exp. #	ΣC_{to}	ΣC_{tp} MATTHEW/ADPIC	Ratio: $\Sigma C_{tp} / S C_{to}$ MATTHEW/ADPIC
8	3718.0	3518.0	0.91
12	1976.0	286.0	0.14
14	10210.0	10620.0	1.04

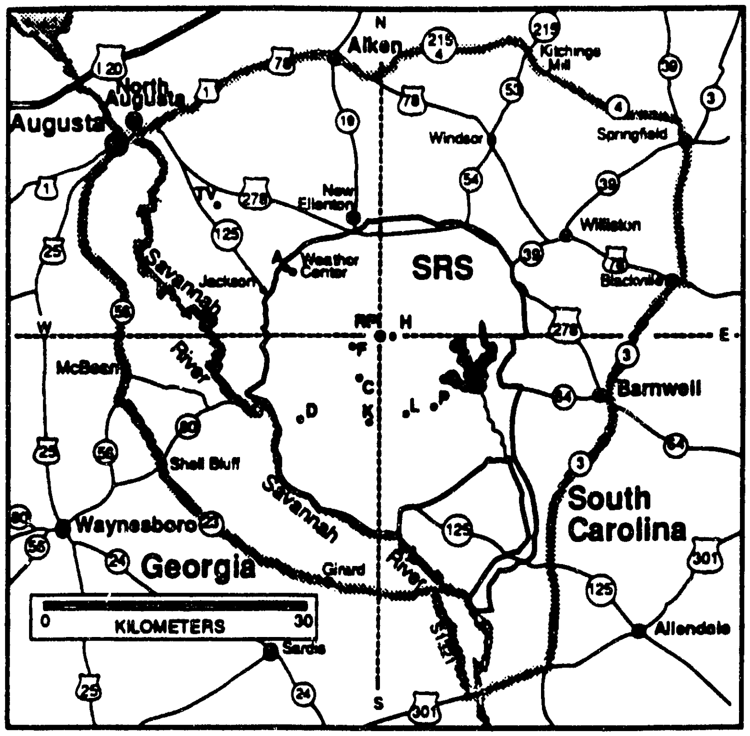

Fig. 1. Locations of the onsite meteorological towers and roads where sampling was done (hatched) for the MATS experiments

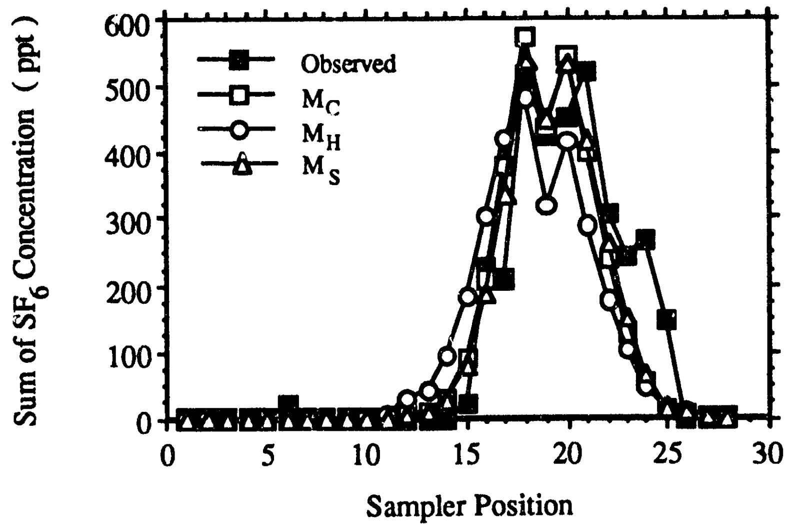

Fig. 2. Sum of the SF_6 concentration that was observed along the sampler arc and predicted by 2DPUF for MATS experiment 24

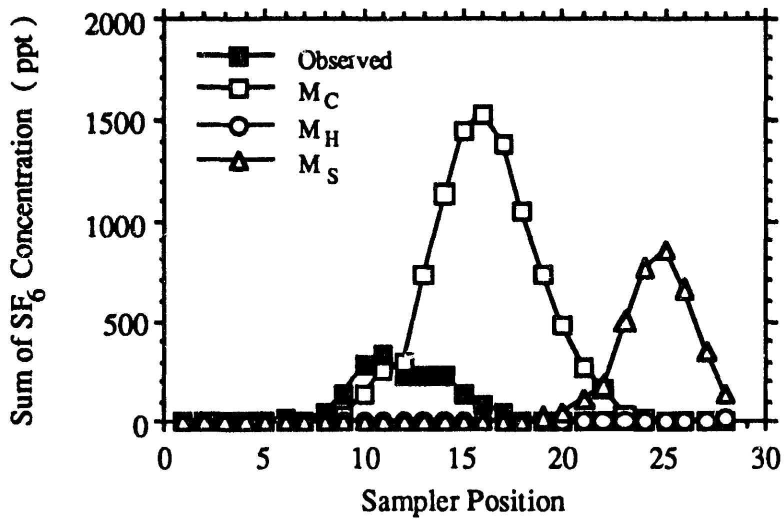

Fig. 3. Same as Fig. 2, except for MATS experiment 31

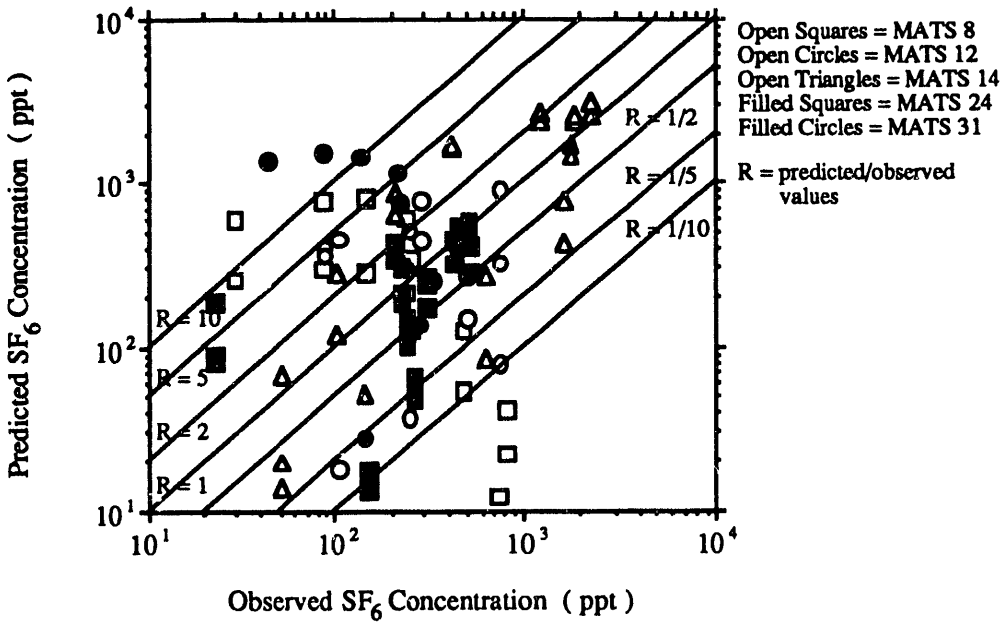

Fig. 4. Sum of the SF_6 concentration that was observed and predicted by 2DPUF, paired in space, for five MATS experiments where open squares denote experiment 8, open circles denote experiment 12, open triangles denote experiment 14, filled squares denote experiment 24, and filled circles denote experiment 31

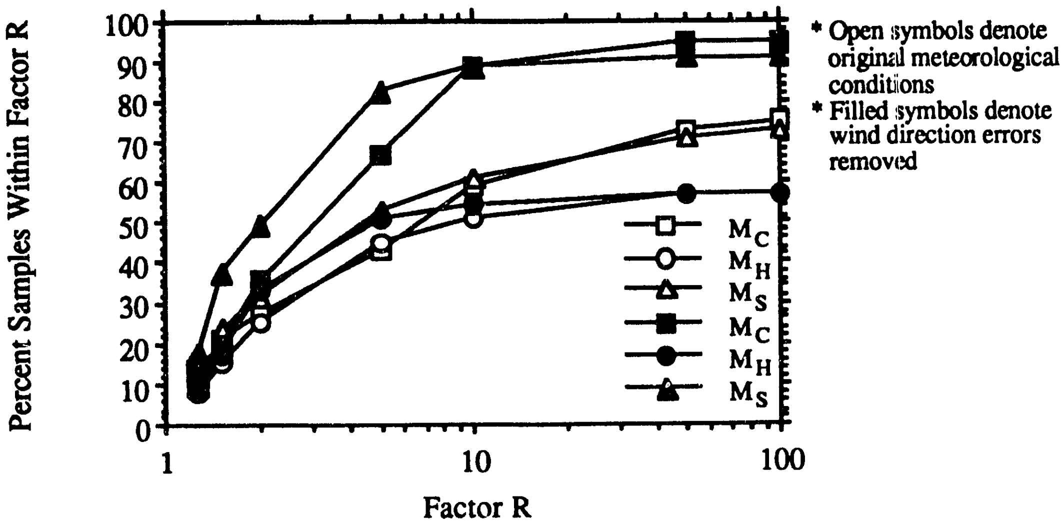

Fig. 5. Percent of the sum of the SF_6 concentrations predicted by 2DPUF within a factor R of the observed values where open symbols denote original meteorological conditions and filled symbols denote wind direction errors removed

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