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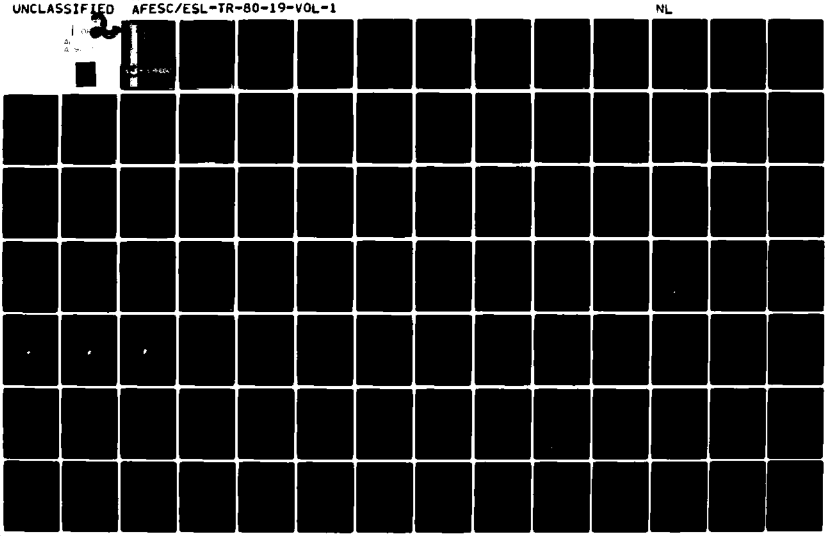

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ANALYSIS FOR THE ACCURACY DEFINITION OF THE AIR QUALITY ASSESSMENT MODEL (AQAM) AT WILLIAMS AIR FORCE BASE, ARIZONA
VOLUME I. TECHNICAL DISCUSSION

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20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

The Air Quality Assessment Model (AQAM) overall predictive accuracy is analyzed using actual air base ambient air quality measurements. These measurements of CO, NO, NO_x, THC, CH_4, and visibility at Williams Air Force Base, Arizona, from June 1976 to June 1977 were compared with AQAM predicted air pollution concentrations to determine AQAM's predictive power. The AQAM accuracy is analyzed on an hour-by-hour basis and statistical basis using accumulative frequency distribution. The conclusions are that AQAM accuracy is well within the accuracy range expected for Gaussian urban dispersion models. Even though

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SECURITY CLASSIFICATION OF THIS PAGE (When Data Entered) an attempt was made to select an isolated base from urban background emissions, the background concentration had to be accounted for in the analysis. Concentrations in the air base vicinity were extremely low when compared with background concentrations resulting from urban transport. Without the background concentration adjustments, the AQAM model tended to underpredict the pollutant concentrations. The results also indicate that AQAM is especially accurate in simulating the potential worst case airbase concentrations associated with morning hours, low wind speeds, stable atmospheric conditions, and high activity.

EXECUTIVE SUMMARY

Objectives

The U.S. Air Force must have an analytical tool which can reliably predict the impact of their airbases on air quality. Such a tool is essential for assessing the significance of existing airbase emissions in relation to National Ambient Air Quality Standards (NAAQS) and for estimating the impact of proposed facilities and missions changes as is required by federal, state and local laws. The Air Quality Assessment Model (AQAM), developed by ANL for the Air Force is such a tool that meets these air quality impact assessment requirements. The AQAM model treats airbase emissions in sufficiently great detail and incorporates a state-of-the-art treatment of pollutant transport and diffusion. However, until now, a suitable data base has not been available for determining the accuracy limits of this mathematical computer-based model.

Ambient air quality measurements of CO, NO, NO_x THC, and CH_4, and visibility were made at Williams AFB, near Phoenix from June 1976 to June 1977. The objectives were (1) to determine the effects of local aircraft operations on air quality and (2) to provide a data base for evaluation of AQAM. In this report model independent statistical analyses of the data and comparisons of AQAM predicted and observed concentrations are performed to determine the accuracy limits of AQAM.

Approach

The AQAM is designed to predict the impact of airbase operations, including aircraft, on the air quality in the vicinity of the airbase. It does not predict background concentrations as such. Hence, it is important from a model evaluation point of view that the influence of the local, modeled sources dominate the measured pollutant levels. Spatial and temporal dependences of these local sources must also be well described. These considerations played a significant role in the selection of Williams AFB as the site meeting these requirements for this model validation effort. Williams AFB had a high volume aircraft operations and is relatively remote from an urban area.

Thirteen months of hourly average concentrations of CO, NMHC, and NO_x monitored at the five-station network, shown in Fig. A, constitutes the data base used for assessing the predictive capabilities of AQAM. Parallel data bases of hour-by-hour meteorology and aircraft activity were utilized, in conjunction with the standard emissions inventory input to AQAM, to compute pollutant concentrations at the locations of interest. To define the incremental AQAM predictive power obtained through the use of higher time resolution aircraft data, AQAM predictions were made based on both the standard AQAM input of annual total aircraft operations (referred to as AQAM I predictions) and on the hour-by-hour aircraft operations mentioned above (referred to as AQAM II predictions).

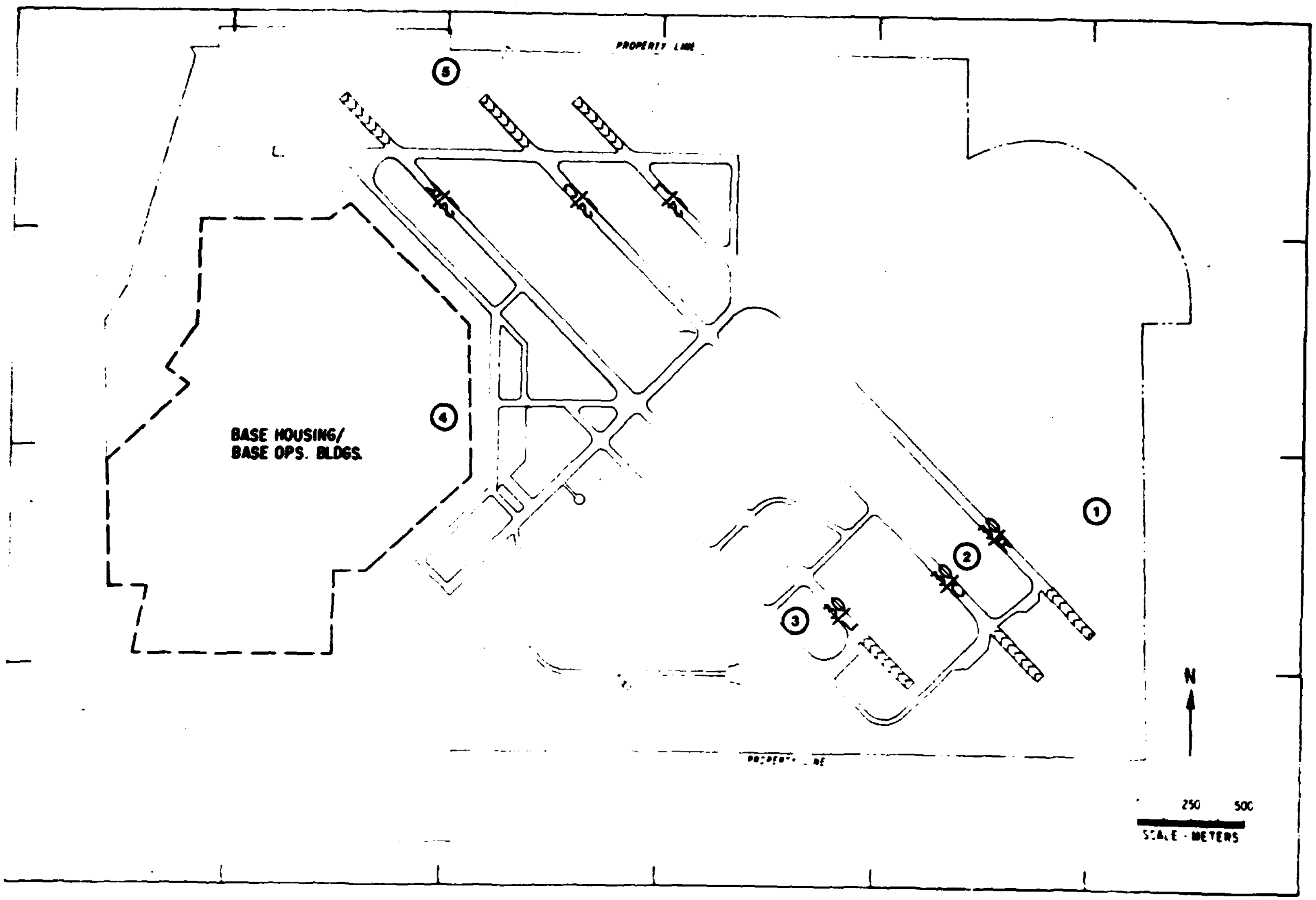

Fig. A. Locations of the Five Ambient Air Quality Monitoring Trailers

Impact of Aircraft on Local Air Quality

As seen in Table A, pollutant levels at several receptors are found to depend in a significant way on aircraft emissions though the average concentration impacts are small relative to the National Ambient Air Quality Standards (NAAQS). In all cases AQAM overpredicts the percentage role of aircraft emissions but much of this is simply due to the background levels not accounted for in AQAM. The fact that AQAM overpredicts the absolute role of aircraft at most stations is thought to be related to the model's neglect of plume rise and plume turbulence enhanced dispersion: two mechanisms which act to reduce concentrations nearby the aircraft. The largest observed average daytime impact of aircraft occurs at station 4 where, on the average, aircraft account for 36% of the CO, 28% of the NMHC and 24% of the NO_x.

Both AQAM predictions and measurements agree that station 4, atypical in the sense of its close proximity to buildings, trees, and automobiles, sees the highest concentrations: a factor of 2-3 higher than station 1, 2, 3, and 5 collectively in the cumulative frequency distribution (CFD) sense. The failure of the AQAM to correctly reproduce the observed rank ordering among stations 1, 2, 3, and 5 is also thought to be due to dynamical factors such as the neglect of aircraft plume rise (which clearly leads to overprediction of CO and NMHC at station 3). Finally, using the computed CFDs for off-base populated areas and allowing for possible underprediction by a factor of 2-3, one concludes that, with the exception of the 6-9 AM National ambient guideline concentration for reactive hydrocarbons, the airbase impact is negligible relative to existing NAAQS.

No significant difference in predictive power between the AQAM I and AQAM II has been found, thus extremely detailed time histories of aircraft operations do not have a significant effect on the model's accuracy (predictive power) and the standard AQAM input of an average diurnal distribution of aircraft operations appears adequate.

Performance of the Model

In the CFD sense, the AQAM predictions for the upper percentile concentration range agree reasonably well in magnitude and slope with the observed concentration distributions (sample case seen in Fig. B), suggesting that the model simulation encompasses a range of emission and dispersion conditions comparable with reality. At the lower concentration percentile levels, the CFDs are often orders-of-magnitude different, reflecting the problem of absence of background levels in the AQAM computations. CFD estimates of the 99.99 percentile concentrations (i.e., highest hourly average concentration per year) of $\approx$ 3 ppm CO, 1-3 ppm NMHC, and 0.1-0.3 ppm NO_x agree surprisingly well with observed values of 2-4 ppm CO, 1-3 ppm NMHC, and 0.08-0.15 ppm NO_x if stations 1, 2, 3, and 5 are considered collectively; however, such estimates for any single station may underpredict the once per year high by as much as a factor of 1.7 for CO and NMHC and 3 for NO_x. The fact that the CFDs of observed concentrations at the different stations converge at the upper percentiles while the individual station curves diverge

Table A. Williams AFB Aircraft Emissions Impact on Annual Average Hourly 6AM-6PM Concentrations

	Total Concentration (ppm)	Concentration Without Aircraft* (ppm)	Aircraft Contribution (ppm)	Percent Aircraft Contribution
		CO		
Station 1				
Observed	0.114	0.105	0.009	8
AQAM II	0.071	0.040	0.031	44
Station 2				
Observed	0.134	0.119	0.015	11
AQAM II	0.106	0.039	0.067	63
Station 3				
Observed	0.108	0.093	0.015	14
AQAM II	0.195	0.064	0.131	67
Station 4				
Observed	0.362	0.230	0.132	36
AQAM II	0.345	0.168	0.177	51
Station 5				
Observed	0.156	0.136	0.020	13
AQAM II	0.099	0.046	0.053	54
		NMHC		
Station 2				
Observed	0.123	0.128	-0.005→ consistent with zero	0
AQAM II	0.039	0.019	0.020	51
Station 4				
Observed	0.215	0.155	0.060	28
AQAM II	0.209	0.071	0.138	66
		NO_x (concentrations in ppb)		
Station 2				
Observed	9.44	8.98	0.46	5
AQAM II	3.68	2.15	1.53	42
Station 4				
Observed	15.1	11.5	3.6	24
AQAM II	8.4	6.6	1.8	41

*Based on regression of pollutant vs AQAM II estimated aircraft emissions on ground level line sources.

slightly for the AQAM predictions, suggests that the most severe pollution episodes actually exist over a spatial domain much larger than the airbase and thus are probably not solely due to specific local sources such as aircraft, as suggested by the model.

In examining the performance of AQAM on an hour-by-hour basis one encounters shortcomings common to Gaussian plume models in general. If no accounting of background pollutant levels is made, hour-by-hour comparisons of AQAM with observations indicate severe underprediction for all three pollutants (a mean factor of 3 for CO and NMHC and a factor of 5 for NO_x). In addition, the standard deviations of these distributions indicate that the unadjusted model falls short of the 50-percent within a factor-of-two criteria for Gaussian models. However, addition of a modest annual mean background (0.09 ppm for CO, 0.08 ppm for NMHC, and 7 ppb for NO_x) leads to a dramatic improvement in predictive power. The background adjusted model yields predictions with a factor-of-two of observation in excess of 65% of the time, while errors in excess of factor-of-ten occur at a tolerable ≈1% level. The reason such order of magnitude discrepancies exist lies with the fundamental limitations of modeling a stocastic process with a deterministic model.

Difficulties with the Theory Versus Observation Comparison

At the time the experiment was being planned (circa 1975), Williams AFB had the highest level of aircraft operations of any airbase in the U.S., and, as Williams is a training base, it was expected that records of aircraft activity would be more accurately maintained than at other bases. While accurate records were available during normal training operations periods, documentation of off-hours activity (e.g. weekends) was incomplete. In addition, as most of the operations involved small twin-engine aircraft (i.e., T37, T38, and F5), selection of the airbase having the highest traffic count was not necessarily compatible with a choice based on highest aircraft pollutant emissions.

It was also thought that the remoteness of the base from other significant sources would render the resolution of airbase and aircraft generated pollution from background levels straightforward. Unfortunately, Phoenix, though some 50 km to the Northwest, contributed high background levels to the measured air quality particularly at night. These so-called background levels often exceeded the local pollutant levels, resulting in a poor signal-to-noise ratio and greatly reducing the effectiveness of the receptor network in sensing local source (i.e., airbase) created pollutant gradients. In addition, the entire Valley of the Sun appears at times to exhibit pollution reservoir characteristics which can not be predicted by a short-range Gaussian plume model such as AQAM. Even the several hour transport and dispersion of pollutant from Phoenix, though included in the AQAM inventory of environ sources, is not adequately treated due to total reliance on the stationary state assumption. Such multihour transport could have been more realistically modeled using a backward trajectory technique, which would select the emission rate for the time period presently impacting the receptors and allow for varying dispersion rates over the trajectory of the plume, but such is not the case in the present AQAM, designed for short-range pollutant

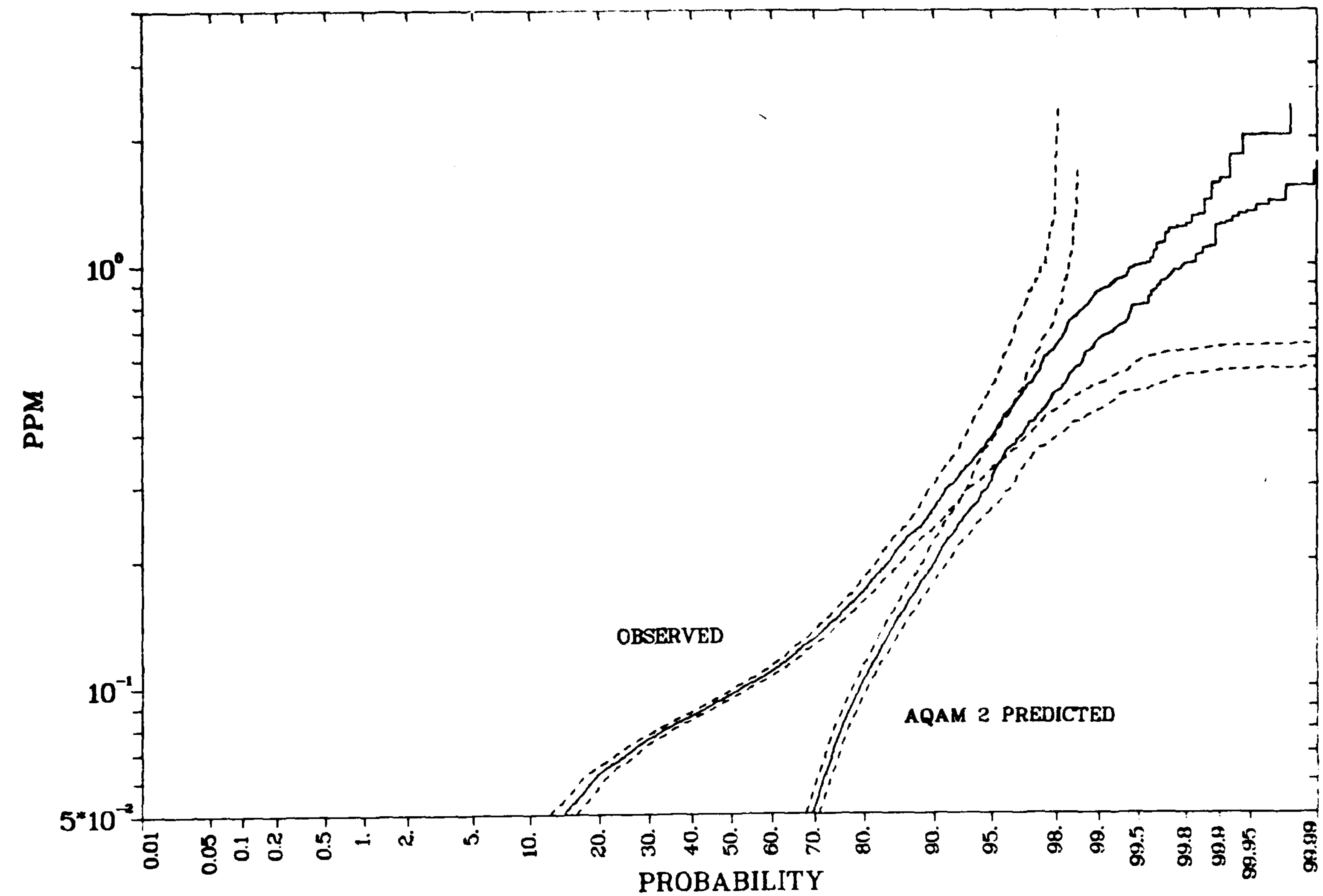

Fig. B. Cumulative Frequency Distribution for Observed and AQAM II Predicted CO at Station 1 -- 95% Confidence Bounds are Indicated transport and dispersion calculations. Thus, it was necessary to attempt to validate the model under conditions where a major portion of the aerometric signal was related to distant, background sources not adequately treated by the model. The presence of five monitors on the base could have been useful in subtracting out these unwanted and poorly described components of the observed concentrations. However, two factors limited the effectiveness of this latter approach to investigating the local (i.e., airbase) contribution to the observed pollutant levels. First, noise in the form of spatial inhomogeneities of the background and, second, inter-instrument random and systematic errors which tended to wash out many of the more subtle effects since local signal components were often small compared to the accuracy limits of the instruments.

All of the studies of model predictive power versus meteorological parameters or time of day suggest that time of day is the most significant variable affecting AQAM performance in that AQAM reproduces the major trends in daytime observed concentrations when local sources dominate but seriously underpredicts at night when more distant sources contribute. This deficiency is probably due to an underestimate of vehicle activity between midnight and 5 a.m. and to a breakdown of the steady-state Gaussian plume assumption used in the model. Major revision of the model to incorporate backward trajectories would probably be required to rectify this latter problem; however, such a revision is perhaps of only academic interest at present since the AQAM is most successful in simulating the potential "worst case" airbase impact situations associated with morning, low wind speed, stable or low inversion height conditions coincident with the commencement of high airbase emissions.

Conclusions

In final summary, we note the major findings of this study as

- the upper concentration-percentile range of the CFD of AQAM predictions agrees well enough with observation to make this a valuable tool for predicting rare worst case situations. As at William AFB, the estimate of worst case (e.g., highest hourly per annum) concentrations at a particular station may be underpredicted by a factor of two or three so that complementary monitoring (for perhaps a few hundred hours) should be performed in questionable situations when concentrations approach 50% of NAAQS.

- the AQAM, adjusted for background levels, provides a predictive tool for hourly average concentrations commensurate in ability (i.e., greater than 50% of predictions within a factor of two of observed concentrations) with well calibrated Gaussian plume models applied to urban areas.

- Without adjustment for background levels, most AQAM results underpredict by more than a factor of two and often by as much as 10 to 100. Without background compensation, AQAM results should be interpreted with caution. Air quality monitoring data sampled in the Air Quality Control Region should be considered when analyzing AQAM results.

- The present AQAM, unadjusted for jet plume rise or other jet plume dynamical factors, tends to overpredict the near field air quality impact of aircraft. Studies at commercial airports suggest that this overprediction becomes negligible beyond a few hundred meters from the aircraft.

- The highest predicted, average hourly aircraft impact of 0.18 ppm CO (51% of total CO) at station 4 only slightly overpredicts the observed impact of 0.13 ppm CO (36% of total CO). [Special instances do exist, however, where aircraft contribute nearly 100% of observed and predicted concentrations.]

- The ability of the AQAM to accurately predict inter-station concentration differences is only weakly confirmed because of large measurement errors relative to these observed concentration differences and because of the unexpectedly high background concentrations.

- The AQAM could benefit from minor revisions such as the incorporation of jet plume rise and turbulence enhanced dispersion and from major revisions such as a backward trajectory calculation for more realistic assessment of the impact from distant sources.

- AQAM is ready for acceptance under EPA Guidelines on Air Quality Modeling.

PREFACE

This final report was prepared by the Energy and Environmental Systems Division of Argonne National Laboratory (ANL) under contract to USAF Engineering and Services Center, Tyndall AFB, Florida. The work was accomplished under Job Order Number 19009004. Lt Col Peter A. Crowley, Majors Dennis F. Naugle and Joseph B. Hooten, and Capt Harold A. Scott were the Air Force project officers.

Contributions were made by many others including Mr Edward P. Durphy, while at the University of New Mexico, Civil Engineering Research Facility (CERF) and subsequently as a statistical consultant to ANL, and Mr Karl F. Zeller, while EPA project officer.

Northrop Environmental Services provided the ambient measurement data used throughout this report.

The authors are also grateful to the following people for their technical assistance: Mr John Connolly, EPA/EMSL; Lt Blair Thisted, USAF; Ms Polly Brown, ANL; Ms Lyn Deacon, ANL; Dr Kenneth Brubaker, ANL; and Mr Simon Bremer, ANL.

A special thanks is given to Ms Louise Benson, Ms Patricia Traczyk, Ms Sally Vargo, and Ms Linda Wulf for typing this and the numerous draft manuscripts.

This report has been reviewed by the Public Affairs Office and is releasable to the National Technical Information Service (NTIS). At NTIS it will be available to the general public and foreign nationals.

This report has been reviewed and is approved for publication.

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LIST OF SYMBOLS

B, C_B	background concentration as defined in text.
C_{oi}, C_{Mi}	observed (i.e., measured) hourly pollutant concentration at the ith station.
C_{Ti}	AQAM predicted hourly concentration at the ith station.
C_O, C_M	observed station averaged, hourly pollutant concentration.
C_T	AQAM predicted, station averaged, hourly pollutant concentration.
q_α	r.m.s. fractional deviation of the subscripted quantities α as defined in the text.
σ	standard deviation.
σ_θ	standard deviation of wind direction about the hourly mean value r.
θ	wind direction
μ	wind speed

SECTION I

INTRODUCTION

A. Motivation

The U.S. Air Force is greatly interested in having an analytical tool which can reliably predict the impact of their airbases on air quality. Such a tool is essential for assessing the significance of existing airbase emissions in relation to National Ambient Air Quality Standards (NAAQS), as well as estimating the impact of proposed facilities as is required in Environmental Impact Statements. The Air Quality Assessment Model (AQAM), developed by ANL for the Air Force, is potentially such a tool in that it treats airbase emissions in sufficiently great detail and incorporates a state of the art treatment of pollutant transport and diffusion. However, until now, a suitable data base has not been available for determining the limits of accuracy of this mathematical computer based model.

B. Rationale

Two basic reasons emerge for wanting to evaluate the accuracy of AQAM under normal airbase operating conditions. The first is the potential for determining the adequacy of the dispersion mechanisms; not from the point of view of the correctness of the atmospheric physics therein but rather on the basis of overall predictive accuracy. Though one may argue that this question might be attacked more directly through tracer experiments, one can envision situations where air quality predictions for an airbase, with its spatially and temporally complex source inventory, might be made with either greater or lesser confidence than one has in the more fundamental tracer results. The second reason is to determine the degree of detail (and thus expense) required in the emissions inventory to achieve a specified predictive accuracy with the model. Thus, one is strongly motivated to evaluate the accuracy and utility of this potentially useful assessment tool in the context of its intended application; that is, at an airbase.

C. The Williams AFB Air Monitoring Experiment

Williams AFB (WAFB) was selected as the site for the experiment intended to provide the database for evaluating AQAM. The reasons for selecting Williams AFB included:

1) high volume of aircraft activity (though the aircraft are small twin-engine trainers, the number of operations make Williams one of the busiest airports in the world).

2) accurate records of aircraft activity (WAFB is a training base and as a result careful records are kept of scheduled flight operations, deviations from planned operations, as well as transient aircraft operations.

3) distance from other major sources, (WAFB is surrounded by farmland for a 15 mile or greater distance and this simplifies, but does not eliminate, the problem of background pollutant level determination).

4) the wide variety of meteorological conditions encountered in the desert environment.

An extensive review of all ambient measurements obtained during the thirteen month experiment is given in Reference 1. Therefore, only a brief summary, including a monitoring site map, station siting rationale, a monitoring station description, and data acquisition and reduction procedures, is given in Appendix A of this report. In addition, Appendix A also contains frequency distributions, statistical summaries, and cumulative frequency distributions of the hourly average, aerometric, and meteorolgical quantities measured by the EPA/EMSL during the thirteen month Williams AFB experiment. Table 1 gives a statistical summary of the aerometric quantities for the thirteen month monitoring experiment.

D. AQAM/Analysis Data Flow

Figure 1 shows the steps involved in the production of final AQAM data analysis tape (DS V) which then serves as input to all analysis programs.

It can be seen that the base meterological data, which was prepared by ETAC/USAF, has been augmented with the acoustic sounder codes supplied by EPA/NORTHROP. The resulting data set (DS IIIb) served as input to FORTRAN coded computer programs formulated to compute the theoretical lid heights, decode the acoustic sounder data (observed lid height), and determine the stability class indices. Operating in parallel was a FORTRAN program that reduced the individual aircraft event times (i.e., takeoff time, landing time, etc. from DS II) into tallies of hourly aircraft activity.

The production of DS IV, to be submitted to the National Technical Information Service (NTIS), involved the mergence of the observed air quality data base (DS IIIa), the observed meteorology (DS IIIb) along with the computed atmospheric parameters, and the observed aircraft activity. This composite hourly data set was then used along with the source emissions inventory (DS I) as input to the AQAM. The analysis tape (DS V) contains the results of these AQAM calculations in addition to the contents of DS IV.

The entire thirteen months of hourly data have been processed in this manner and serve as the basis for the analyses in this report. A detailed description of the approximately 600-word DS V record structure will be given in a later technical report.

E. AQAM Calculations

Before consideration of the comparisons between AQAM predictions and observed concentrations, it is worthwhile to consider the assumptions used in AQAM and the differences between the AQAM I and AQAM II models.

Table 1. Williams Air Force Base Aerometric Data Summary for the Period June 1, 1976 to June 30, 1977. Concentrations are in ppm for all gaseous pollutants and in units of $10^{-4} m^{-1}$ for b_{SCAT}.

	NITRIC OXIDE (NO)	NITROGEN DIOXIDE (NO2)	OXIDES OF NITROGEN (NOX)	METHANE (CH4)	TOTAL HYDROCARBON (THC)	NONMETHANE HYDROCARBON (NMHC)	CARBON MONOXIDE (CO)	NEPHELOMETER READING (BSCAT)
STATION NUMBER ... 1								
NO. VALUES	6197	6125	6378	4568	5022	4537	5055	6293
ARITHMETIC MEAN	2.5000E-03	7.3019E-03	1.0[illegible]E-02	1.6921E+00	1.6360E+00	6.4124E-02	1.3[illegible]E-01	5.4[illegible]E-01
STD. ARITH. DEVIATION	3.3112E-03	8.0000E-03	1.0179E-02	1.4106E-01	2.0730E-01	9.8957E-02	1.5310E-01	3.8313E-01
GEOMETRIC MEAN	1.2211E-03	5.0300E-03	7.3036E-03	1.5973E+00	1.6260E+00	4.0100E-02	1.0211E-01	4.5135E-01
STD. GEOM. DEVIATION	2.5437E+00	2.5134E+00	2.2224E+00	1.0[illegible]E+00	1.1201E+00	3.1000E+00	2.1090E+00	1.8832E+00
MINIMUM VALUE	-1.0100E-02	-2.0000E-02	-4.5000E-03	1.2[illegible]E+00	1.2035E+00	-1.7630E-01	0.0	0.0
MEDIAN VALUE	1.9000E-03	5.3000E-03	7.6000E-03	1.6147E+00	1.6510E+00	4.0700E-02	9.6100E-02	4.6310E-01
MAXIMUM VALUE	6.0100E-02	9.5600E-02	2.6670E-01	3.3307E+00	4.4430E+00	1.5343E+00	2.3014E+00	6.0130E+00
STATION NUMBER ... 2								
NO. VALUES	7371	7324	7411	7003	6312	6019	6994	7621
ARITHMETIC MEAN	2.8054E-03	8.7350E-03	1.1737E-02	1.6231E+00	1.6906E+00	7.6546E-02	1.6733E-01	5.8640E-01
STD. ARITH. DEVIATION	3.3039E-03	8.9235E-03	1.0659E-02	1.1703E-01	2.0976E-01	1.3049E-01	1.6151E-01	4.5142E-01
GEOMETRIC MEAN	2.5223E-03	5.8491E-03	9.0031E-03	1.6210E+00	1.6003E+00	5.4552E-02	1.2940E-01	4.6540E-01
STD. GEOM. DEVIATION	2.0564E+00	2.6405E+00	2.0700E+00	1.0727E+00	1.1[illegible]E+00	3.7410E+00	2.0114E+00	2.0223E+00
MINIMUM VALUE	-1.0500E-02	-1.1500E-02	-8.0000E-03	1.2271E+00	1.2797E+00	-2.0000E-01	0.0	0.0
MEDIAN VALUE	2.6000E-03	6.3000E-03	9.0000E-03	1.6034E+00	1.7016E+00	7.9500E-02	1.2195E-01	4.9200E-01
MAXIMUM VALUE	6.5400E-02	9.7700E-02	2.9150E-01	3.1203E+00	4.3471E+00	1.3517E+00	3.8692E+00	7.4879E+00
STATION NUMBER ... 3								
NO. VALUES	7292	7243	7256	7212	7167	7005	6614	7315
ARITHMETIC MEAN	2.4443E-03	1.0057E-02	1.2650E-02	1.5074E+00	1.6693E+00	8.2376E-02	1.2940E-01	5.8[illegible]E-01
STD. ARITH. DEVIATION	2.9253E-03	9.6327E-03	1.1669E-02	1.2031E-01	1.8937E-01	1.1379E-01	1.5327E-01	3.37[illegible]E-01
GEOMETRIC MEAN	2.0346E-03	7.3715E-03	9.6375E-03	1.5914E+00	1.6613E+00	4.9672E-02	8.8570E-02	5.0103E-01
STD. GEOM. DEVIATION	2.2409E+00	2.2350E+00	2.0021E+00	1.0721E+00	1.0923E+00	3.3357E+00	2.2770E+00	1.7812E+00
MINIMUM VALUE	-6.2000E-03	-1.3200E-02	-9.7000E-03	1.3061E+00	1.3043E+00	-1.0310E-01	0.0	0.0
MEDIAN VALUE	2.0000E-03	7.3000E-03	9.3000E-03	1.5006E+00	1.6367E+00	6.4300E-02	8.3600E-02	5.1120E-01
MAXIMUM VALUE	5.3000E-02	1.1360E-01	2.4120E-01	3.7740E+00	5.1778E+00	3.5704E+00	3.6703E+00	5.9621E+00
STATION NUMBER ... 4								
NO. VALUES	6762	6262	6331	6768	6739	6697	6595	6935
ARITHMETIC MEAN	5.2055E-03	1.2350E-02	1.7227E-02	1.6713E+00	1.8927E+00	1.9[illegible]E-01	3.5033E-01	5.7123E-01
STD. ARITH. DEVIATION	7.4459E-03	1.2745E-02	1.62[illegible]E-02	1.9710E-01	3.5371E-01	2.3260E-01	3.6460E-01	4.1361E-01
GEOMETRIC MEAN	3.4074E-03	8.5994E-03	1.2295E-02	1.6633E+00	1.8300E+00	1.1[illegible]E-01	2.02[illegible]E-01	4.6559E-01
STD. GEOM. DEVIATION	2.7377E+00	2.6060E+00	2.4000E+00	1.103[illegible]E+00	1.1677E+00	3.5[illegible]E+00	3.5033E+00	1.9049E+00
MINIMUM VALUE	-9.2000E-03	-1.8000E-02	-1.7[illegible]E-02	1.3151E+00	1.3364E+00	-1.9630E-01	0.0	0.0
MEDIAN VALUE	3.3000E-03	9.3000E-03	1.3[illegible]E-02	1.6227E+00	1.7754E+00	1.5120E-01	2.4290E-01	4.7550E-01
MAXIMUM VALUE	9.6900E-02	1.5020E-01	1.5[illegible]E-01	4.2962E+00	7.1507E+00	4.9516E+00	3.9774E+00	5.7665E+00
STATION NUMBER ... 5								
NO. VALUES	6416	6403	6570	6939	6951	6797	7020	7215
ARITHMETIC MEAN	3.2124E-03	8.1537E-03	1.1236E-02	1.6573E+00	1.7223E+00	6.4537E-02	1.9907E-01	5.6312E-01
STD. ARITH. DEVIATION	3.9133E-03	1.0[illegible]E-02	1.1369E-02	1.4921E-01	2.1953E-01	1.1[illegible]E-01	1.9[illegible]E-01	3.9305E-01
GEOMETRIC MEAN	2.5619E-03	5.3[illegible]E-03	7.0[illegible]E-03	1.6335E+00	1.7107E+00	4.4[illegible]E-02	1.5002E-01	4.6717E-01
STD. GEOM. DEVIATION	2.3029E+00	2.7174E+00	2.[illegible]E+00	1.07[illegible]E+00	1.1137E+00	3.1[illegible]E+00	2.0[illegible]E+00	1.9030E+00
MINIMUM VALUE	-1.0000E-02	-1.8600E-02	-5.4000E-03	1.3619E+00	1.30[illegible]E+00	-1.9[illegible]E-01	0.0	0.0
MEDIAN VALUE	2.4000E-03	5.5000E-03	[illegible]	1.62[illegible]E+00	1.6[illegible]E+00	5.8[illegible]E-02	1.3320E-01	4.7[illegible]E-01
MAXIMUM VALUE	6.4000E-02	1.0320E-01	1.1119E-01	3.[illegible]E+00	6.3740E+00	3.6[illegible]E+00	2.17[illegible]E+00	4.7253E+00

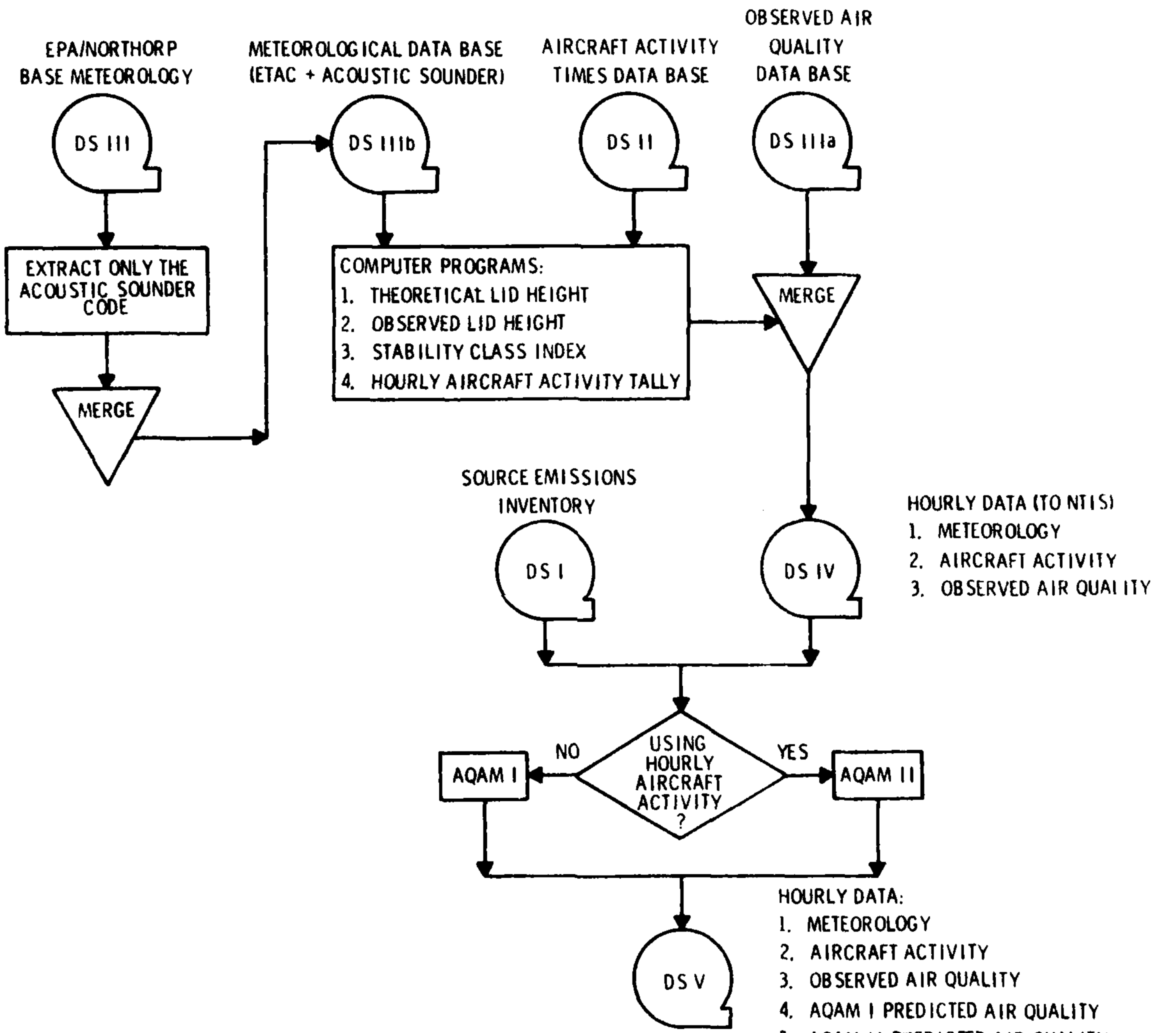


Fig. 1. AQAM/Analysis Data Flow

AQAM[2] is a Gaussian plume type model which utilizes the dispersion curves given in Turner's Workbook.[3] Stability class is determined on the basis of solar angle, ETAC determined cloud cover and ceiling height, and surface wind speed, and the method of determination and approximations used are discussed in Appendix B. AQAM also requires input of the mixing depth and the Air Force requires that any such mixing depth determination be based on readily obtainable ETAC meteorological data. This constraint at Williams AFB required the development of a mixing depth algorithm based solely on surface observations. This algorithm, based primarily on surface temperature trends but also somewhat dependent on solar angle and wind speed, is given in Appendix B and compared with approximately 1000 acoustic sounder determinations of mixing depth.

AQAM also requires a detailed emissions inventory, certain facets of which are discussed in Appendix C. Usually, aircraft emissions in any given hour are based on total annual aircraft emissions and some simple approximation regarding the time dependence of aircraft operations at the base. In the AQAM I, it is assumed that aircraft operate Monday thru Friday from 0600 to 1800 at a constant activity rate with zero activity at other times. This assumption is sufficient to specify aircraft emissions. However, in the AQAM II, use is made of the detailed, minute-by-minute tally of aircraft operations at Williams AFB during the thirteen month air quality monitoring program. This data base is described in Appendix D, but from the wide variability of CO emission rates (for aircraft ground level lines only) seen in Figure 2, it would appear that the simple assumption of constant (i.e., either on or off) aircraft activity might be a gross oversimplification. However, examination of the actual time dependence of this emission rate (Figure 3) indicates that the simple AQAM I approximation of 80 gms CO/sec between 0600 and 1800 may not be unreasonable on the average during much of the day though AQAM I clearly overestimates emissions during the initial startup of airbase activities (0600-0800) and during late afternoon (1400-1800), while totally ignoring evening emissions (1800-2400) associated with night training operations.

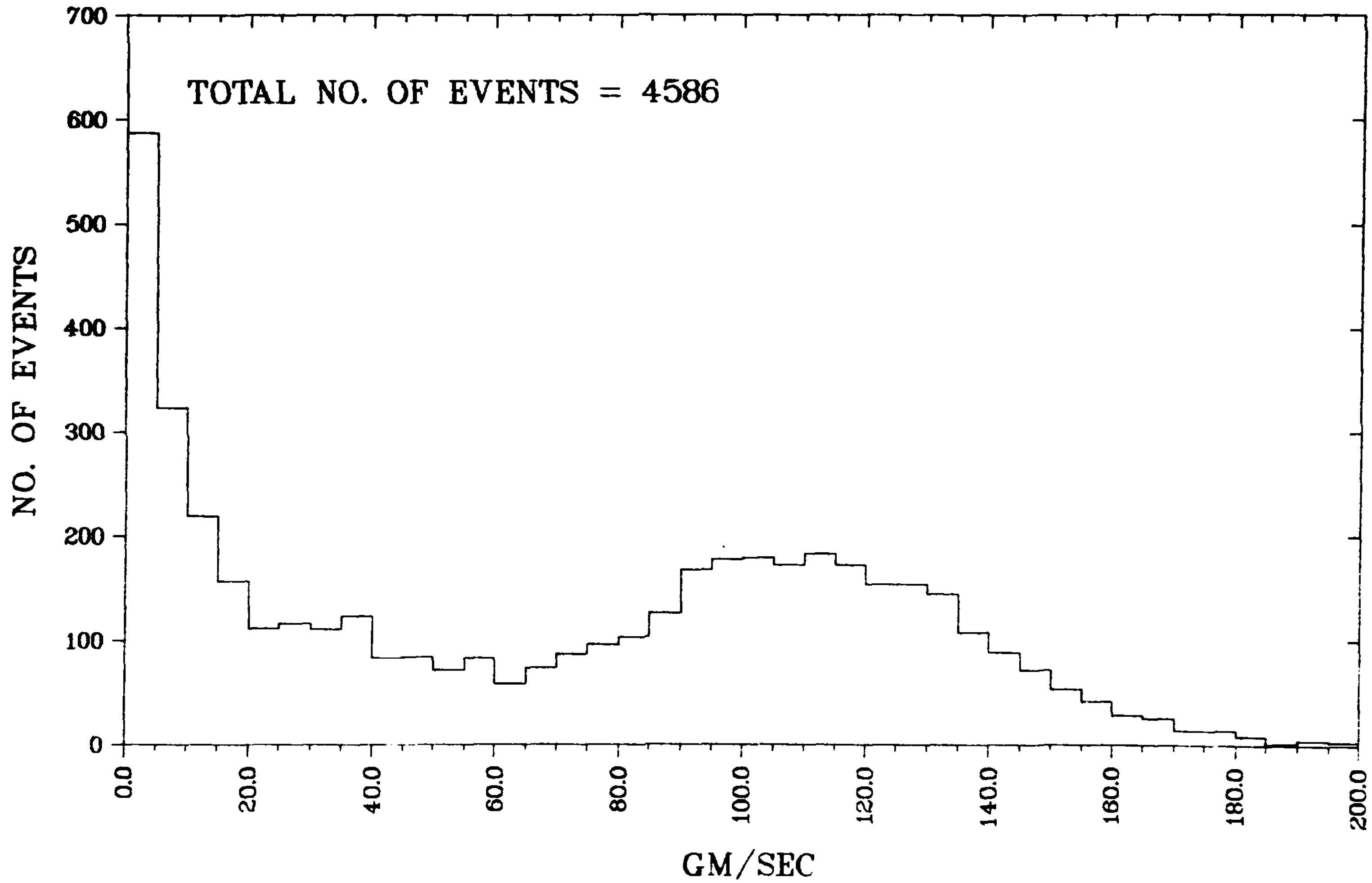


Fig. 2. Frequency Distribution of Non-Zero, Ground-Level Line, Aircraft Emission Rates Based on Hourly Aircraft Operations

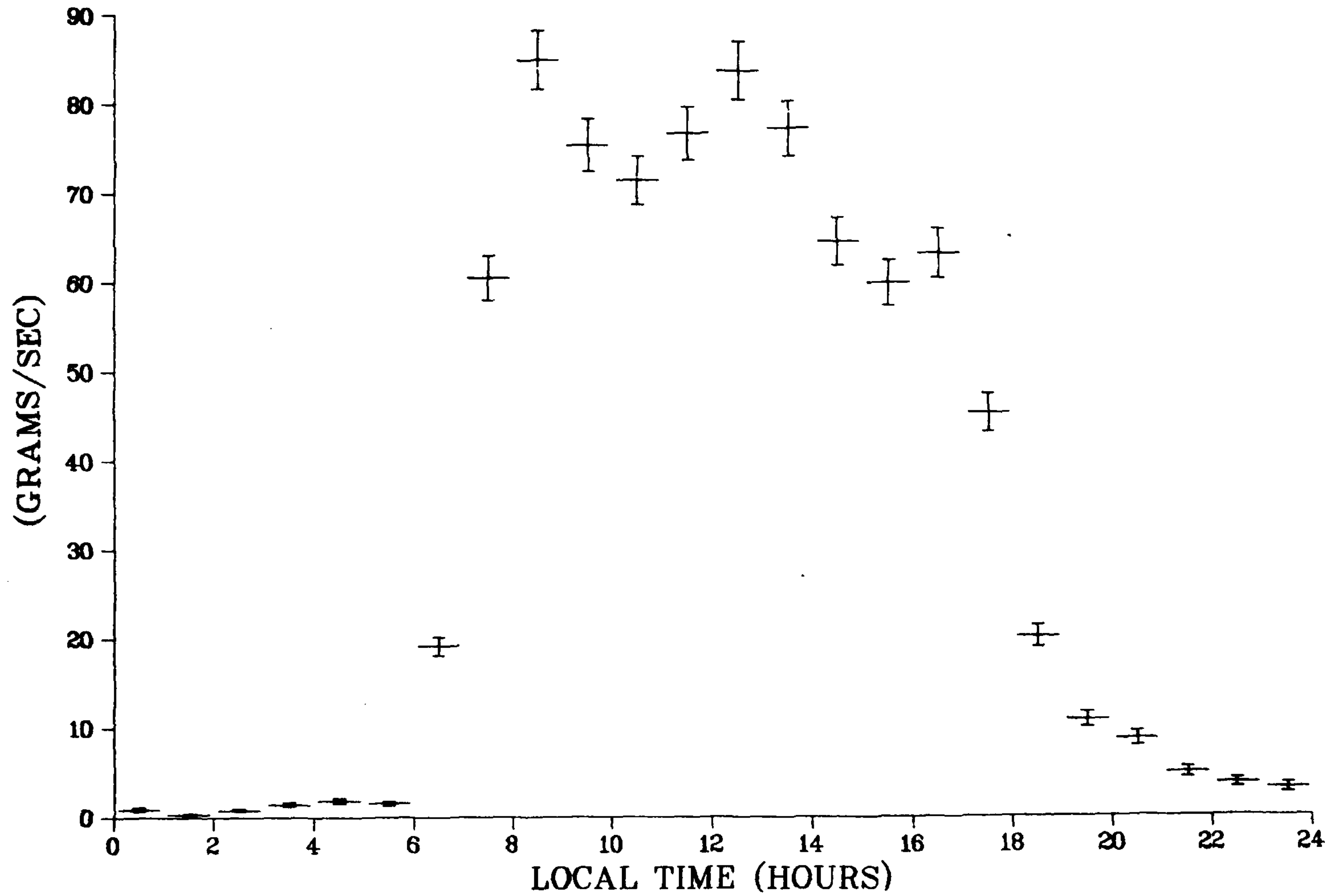


Fig. 3. AQAM II Assumed Aircraft CO Emission Rate on Ground-Level Lines vs Time of Day. AQAM I Assumes a Constant Value of 80 gms CO/sec Between 0600 and 1800 hrs

SECTION II

OVERALL AQAM ACCURACY DEFINITION

A. Statistical Measures

The question of assessing a model's overall accuracy can and has been addressed in a number of ways, such as:

1. Cumulative Frequency Distributions (i.e., the percentage of the time a given hourly concentration is exceeded.) These are given for each of the observed pollutants at each station in Appenix A, and again in Appendix G for CO, NO_x, and NMHC along with the theoretical predictions of AQAM I and AQAM II. One observed close correspondence of the AQAM I and II distributions and rather good agreement with observations particularly in the region of greatest interest, the upper percentiles of the cumulative frequency distribution (CFD). The goodness of agreement between theory and experiment should be judged relative to the distribution-free, Kolmogorov-Smirnov bounds (95% bounds are indicated in Appendix G) around the observation CFD.

   Figures 4 and 5 show the CFD's for (a) CO, (b) NMHC, and (c) NO_x at each station for observation and AQAM II prediction, respectively. Comparison of these two sets of figures indicate that AQAM correctly predicted station 4 to have the highest concentrations of each pollutant and stations 1, 2, 3, and 5 to be closely grouped. The only clear failing is the overprediction of CO and NMHC at station 3 (alongside the main taxiway) probably due to a failure to incorporate jet plume rise into AQAM. The somewhat flatter slopes of the observed CFDs is due, at least in part, to the presence of backgrounds not included in AQAM.

   Finally, we note that the observed convergence of the observed CFDs at the highest concentrations suggest that the highest pollution episodes might be associated with area wide phenomena rather than local emissions as suggested by diverging CFDs for AQAM II predicted CO and NMHC.

   Figures 6-7 show just how dramatic a difference an assumed background can make on the inference one draws from a CFD. In Figure 6, no CO background is assumed, and the observations lie above the predictions. In Figure 7, the minimum one-minute reading within each hour is taken as background and subtracted from the hourly concentration. The effect of such a background subtraction is to cause the curves to cross over for all concentrations above the ∿50 ppb measurement threshold.

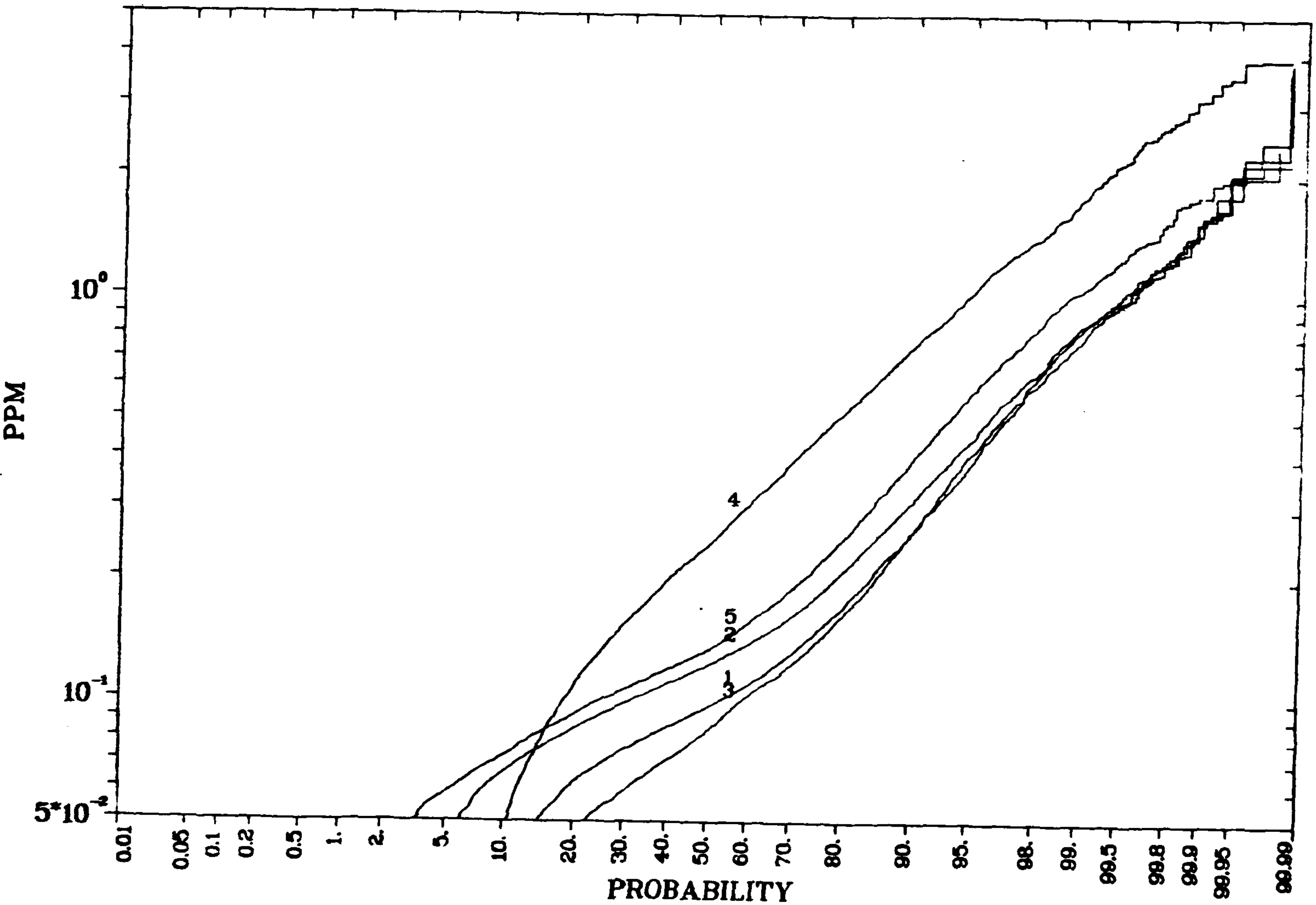


Fig. 4a. Cumulative Frequency Distribution for Hourly Observed CO Concentrations at each Station

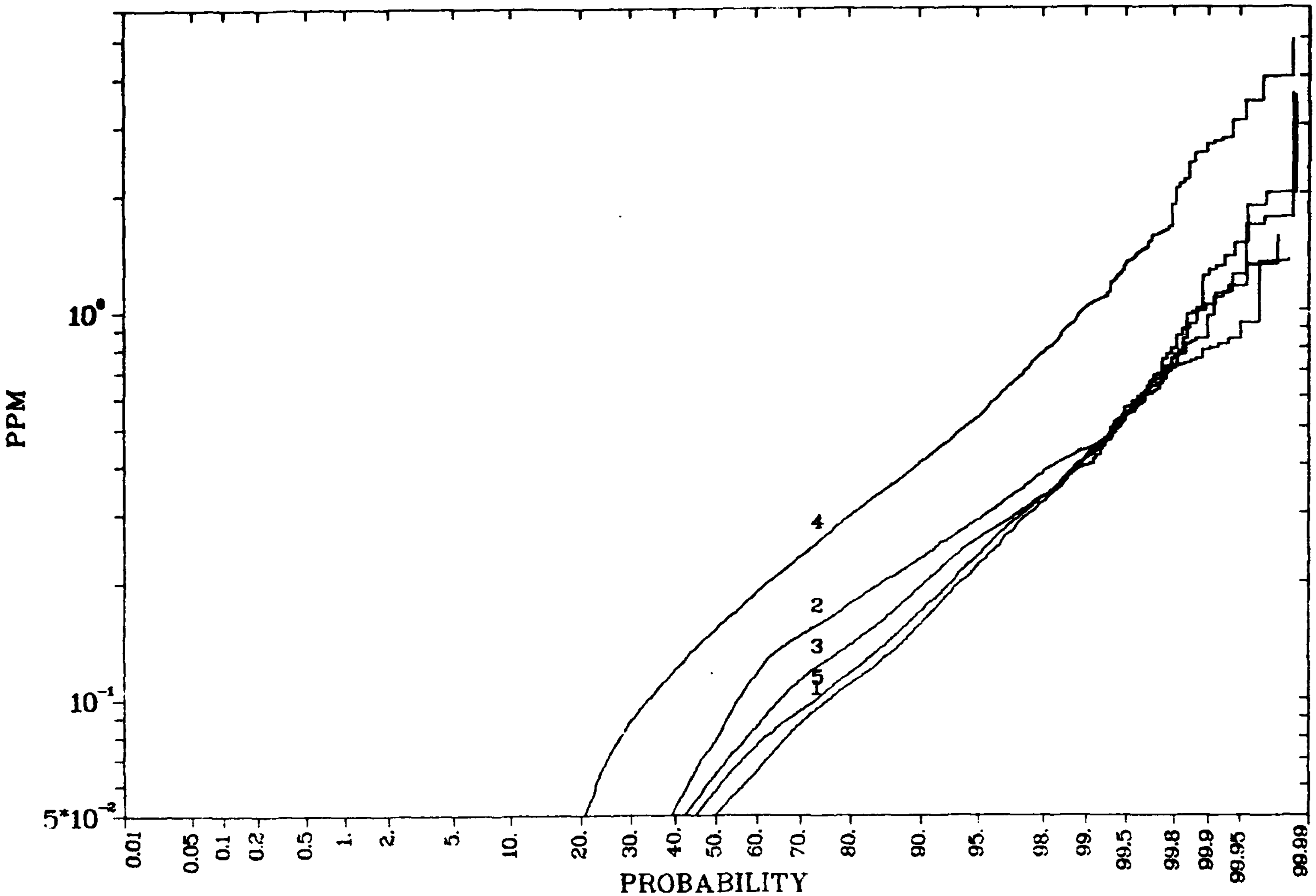


Fig. 4b. Cumulative Frequency Distribution for Hourly Observed NMHC Concentrations at each Station

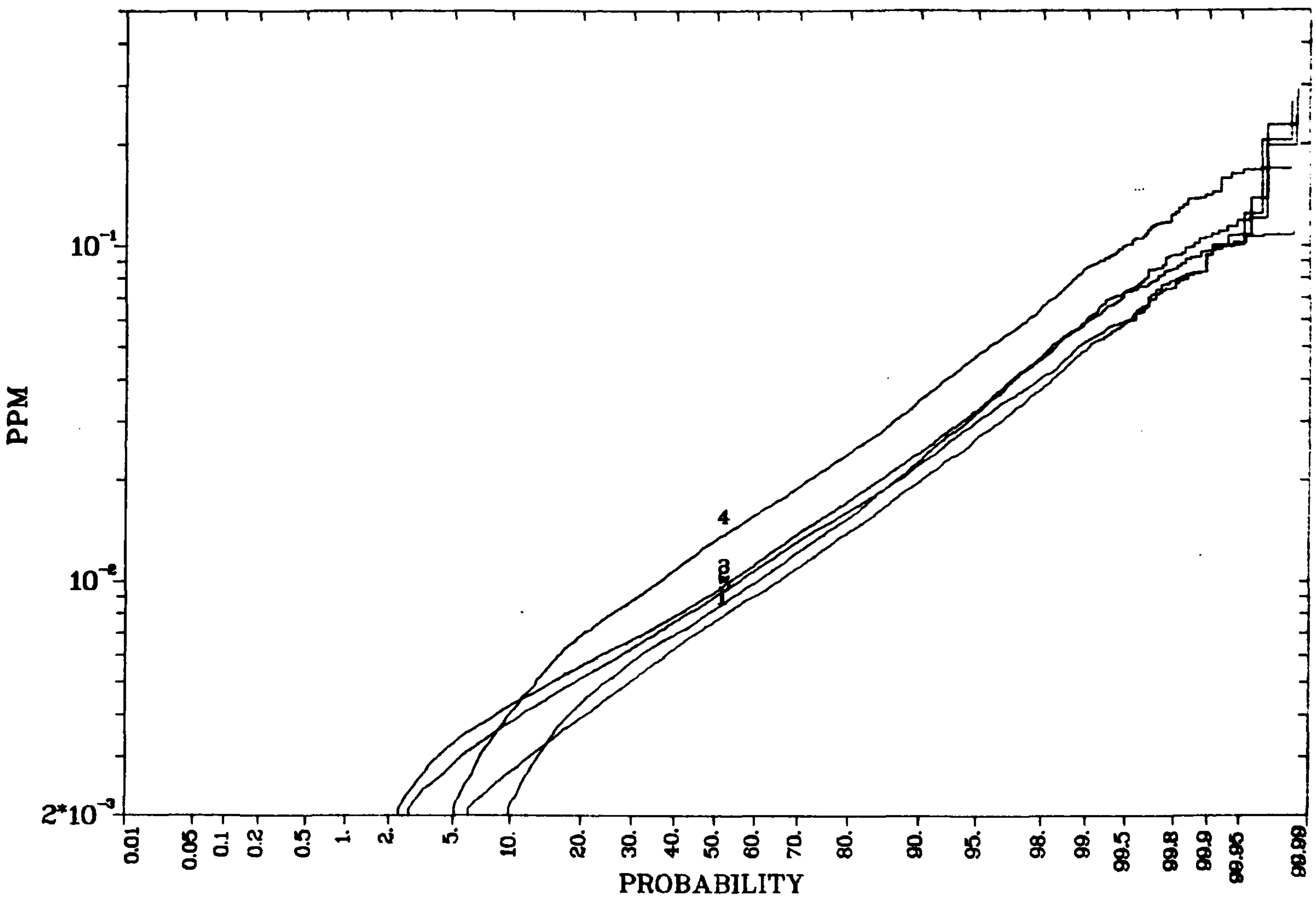


Fig. 4c. Cumulative Frequency Distribution for Hourly Observed NO_x Concentrations at each Station

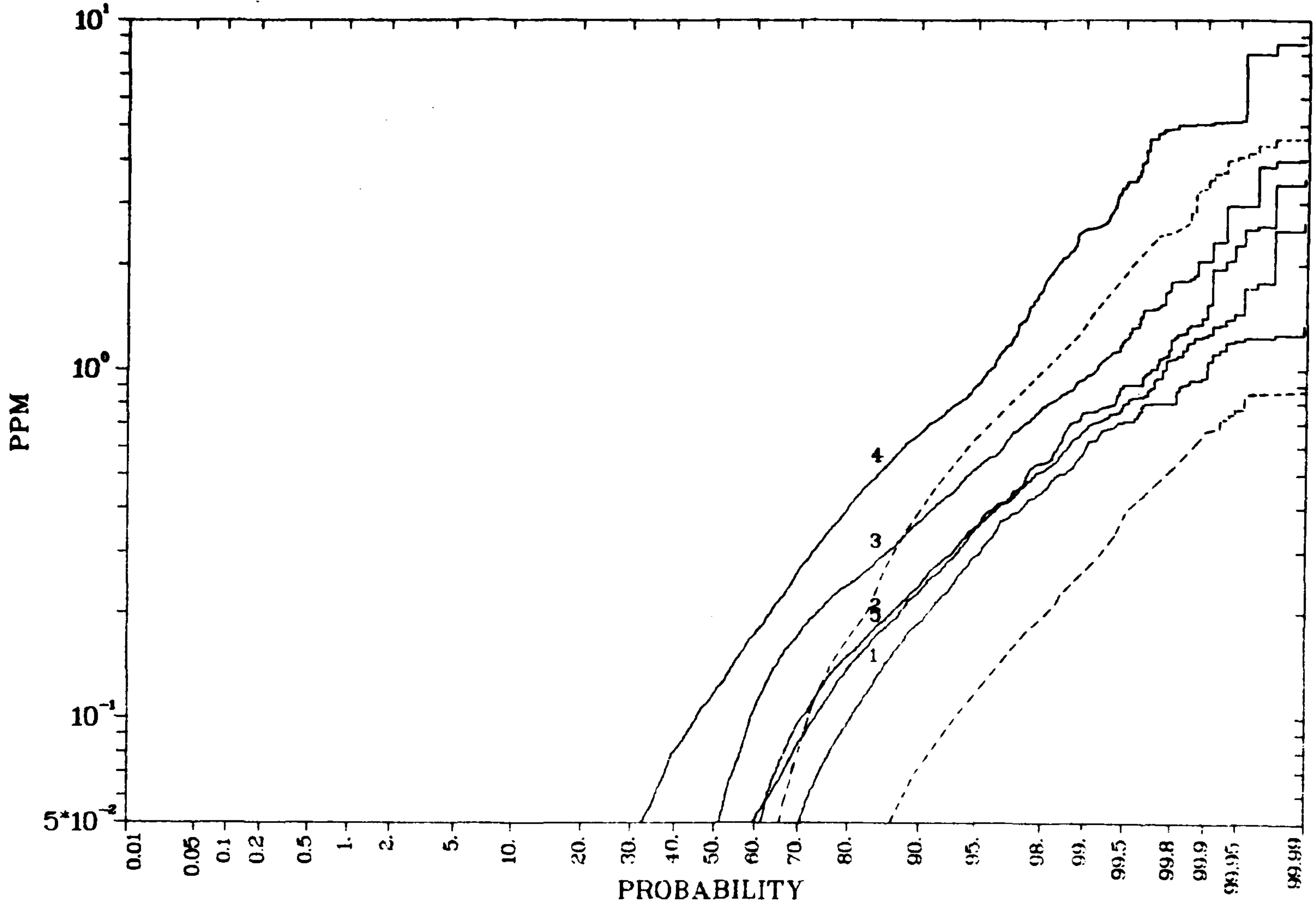


Fig. 5a. Cumulative Frequency Distribution for Hourly AQAM II Predicted CO Concentrations at each Station. Dotted lines indicate the range of aircraft contribution with the upper curve generally representing station 4 and the lower curve station 1

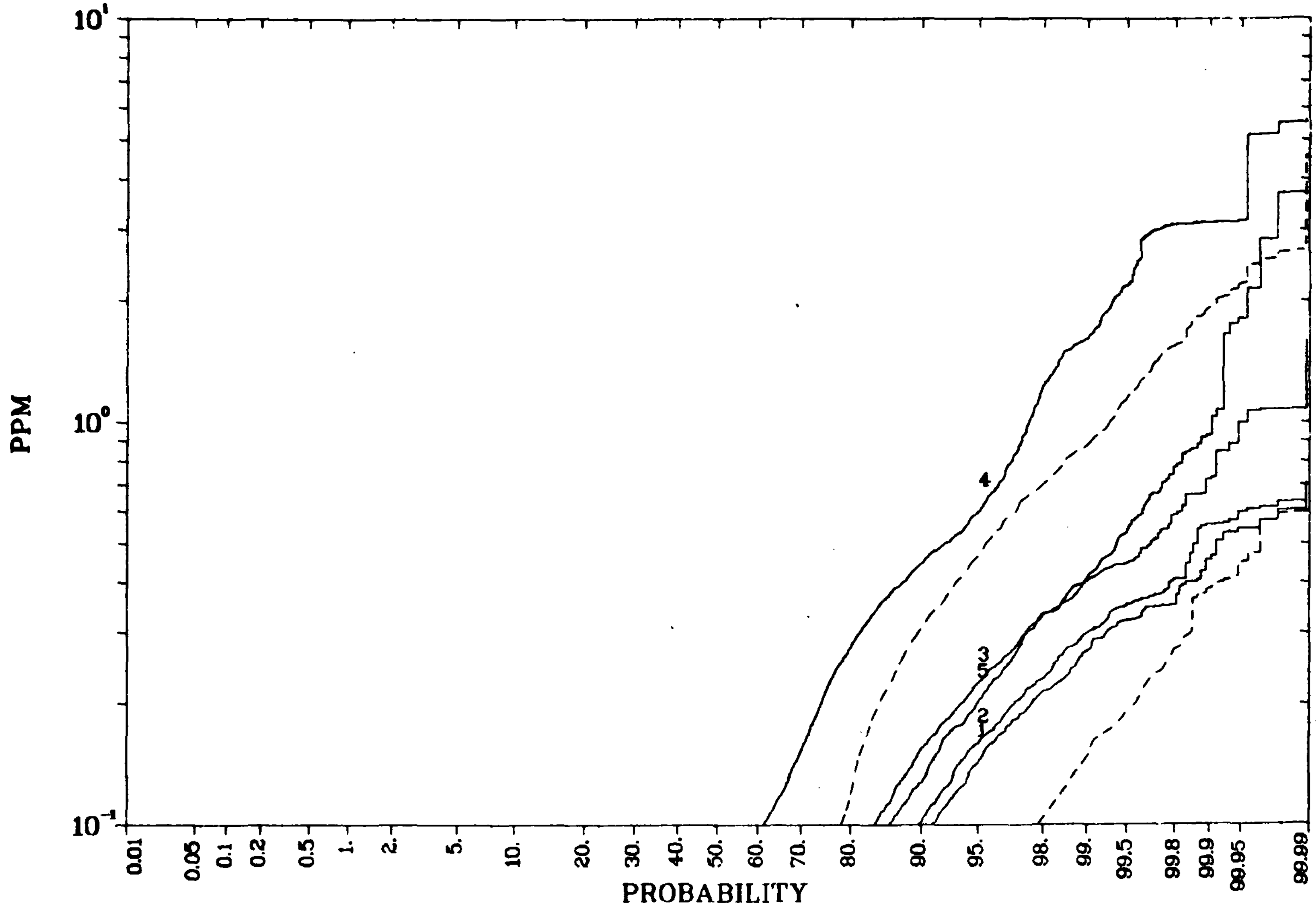


Fig. 5b. Cumulative Frequency Distribution for Hourly AQAM II Predicted TCH Concentrations at each Station. Dotted lines indicate the range of aircraft contribution with the upper curve generally representing station 4 and the lower curve station 1

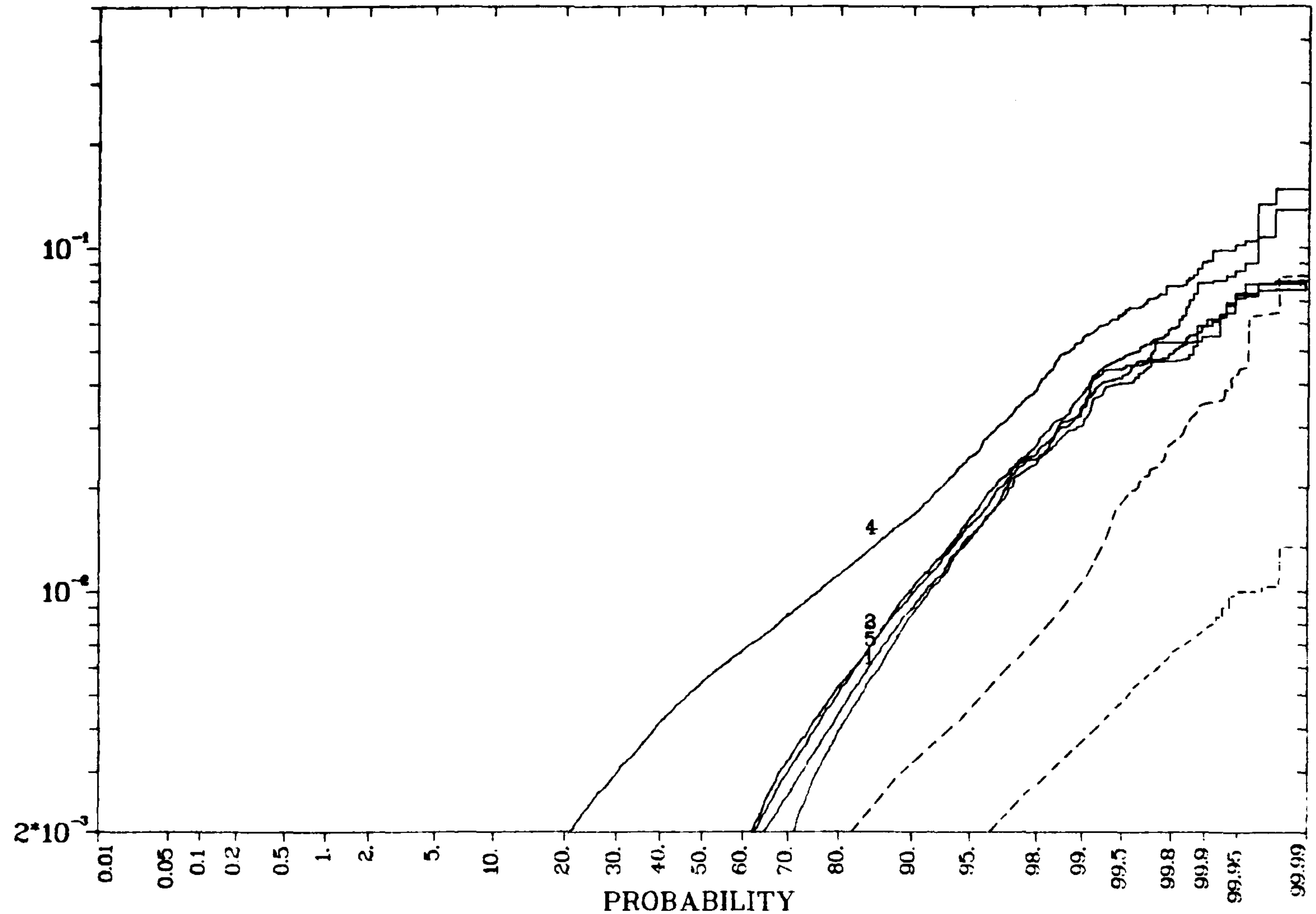


Fig. 5c. Cumulative Frequency Distribution for Hourly AQAM II Predicted NO_x Concentrations at each Station. Dotted lines indicate the range of aircraft contribution with the upper curve generally representing station 4 and the lower curve station 1

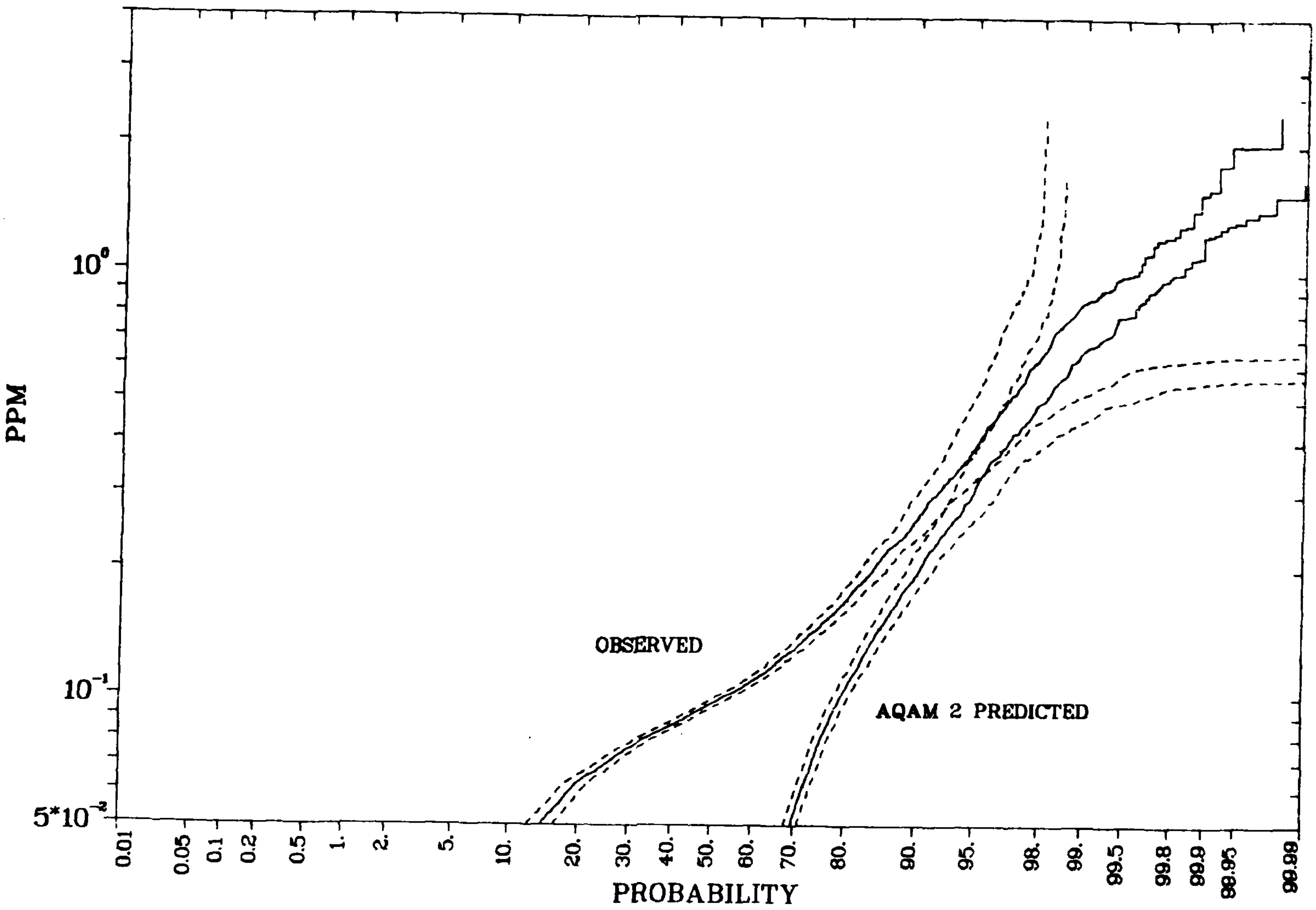


Fig. 6. Cumulative Frequency Distributions for Observed and AQAM II Predicted CO at Station 1.95% Confidence Bounds are Indicated

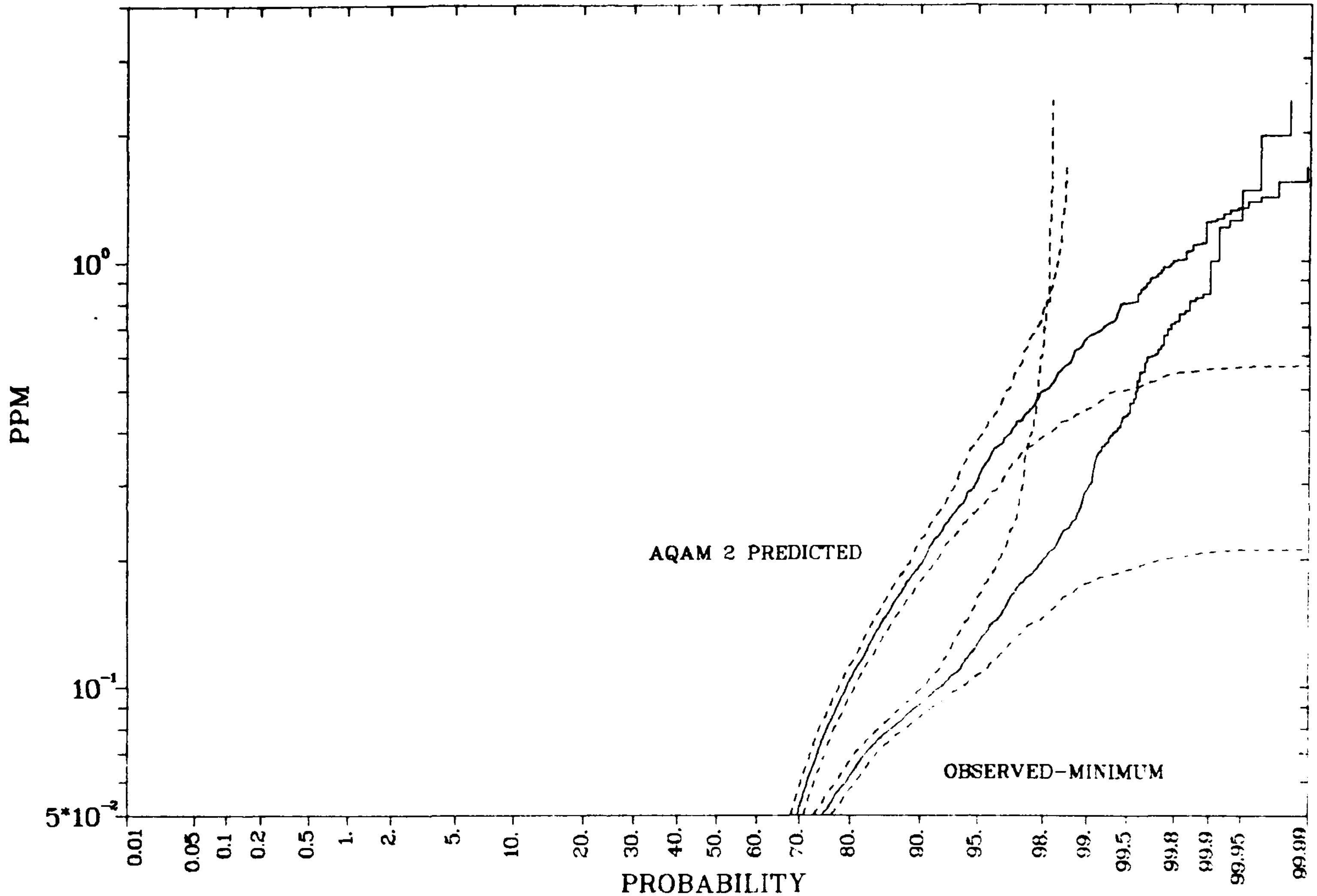


Fig. 7. Cumulative Frequency Distributions for (Observed-Minimum) and AQAM II Predicted CO at Station 1. The minimum is the minimum at that station during the hour (i.e. out of 60 samples). 95% confidence bounds are indicated

2. Frequency Distributions - Comparison of the theoretical and experimental means and standard deviations via a t-test will also provide a confidence level measure; however, robust computation of the moments would be required to avoid the issue of the distribution-dependent nature of the t-test and confidence level estimates. The approach seems, in retrospect, to provide no additional insights over those provided by the CFD and, in fact, would seem to place undue emphasis on the regime where one would expect maximum background interference.

3. Scatter Plots - Figures 8a, b, and c show the comparison of AQAM II predicted hourly concentrations with the upper ~10% of concentrations observed at Williams for CO, NMHC, and NO_x, respectively. Though considerable deviation from perfect agreement is apparent, one also notes that at these higher concentrations shown, a fraction exceeding 75% of the cases appear to fall within the lines denoting the frequently cited factor-of-two level of agreement[4] between theory and hourly average observation. Agreement is usually within a factor of 5 and nearly always within a factor of 10. The scatter plot provides instant intuitive insight into the data, and whether it be viewed as an advantage or liability, gives to the observer the freedom of judging the significance of "outlier" points and also shows any clustering of points in the data; however, this type of plot can also lead to gross misrepresentation of model performance since one can only observe those cases which fall within the plot and not the substantial number of cases where the model underpredicts so badly (excessive overprediction is generally not a problem) that the points fall outside the plot boundary.

4. Frequency Distribution of Residuals - Examination of the appropriately normalized histogram of the difference, $\Delta \equiv \chi_{EXP} - \chi_{THEORY}$, between experimental and theoretical concentrations answers the question "What percentage of the time is the prediction good to within x ppm?" Though the question "How often is the prediction within x percent?" can be addressed by considering histograms of Δ/χ_{EXP}, the first question may be of more direct significance from the point of view of achieving desired ambient air quality goals. Figures 9a-c present somewhat of a compromise between these two approaches. The $\log_{10}$ (AQAM II/observed) frequency distribution is plotted for the upper ~10-15% of the observed concentrations for CO, NMHC, and NO_x. In each case, one observes instances where AQAM underpredicts by more than two orders-of magnitude as well as a general tendency toward underprediction. Twenty to twenty-five percent of the

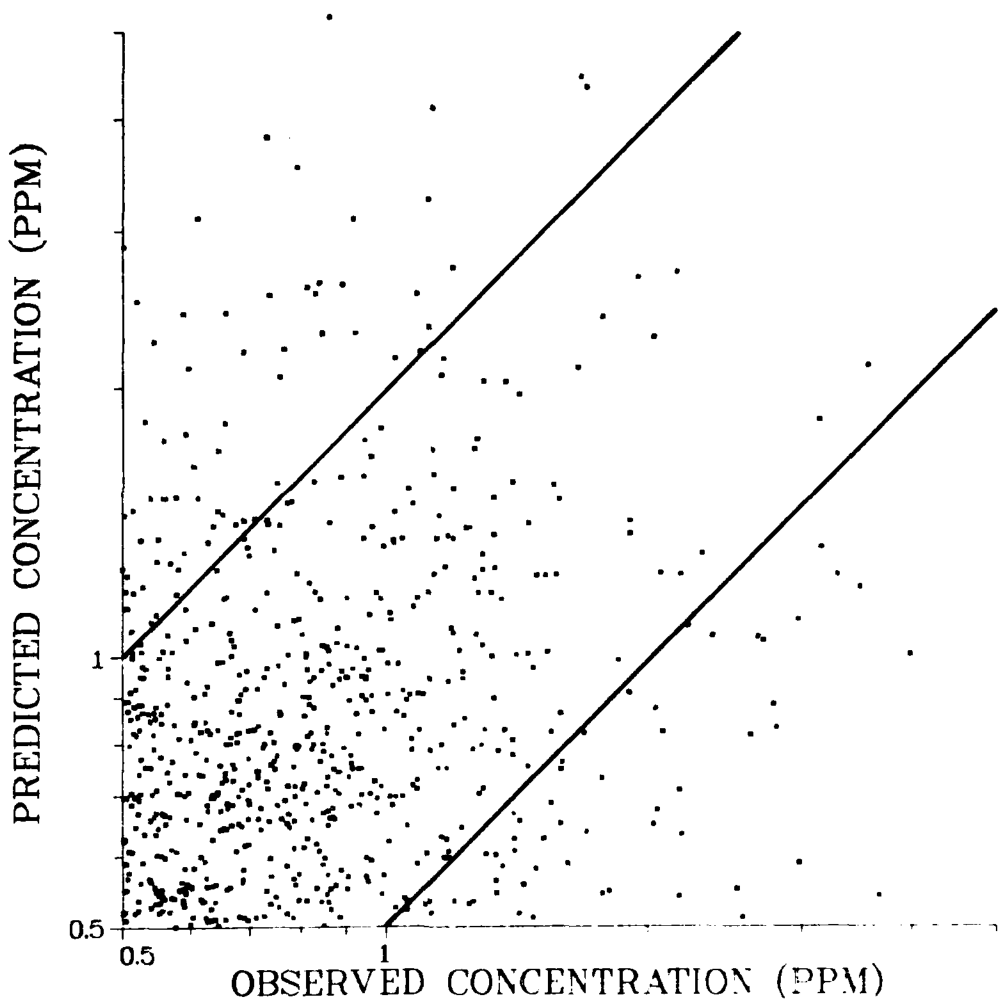


Fig. 8a. AQAM II Predicted vs Observed Hourly Average CO Concentrations for Values Above 0.5 ppm -- Williams AFB, 1976 - 1977.

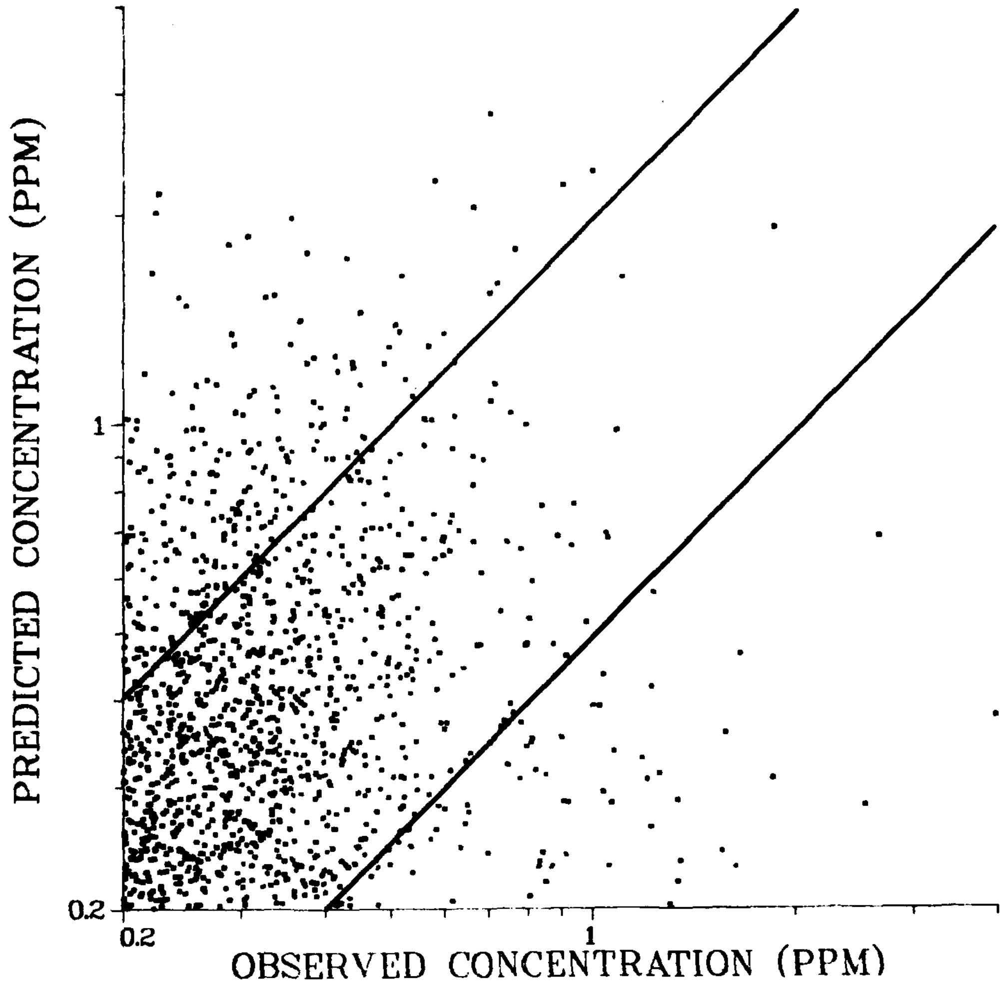


Fig. 8b. AQAM II Predicted vs Observed Hourly Average NMHC Concentrations for Values above 0.2 ppm -- Williams AFB, 1976-1977.

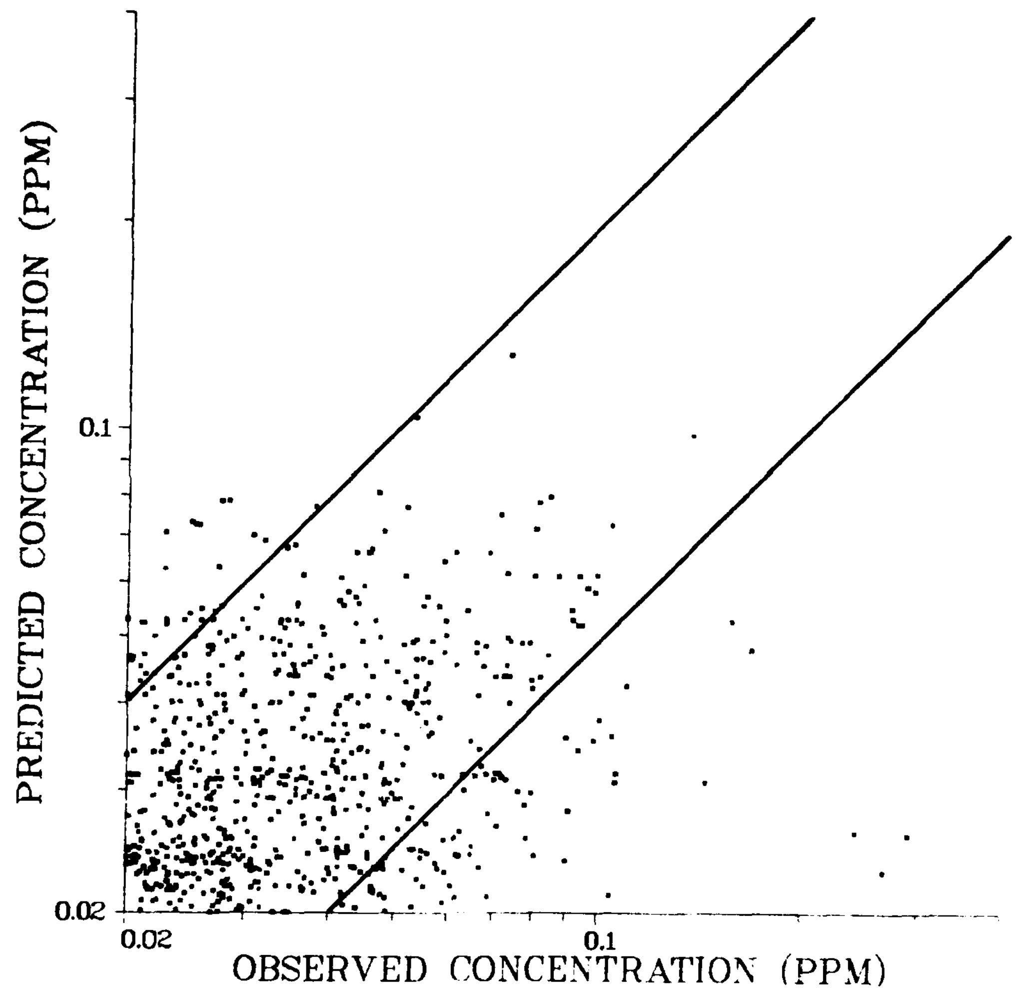


Fig. 8c. AQAM II Predicted vs Observed Hourly Average NO_x Concentrations for Values Above 0.02 ppm -- Williams AFB, 1976-1977

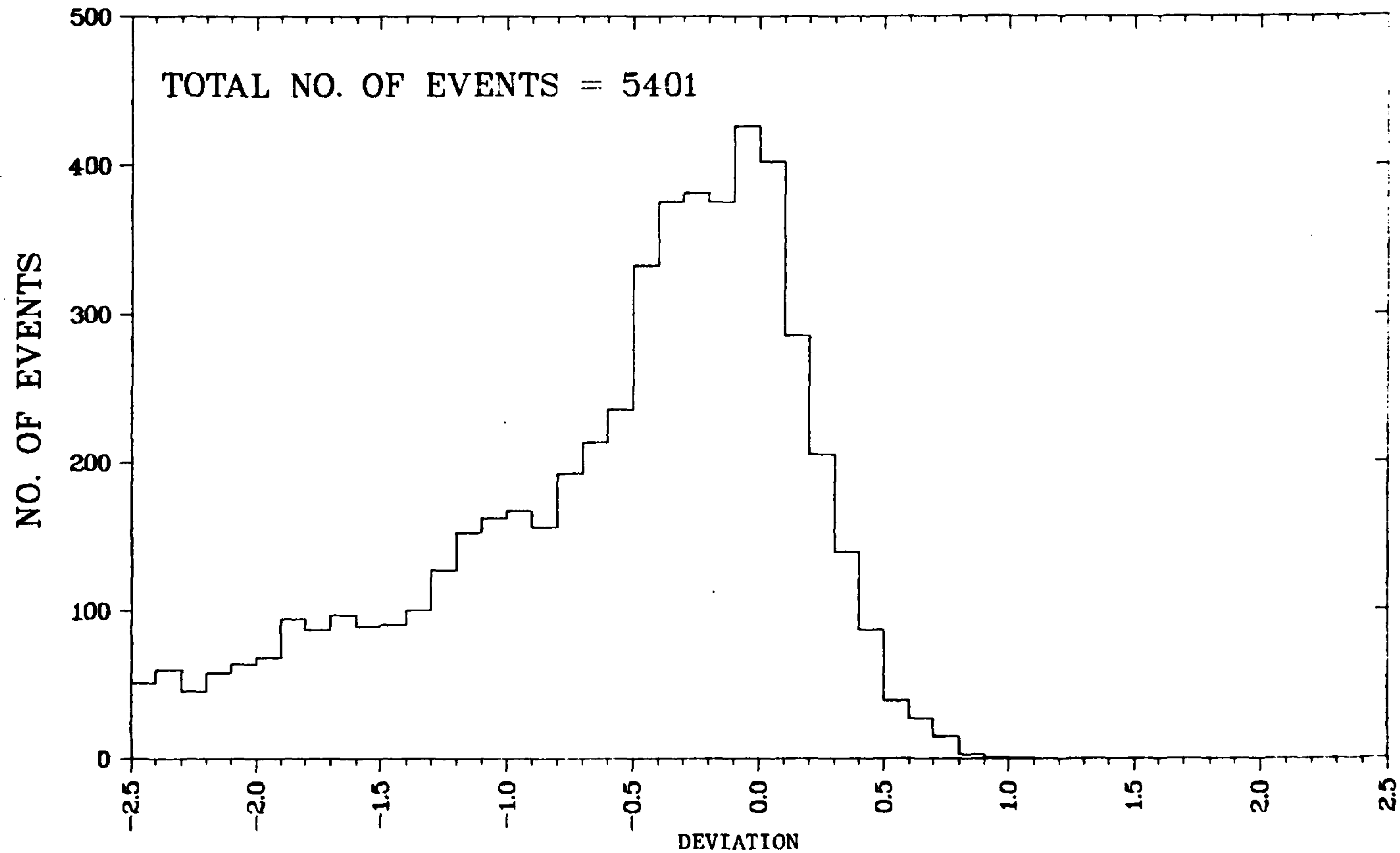


Fig. 9a. Frequency Distribution of Log_{10} (AQAM II/Observation) for the Upper ~10% of Observed Concentrations of CO. Willimas AFB Hourly Rate.

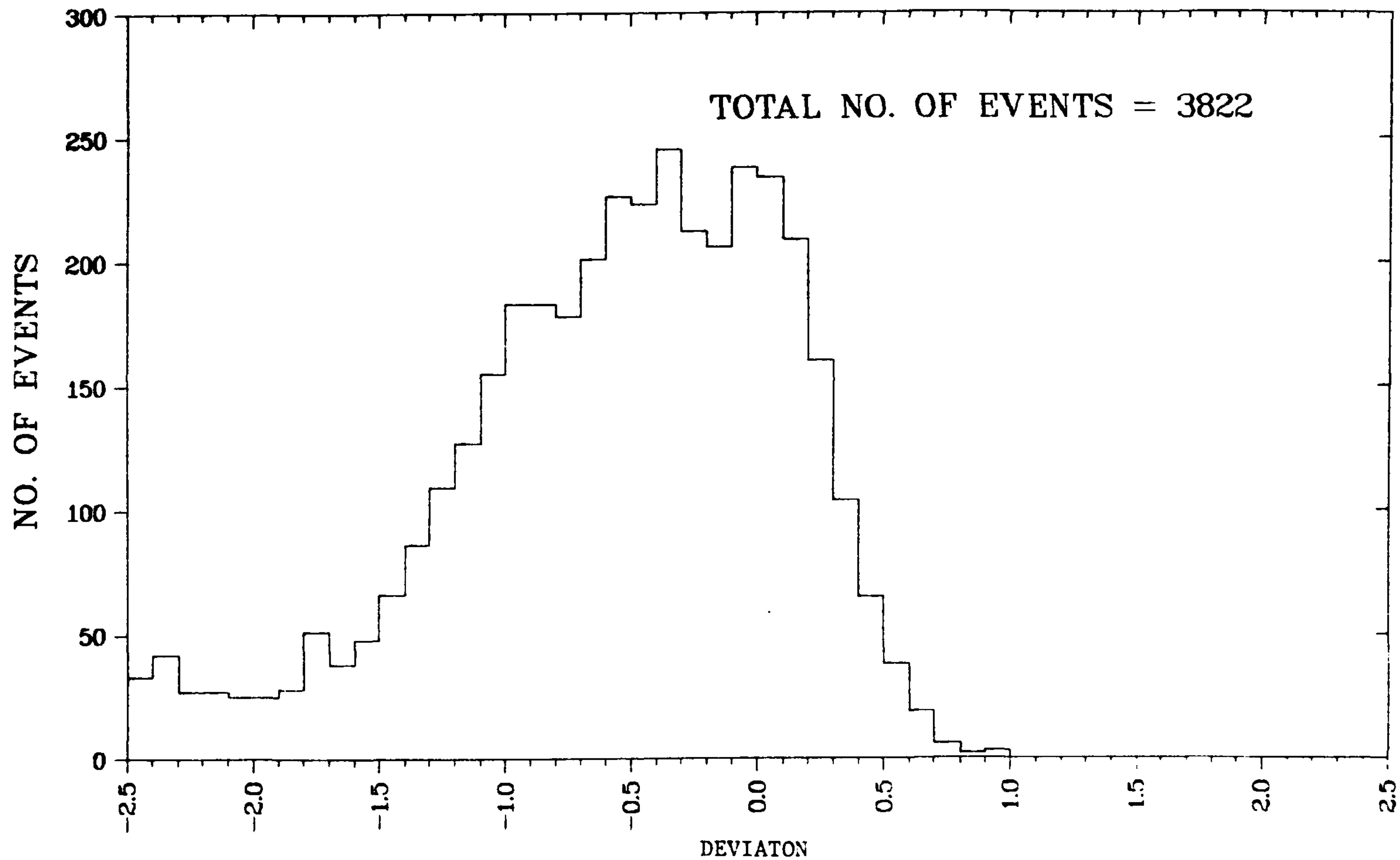


Fig. 9b. Frequency Distribution of Log_{10} (AQAM II/Observation) for the Upper ~10% of Observed Concentrations of NMHC. Williams AFB Hourly Data.

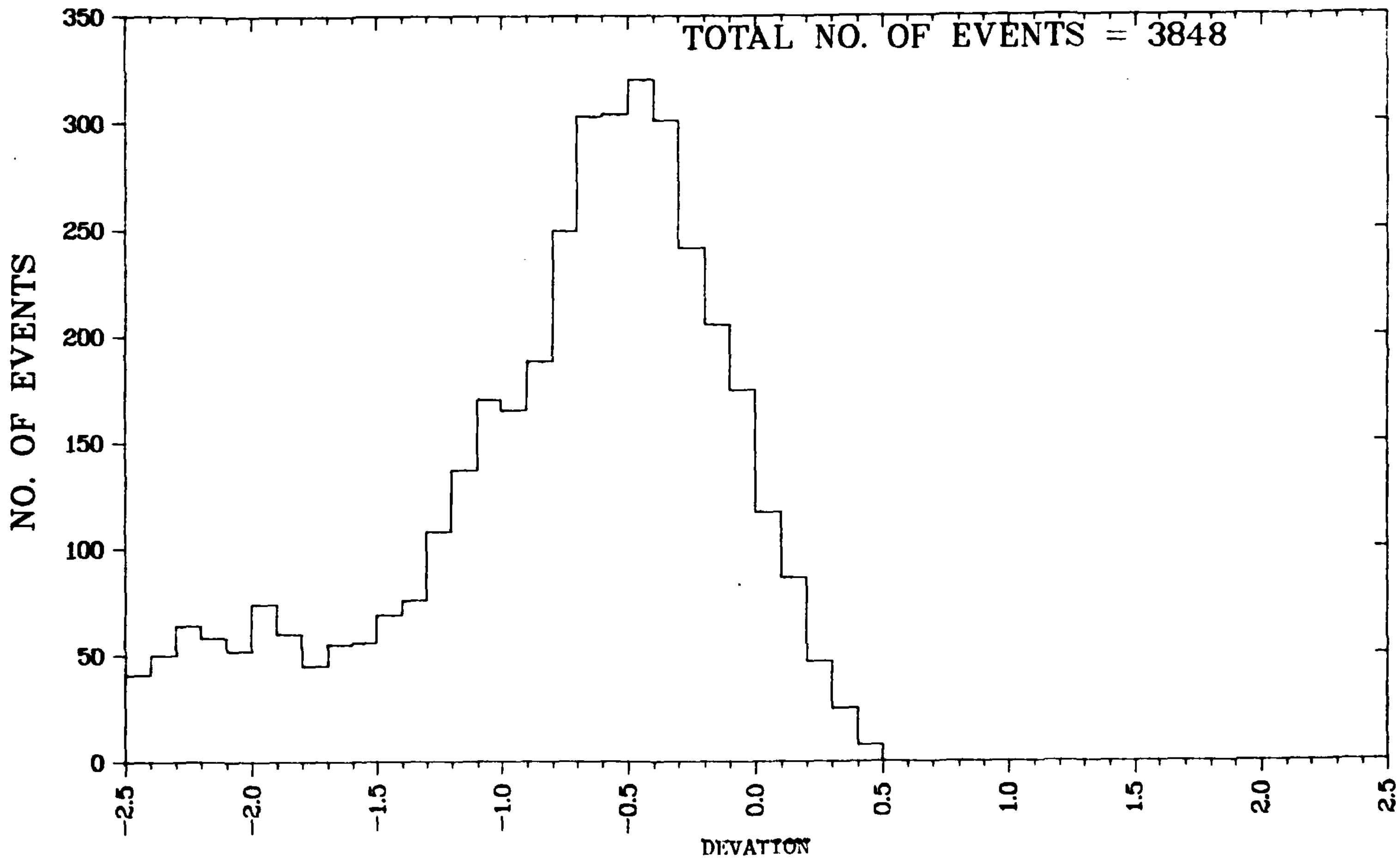


Fig. 9c. Frequency Distribution of Log_{10} (AQAM II/Observation) for the Upper ∿10% of the Observed Concentrations of NO_x. Williams AFB Hourly Rate.

predictions are in error by more than a factor of ten and standard deviations of $\sim 2/3$ are substantially larger than the value of $\sigma = 0.446$ expected if the factor-of-two rule holds for lognormal distributions. Such plots for each station separately are presented in Appendix G.

Table 2 sumarizes the performance of both AQAM I and AQAM II in this logarithmic sense. Several general characteristics can be observed.

1) Both AQAM I and II have slightly better predictive power when only the higher observed concentrations are considered, but this performance, measured in terms of the standard deviation of the log distribution, falls short of the factor-of-two rule. This predictive power is nearly the same for all pollutants considered.

2) When all observations are considered, AQAM II performs slightly better than AQAM I both on mean level of agreement and scatter about that mean value; however, when only the upper 10-15% of all concentration data are considered, AQAM II shows no superiority over AQAM I in the mean and is even slightly inferior in terms of the standard deviation.

3) Both AQAM and I and II underpredict on the average for each of the three pollutants considered. This degree of underprediction is nearly the same for each station and of approximately the same order for each of the pollutants and is most likely due to the presence of background concentrations not accounted for by the model.

4) Tremendous improvement is realized when a appropriate annual average background is added to the AQAM concentrations. This fact is evident from the greatly reduced standard deviations of the log residuals presented in Table 2. Method of background selection and further details regarding model performance will be discussed along with Hypothesis D12.

5) Correlation Coefficients - There are many possible measures of success which might be aptly termed correlation coefficients. Though the data itself will impose constraints on the appropriateness of choosing a particular correlation coefficient, one may generally consider the following.

   a. Non-parametric or distribution-free measures such as the Spearman rank correlation coefficient, or

Table 2. Distributional Characteristics of $\log_{10}$ ((AQAM+B)/Measured Concentration) for Hourly Data at all Five Williams AFB Monitoring Sites using different data samples and AQAM Background (B) Assumptions. Mean, Standard Deviation and Number of Cases are given for both AQAM I and AQAM II Predictions. Only cases where $|\log_{10}| \leq 2.5$ are included

	a) All Observations with $\chi_M \geq \chi_c$ and* $B \approx 0$		b) All Observations with $\chi_M \geq$ XTHRESH** AND $B \approx 0$		c) All Observations with $\chi_M >$ XTHRESH** and B as given	
	AQAM I	AQAM II	AQAM I	AQAM II	AQAM I	AQAM II
CO						
M	-0.5712	-0.5649	-0.4508	-0.4485	-0.0046	0.0082
σ^+	0.7110	0.7107	0.7774	0.7779	0.3684	0.3630
N	5237	5401	20734	20902	28655	28654
NMHC						
M	-0.5562	-0.5605	-0.5354	-0.5224	-0.0176	-0.0174
σ^+	0.6486	0.6629	0.7176	0.6936	0.3175	0.3092
N	3744	3822	14006	13934	19263	19262
NOx						
M	-0.7486	-0.7672	-0.6817	-0.6852	-0.0043	-0.0052
σ^+	0.6106	0.6397	0.7418	0.7302	0.3225	0.3207
N	3709	3848	23545	23599	32414	32413

* **

	χ_c (ppm)	χ_{THRESH} (ppm)	B (ppm)
CO	0.25	0.05	0.09
NMHC	0.20	0.05	0.08
NO_x	0.02	0.002	0.007

+Relation between standard deviation and percentage within a factor of two

σ	%	σ	%
1.19	20	0.446	50
0.781	30	0.358	60
0.574	40	0.290	70

b. Correlation coefficients which assume normally distributed (or at least strongly peaked) population distributions. In such cases, we can define the linear correlation coefficient:

$$r_2 = \frac{\frac{1}{N}\sum x_i y_i - \bar{x}\,\bar{y}}{\sigma_x \sigma_y}, \text{ where } \bar{x} = \frac{1}{N}\sum x_i ,$$

and

$$\sigma_x = \left[\frac{1}{N}\sum x_i^2 - \bar{x}^2\right]^{1/2}$$

or, the one-parameter linear correlation coefficient

$$r_1 = \frac{\sum x_i y_i}{\left[\sum x_i^2 \sum y_i^2\right]^{1/2}} ,$$

in cases where we can confidently assume that the zero is well pinned down (i.e., $x_i = 0$ always implies $y_i = 0$). In addition the slope of the associated regression lines provides insight into the adequacy of the model's overall normalization. Confidence limits for the correlation coefficient and the regression coefficients may also be computed.

The chief drawbacks of the use of these product-moment correlation measures are that:

i. Parametric estimates may be very sensitive to outliners (this may be alleviated, for example, by working with the logs of the concentrations), and that

ii. The inferences are strongly dependent on initial assumptions concerning the distributional nature of the data and the subsequent choice of normalizing transformation.

6) Time Series - Visual comparison of the observed and predicted concentration time series should indicate whether the AQAM predictions follow the observations. Coupled with this intuitive insight, one may compute the coefficient of coherence via appropriate normalization of the Fourier transform of the cross-covariance function. This technique may prove even more useful in the assessment of the significance of independent variables (e.g., aircraft activity, wind speed, stability) on observed concentrations and predictive accuracy. Preliminary results of such time series investigations are presented in Appendix I. Figures 10a and b are

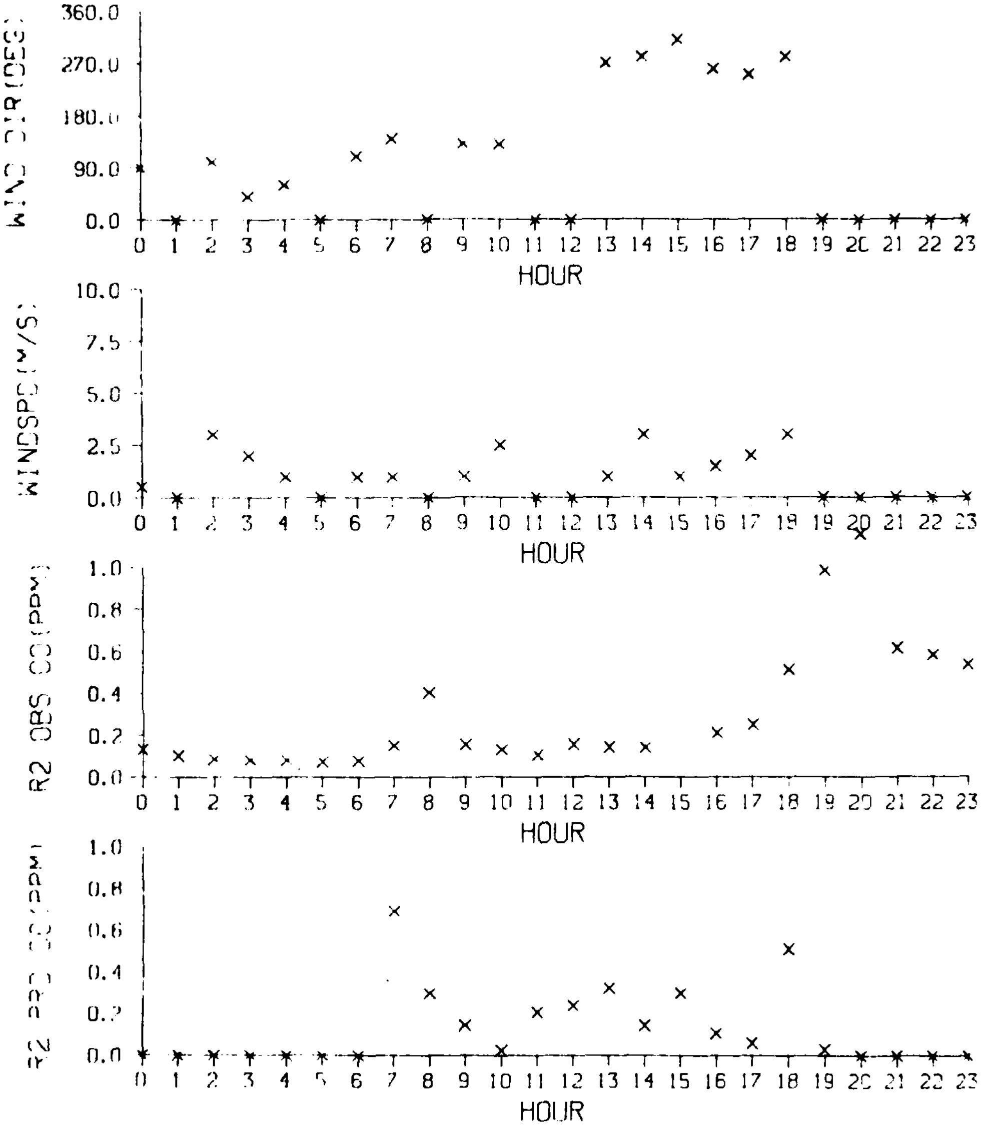


Fig. 10a. Twenty-four Hour Time Series of Airbase Wind Direction, Airbase Wind Speed, Observed CO Concentration at Receptor 2, and AQAM II Predicted Concentration at Receptor 2. January 10, 1977

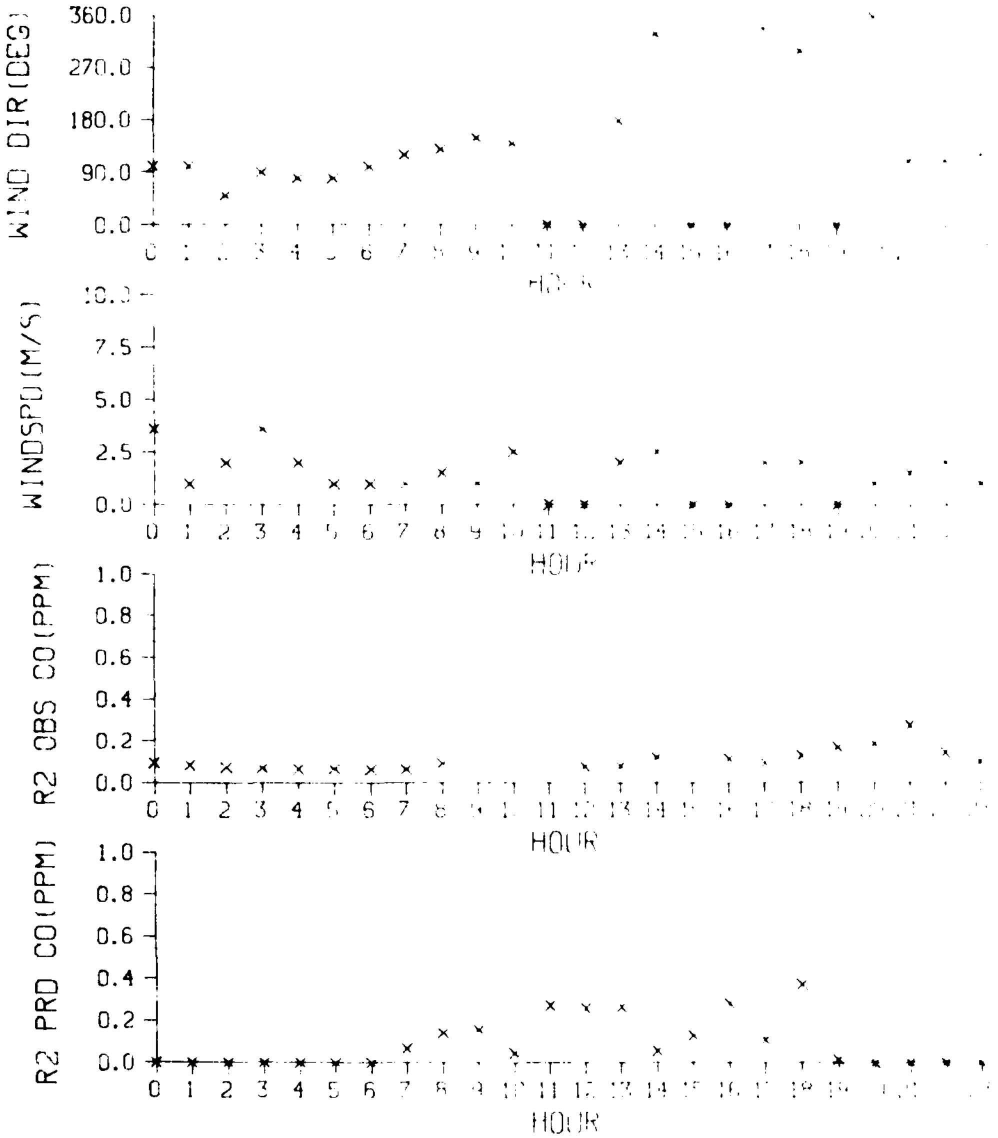


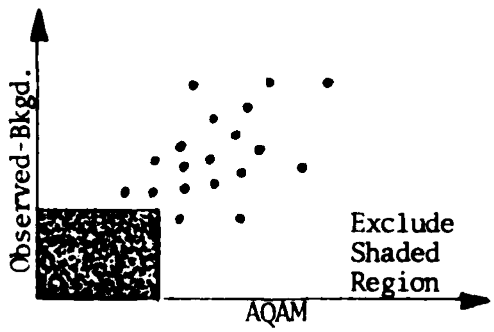
Fig. 10b. Twenty-four Hour Time Series of Airbase Wind Direction, Airbase Wind Speed, Observed CO Concentration at Receptor 2, and AOAM II Predicted Concentration at Receptor 2. January 31, 1977

typical examples of multiple time series plots produced from the January 1977 Williams AFB data. Base Weather station wind speed and direction are shown along with observed and AQAM II predicted CO levels for station 2 for two days. As can be seen, the model is generally successful in predicting the 8 a.m. enhancement, tends to overpredict afternoon levels, and understandably fails to predict the elevated nighttime levels thought to be associated background air from Phoenix.

Several additional techniques for addressing the question to overall model performance assessment have been suggested by Karl Zeller (EPA/EMSL), reviewed by other experts within the EPA, and are contained in Appendix E.

B. Data Selection Criteria for the Overall AQAM Accuracy Definition

Since the utlimate purpose of AQAM is to predict air quality levels which are of health or welfare significance, it would be reasonable to make the accuracy definition at higher concentrations rather than over the total spectrum. If indeed one could confidently prescribe a procedure that would reliably isolate periods of high, background subtracted pollutant levels, then one could evaluate AQAM for those select periods; however, this procedure may not be unique. Even if one could accomplish this, it is not apriori clear that AQAM will correctly predict the higher concentrations for these periods. Thus, one should run AQAM for all hours, irrespective of observed pollutant levels. Selection of data for the overall accuracy definition might then consist of eliminating some region in the lower left corner of the scatter plot of (Observed-Backround) concentrations versus AQAM predicted concentrations, as shown in the sketch below. The actual size of this excluded region, preferably with identical cutoffs on both axes, might be defined in terms of eliminating some fraction of the data or at some concentration related to the NAAQS.



Though such a data cut appears not to bias interpretation of the cumulative frequency distributions, provided some accounting is made of the number of points below the cutoff concentration, one should realize that equality of cumulative frequency distributions does not assure any predictive power of the model on an hour-by-hour basis. Other measures of overall AQAM accuracy, such as regression fits, could be substantially distorted by such data cuts. Hence, cuts of this nature should be considered carefully.

It should be mentioned that the desired insight into any concentration dependent nature of the model's predictive power might be obtained via examination of the concentration residuals (i.e., Observed-Background-AQAM) as a function of various concentration measures.

It will become evident in the following section that definition of the background as the n-station (where n=5 in this experiment) arithmetic mean, $\bar{C}_o$, leads naturally to a mechanism for selecting a subset of periods for which AQAM must perform best. Just as comparison of the r.m.s. signal to the average signal for a given hour at a single station lends insight into nearby source activity, consideration of the normalized variance, q^2, given as

$$q^2 \equiv \frac{1}{N} \sum_{i}^{n} \frac{(C_{oi} - \bar{C}_o)^2}{\sigma^2(C_{oi})}$$

where $\sigma^2(C_{oi})$ is the experimental variance, provides one measure of the degree of observed station-to-station variation in a given hour. Failure of AQAM at high levels of q implies failure at lower q levels while success at low q suggests success at high q. Thus, it becomes reasonable to examine AQAM success as a function of q.

C. Determination of Background

Much of the proposed analysis strategy rests on a presumed ability to compute background pollutant levels. An inability to do this accurately, while of little consequence if the background is a small contribution to the total observed signal, may be a very serious problem if backgrounds are as large as some[5] estimates (up to ~80%).

We now consider several possible schemes for computing the background and the extent to which the true background must be separated out in order to assess AQAM. For example:

a) Let the observed concentration, C_{oi}, at the most upwind station be considered the background, C_B.

Problems: i) $C_{oj} - C_B < 0$ is possible

ii) ignores AQAM consideration of environ sources.

b) Consider the most upwind station but define $C_B = C_{oi} - C_{Ti}$, where the subscript T indicates theory prediction (AQAM).

Problems: i) $C_{oj} - C_B < 0$ still possible

ii) correctly accounts for AQAM environ source impacts but now couples theory and experiment in a new way that can lead to fake correlations.

c) Pick the station with the lowest hourly average concentration and call that the background. Though this avoids negative background subtracted concentrations it is an arbitrary and capricious procedure. With or without any "theory correction", as described above, potential problems include:

   i) the background station may be different for different pollutant species

   ii) theory and experiment may not agree on the choice of background station

   iii) makes background station choice subject to single instrument fluctuations or drift.

d) Let AQAM dictate which station should be measuring the minimum signal and define that to be background.

   Problems: i) presupposes a correct theory

   ii) $C_{oj} - C_B < 0$ possible

   iii) background station may vary with pollutant species.

e) Finally we might consider a more general background.

$$C_B = \sum_{i=1}^{5} (C_{oi} - C_{Ti}) w_i \Big/ \sum_{i=1}^{5} w_i$$

where the weights w_i may result from experimental and/or theoretical considerations. Problems include a mixture of those previously mentioned. Though this approach is not without its merits, the potential for abuse is clearly present.

Irrespective of the method used to determine background, the resulting distributions of background concentrations should be compared with measurements from sites well isolated from local source influence.

The above discussion should suggest that any procedure to determine the true background is likely to have its problems and, given that this experiment may likely have high background concentrations, the problems may be severe. On the other hand, comparison of experiment and theory with the isotropic signal component removed from each signal separately should provide an unbiased approach to AQAM accuracy definition. By isotropic component we mean simply the five station arithmetic mean signal levels, C_o or $\bar{C}_T$. The background is then given by, $C_B = \bar{C}_o$ - "unknown constant", but the fact that this "offset" is unknown is inconsequential*. Removal of the isotropic or mean components from both the predicted and observed concentrations can be justified by symmetry considerations and leads to new insights into model/observation comparison. In particular, Figures 11a-c, point out that,

*Provided that in any statistical measures one accounts correctly for the reduced number of degrees of freedom.

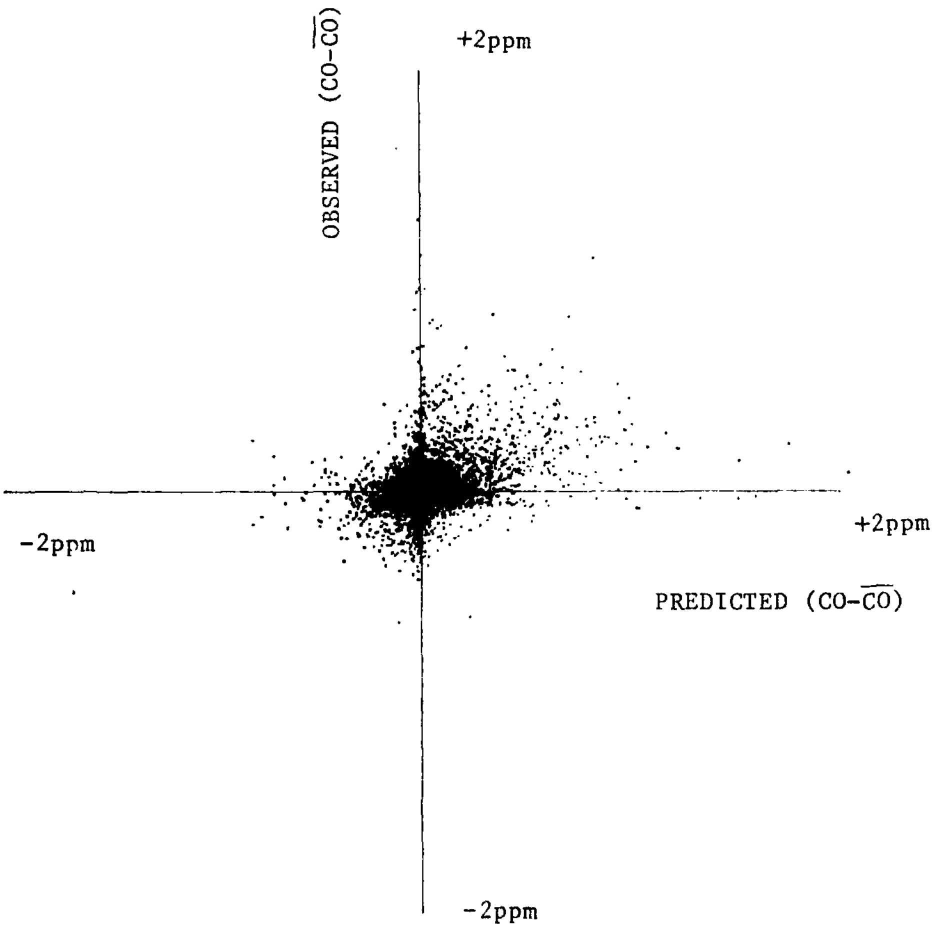


Fig. 11a. Observed vs AQAM II Predicted "Background Subtracted" CO Levels. **Williams AFB**, 1976-1977. Background is defined separately for observed and predicted concentrations as the five station arithmetic mean for the hour.

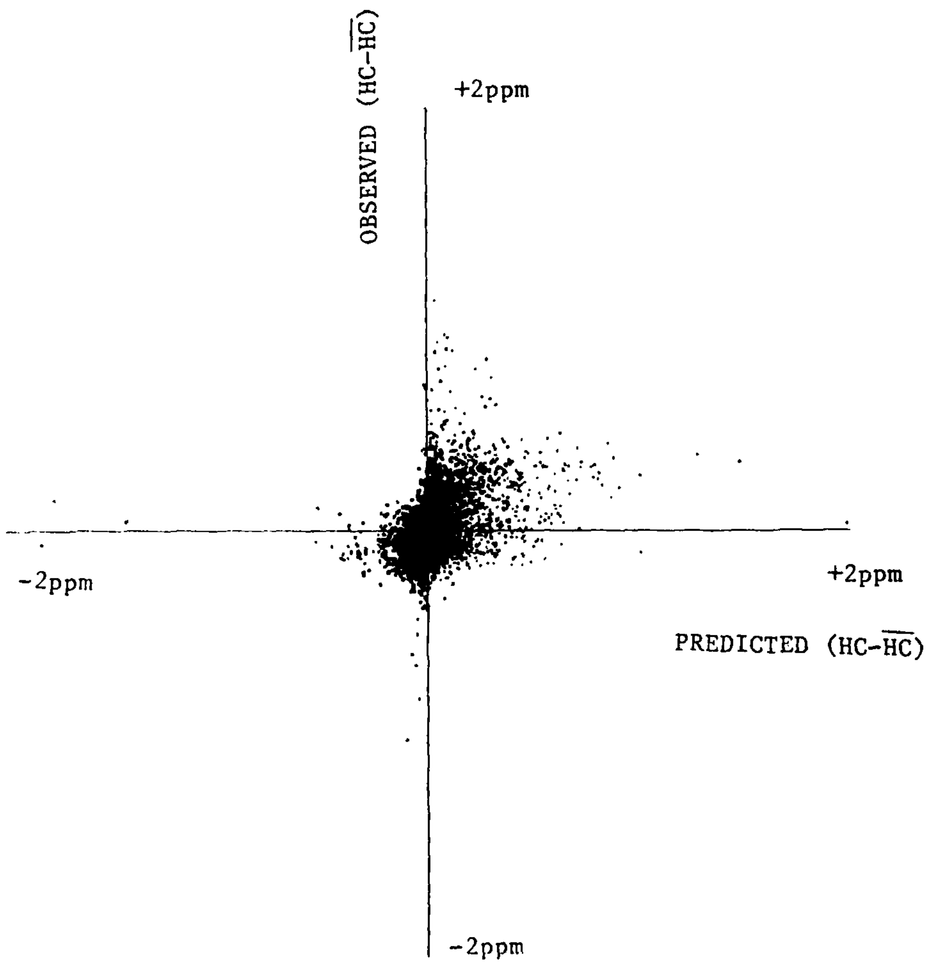


Fig. 11b. Observed vs AQAM II Predicted "Background Subtracted" NMHC Levels. Williams AFB, 1976-1977. Background is defined separately for observed and predicted concentrations as the five station arithmetic mean for the hour.

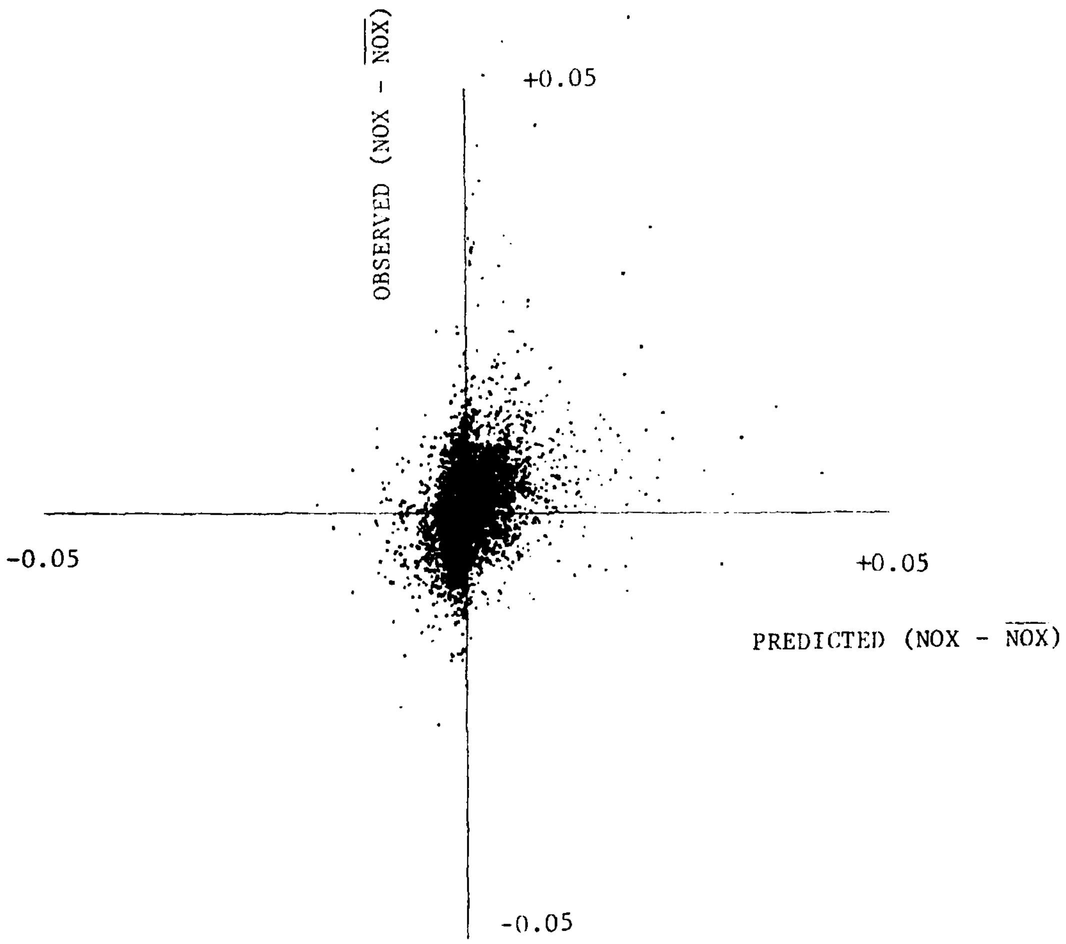


Fig. 11c. Observed vs AQAM II Predicted "Background Subtracted" NO_x. Levels. Williams AFB, 1976-1977. Background is defined separately for observed and predicted concentrations as the five station arithmetic mean for the hour. Not shown are two points predicted near 0.1 ppm amd observed near 0.003 ppm.

although substantial scatter away from perfect agreement between AQAM II theoretical and observed concentrations still persists after background adjustment, theory and experiment essentially agree on the pollutant rank ordering of the stations as suggested by the relative absence of entries in the second and fourth quadrants.

However, much of this apparent correctness in this station rank ordering is due to the dominance of station 4 relative to the other four stations. The large majority of the differences from the 5-station mean are seen to be strongly clustered around the origin and most are visibly within the inter-station resolutions of 0.02 ppm for CO and NMHC and 20 ppb for NO_x. This lack of significant deviation from the 5-station mean is further refelcted in fact that the correlation coefficients, accompanying linear regressions on the mean subtracted quantities, are less than 0.1 for each of the three pollutants. Requiring deviations from the 5-station mean to exceed 0.1 ppm for CO and NMHC (10 ppb for NO_x) one obtains correlation coefficients of 0.43 for CO (12803 cases) and 0.34 for NMHC (10361 cases) and accompanying regression slopes of $\sim$0.4. Unfortunately, the greater than 10 ppb criteria for NO_x reduces this sample size by more than 90% (i.e., only 3483 cases) and yet yields no significant improvement in the correlation coefficient.

SECTION III

STUDIES OF PARAMETER SIGNIFICANCE

Once the overall accuracy of AQAM is assessed, the individual parameters which are most significant need to be investigated. Significance in this context is taken to mean significance of a variable with respect to that variable's contribution to the concentration residuals (e.g., Observed-Background-AQAM). Significance of a variable in terms of a model's sensitivity to that variable does not generally require an experimental effort and falls into the broad category of effects analysis. Such a study has already been carried out for AQAM[6].

Returning now to the concept of significance with respect to residuals, consider first an experiment with only one independent variable, x. The residuals, Δ, may possess a standard deviation, σ_Δ, which is independent of x (e.g., Fig. 12a) or is some function of x (e.g., Fig. 12b). If the theory is reasonably correct and optimized, we expect the average residual, $\overline{\Delta}$, to be zero and σ_Δ to be at some minimal value. The fact that the mean residual, $\overline{\Delta}(x)$, is a function of x in Fig. 12b indicates a deficiency in the theory though the lack of such dependence in Fig. 12a cannot be taken as a proof of the correctness of the theory. Thus, one may learn a fair amount about a theory, particularly its shortcomings, by studying the residuals.

In the case of N independent variables the residuals populate an N + 1 dimensional space and one is often forced to abandon the intuitively simple technique of examining the one-dimensional projections of the residuals onto the various independent variable axes and instead utilize an approach such as multiple linear regression (stepwise linear regression in particular) to determine which variables (or combination of variables) are responsible for the majority of the variance σ_Δ.

Hence, in order to investigate the significance of variables such as on-base emissions, aircraft activity, background emissions and concentrations, wind speed, stability class, wind direction, mixing depth, and time of day one should

1) first examine simple, single variable projections and dependences of the residuals and if this proves inadequate

2) move on to various regression techniques to determine the absolute and relative significance of various independent variables and combinations of variables.

We note that the quantity q, introduced in Section II B, suggests a method which should enable stratification of conditions under which the AQAM model should perform within a certain range of reliability. Consider, for example, the uniform wind field assumption implicit in most Gaussian plume formulations (including AQAM). The quantities q_u and q_θ,

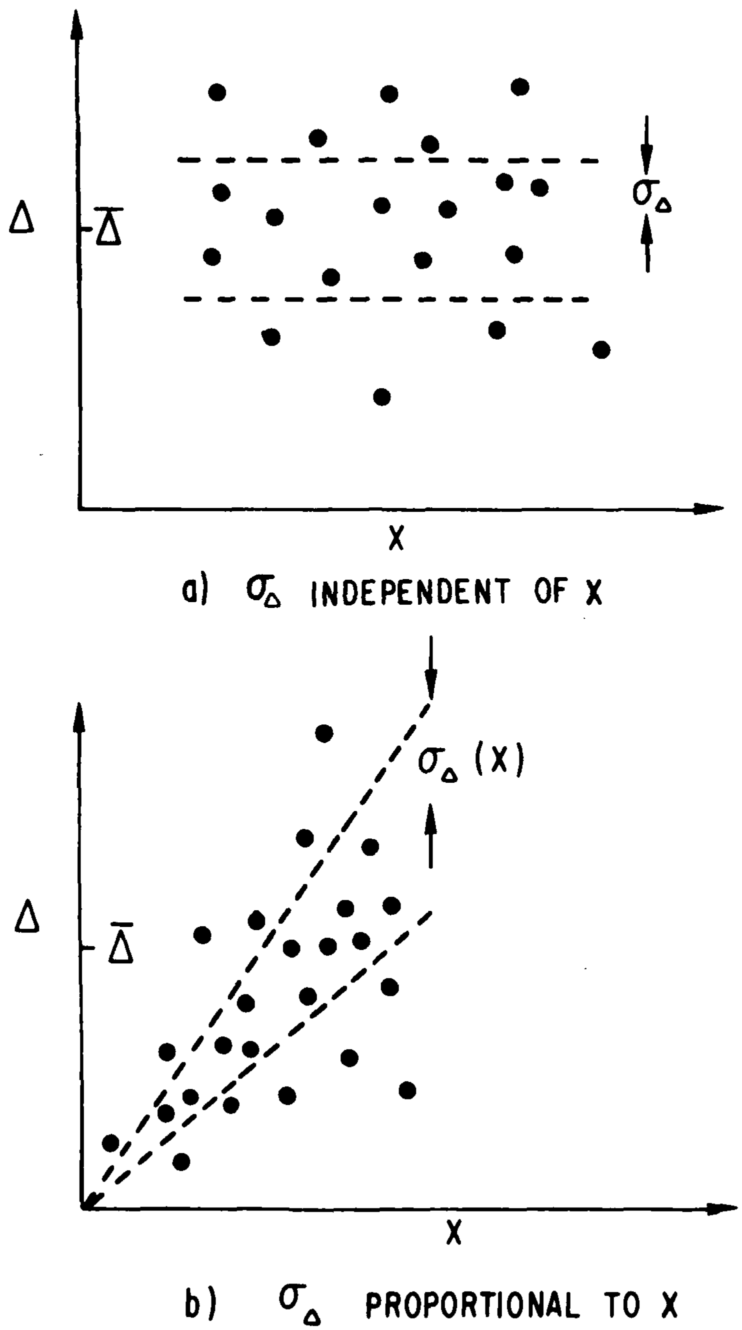


Fig. 12. Two Examples of Possible Residual Distributions

where $$q_u^2 = \frac{1}{n} \sum_{i=1}^{n} \frac{(u_i - \bar{u})^2}{\bar{u}^2} ,$$

$$q_\theta^2 = \frac{1}{n} \sum_{i=1}^{n} \frac{(\theta_i - \bar{\theta})^2}{\bar{\sigma}_\theta^2} ,$$

and where u_i and θ_i are the wind speed and direction at the ith station, $\bar{u}$ and $\bar{\theta}$ are their n station means, and $\bar{\sigma}_\theta$ is the n station mean standard deviation of wind direction within the hour,

essentially measure the degree to which this basic assumption of model applicability is satisfied. One would expect better model performance with q_u, $q_\theta << 1$ than in the case q_u, $q_\theta << 1$. Thus, one might think in terms of a functional relationship,

$$\sigma_\Delta = f(q_u, q_\theta, q_{\sigma_\theta}, q_{cm}, q_{ct}, \ldots) ,$$

where q_{σ_θ}, q_{cm}, and q_{ct} measure the spatial variability of the turbulence, measured concentration, and theoretical concentration fields respectively. Other q-type factors might include temporal persistence of the wind speed and turbulence averaged over the network. One is limited only by the quantities measured and the number of assumptions implicit in the model.

Frequency distributions of the dimensionless variable q_θ are presented in Figures 13a and b. Figure 13a indicates that for almost all hours, the r.m.s. difference in wind direction between stations 1, 2, 3, and 5 is less than one unit of σ_θ, while Figure 13b shows that wind directions at station 4 often differ from the mean wind direction (i.e., stations 1, 2, 3, and 5 only) by more than one unit of σ_θ. Similar results are obtained for the q_u distribution. This is intuitively quite reasonable as the airfield stations (i.e., 1, 2, 3, and 5) are in flat open terrain where uniform flow might be anticipated while station 4 is surrounded by airbase buildings and trees which could, and clearly do, significantly alter the mean wind flow.

Now consider the residual R^2 between the anistropic observed and AQAM II concentrations, defined as

$$R^2 = \frac{1}{m} \sum_{i=1}^{m} \left[(C_{Mi} - \bar{C}_M) - (C_{Ti} - \bar{C}_T) \right]^2 .$$

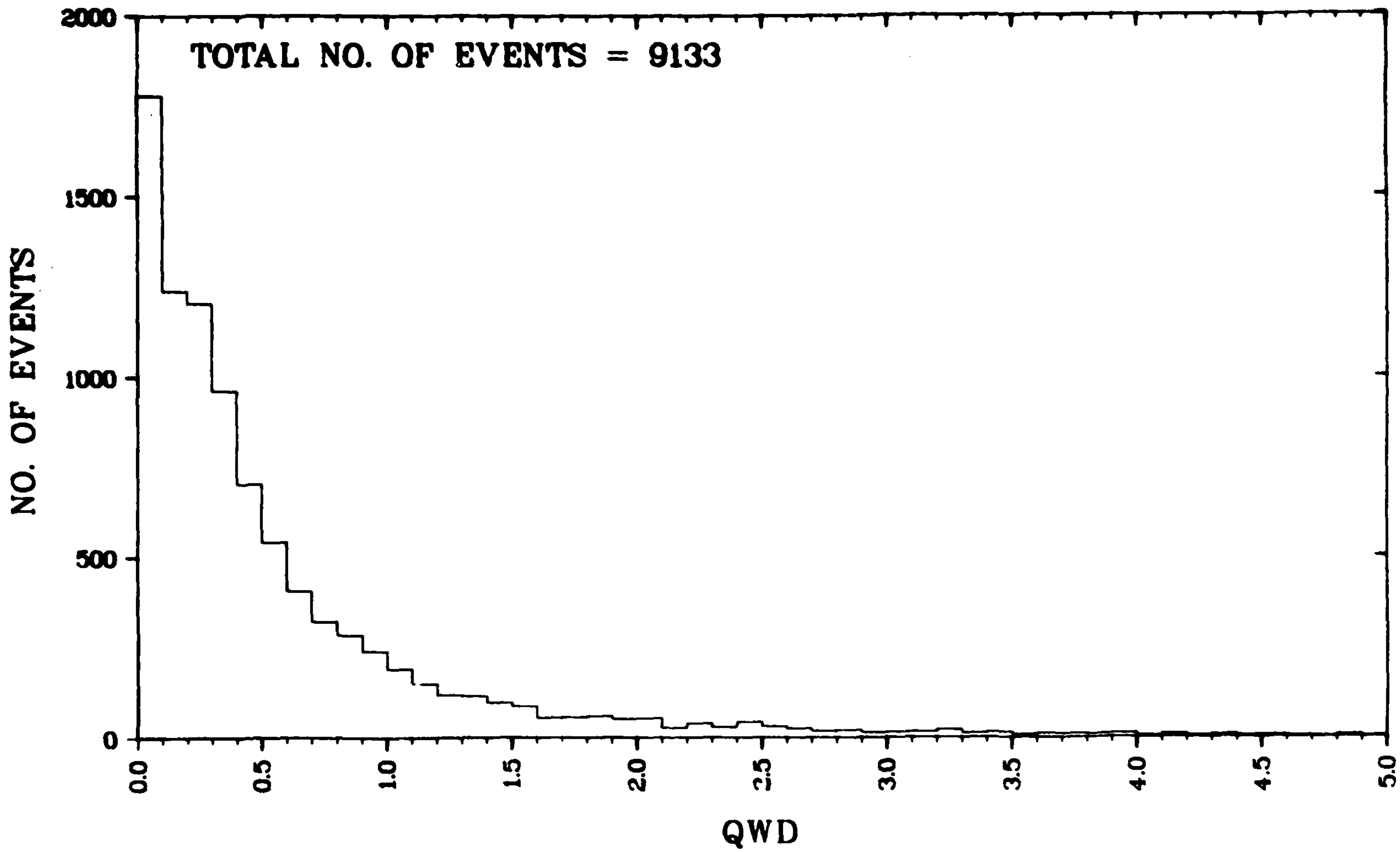


Fig. 13a. Wind Direction q Factor for Stations 1, 2, 3, and 5 Combined, Based on Deviations of the Wind Direction from the Four Station (i.e., station 4 excluded) Average Wind Direction. Data for the Period June 1976–June 1977 are included

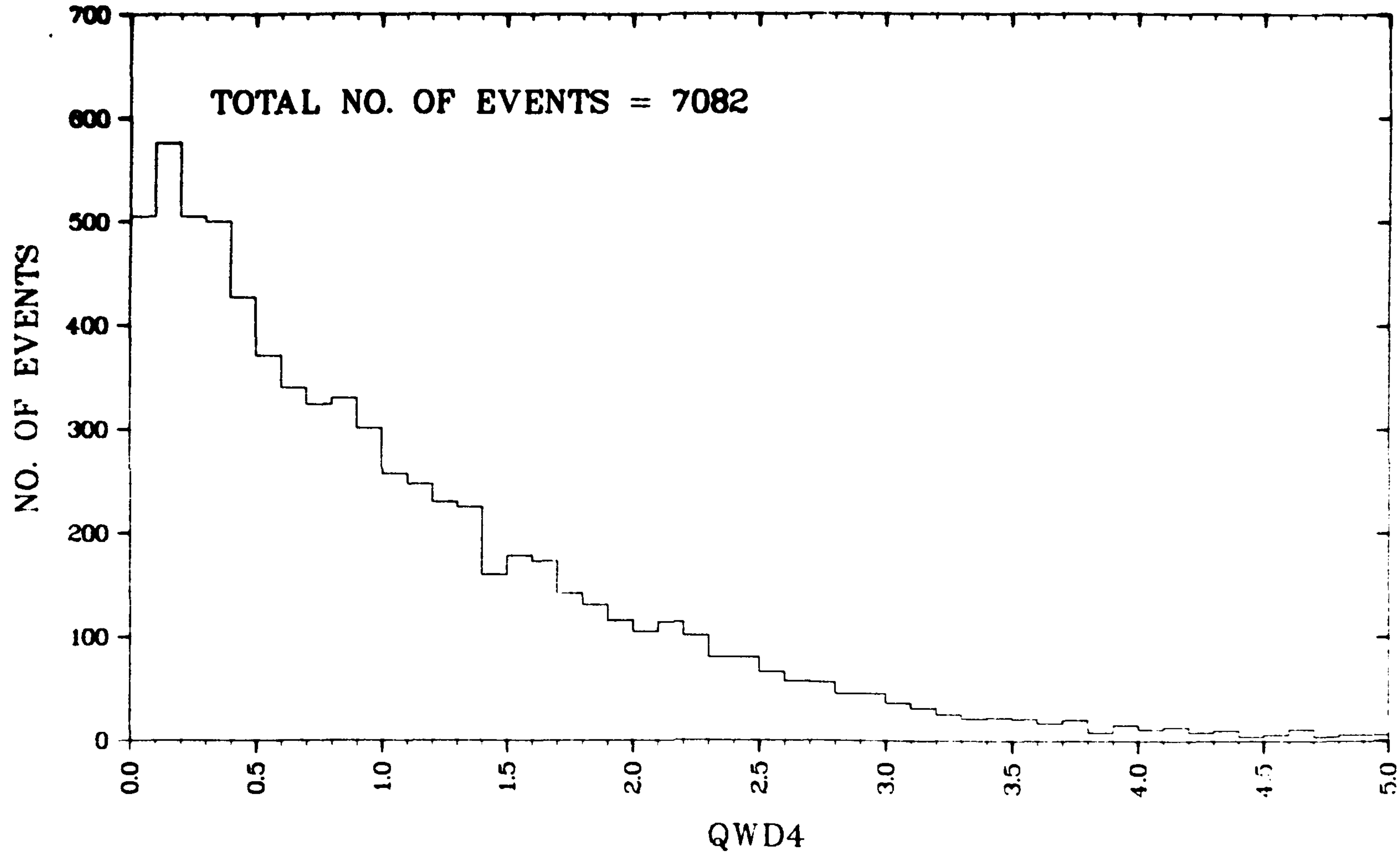


Fig. 13b. Wind Direction q Factor for Station 4, Based on Deviations of the Wind Direction from the Four Station (i.e., station 4 exluded) Average Wind Direction. Data for the Period June 1976-June 1977 are included

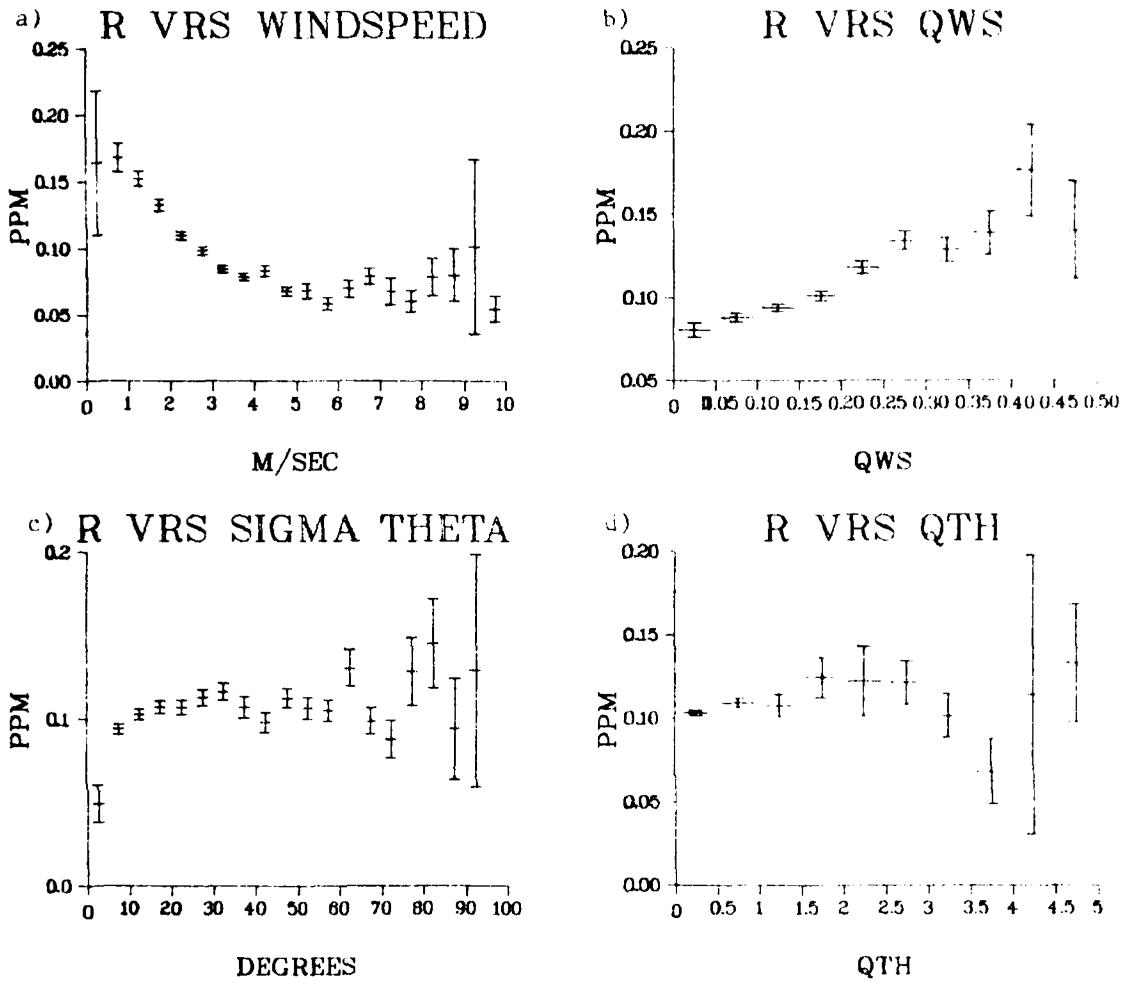
Figure 14 shows plots of the residual R vs windspeed (u), q_u, σ_θ, q_θ, Turner stability class, C_M, q_{CM}, C_T, q_{CT}, and time of day. Figure 15 represents the logarithmic residual

$$R_L \equiv \frac{1}{n} \sum_{i=1}^{n} \log_{10}(C_{Ti}/C_{Mi})$$

for each of the same variables and together these two residuals enable one to uncover basic trends in the model's goodness of fit. For example: i) R decreases with u but since C_T amd C_M also decrease with windspeed, the independence of R_L on u shows that model performance is independent of windspeed, ii) The model underpredicts more seriously at higher q_u, iii) The model underpredicts more seriously at low σ_θ and stable conditions. (This failing could be directly related to stability or indirectly through time of day.), iv) The degree of model underprediction is nearly independent of measured concentrations and yet is more serious at lower values of AOAM concentrations and when larger percentage interstation differences are predicted. These three factors coupled together suggest that much of the underprediction is due to the presence of background concentrations that are neglected by AQAM, v) While R follows the time of day dependence of $\overline{C_M}$ (see Figure 26j), the degree of underprediction is severe at night and mild during the day. This suggests a failing of the model during times when local sources are turned off and concentrations result from background and/or longer pollutant transport times (i.e., during periods when the "steady state" assumption is less valid); although much of this underprediction is now considered related to an underestimate (discovered only after report in press) of vehicle activity between midnight and 5AM.

One should be aware, however, that other interpretations of these dependences is possible due to the interrelated, phase-locked nature of most of these variable with time of day.

Multivariate analysis using the stepwise multilinear regression codes in SPSS[7] have yielded no additional information, regarding the dependences of the residual R^2, that was not apparent from the univariate analyses.



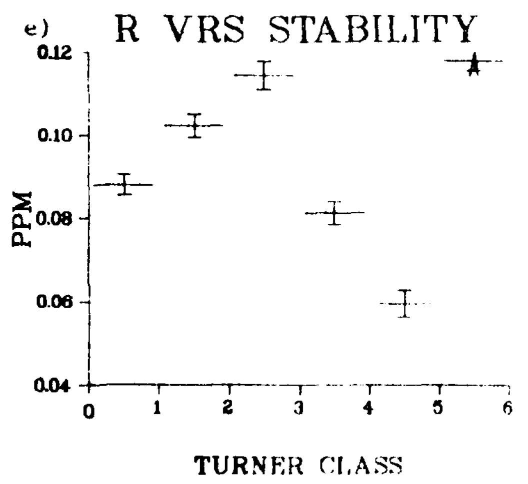
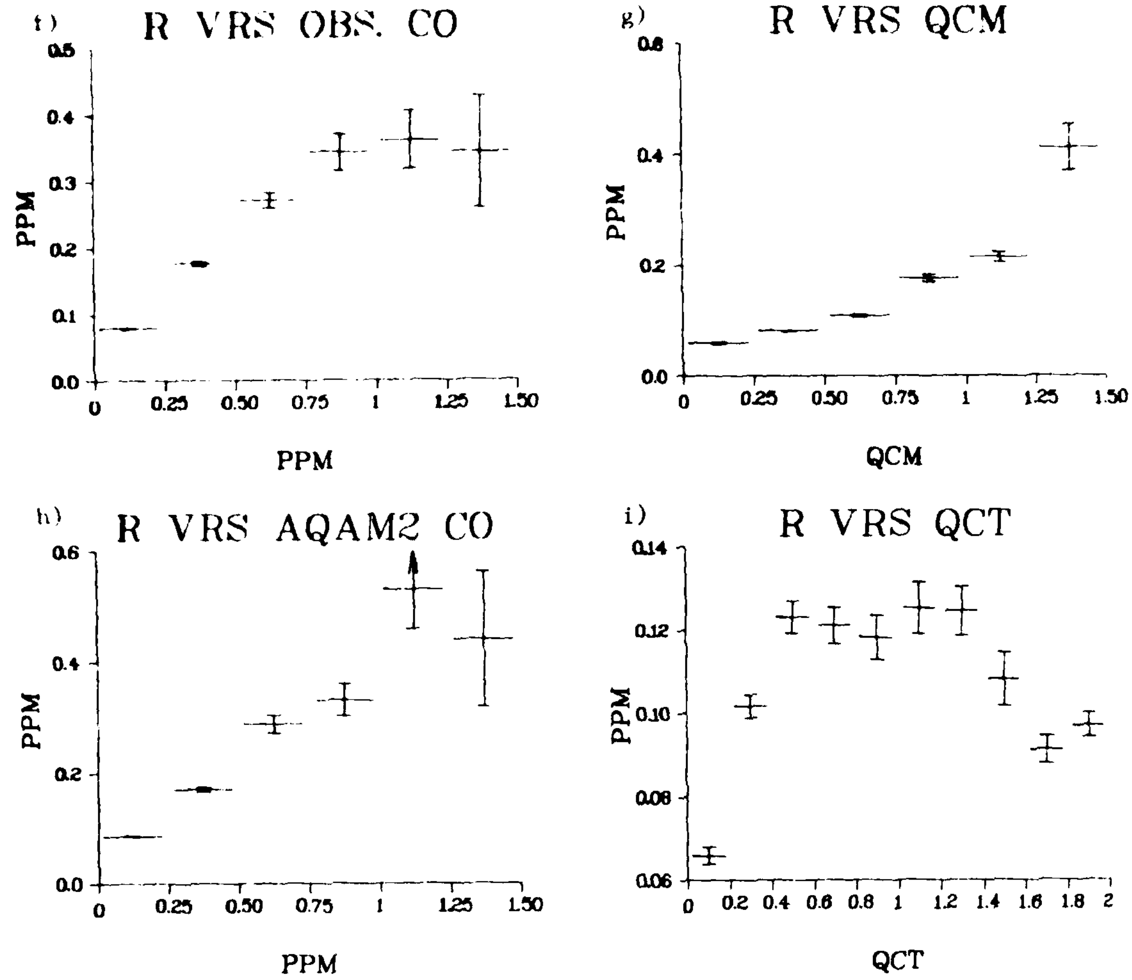


Fig. 14a-e. The Residual R Between the Anisotropic Observed and AQAM II CO Concentrations vs

a) windpseed (u)
b) q_u
c) σ_θ
d) q_θ
e) Turner stability class

Error bars indicate the standard deviation of the mean



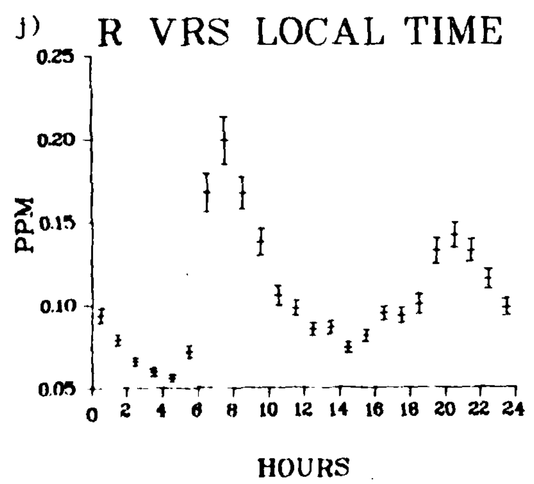
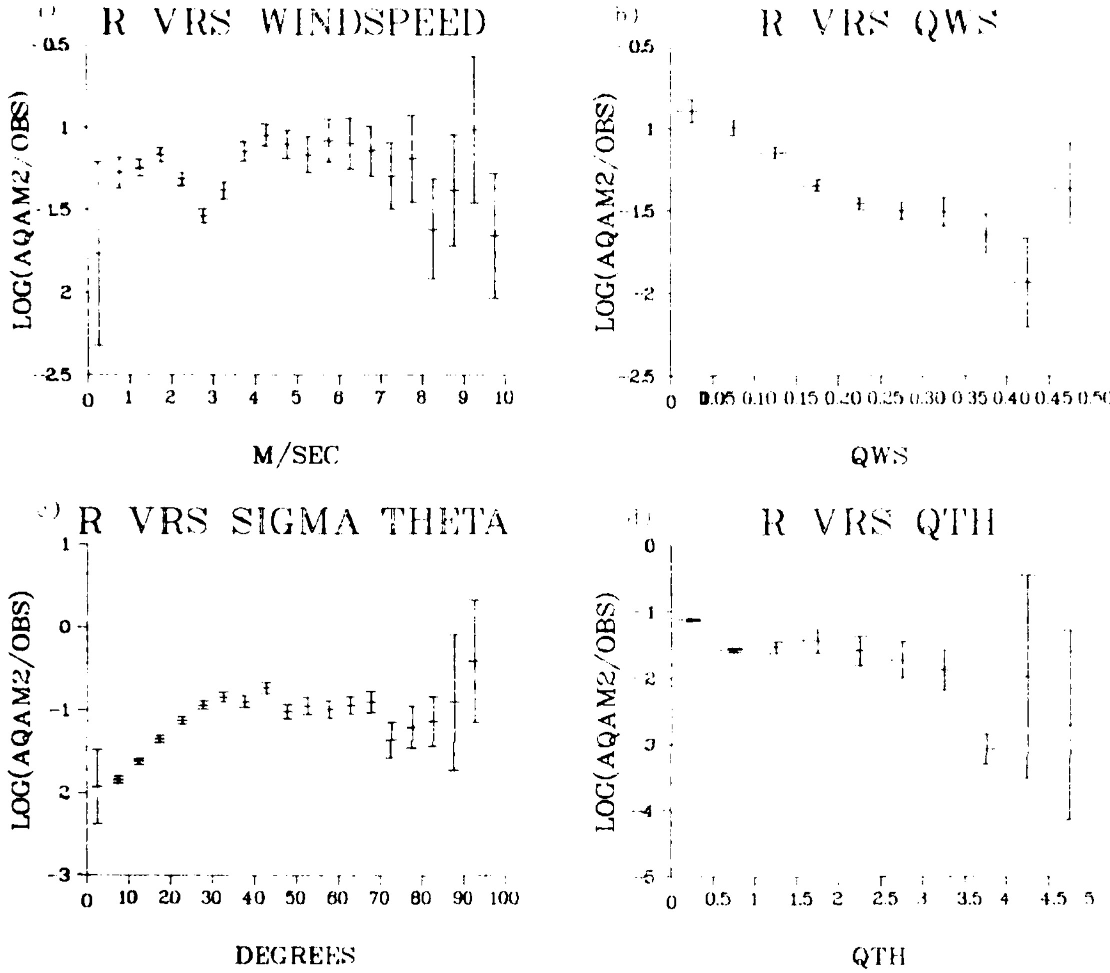


Fig. 14f-j. The Residual R Between the Anisotropic Observed and AQAM II CO Concentrations vs

- f) $\bar{C}_M$
- g) q_{CM}
- h) $\bar{C}_T$
- i) q_{CT}
- j) local time

Error bars indicate the standard deviation of the mean



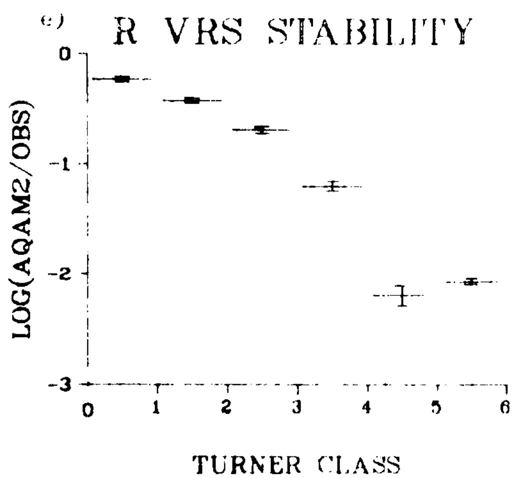
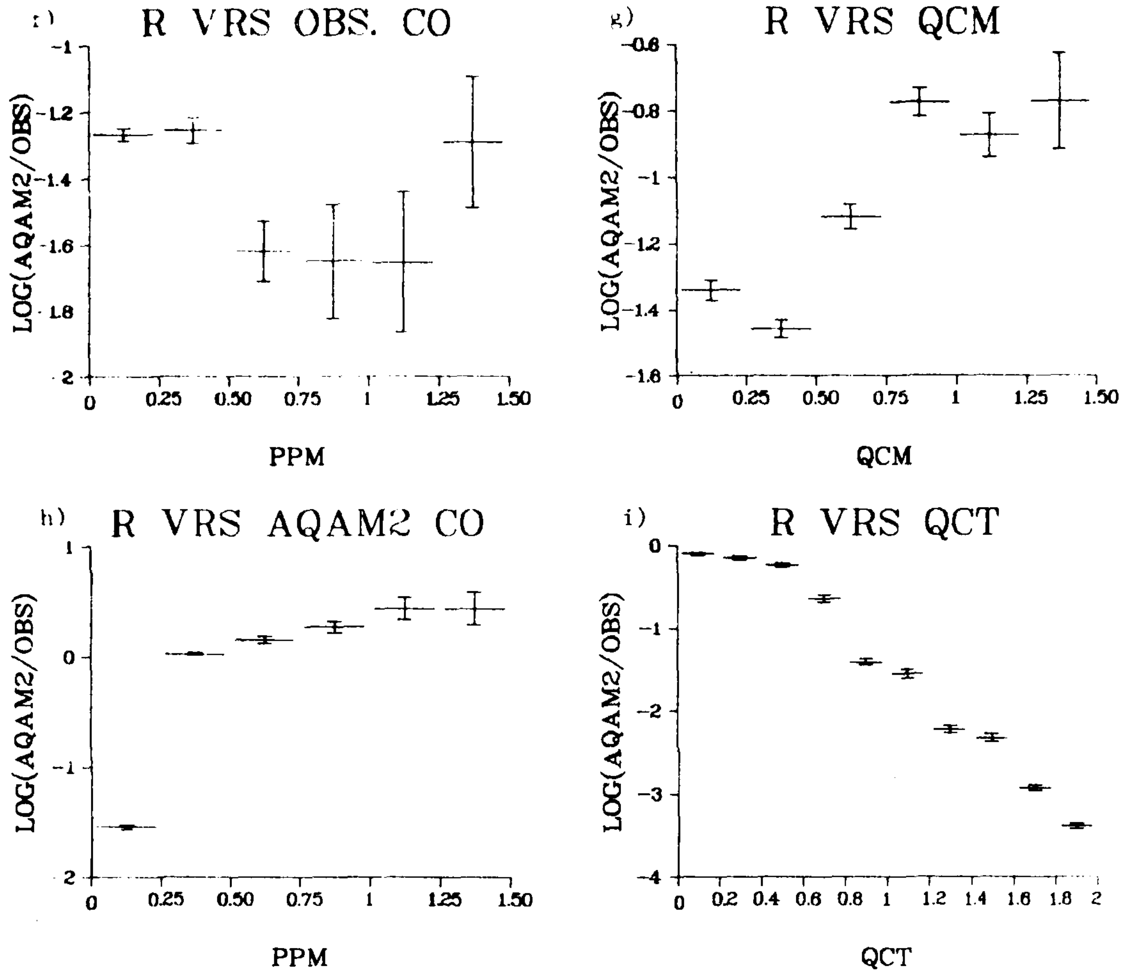


Fig. 15a-e. The Log Residual, $R \equiv \log_{10}$ (AQAM II/Observed), averaged over all stations, between the Observed and AQAM II CO Concentrations vs

a) windspeed (u)
b) q_u
c) σ_θ
d) q_θ
e) Turner stability class

Error bars indicate the standard deviation of the mean



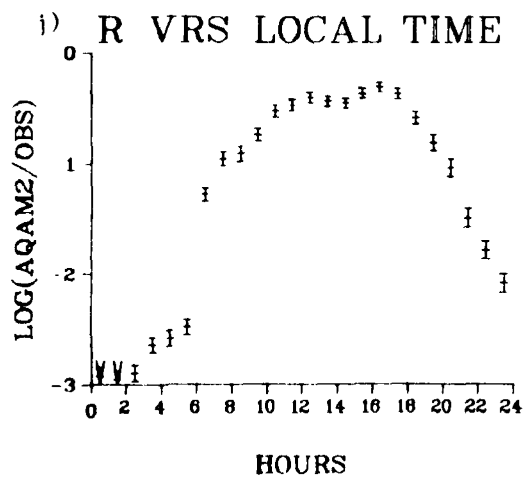


Fig. 15f-j. The Log-Residual, $R \equiv \log_{10}$ (AQAM II/Observed), averaged over all stations, between the Observed and AQAM II CO Concentrations vs

- f) $\bar{C}_M$
- g) q_{CM}
- h) $\bar{C}_T$
- i) q_{CT}
- j) local time

Error bars indicate the standard deviation of the mean

SECTION IV

SPECIFIC TESTS OF HYPOTHESES

A. Introduction and Strategy

Assumptions, hypotheses, and questions regarding the Williams Air Force Base air pollution monitoring program, the Air Quality Assessment Model, and the comparison of the AQAM to the Williams Air Force Base air pollution monitoring program evolved during the early phases of the experiment from a joint effort between EES/ANL and CERF/UNM.

In this section we present these hypotheses, the initally proposed methods for investigating these hypotheses, and results of examining these hypotheses. Often there are several methods, of varying difficulty to carry out, for investigating or testing a specific hypothesis. Thus it was difficult to assess the effort required to evaluate a given hypothesis in advance of examining the data. A reasonable strategy was to address those hypotheses which were easiest to make a clear definitive statement about. Often such a statement results from a single plot or simple linear regression, while in other not so transparent cases one must utilize multiple linear regression, non-linear optimization, or multiple time series analysis techniques. The specific hypotheses and tests which follow were designed to span the widest range consistent with the scope of the experimental effort.

B. Assumptions and Hypotheses about the Williams AFB Air Monitoring Program

ASSUMPTIONS

1. All instrumentation systems and data adquisition systems are functioning properly and reliably. Extensive checking of data by Northrop and EPA personnel have ensured the reliability of these data as documented in Reference 1. The overall data recovery rate is about 70%.

2. The sampling rates for meteorology and pollutants are sufficiently high. This has been confirmed by higher repetition rate sampling and is reported in Appendix H.

3. The data sample is sufficiently large and covers a wide enough range of meteorological and source activity conditions to test the hypotheses stated below. The 13-month sample under consideration provides adequate coverage except with respect to rare event situations (i.e., once per year or less).

4. The observed hourly average concentrations (aerometric signals) are insensitive to minor perturbations (e.g., a shift of tens of meters) in trailer locations. No tests of this assumption were performed in the field, though modeling exercises suggest that stations 2 and 3 are quite sensitive to uncertainties in the jet plume dynamics.

5. The reproducibility and repeatability* errors associated with the sampling system are known. These are reported in Reference 1.

HYPOTHESES

B1. The hour-to-hour variations in signal strength are significant with respect to system repeatability noise for all instruments. This hypothesis is tested by direct comparison of mean single strength to instrument threshold and the standard deviation of hourly fluctuations about the mean to repeatability noise as determined by the EPA or instrument manufacturer. The statistical summaries and cumulative frequency distributions in Appendix A suggest that reasonable fraction of the data (e.g., > 80% for CO, > 50% for NMHC, and > 90% for NO_x) lie well above instrument threshold and noise levels for all stations. Further insight into the hour-to-hour variations can be obtained from typical 3-d concentration time histories (Figures 16a-c) and from displays of the diurnal variation of mean concentration levels (Figures 17a-c). The average hour-to-hour variations are also clearly significant relative to the standard deviation of the mean, also shown in Figure 17.

B2. The station-to-station variations in signal strength are significant with respect to reproducibility errors a reasonable fraction of the time (so as to provide adequate statistics). This is tested by comparing the root-mean-square residual between hourly average concentrations at a single station and the five station hourly mean to the instrument reproducibility errors as determined by the EPA or instrument manufacturer. This hypothesis may also be tested by visual examination of the frequency distributions (Figs. 18a-h) of pollutant level minus the minimum hourly average for the five-station network. For CO, about 65% of these background subtracted concentrations exceed 50 ppb (40% above 0.2 ppm) while for NMHC this percentage climbs to 70% (45% above 0.1 ppm). Unfortunately for NO_x only 40% of the minimum-subtracted values lie above a marginally significant 5 ppb, with only 20% above 10 ppb.

*Reproducibility refers to observed differences between similar instruments measuring the same quantity while repeatability refers to the differences observed when a single instrument measures the same quantity many times.

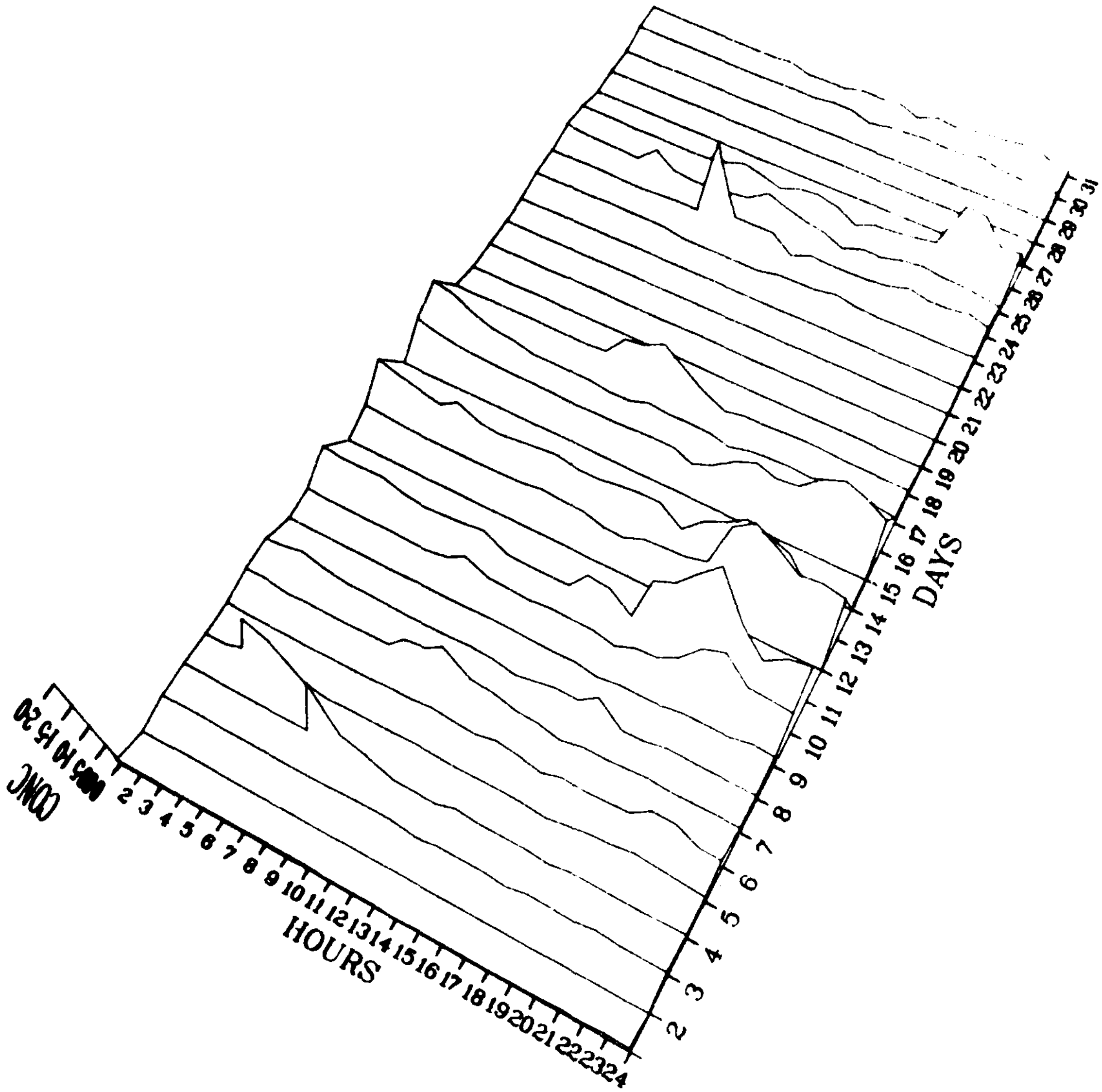


Fig. 16a. Three-Dimensional Time History of Observed CO Concentrations at Station 2 During January 1977

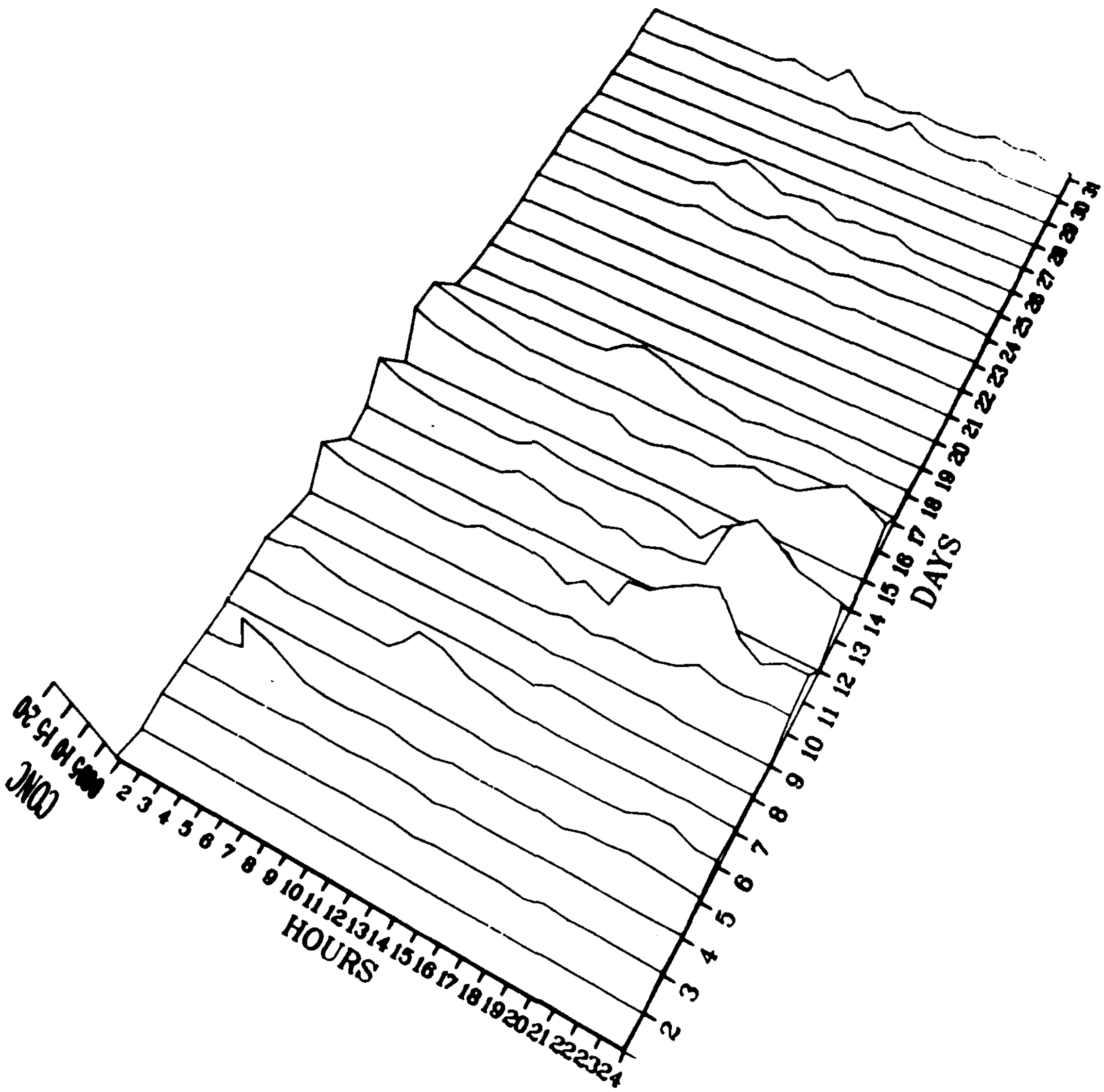


Fig. 16b. Three-Dimensional Time History of Observed CO Concentrations at Station 3 During January 1977

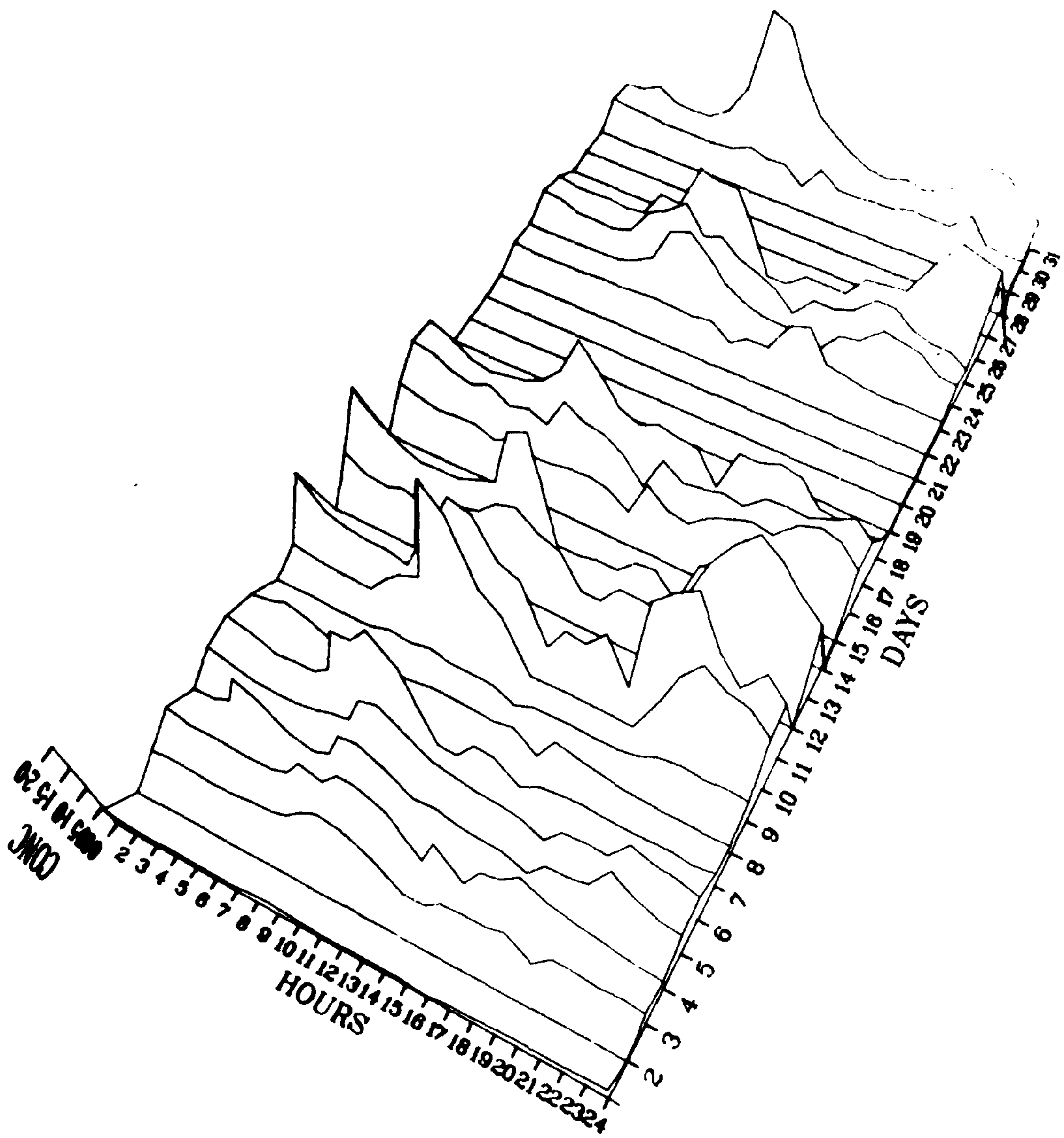
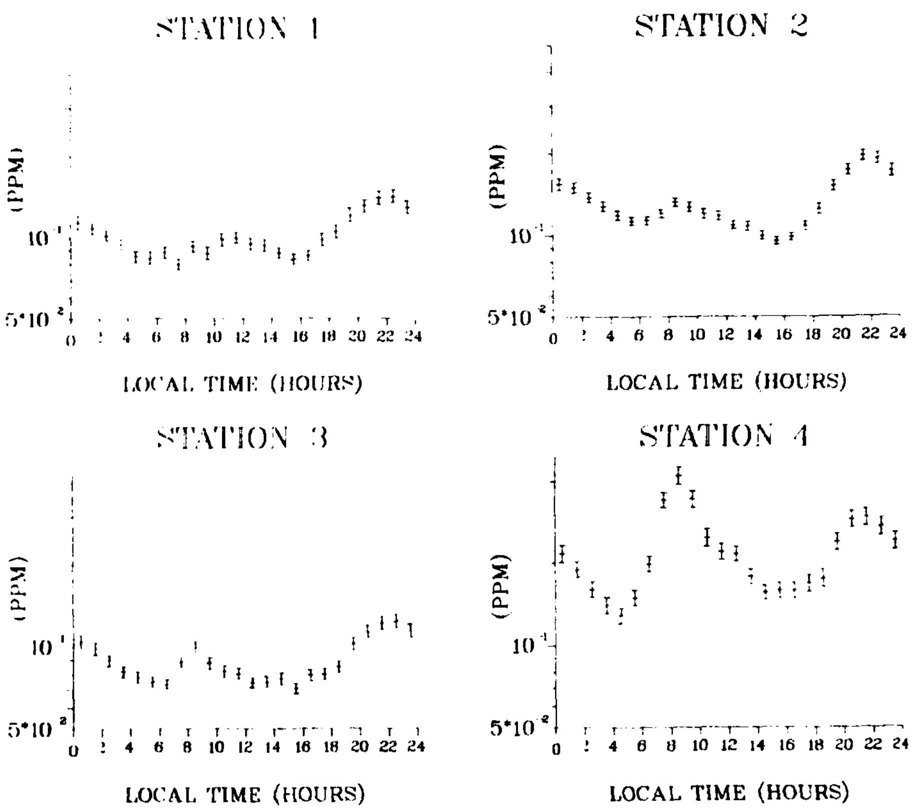


Fig. 16c. Three-Dimensional Time History of Observed CO Concentrations at Station 4 During January 1977



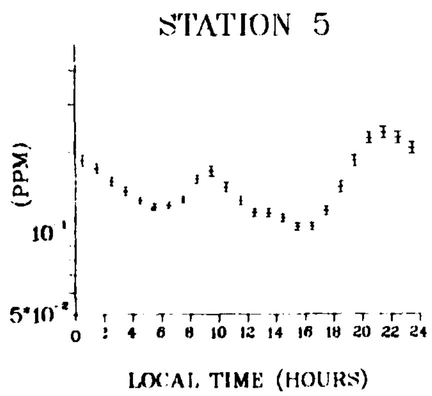
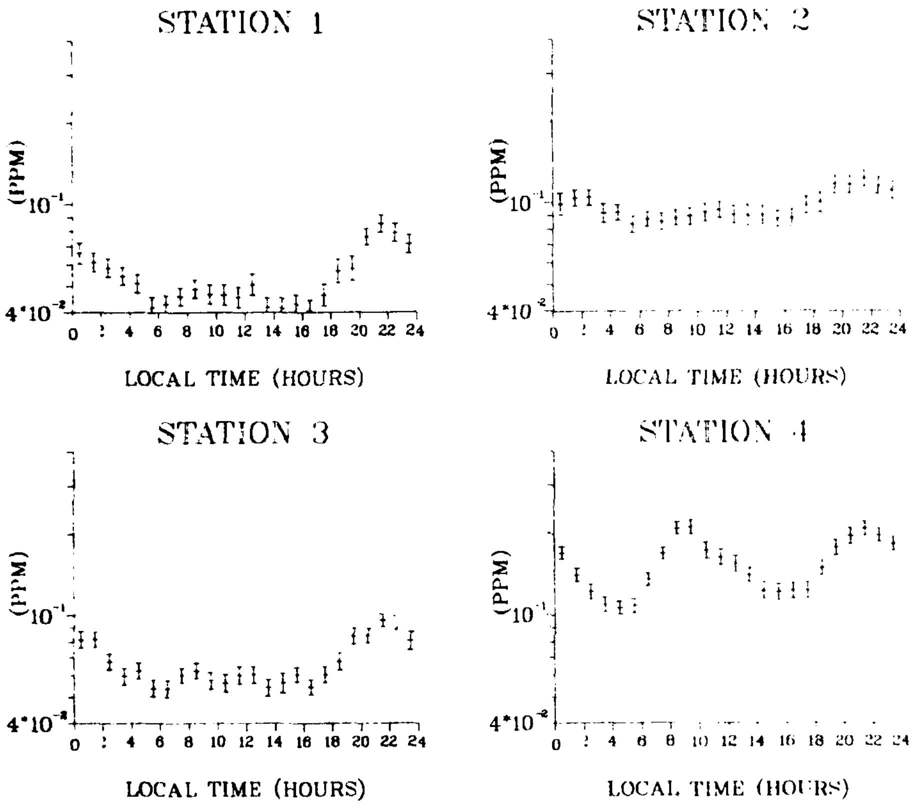


Fig. 17a. Average CO concentration at each receptor vs time of day. Data for the period June 1976-June 1977 are included. Error bars indicate the standard deviation of the geometric mean for the given hour. The actual range of concentrations is, of course, much greater than indicated by these error bars. Instrument threshold is about 50 ppb.



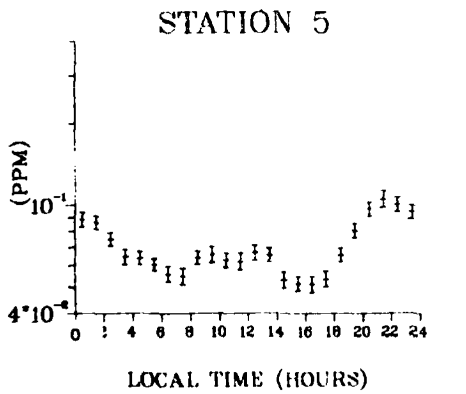
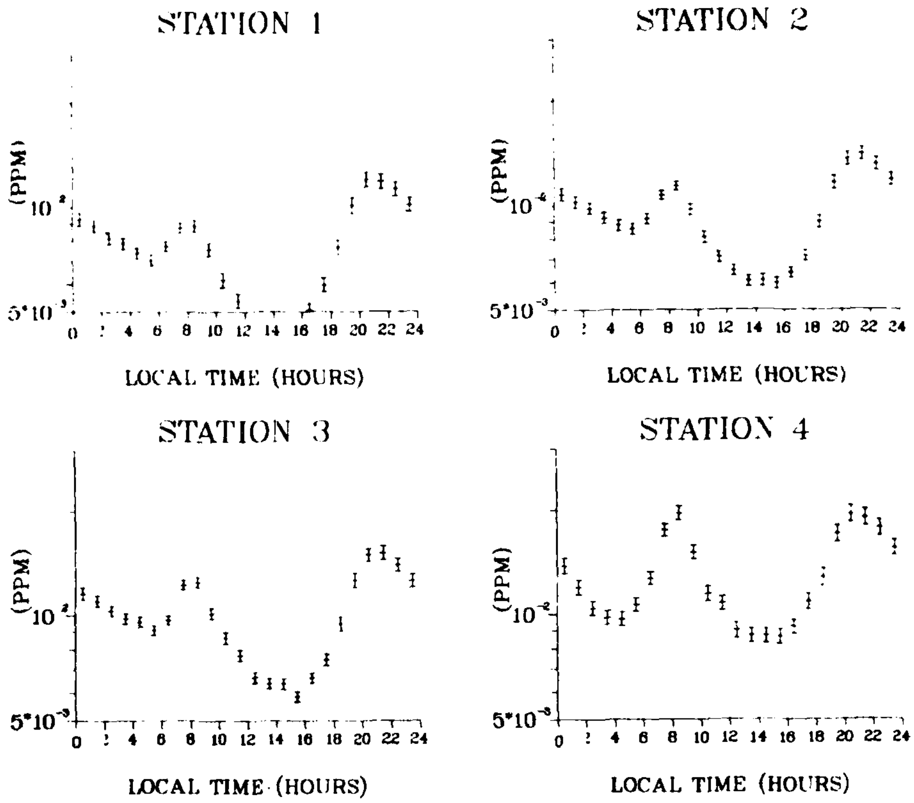


Fig. 17b. Average NMHC concentration at each receptor vs time of day. Data for the period June 1976-June 1977 are included. Error bars indicate the standard deviation of the geometric mean for the given hour. The actual range of concentrations is, of course, much greater than indicated by these error bars. Instrument threshold is about 50 ppb.



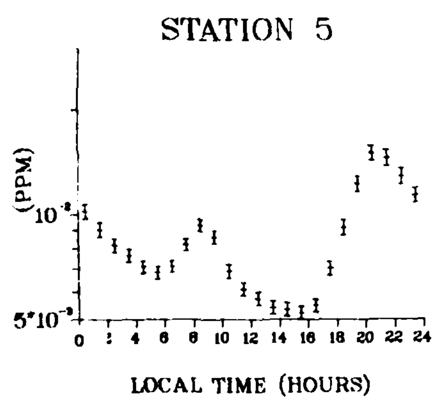


Fig. 17c. Average NO_x concentration at each receptor vs time of day. Data for the period June 1976-June 1977 are included. Error bars indicate the standard deviation of the geometric mean for the given hour. The actual range of concentrations is, of course, much greater than indicated by these error bars. Instrument threshold is about 2-5 ppb.

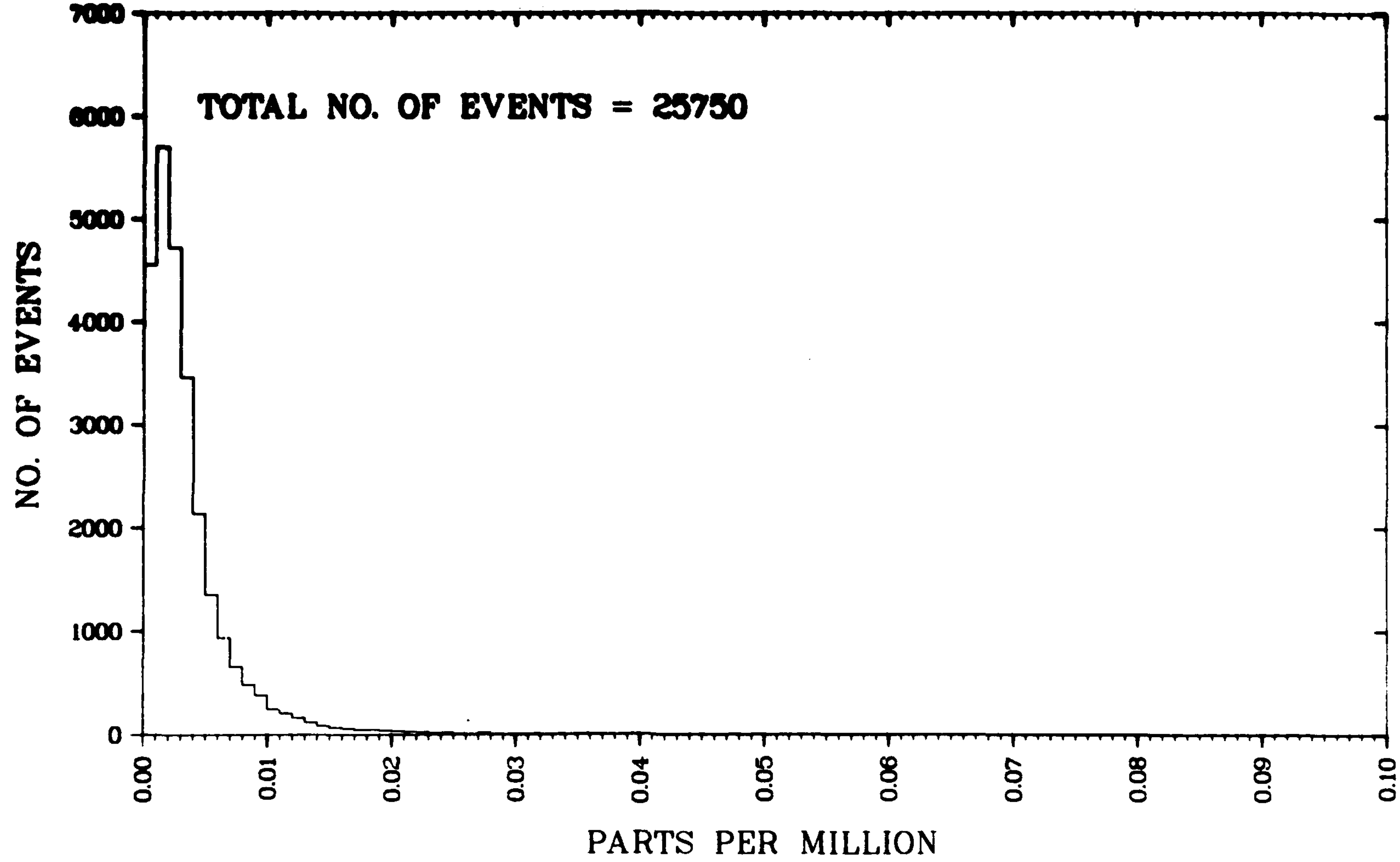


Fig. 18a. Background Subtracted Concentration Frequency Distribution for NO. All Stations Included. Background is Defined as the Minimum Hourly Average Concentration for the Five Station Network

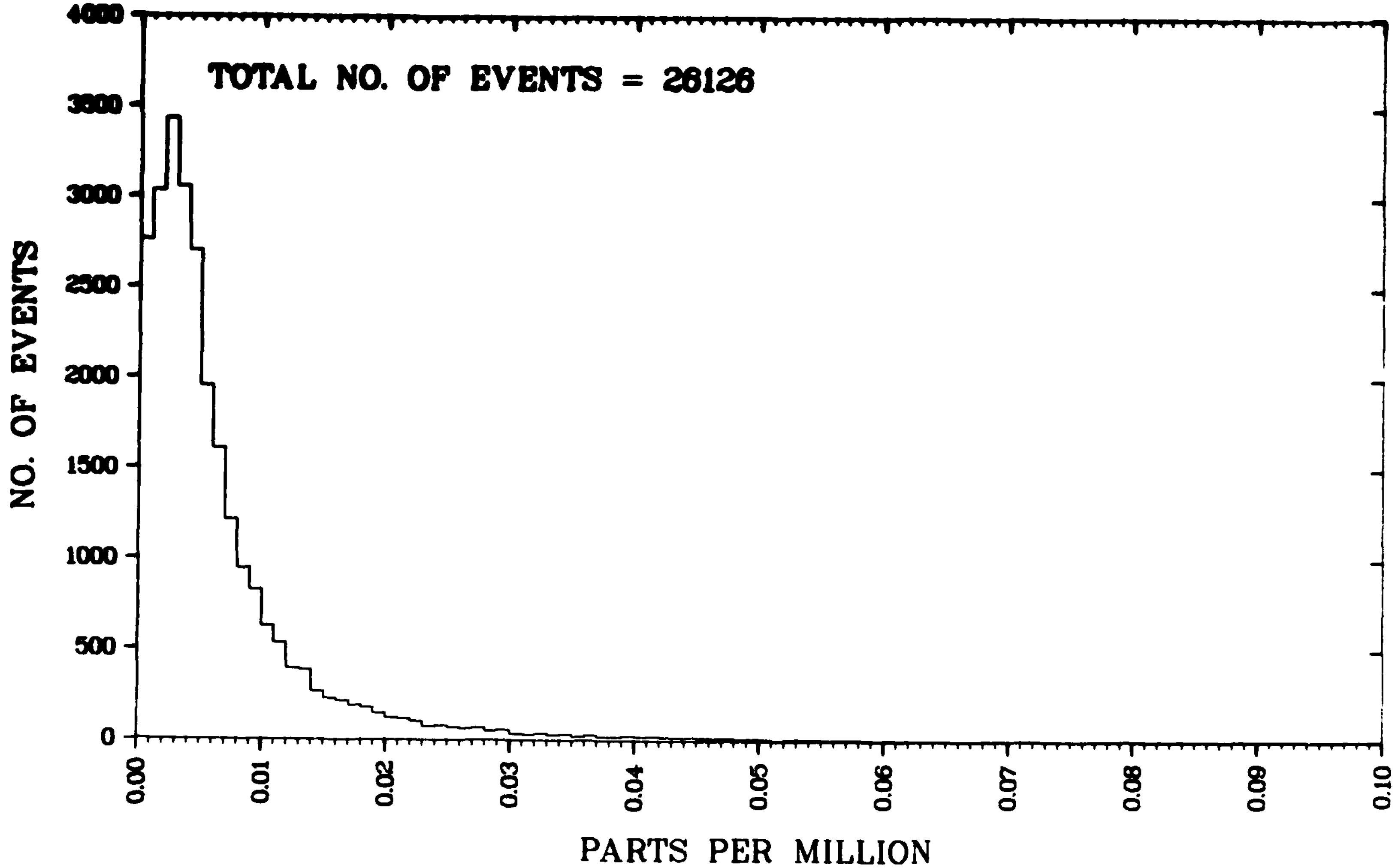


Fig. 18b. Background Subtracted Concentration Frequency Distribution for NO_x. All Stations Included. Background is Defined as the Minimum Hourly Average Concentration for the Five Station Network

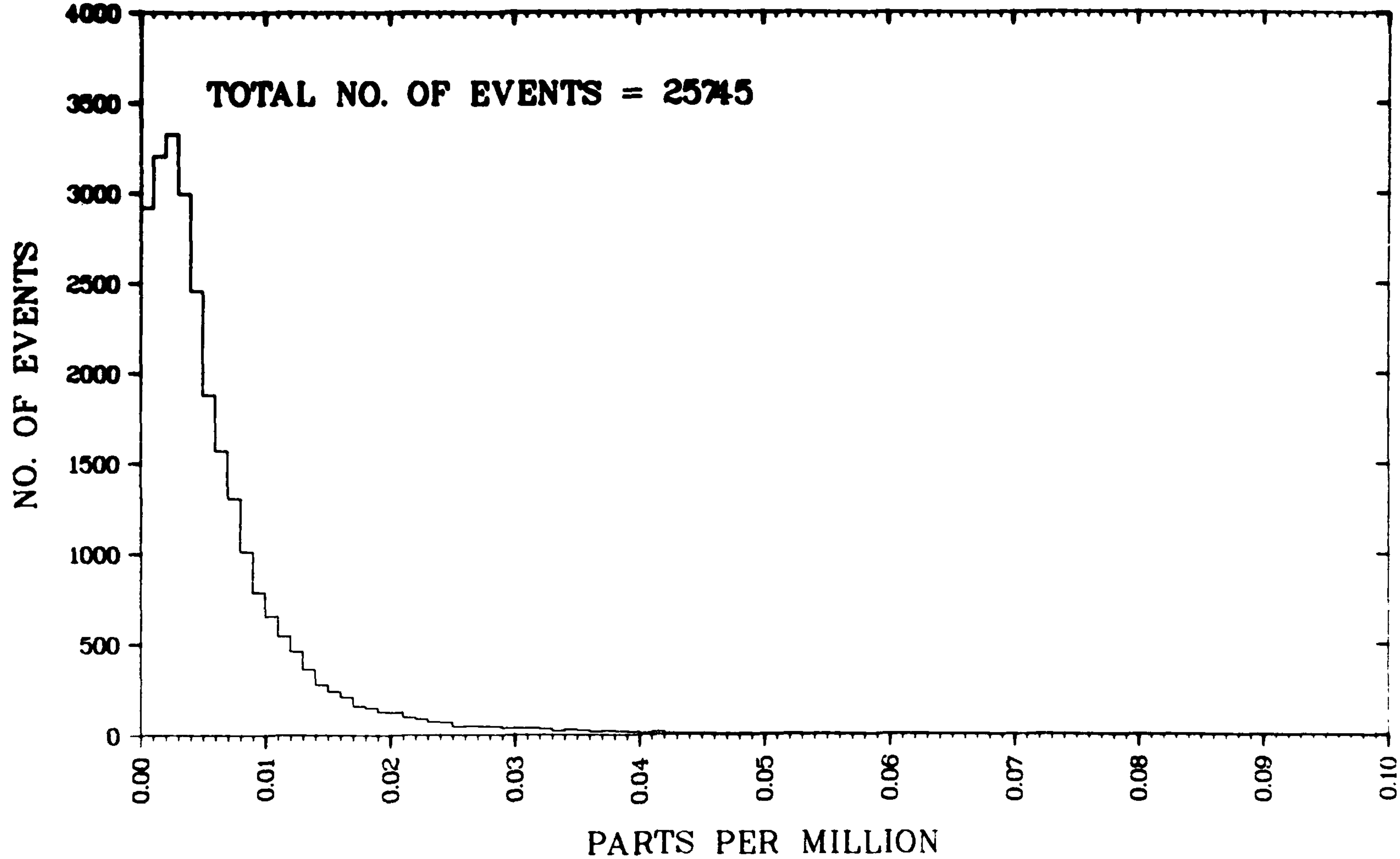


Fig. 18c. Background Subtracted Concentration Frequency Distribution for NO_2. All Stations Included. Background is Defined as the Minimum Hourly Average Concentration for the Five Station Network

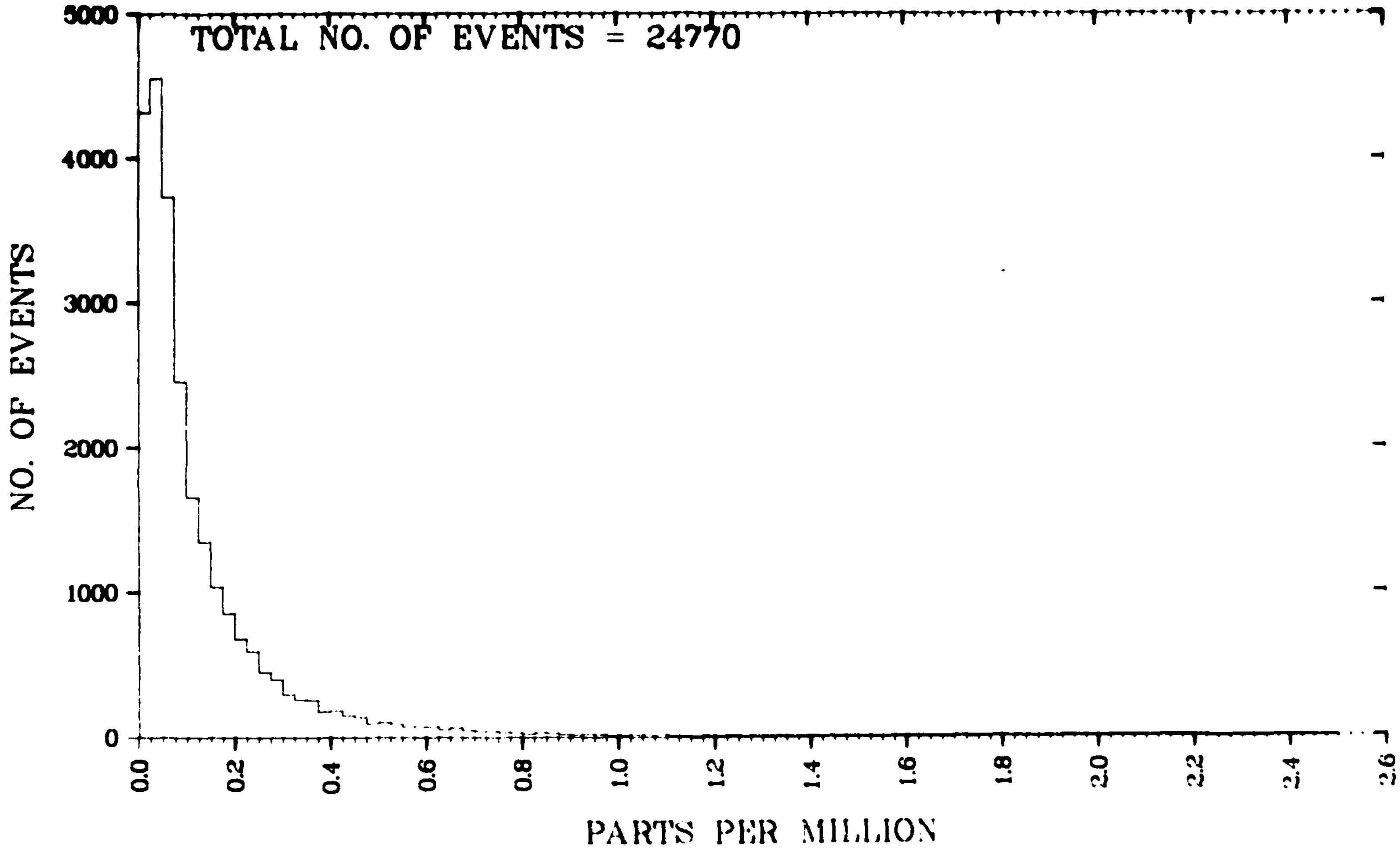


Fig. 18d. Background Subtracted Concentration Frequency Distribution for CO. All Stations Included. Background is Defined as the Minimum Hourly Average Concentration for the Five Station Network

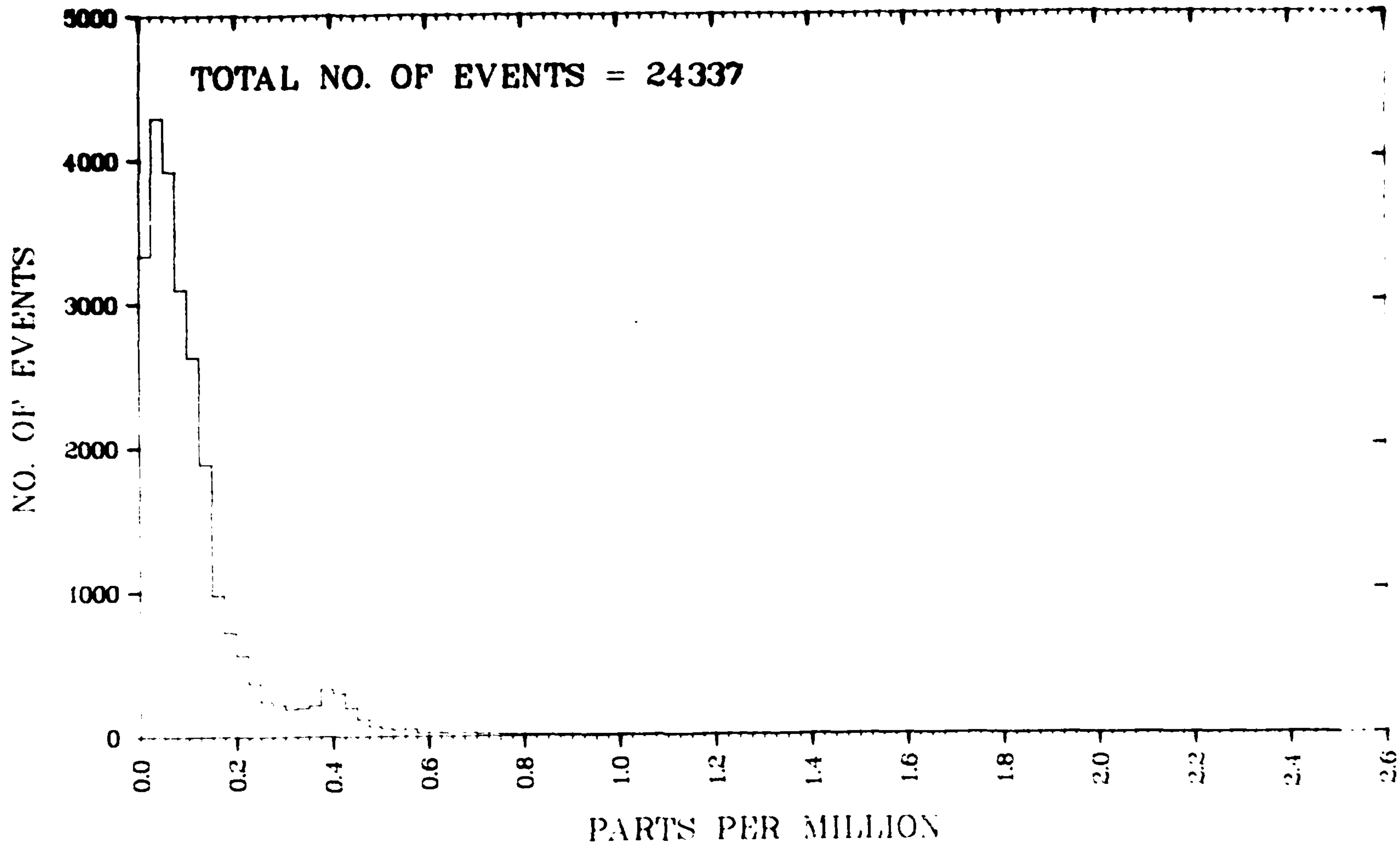


Fig. 18e. Background Subtracted Concentration Frequency Distribution for CH_4. All Stations Included. Background is Defined as the Minimum Hourly Average Concentration for the Five Station Network

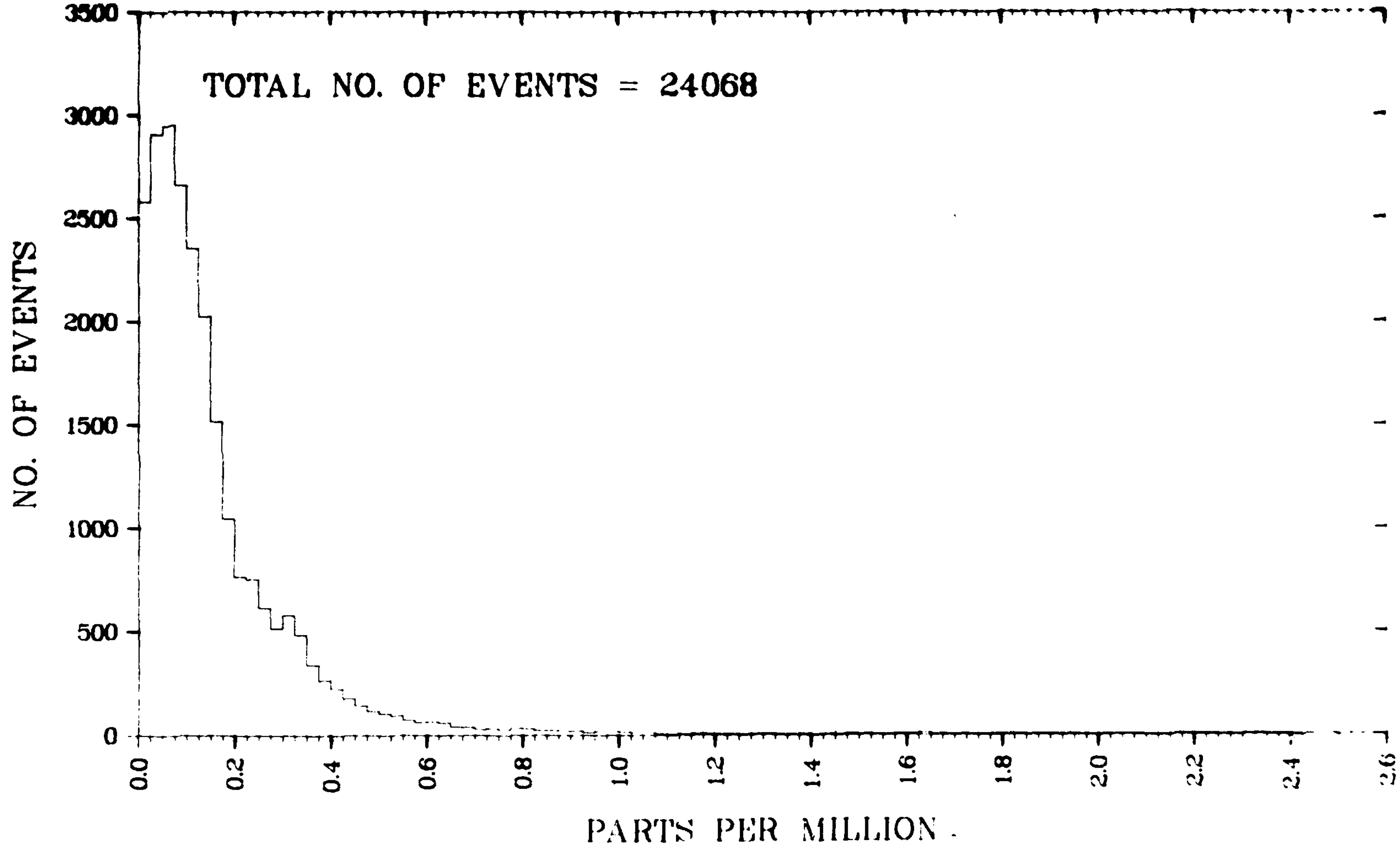


Fig. 18f. Background Subtracted Concentration Frequency Distribution for THC. All Stations Included. Background is Defined as the Minimum Hourly Average Concentration for the Five Station Network

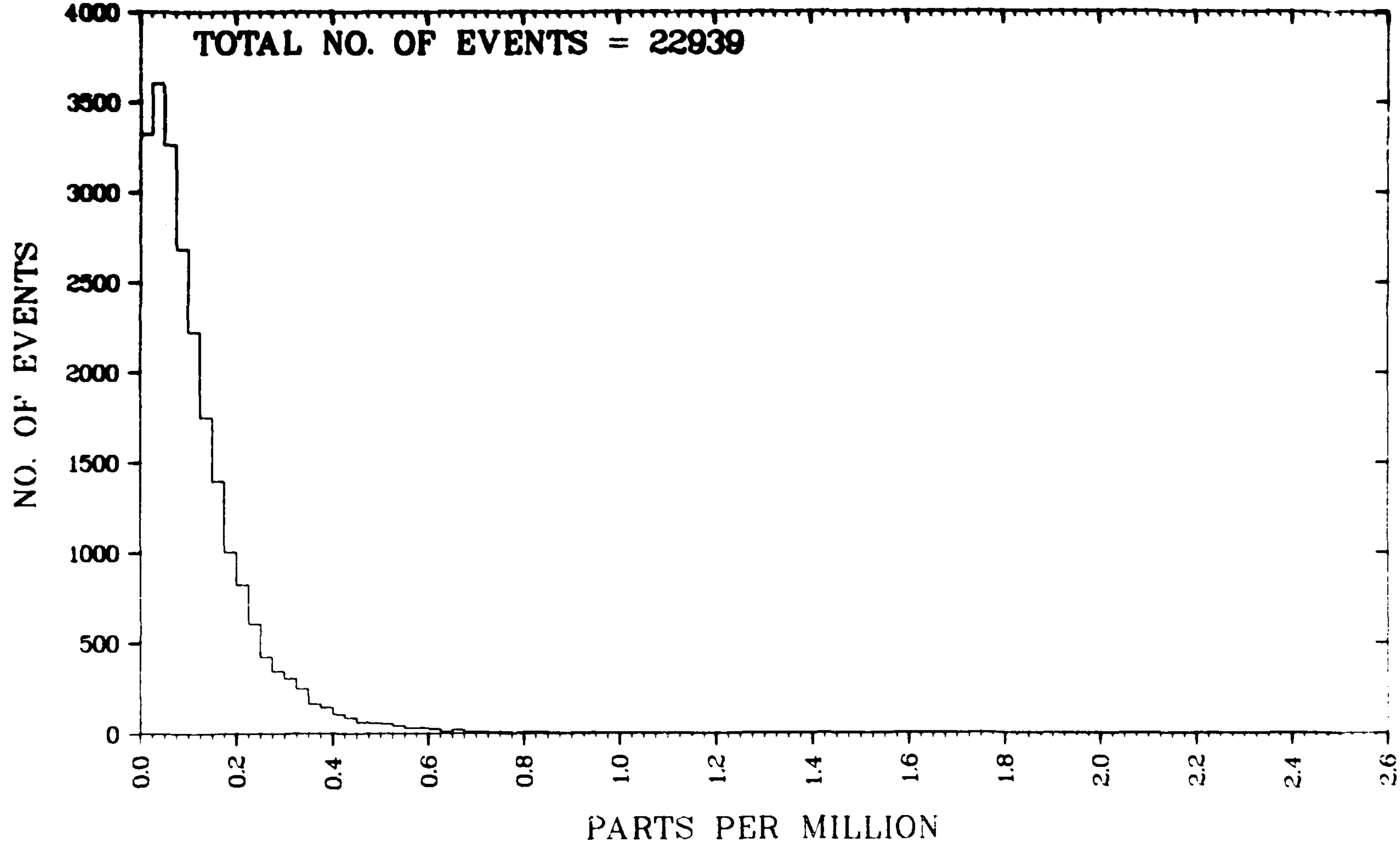


Fig. 18g. Background Subtracted Concentration Frequency Distribution for NMHC. All Stations Included. Background is Defined as the Minimum Hourly Average Concentration for the Five Station Network

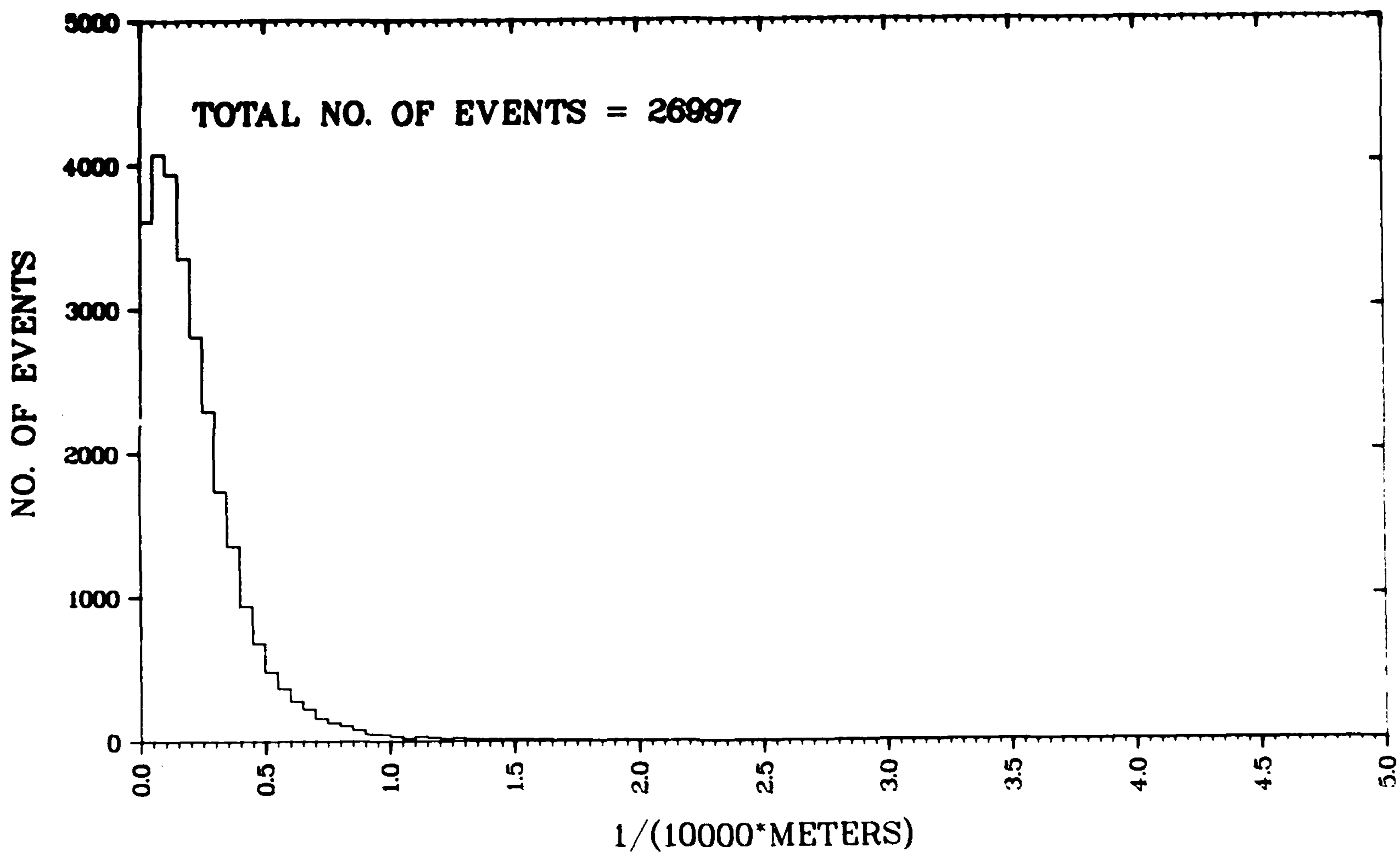


Fig. 18h. Background Subtracted Concentration Frequency Distribution for b_{SCAT}. All Stations Included. Background is Defined as the Minimum Hourly Average Concentration for the Five Station Network

B3. The aerometric signals are correlated with aircraft operations activity information. Simple scatter diagrams of level of aircraft activity versus hourly average pollution concentration or peak concentration suggest that meteorological dependences severely mask any visually observable effect. This hypothesis is examined further by using bivariate spectral analysis to determine the coherence between the various aerometric signals and the ensemble of aircraft operations. Rather significant coherence between CO observations at station 2 and aircraft CO emission rates (on all ground level lines based on actual hourly aircraft operations) is reported in Appendix I.

Another approach is to test the null hypothesis of no significant difference in pollutant concentrations for different levels of aircraft activity. Preliminary investigations suggest this is a reasonable procedure. The regression line through the plot of observed, station 2 daytime CO versus hourly aircraft emissions (Fig. 19) has a non-zero slope at the 7.2 standard deviation (SD) significance level (i.e., the ratio of the regression slope to the error in the slope equals 7.2). A plot of AQAM II predicted, station 2 CO versus hourly aircraft emissions (Fig. 20), with its non-zero regression slope of 31 SD of significance, is included for comparison and will be further considered in hypothesis D4.

Converting the results of these regressions into percentage influence of aircraft on station 2 CO levels, one finds average observed aircraft impacts of 11% at average emission rates and 29% at peak emission rates of 200 gms CO/sec.

A similar analysis for daytime THC indicates that observed levels at station 2 were found consistent (i.e, regression slope = -0.46 ± 0.33 ppb sec/gm) with the null hypothesis of no significant difference as might be expected since little NMHC is expected from the adjacent runways.

For NO_x at station 2, a non-zero regression slope of 3.1 SD of significance was found in the observed data yielding average aircraft percentage influences of 5% at average emission rates and 12% at peak emission rates. This level of influence seems rather low considering the proximity of runways 30C and 30R.

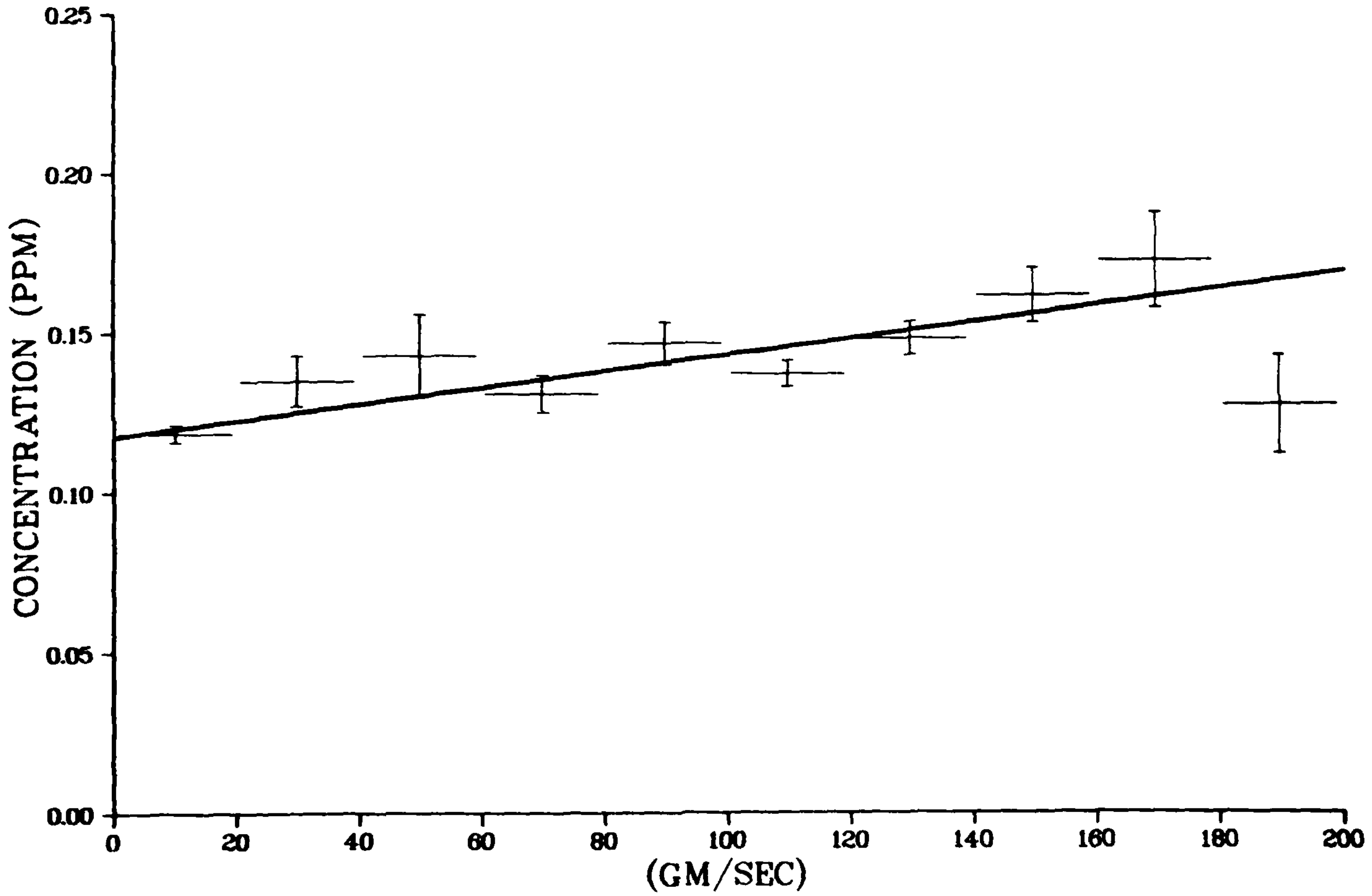


Fig. 19. Observed CO Concentrations at Station 2 During Daytime Hours (6 AM - 6 PM) Versus Hourly Average Aircraft Emission Rate (gm/sec) at Ground Level in the Taxi/Idle Mode. Williams AFB

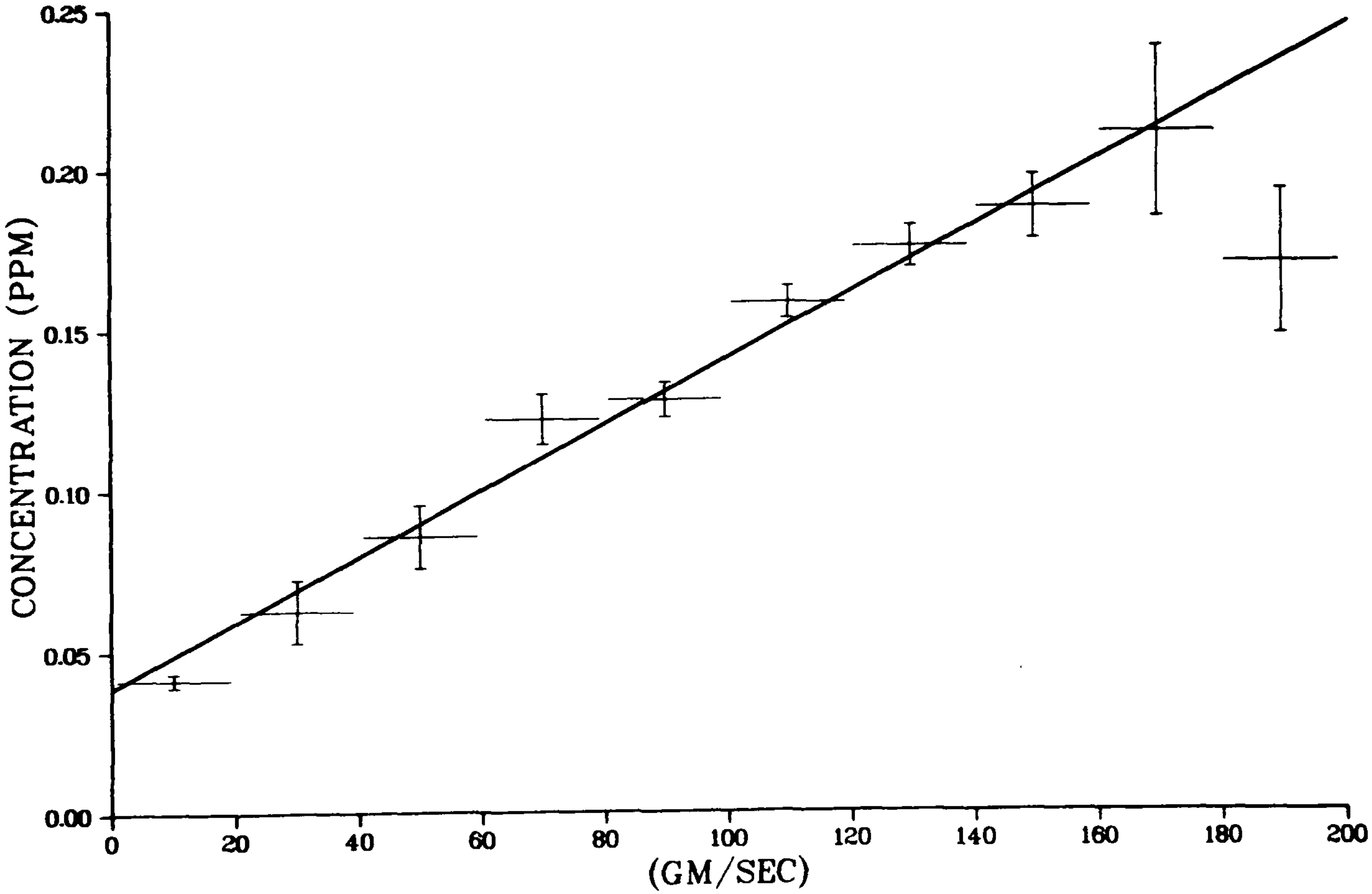


Fig. 20. AQAM II Predicted Concentrations at Station 2 During Daytime Hours (6 AM - 6 PM) Vs Hourly Average Aircraft Emission Rate (gm/sec) at Ground Level in the Taxi/Idle Mode Williams AFB

Additional aircraft emissions impacts on observed and predicted concentrations are given in Table 3.

B4. A non-airbase background can be extracted from the aerometric signals (for a reasonable number of hourly average observations) so that the airbase contributions can be distinguhished from the background contributions. As described in Section II C, there are many schemes for defining and extracting a background, though none of these schemes guarantee extraction of the true background. In addition, the more reasonable estimators of background involve use of AQAM results and are thus model-dependent: A fact which renders them unsuitable for this particular hypothesis.

If the minimum of the five-station hourly averages is chosen as background, then the remainder of this hypothesis, that is the question of distinguishing airbase contributions from background, reduces to hypothesis B2. In this case one finds that, depending on pollutant and assumed instrumental accuracy, between 20-65% of the data lie more than one standard deviation of interstation instrument uncertainty above background. One further notes that a level of 20% could be obtained merely by having one station (e.g., station 4) read above background while the other four stations read background.

In conclusion, a background (as distinct from the background) may be extracted for a reasonable number of hours so that airbase contributions can be distinguished from this assumed background.

The time series and distributional nature of the extracted background may then be compared with known characteristics of background concentrations; however, the complexities introduced by having strong correlations between wind direction and time of day and the presence of a large metropolitan area (Phoenix) a few hours of transport away, make such a comparison difficult at best. We note from Figures 17a-c that, in the mean, stations 1 and/or 3 see the lowest levels at all times of day and for all pollutants. These data and Table A4 suggest annual geometric mean backgrounds of $\sim$0.1 ppm for CO, $\sim$0.04 ppm for NMHC, and $\sim$7.4 ppb for NO_x. Nighttime levels for all pollutants are clearly elevated as much as a factor of two (up to three for NO_x) above daytime levels. The morning peak (8-10 AM) which is seen in CO and NO_x is probably not a true background peak but merely a reflection of rush hour being observed at all five stations.

Table 3. Williams AFB Aircraft Emissions Impact on Annual Average Hourly 6AM-6PM Concentrations

	Total Concentration (ppm)	Concentration Without Aircraft* (ppm)	Aircraft Contribution (ppm)	Percent Aircraft Contribution
		CO		
Station 1				
Observed	0.114	0.105	0.009	8
AQAM II	0.071	0.040	0.031	44
Station 2				
Observed	0.134	0.119	0.015	11
AQAM II	0.106	0.039	0.067	63
Station 3				
Observed	0.108	0.093	0.015	14
AQAM II	0.195	0.064	0.131	67
Station 4				
Observed	0.362	0.230	0.132	36
AQAM II	0.345	0.168	0.177	51
Station 5				
Observed	0.156	0.136	0.020	13
AQAM II	0.099	0.046	0.053	54
		NMHC		
Station 2				
Observed	0.123	0.128	-0.005→ consistent with zero	0
AQAM II	0.039	0.019	0.020	51
Station 4				
Observed	0.215	0.155	0.060	28
AQAM II	0.209	0.071	0.138	66
		NO_x (concentrations in ppb)		
Station 2				
Observed	9.44	8.98	0.46	5
AQAM II	3.68	2.15	1.53	42
Station 4				
Observed	15.1	11.5	3.6	24
AQAM II	8.4	6.6	1.8	41

*Based on regression of pollutant vs AQAM II estimated aircraft emissions on ground level line sources.

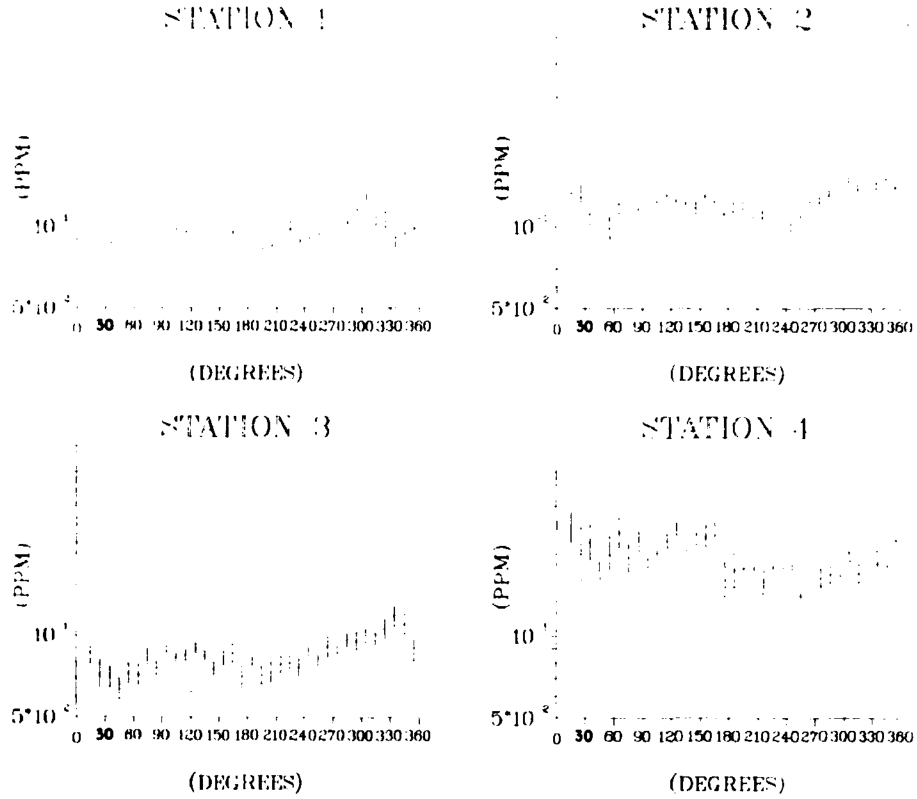
B5. The spatial inhomogeneities in the background over the sampling network are negligible for the averaging times of interest (i.e., that the coherence length of the background is large compared to the network size). This can be investigated by examining signal variance between stations during periods of minimal airbase activity. Whether a single coherence length can even be defined, as opposed to alongwind and crosswind coherence lengths, which are functions of meteorlogical variables, is debatable.

Unfortunately, in situ reproducibility tests on the Beckmann 6800 and Monitor Labs 8440 instruments were not performed during the course of the 13 month experiment. The resulting large interstation uncertainties (see ref. 1) of $\sim$0.2 ppm for CO, THC, and CH_4 and $\sim$20 ppb for NO and NO_x are of the same magnitude as expected background levels for all pollutants except methane, thus, rendering an analysis in terms of background coherence lengths beyond the resolution of this data base.

B6. The background-subtracted aerometric signals are significant with respect to the relevant errors and are correlated in space and time with aircraft activity. Contingent on success in extracting a non-airbase background signal (see hypothesis B4), the techniques used in testing hypothesis B3 may be used in this case also. Though more difficult to approach than the closely related hypothesis B3, this hypothesis should be less subject to interference than B3, where the principal interference stems from the essentially phase-locked nature of the aircraft activity, meteorological and background concentration dirunal cycles. However, regressing background subtracted hourly pollutant concentrations (where background is taken as the minimum hourly average of the five stations) against the AQAM II emission rate on all aircraft ground level lines leads to the surprising result that the regression slopes are less steep and less significant than when using unsubstracted concentrations (hypothesis B3). This result suggests that the defined background may itself be positively driven by aircraft activity and thus not really a background at all. In the case that all five stations are influenced by aircraft activity, it becomes impossible to define a model independent background. Such may indeed be the case under worst case conditions (i.e., high activity with low wind speed, stable conditions).

B7. <u>The aircraft source activity is the dominant contributor to the airbase portion of the aerometric signal.</u> Testing this hypothesis would be equivalent to demonstrating that the aircraft activity is among the most significant contributors to the variance in the airbase portion of the aerometric signal. A multiple linear regression analysis would indicate the relative significance of aircraft source activity in explaining the variance of the airbase signal. The simple linear regression described in hypothesis B3 (see also Figure 19) suggests that this hypothesis might be easily tested. For example, the regression line on Figure 19 indicates that at average levels of aircraft operations, aircraft account for 11% or 15 ppb (29% or 48 ppb at peak aircraft operating levels) of the average observed daytime CO level at station 2. For daytime NO_x at station 2 the regression yielded an average aircraft percentage impact of 5% (0.5 ppb) at average emission rates and 12% (1.2 ppb) at peak aircraft operating levels. Aircraft emissions impacts tend to be small at most other stations with two noticeable exceptions. Absolute and percentage impact of aircraft on station 3 CO is nearly identical to their impact on station 2 CO while aircraft show their largest impact on all station 4 pollutants, with average influences at average operations levels of 36% (0.13 ppm) on CO, 28% (0.06 ppm) on NMHC, and 24% (3.6 ppb) on NO_x as given in Table 3. Noting that large deviations from these average impacts can and do exist, one concludes that on the average aircraft are not the dominant contributor to the total aerometric signal. However, if one subtracts presumed background levels of 0.1 ppm CO, 0.04 ppm NMHC, and ppb NO_x from station 4 concentrations without aircraft (see Table B3), one observes that the aircraft portion of the aerometric signal can approximately equal the airbase non-aircraft portion under average aircraft operations levels. Thus, dominance of aircraft in the airbase portion of the aerometric signals for CO, NMHC, and NO_x may be expected during greater-than-average, aircraft activity levels.

B8. <u>The observed average concentrations as a function of wind direction show a dependence corresponding to the locations of known sources.</u> Pollutant roses (Figs. 21a-c) are quite useful in addressing this hypothesis; however, the strong correlation which exists between wind direction and time of day (see Figure 22) renders interpretation regarding source strengths and locations somewhat dubious. Background subtracted pollutant roses (Figs. 23a-c) represent an attempt to circumvent this bias; however, the process of averaging over all meteorological conditions tends to wash-out the capability of pinpointing pollution sources. An effective source-mapping technique has been developed and applied[8] to the



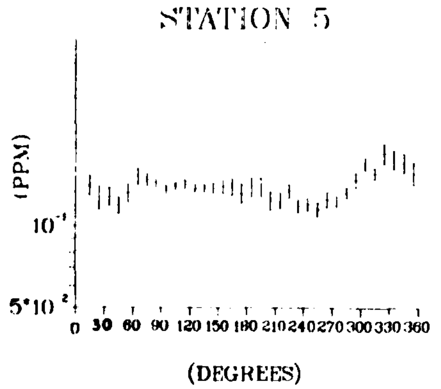
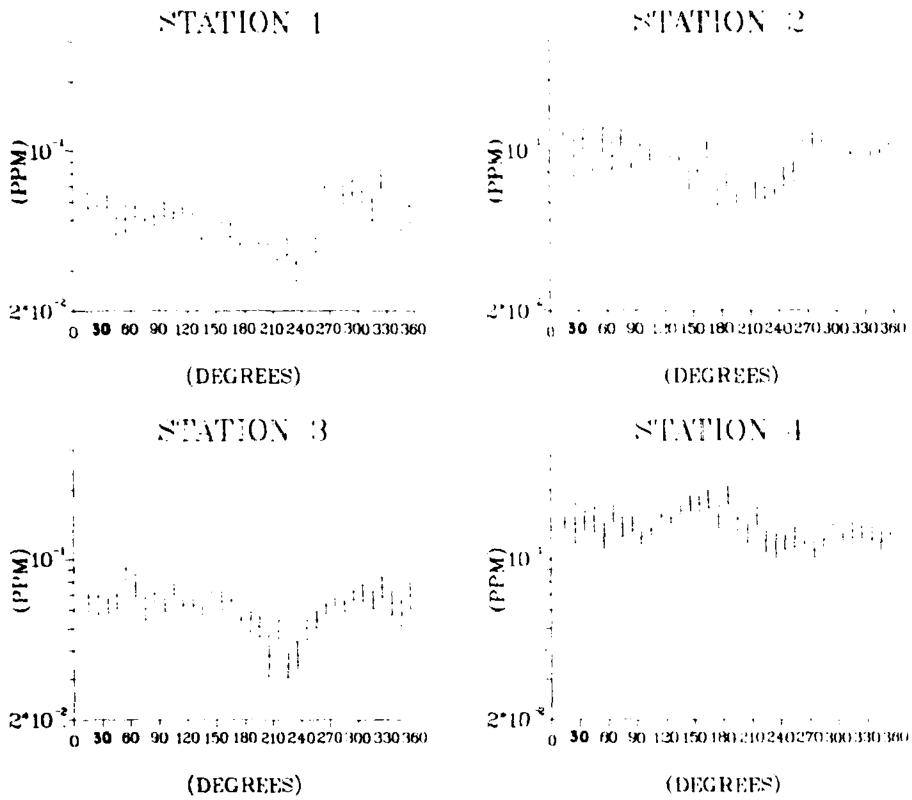


Fig. 21a. Hourly Mean CO Concentration at Each Receptor Vs Wind Direction. Data for the period June 1976-June 1977 are included. Error bars indicate the standard deviation of the geometric mean. The actual range of concentrations is, of course, much greater than indicated by these error bars.



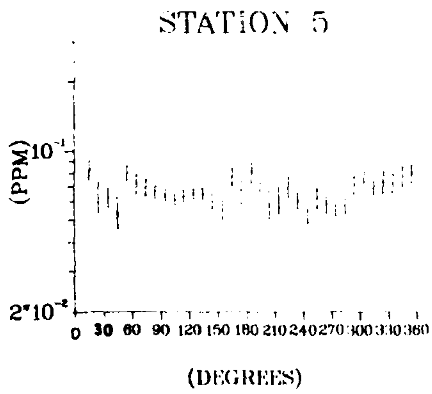
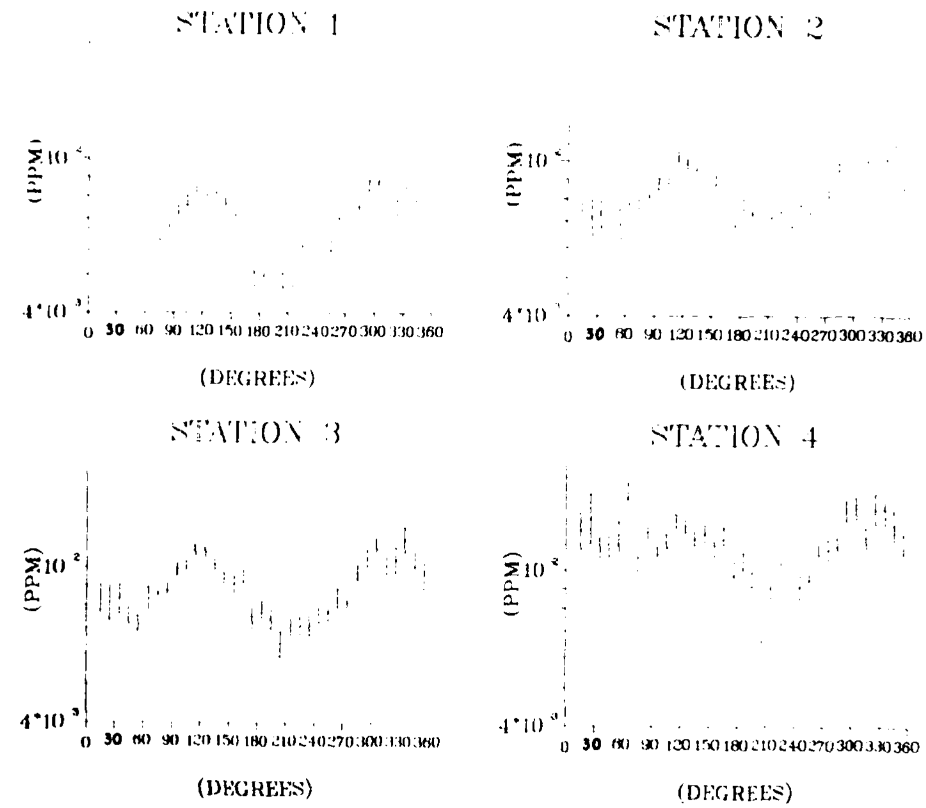


Fig. 21b. Hourly Mean NMHC Concentration at Each Receptor Vs. Wind Direction. Data for the period Jun 76-Jun 77 are included. Error bars indicate the standard deviation of the geometric mean. The actual range of concentrations is, of course, much greater than indicated by these error bars.



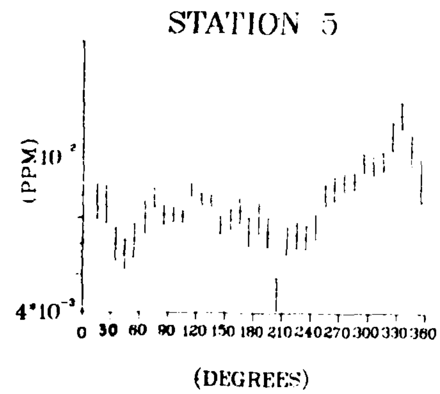


Fig. 21c. Hourly Mean NO_x Concentration at Each Receptor Vs Wind Direction. Data for the period Jun 76–Jun 77 are included. Error bars indicate the standard deviation of the geometric mean. The actual range of concentrations is, of course, much greater than indicated by these error bars.

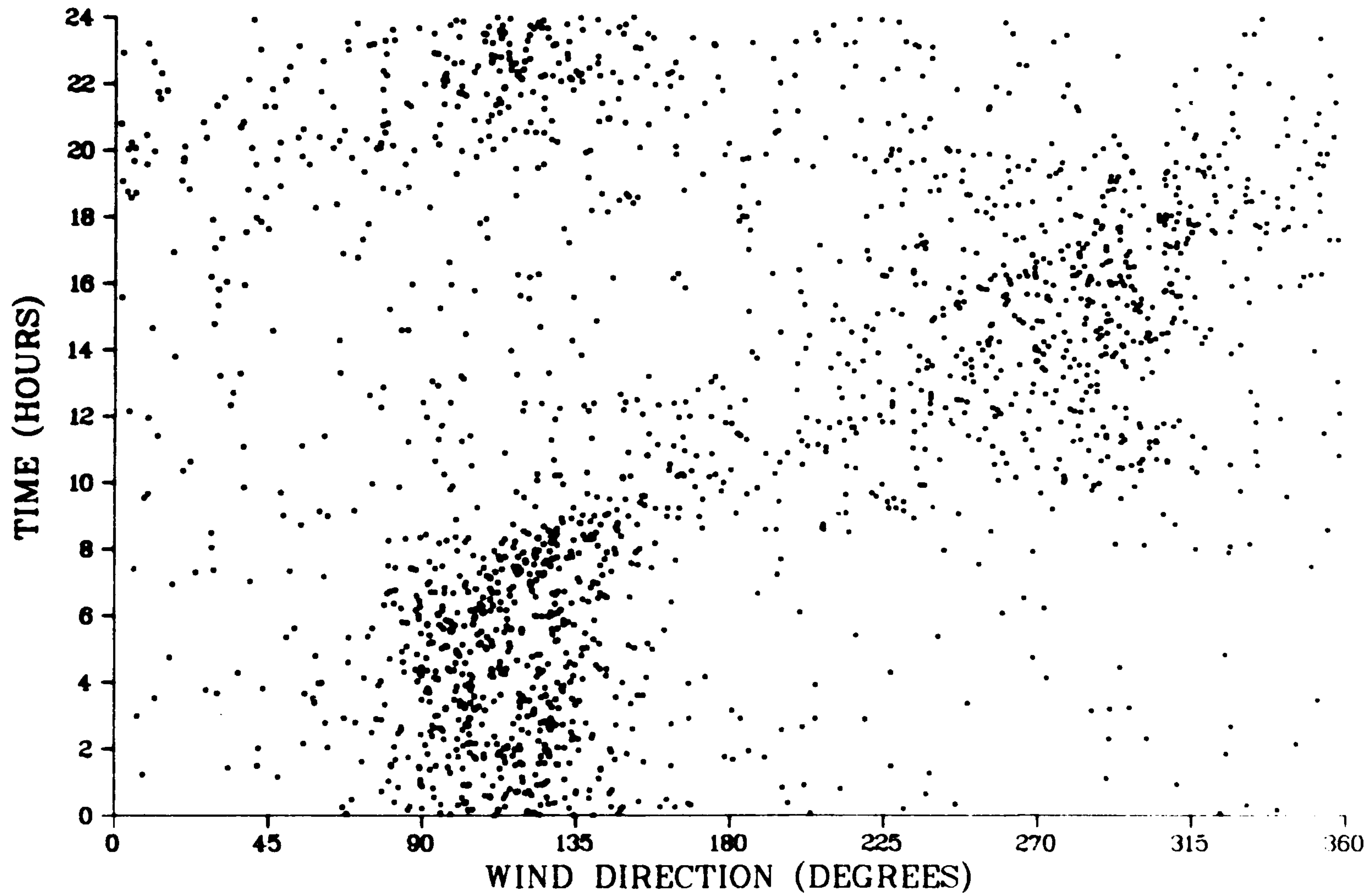


Fig. 22. Wind Direction at Station 2 Versus Time of Day (June 1976-June 1977)

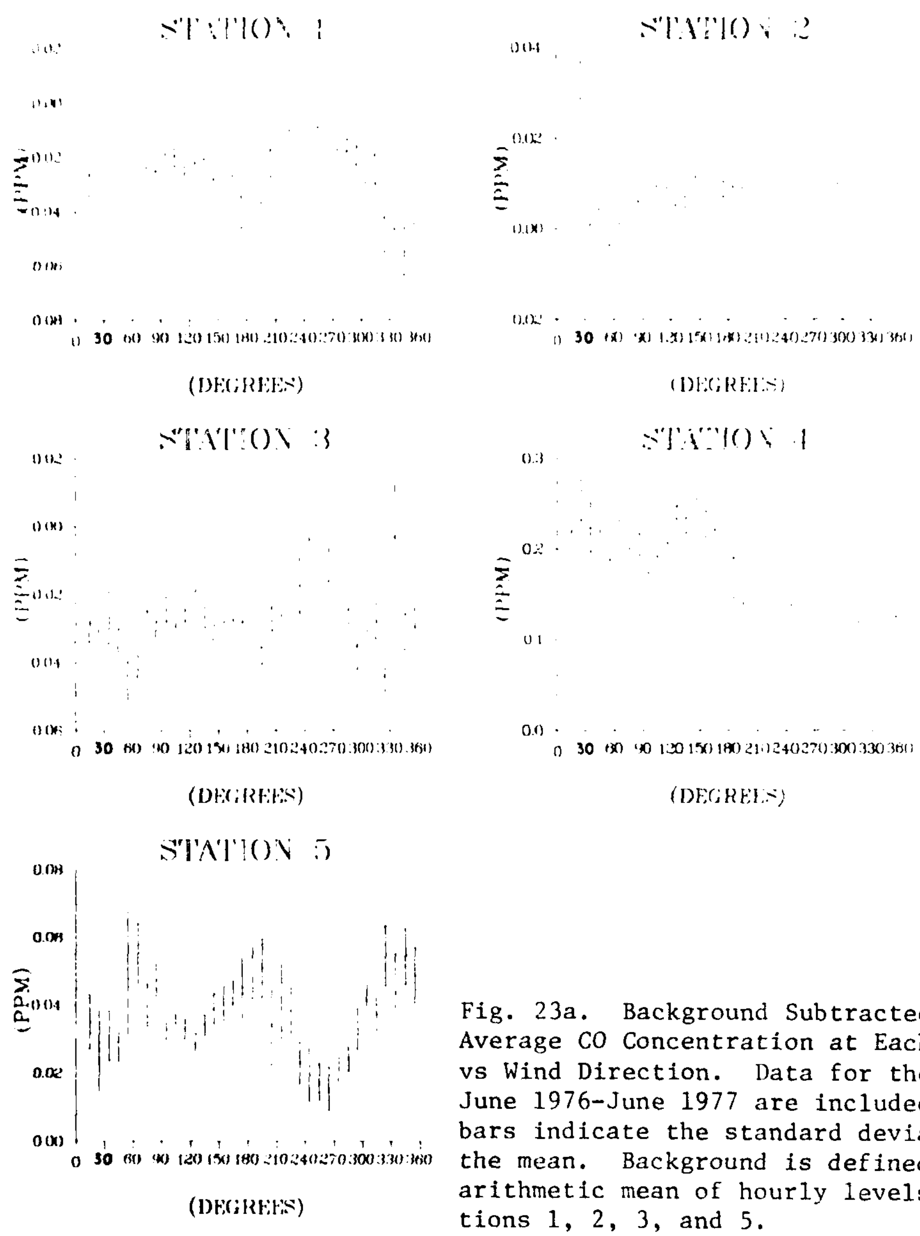


Fig. 23a. Background Subtracted Hourly Average CO Concentration at Each Receptor vs Wind Direction. Data for the period June 1976-June 1977 are included. Error bars indicate the standard deviation of the mean. Background is defined as the arithmetic mean of hourly levels at stations 1, 2, 3, and 5.

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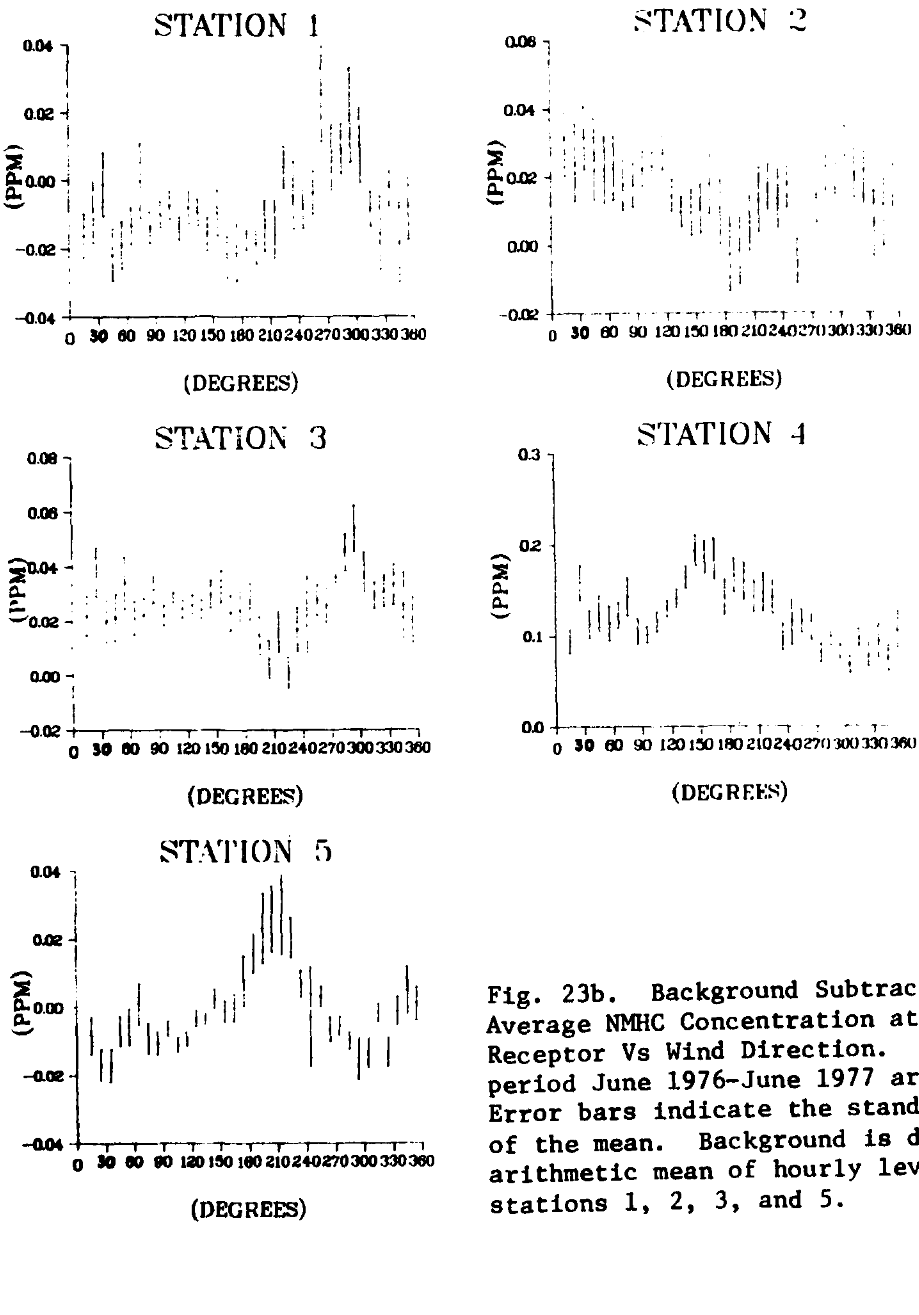
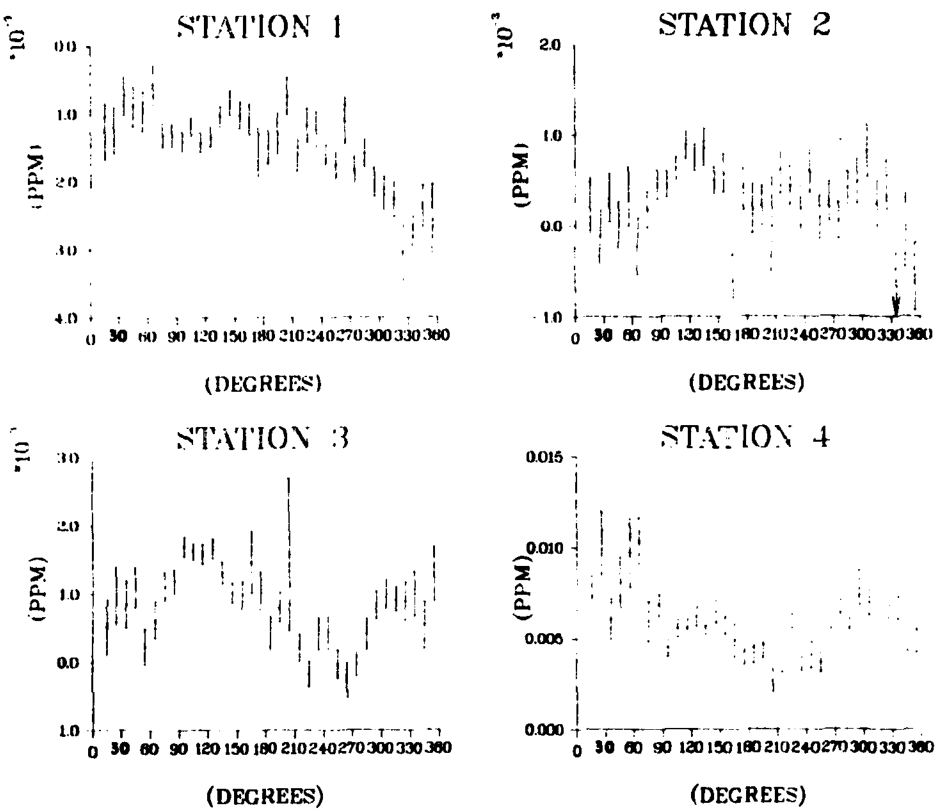


Fig. 23b. Background Subtracted Hourly Average NMHC Concentration at Each Receptor Vs Wind Direction. Data for the period June 1976–June 1977 are included. Error bars indicate the standard deviation of the mean. Background is defined as the arithmetic mean of hourly levels at stations 1, 2, 3, and 5.



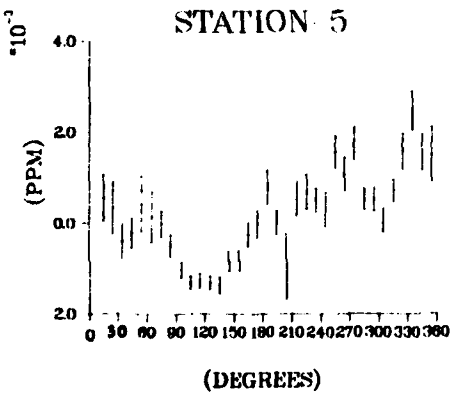


Fig. 23c. Background Subtracted Hourly Average NO_x Concentration at Each Receptor Vs Wind Direction. Data for the period June 1976–June 1977 are included. Error bars indicate the standard deviation of the mean. Background is defined as the arithmetic mean of hourly levels at stations 1, 2, 3, and 5.

CO observations at Williams AFB. The solution, plotted in Figure 24 as contours proportional to the logarithm of the source strength, corresponds well with the locations of known aircraft sources.

B9. There is an overall diurnal pattern in the data related to the characteristic diurnal variation in atmospheric ventilation (ventilation $\sim 1/uL$). This hypothesis could be verified by performing univariate spectral analysis on a segment of data of appropriate length and examining the power spectral density function; however, the acoustic sounder measured mixing depth data is generally only available for the few hours following sunrise. This sparsity of data would greatly impede any spectral analysis. In addition, we note that unless the pollution is well mixed within the layer of depth L, the influence of the mixing depth may be small.

Figure 25 shows the diurnal variation in station 2 windspeed while Figures 26a and 26j show the influence of wind speed and time of day respectively on the receptor averaged CO concentration. In addition, some insight into the dependence of mixing depth on time of day can be obtained from Figures B7 and B8. One observes that i) concentrations fall with increasing windspeed, ii) the 9 AM low and 4 PM high in windspeed corresponds to a high and low respectively in observed concentration (the fact that the concentration exhibits a much stronger dependence than shown by the windspeed alone might suggest the significance of the mixing depth but it could also result from the pronounced morning rush hour peak in source activity), and iii) the nighttime behavior of the concentration requires additional variables to describe its behavior.

Unfortunately, the strong diurnal dependence in source emissions leaves us unable to more rigorously confirm the ventilation hypothesis.

B10. The spatial variations in hourly average wind speed and wind direction over the airbase are negligible. Testing this hypothesis shoud help to support the assumption of a uniform wind field over the receptor network, a necessary assumption in the AQAM. Comparison of interstation variance in average wind speed and direction, normalized by the average windspeed and average hourly standard deviation of the wind direction respectively, should adequately address this hypothesis. As has been shown in Figure 13b, Station 4 often measures a wind direction which deviates more than one unit of σ_θ away from the average of wind directions measured at stations 1, 2, 3, and 5. Figure 13a indicated close agreement between wind direction measurements at stations 1, 2, 3, and 5. This same result has been found for wind speeds.[9]

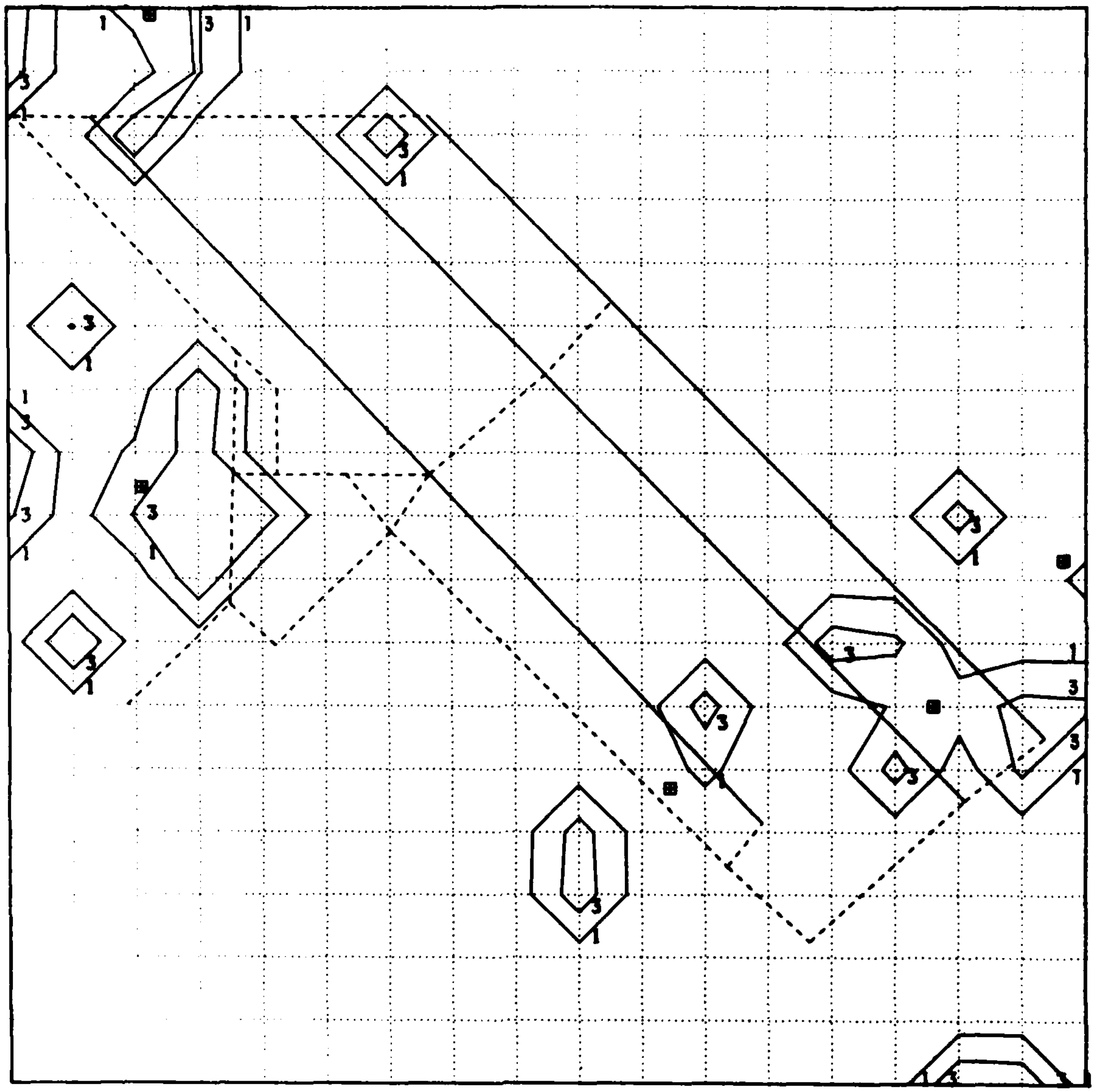


Fig. 24. Contours proportional to the logarithm of the source strength for the solution obtained by applying the exact source finding method to 13 months of hourly CO concentrations data from the five-station network at Williams AFB

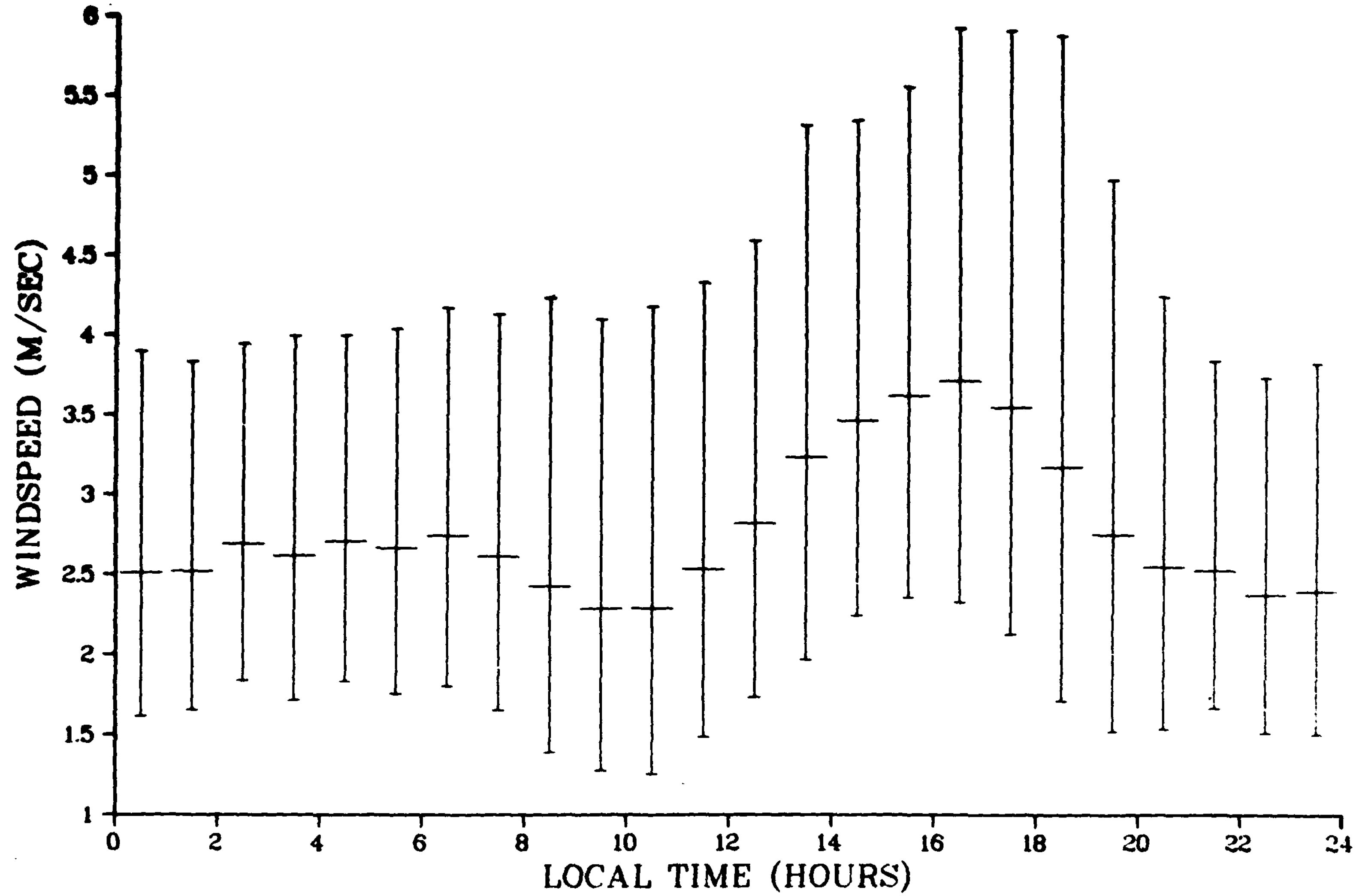
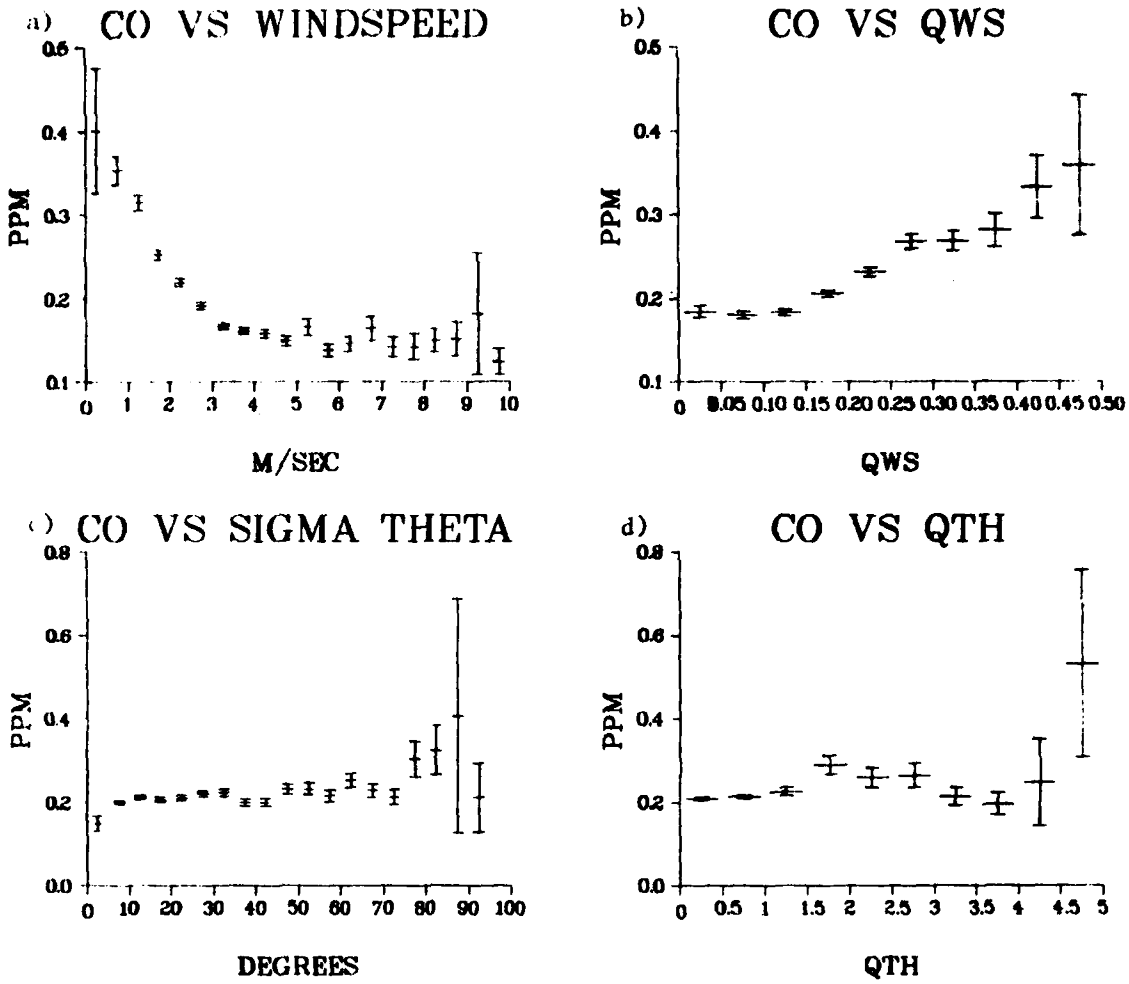


Fig. 25. Wind Speed at Station 2 Versus Time of Day. June 1976-June 1977. Error Bars Indicate the Standard Deviation of Speeds Within Each Hour



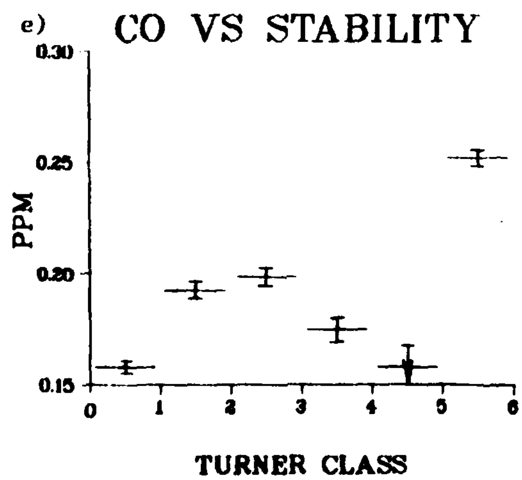


Fig. 26 a-e. Receptor Averaged Observed CO Concentration vs

a) u

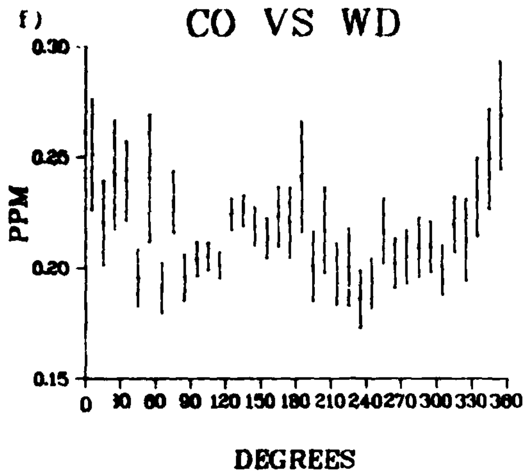
b) q_u

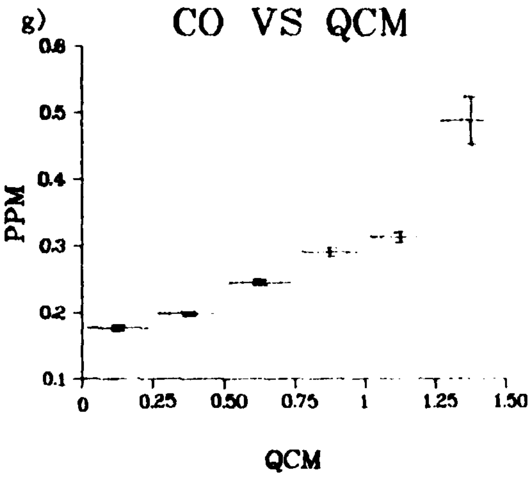
c) σ_θ

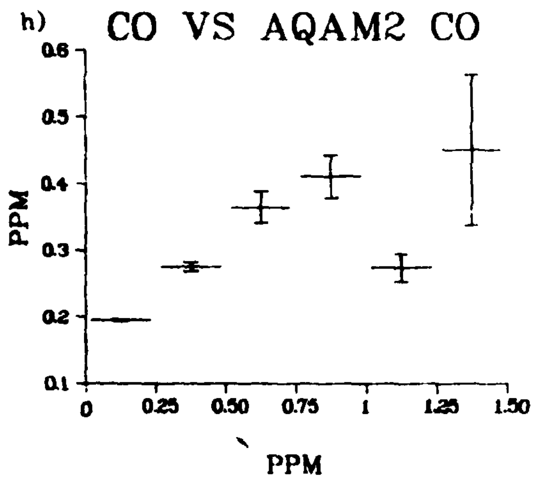
d) q_θ

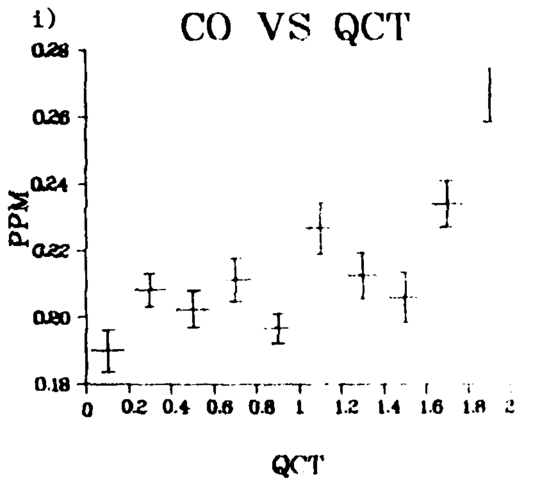
e) Turner stability class

Error bars indicate the standard deviation of the mean.









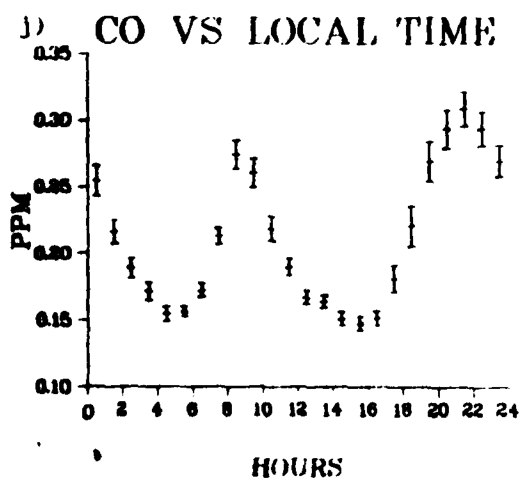


Fig. 26 f-j. Receptor Averaged Observed CO Concentration vs

f) θ

g) q_{CM}

h) $\overline{C}_T$

i) q_{CT}

j) local time

Error bars indicate the standard deviation of the mean.

Again, this fact follows intuitively from the fact that stations 1, 2, 3, and 5 are located in flat, open terrain while station 4 is surrounded by airbase buildings and trees.

It is interesting to note further that while CO concentrations increase with increasing q_u (see Figure 26b), since q_u increases at lower windspeeds, concentrations are quite independent of q_θ (see Figure 26d).

QUESTIONS

1. Is the plume rise from aircraft a significant factor when the trailer site is in close proximity to a taxiway/runway?

2. Under what meteorological conditions will the selcted trailer sites provide adequate data on background levels?

3. Which weather station provides wind speed and wind direction data most representative of conditions throughout the airbase?

C. Assumptions and Hypotheses about the Air Quality Assessment Model

ASSUMPTIONS

1. The conditions of applicability of AQAM are satisfied (see Q1, below).

2. The various numerical algorithms used in the model are adequate (e.g., area source integrations, line source segmenting, pseudo downwind distance computations, etc.). We note that the version of AQAM used in these simulations differs from the original AQAM[2] in the following ways.

   a) A faster, numerical quadrature scheme is used in place of the piecewise, quasi-analytic solution for line source concentration calculations. This new line source source algorithm continues to exhibit pathological behavior at the approximate one in 10,000 rate.

   b) The zero wind speed cases are handled using an integrated Gaussian-puff algorithm[10] with time dependent dispersion coefficients.

   c) The transition from distance dependent[3] to time dependent dispersion coefficients,[2,11] which normally occurred in AQAM for wind speeds below about 4 m/sec., has been inhibited for the vertical dispersion coefficient under E and F stabilities.

3. The fuel flow rates and emissions factors for various aircraft modes used in the model are adequate and are based on the latest available data.

HYPOTHESES

C1. The accumulated short-term model predictions are not significantly different from the long-term predictions. This hypothesis could be addressed first by comparing the long-term predictions to the averaged short-term predictions and their 95% confidence interval estimates. Since a relatively small number of long term predictions are required, it may be of some interest to run several long term predictions in order to see how sensitive the long term model is to perturbations in the input data within the context of the Williams AFB experiment. In this fashion, several long term predictions could be compared with the confidence interval for the accumulated short term predictions. Long-term AQAM simulations have not yet been performed.

C2. There are no significant differences between predictions based on the use of hourly aircraft operational activity information compared with predictions based on the use of fractional distributions of annual aircraft activity. The use of discrete aircraft activity information provides a control in defining the accuracy of the fractional, temporal distributions routinely used in modeling aircraft activity. The residuals between predictions could be analyzed using univariate spectral analysis to indicate which frequency components are subject to greatest errors; to date, very little difference between AQAM I and AQAM II predictions or predictive power has been observed. The cumulative frequency distributions of Appendix G are nearly identical for the two modeling approaches. In addition, examination of the residuals between AQAM I and observed concentrations gives rise to residual distributions nearly indistinguishable from the AQAM II/observed concentration residuals shown in Figures 9a-c.

Table 4 presents a summary of AQAM I and II predictions for each of the five stations plus an additional four hypothetical receptor points. One notes that differences between AQAM I and AQAM II predicted total concentrations on an annual average or geometric mean basis are confined to ±10%. Differences in the maximum hourly concentration predicted for the year are as large as ±30% for CO and NMHC (±45% for NO_x) and not necessarily associated with the same hour.

Table 4. Summary of AQAM I and AQAM II Computed Concentrations at Williams AFB. All Gaseous Concentrations in ppm. Particulates expressed as μg/m^3

	STATION 1	STATION 2	STATION 3	STATION 4	STATION 5
AQAM I AIRCRAFT ONLY					
POLLUTANT CO					
ARITHMETIC MEAN	0.162E-01	0.377E-01	0.876E-01	0.129E 00	0.303E-01
GEOMETRIC MEAN	0.431E-04	0.352E-02	0.726E-02	0.189E-03	0.559E-03
MAXIMUM VALUE	0.876E 00	0.264E 01	0.396E 01	0.757E 01	0.286E 01
POLLUTANT THC					
ARITHMETIC MEAN	0.764E-02	0.114E-01	0.286E-01	0.104E 00	0.215E-01
GEOMETRIC MEAN	0.320E-04	0.224E-02	0.520E-02	0.254E-03	0.447E-03
MAXIMUM VALUE	0.304E 00	0.633E 00	0.108E 01	0.520E 01	0.338E 01
POLLUTANT NOX					
ARITHMETIC MEAN	0.268E-03	0.916E-03	0.101E-02	0.910E-03	0.282E-03
GEOMETRIC MEAN	0.458E-05	0.393E-03	0.563E-03	0.166E-04	0.683E-04
MAXIMUM VALUE	0.161E-01	0.500E-01	0.492E-01	0.511E-01	0.170E-01
POLLUTANT PART					
ARITHMETIC MEAN	0.312E-01	0.869E-01	0.155E 00	0.297E 00	0.517E-01
GEOMETRIC MEAN	0.168E-02	0.135E 00	0.342E 00	0.150E-01	0.348E-01
MAXIMUM VALUE	0.230E 01	0.720E 01	0.657E 01	0.163E 02	0.648E 01
POLLUTANT SOX					
ARITHMETIC MEAN	0.969E-04	0.311E-03	0.360E-03	0.386E-03	0.118E-03
GEOMETRIC MEAN	0.251E-05	0.203E-03	0.308E-03	0.874E-05	0.341E-04
MAXIMUM VALUE	0.555E-02	0.175E-01	0.161E-01	0.221E-01	0.795E-02
AQAM I ALL SOURCES					
POLLUTANT CO					
ARITHMETIC MEAN	0.595E-01	0.819E-01	0.135E 00	0.271E 00	0.842E-01
GEOMETRIC MEAN	0.117E-02	0.180E-02	0.319E-02	0.948E-01	0.936E-02
MAXIMUM VALUE	0.134E 01	0.264E 01	0.396E 01	0.858E 01	0.353E 01
POLLUTANT THC					
ARITHMETIC MEAN	0.274E-01	0.318E-01	0.512E-01	0.182E 00	0.468E-01
GEOMETRIC MEAN	0.373E-03	0.520E-03	0.104E-02	0.807E-01	0.494E-02
MAXIMUM VALUE	0.636E 00	0.708E 00	0.160E 01	0.563E 01	0.372E 01
POLLUTANT NOX					
ARITHMETIC MEAN	0.262E-02	0.329E-02	0.350E-02	0.780E-02	0.315E-02
GEOMETRIC MEAN	0.770E-04	0.103E-03	0.128E-03	0.423E-02	0.433E-03
MAXIMUM VALUE	0.754E-01	0.751E-01	0.765E-01	0.124E 00	0.757E-01
POLLUTANT PART					
ARITHMETIC MEAN	0.381E 01	0.382E 01	0.394E 01	0.544E 01	0.444E 01
GEOMETRIC MEAN	0.673E-01	0.789E-01	0.153E 00	0.170E 01	0.323E 00
MAXIMUM VALUE	0.122E 03	0.121E 03	0.120E 03	0.123E 03	0.125E 03
POLLUTANT SOX					
ARITHMETIC MEAN	0.365E-03	0.636E-03	0.812E-03	0.398E-02	0.575E-03
GEOMETRIC MEAN	0.649E-05	0.150E-04	0.227E-04	0.192E-02	0.588E-04
MAXIMUM VALUE	0.175E-01	0.178E-01	0.203E-01	0.570E-01	0.312E-01

Table 4. (Cont'd)

	STATION 1	STATION 2	STATION 3	STATION 4	STATION 5
AQAM II AIRCRAFT ONLY					
POLLUTANT CO					
ARITHMETIC MEAN	0.206E-01	0.406E-01	0.878E-01	0.112E 00	0.297E-01
GEOMETRIC MEAN	0.163E-03	0.165E-02	0.635E-02	0.487E-03	0.130E-02
MAXIMUM VALUE	0.863E 00	0.125E 01	0.315E 01	0.459E 01	0.235E 01
POLLUTANT THC					
ARITHMETIC MEAN	0.971E-02	0.135E-01	0.317E-01	0.841E-01	0.194E-01
GEOMETRIC MEAN	0.131E-03	0.106E-02	0.479E-02	0.637E-03	0.117E-02
MAXIMUM VALUE	0.683E 00	0.745E 00	0.140E 01	0.460E 01	0.193E 01
POLLUTANT NOX					
ARITHMETIC MEAN	0.313E-03	0.908E-03	0.942E-03	0.779E-03	0.262E-03
GEOMETRIC MEAN	0.210E-04	0.199E-03	0.517E-03	0.405E-04	0.161E-03
MAXIMUM VALUE	0.184E-01	0.446E-01	0.863E-01	0.290E-01	0.191E-01
POLLUTANT PART					
ARITHMETIC MEAN	0.283E-01	0.688E-01	0.145E 00	0.250E 00	0.436E-01
GEOMETRIC MEAN	0.785E-02	0.550E-01	0.251E 00	0.372E-01	0.911E-01
MAXIMUM VALUE	0.374E 01	0.180E 02	0.130E 02	0.133E 02	0.394E 01
POLLUTANT SOX					
ARITHMETIC MEAN	0.120E-03	0.323E-03	0.341E-03	0.333E-03	0.113E-03
GEOMETRIC MEAN	0.119E-04	0.105E-03	0.287E-03	0.235E-04	0.973E-04
MAXIMUM VALUE	0.559E-02	0.133E-01	0.127E-01	0.129E-01	0.749E-02
AQAM II ALL SOURCES					
POLLUTANT CO					
ARITHMETIC MEAN	0.639E-01	0.847E-01	0.136E 00	0.254E 00	0.835E-01
GEOMETRIC MEAN	0.123E-02	0.188E-02	0.305E-02	0.995E-01	0.945E-02
MAXIMUM VALUE	0.166E 01	0.184E 01	0.355E 01	0.590E 01	0.277E 01
POLLUTANT THC					
ARITHMETIC MEAN	0.295E-01	0.339E-01	0.542E-01	0.161E 00	0.447E-01
GEOMETRIC MEAN	0.412E-03	0.557E-03	0.103E-02	0.811E-01	0.479E-02
MAXIMUM VALUE	0.921E 00	0.102E 01	0.131E 01	0.477E 01	0.215E 01
POLLUTANT NOX					
ARITHMETIC MEAN	0.267E-02	0.328E-02	0.344E-02	0.767E-02	0.313E-02
GEOMETRIC MEAN	0.868E-04	0.113E-03	0.132E-03	0.432E-02	0.440E-03
MAXIMUM VALUE	0.753E-01	0.765E-01	0.863E-01	0.125E 00	0.757E-01
POLLUTANT PART					
ARITHMETIC MEAN	0.380E 01	0.381E 01	0.393E 01	0.539E 01	0.444E 01
GEOMETRIC MEAN	0.662E-01	0.702E-01	0.140E 00	0.174E 01	0.314E 00
MAXIMUM VALUE	0.122E 03	0.121E 03	0.120E 03	0.123E 03	0.125E 03
POLLUTANT SOX					
ARITHMETIC MEAN	0.388E-03	0.649E-03	0.793E-03	0.393E-02	0.569E-03
GEOMETRIC MEAN	0.706E-05	0.142E-04	0.206E-04	0.193E-02	[illegible]
MAXIMUM VALUE	0.184E-01	0.178E-01	0.203E-01	0.515E-01	0.312E-01

ADDITIONAL COMPUTATION POINTS

	HIGLEY	LEISURE WORLD	QUEEN CREEK	BASE HOUSING
AQAM I TOTAL CONCENTRATIONS				
POLLUTANT CO				
ARITHMETIC MEAN	0.672E-01	0.146E 00	0.310E-01	0.199E 00
GEOMETRIC MEAN	0.236E-02	0.318E-01	0.517E-03	0.924E-01
MAXIMUM VALUE	0.159E 01	0.222E 01	0.147E 01	0.664E 01
POLLUTANT THC				
ARITHMETIC MEAN	0.342E-01	0.639E-01	0.144E-01	0.102E 00
GEOMETRIC MEAN	0.111E-02	0.143E-01	0.162E-03	0.547E-01
MAXIMUM VALUE	0.755E 00	0.970E 00	0.692E 00	0.346E 01
POLLUTANT NOX				
ARITHMETIC MEAN	0.324E-02	0.817E-02	0.166E-02	0.669E-02
GEOMETRIC MEAN	0.157E-03	0.186E-02	0.609E-04	0.330E-02
MAXIMUM VALUE	0.891E-01	0.124E 00	0.732E-01	0.140E 00
POLLUTANT PART				
ARITHMETIC MEAN	0.510E 01	0.128E 02	0.321E 01	0.546E 01
GEOMETRIC MEAN	0.847E 00	0.287E 01	0.260E 00	0.200E 01
MAXIMUM VALUE	0.144E 03	0.199E 03	0.112E 03	0.128E 03
POLLUTANT SOX				
ARITHMETIC MEAN	0.837E-03	0.378E-03	0.183E-03	0.994E-02
GEOMETRIC MEAN	0.318E-04	0.929E-04	0.134E-04	0.255E-02
MAXIMUM VALUE	0.185E-01	0.500E-02	0.945E-02	0.221E 00
AQAM II TOTAL CONCENTRATIONS				
POLLUTANT CO				
ARITHMETIC MEAN	0.652E-01	0.146E 00	0.316E-01	0.194E 00
GEOMETRIC MEAN	0.252E-02	0.329E-01	0.345E-03	0.931E-01
MAXIMUM VALUE	0.159E 01	0.222E 01	0.148E 01	0.433E 01
POLLUTANT THC				
ARITHMETIC MEAN	0.316E-01	0.639E-01	0.149E-01	0.967E-01
GEOMETRIC MEAN	0.116E-02	0.147E-01	0.118E-03	0.545E-01
MAXIMUM VALUE	0.686E 00	0.970E 00	0.653E 00	0.176E 01
POLLUTANT NOX				
ARITHMETIC MEAN	0.322E-02	0.817E-02	0.166E-02	0.665E-02
GEOMETRIC MEAN	0.163E-03	0.189E-02	0.403E-04	0.331E-02
MAXIMUM VALUE	0.891E-01	0.124E 00	0.733E-01	0.123E 00
POLLUTANT PART				
ARITHMETIC MEAN	0.510E 01	0.128E 02	0.321E 01	0.545E 01
GEOMETRIC MEAN	0.852E 00	0.287E 01	0.261E 00	0.200E 01
MAXIMUM VALUE	0.144E 03	0.199E 03	0.112E 03	0.128E 03
POLLUTANT SOX				
ARITHMETIC MEAN	0.829E-03	0.378E-03	0.185E-03	0.992E-02
GEOMETRIC MEAN	0.335E-04	0.960E-04	0.960E-05	0.255E-02
MAXIMUM VALUE	0.178E-01	0.501E-02	0.942E-02	0.213E 00

Table 4. (Cont'd)

CONCENTRATIONS DUE TO ENVIRON SOURCES

	STATION 1	STATION 2	STATION 3	STATION 4	STATION 5	HIGLEY	LEISURE WORLD	QUEEN CREEK	BASE HOUSING
POLLUTANT CO									
ARITHMETIC MEAN	0.382E-01	0.375E-01	0.374E-01	0.408E-01	0.448E-01	0.478E-01	0.143E 00	0.276E-01	0.403E-01
GEOMETRIC MEAN	0.304E-03	0.157E-03	0.170E-03	0.414E-03	0.583E-03	0.675E-03	0.236E-01	0.420E-03	0.639E-03
MAXIMUM VALUE	0.129E 01	0.128E 01	0.126E 01	0.130E 01	0.135E 01	0.159E 01	0.222E 01	0.120E 01	0.137E 01
POLLUTANT THC									
ARITHMETIC MEAN	0.167E-01	0.165E-01	0.165E-01	0.179E-01	0.196E-01	0.210E-01	0.619E-01	0.123E-01	0.177E-01
GEOMETRIC MEAN	0.104E-03	0.533E-04	0.598E-04	0.213E-03	0.307E-03	0.273E-03	0.990E-02	0.351E-03	0.336E-03
MAXIMUM VALUE	0.568E 00	0.561E 00	0.556E 00	0.570E 00	0.592E 00	0.686E 00	0.970E 00	0.515E 00	0.585E 00
POLLUTANT NOX									
ARITHMETIC MEAN	0.218E-02	0.213E-02	0.213E-02	0.233E-02	0.255E-02	0.274E-02	0.811E-02	0.158E-02	0.231E-02
GEOMETRIC MEAN	0.358E-04	0.185E-04	0.201E-04	0.509E-04	0.713E-04	0.759E-04	0.159E-02	0.553E-04	0.648E-04
MAXIMUM VALUE	0.727E-01	0.717E-01	0.710E-01	0.727E-01	0.757E-01	0.891E-01	0.124E 00	0.676E-01	0.790E-01
POLLUTANT PART									
ARITHMETIC MEAN	0.373E 01	0.369E 01	0.371E 01	0.403E 01	0.432E 01	0.499E 01	0.128E 02	0.320E 01	0.406E 01
GEOMETRIC MEAN	0.405E-01	0.260E-01	0.260E-01	0.143E 00	0.129E 00	0.456E 00	0.277E 01	0.260E 00	0.922E-01
MAXIMUM VALUE	0.121E 03	0.120E 03	0.119E 03	0.121E 03	0.125E 03	0.144E 03	0.199E 03	0.110E 03	0.125E 03
POLLUTANT SOX									
ARITHMETIC MEAN	0.106E-03	0.105E-03	0.107E-03	0.115E-03	0.116E-03	0.149E-03	0.332E-03	0.115E-03	0.120E-03
GEOMETRIC MEAN	0.874E-06	0.460E-06	0.990E-06	0.650E-05	0.334E-05	0.238E-05	0.574E-04	0.715E-05	0.108E-04
MAXIMUM VALUE	0.435E-02	0.463E-02	0.497E-02	0.535E-02	0.510E-02	0.904E-02	0.500E-02	0.438E-02	0.579E-02

Thus, while AQAM I and II predictions may be vastly different for any single hour, especially for hours when AQAM I assumes no aircraft operations, typical statistical estimators do not differ significantly compared to errors involved in the overall modeling process.

C3. The AQAM predictions are insensitive to minor perturbations in the exact trailer locations. This hypothesis was examined within the context of the Williams AFB air pollution program to indicate the sensitivity of model predictions to source-receptor location proximity. This could prove useful in explaining relative errors in predictions for stations with different spatial relationships to modeled emissions such as area and line sources; however, uncertainties in the modeling approach which best represents reality can substantially distort the result of such an analysis. For example, the location of station 3 is found to be quite sensitive to its distance from the main taxiway (i.e. since $\delta\chi/\chi \approx -\delta x/x$); however, inclusion of a more realistic plume rise algorithm not only greatly reduces modeled concentrations but diminishes the percentage sensitivity on distance from the main taxiway. Hence, the decreased predictive power at station 3 might be attributed to this distance sensitivity but is more probably due to uncertainty in the modeling of the jet plume dynamics.

C4. The incorporation of the correct total emissions, based on data obtained during the queueing studies, will have significant impact on receptors near the taxiways; while the exact spatial distribution of these emissions, though significant will be of secondary importance except for those receptors very close (< 1/2 km.) to the affected taxiway segments. The effects on AQAM predictions from the incorporation of correct total emissions for abort and queueing situations can be studied for line, area, and point source sensitivity using appropriate experimental designs and the methods of multiple linear regression analysis. Such analysis could have been carried out within the context of the Williams AFB air pollution monitoring program for observed values of pollutant concentrations and frequency of aircraft operations; however, results of the queueing studies were instead utilized in both AQAM I and II to improve the modeled spatial distribution of pollutant emissions. These spatial redistribution factors were incorporated chiefly through slightly modified, line segment dependent, taxi speeds, and the resulting changes are estimated as being less significant than the differences between AQAM I and II (i.e. see hypothesis C2).

QUESTIONS

1. How well are the conditions of applicability of AQAM satisfied at Williams AFB?

   a. Are the Pasquill-Gifford stability classes applicable? (One must remember that the dispersion coefficients have been measured over grasslands and urban areas. The altered albedo and surface heating characteristics of both desert sand and airport runways suggest that convective transport may be more significant than in the urban or grasslands situations.) Additional meteorological measurements will be necessary to address this question.

   b. Are the inhomogeneities in the wind field significant over an airbase?

   c. Are stability class, mixing depth, or wind speed over a desert environement sufficiently persistent to warrant the steady-state assumption?

   d. Are the fluctuations in wind direction adequately accounted for in the dispersion coefficients?

   e. Do meteorological and aerometric observations suggest a more reasonable averaging time over which steady-state conditions may be assumed?

D. <u>Assumptions and Hypotheses Concerning the Comparison of the AQAM to the Williams AFB Air Pollution Monitoring Program</u>

ASSUMPTIONS

1. The observed air quality concentrations and the AQAM predictions are independent.

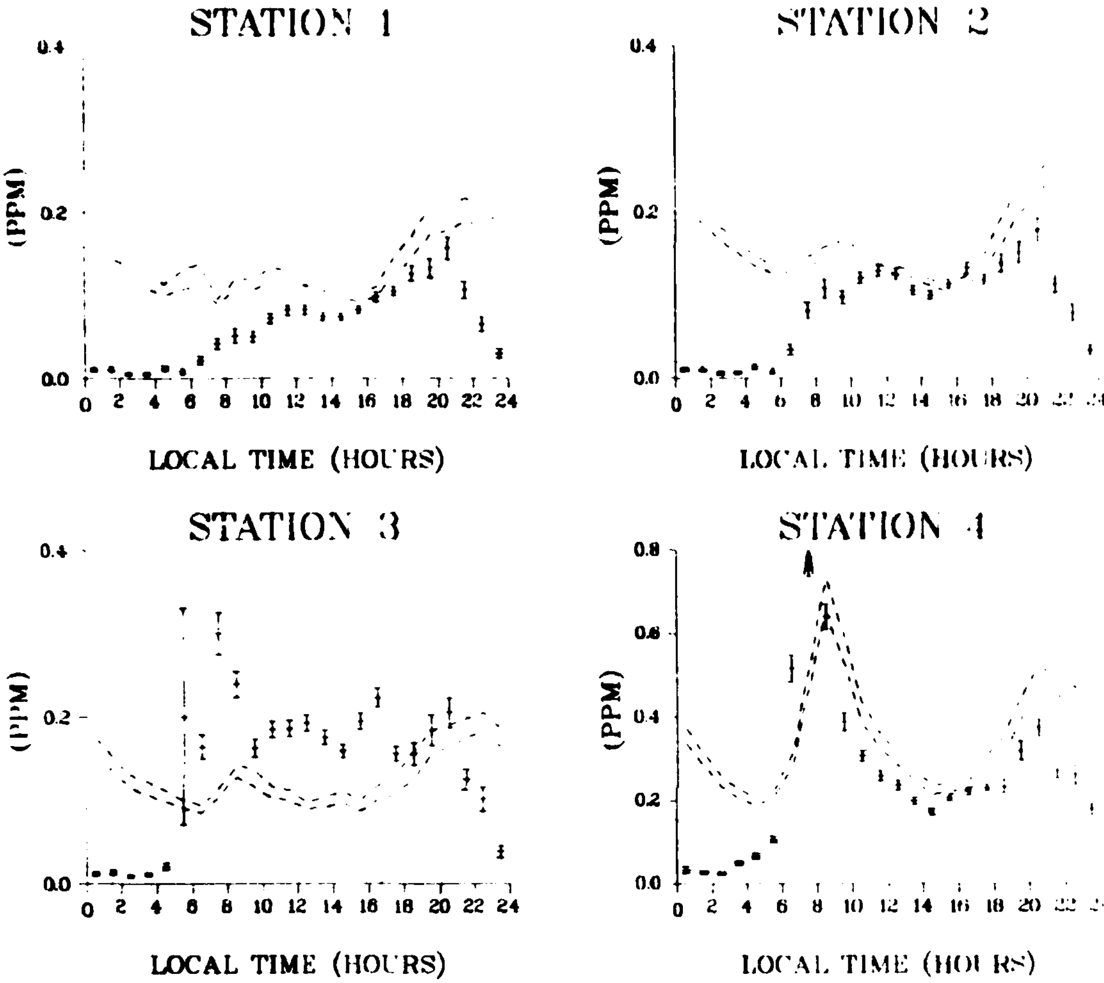
2. A proper evaluation of AQAM requires that comparisons be made of AQAM predictions with both the air quality observations and the air quality observations with background components removed.

HYPOTHESES

D1. <u>The hourly short-term predictions and hourly ambient observations can be reduced to longer time periods with better agreement between observed and predicted aerometric concentrations</u>. Testing this hypothesis involves the same techniques discussed in Section II on the Overall AQAM Accuracy Definition. Comparison can be made between the various statistical measures as a function of averaging time. Taking the limiting case of the annual estimators, comparison of Tables 1 and 4 with subsequent comparison to the mean hourly predictive power given in Table 2, one finds that the reduction to longer averaging time periods does not uniformly improve model predictive power in the mean. However, reduction of the standard deviations given in Table 2 with increased averaging time appears to follow consistently, though thorough verification has not been completed.

D2. The frequency distributions of the observations and predictions are not significantly different. As discussed in Section IIA and shown in Appendix G, the cumulative frequency distributions do not differ significantly (i.e., the model predictions fall within the 95% confidence level bounds about the data distribution) in the upper concentration regimes. The disagreement is significant at lower concentration levels but this is seen, by comparison of Table 2b and c, to be due to the presence of background levels not explicitly treated in AQAM. This same background becomes a negligible fraction of the total prediction at higher concentrations.

D3. The differences between predictions and observations for appropriate stratifications of the data are not statistically significant. Data resulting from stratifications may in practice not be independent. Care must be exercised to ensure that the assumptions of tests of significance are satisfied by performing diagnostic investigations on these data sets. When the stratifications preserve time dependence, time series will provide insight regarding serial correlations for different averaging times. When the stratifications are based on other factors, the underlying distributions are first explored via a moments analysis (the boxplot technique has also been suggested for this purpose). Various measures of correlation and tests of significance may be indicative subsequent to such investigations. The comparison of frequency distributions and direct comparison of descriptive measures should also be performed. The time dependence of mean hourly AQAM II predictions is shown in Figures 27a-c. Comparison with Figures 17a-c, the ± 1 S.D.M. bounds of which are superimposed on Fig. 26, reveals some striking similarities, particularly at station 4, but many contrasts remain and are thought to be partially attributable to background considerations. Figures 28a-c and 29a-c present the parallel situation but with background (defined as the arithmetic mean of stations 1, 2, 3, and 5) subtracted concentrations for observation and theory respectively. The number of similarities increase sharply, especially during the daytime hours when local sources dominate, lending credence to the hypothesis that background uncertainties present the major obstacle to meaningful



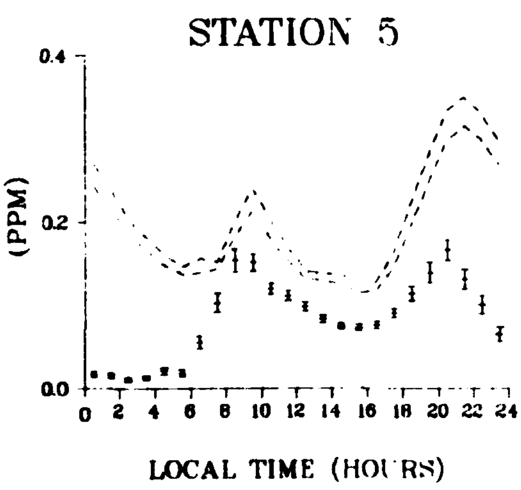
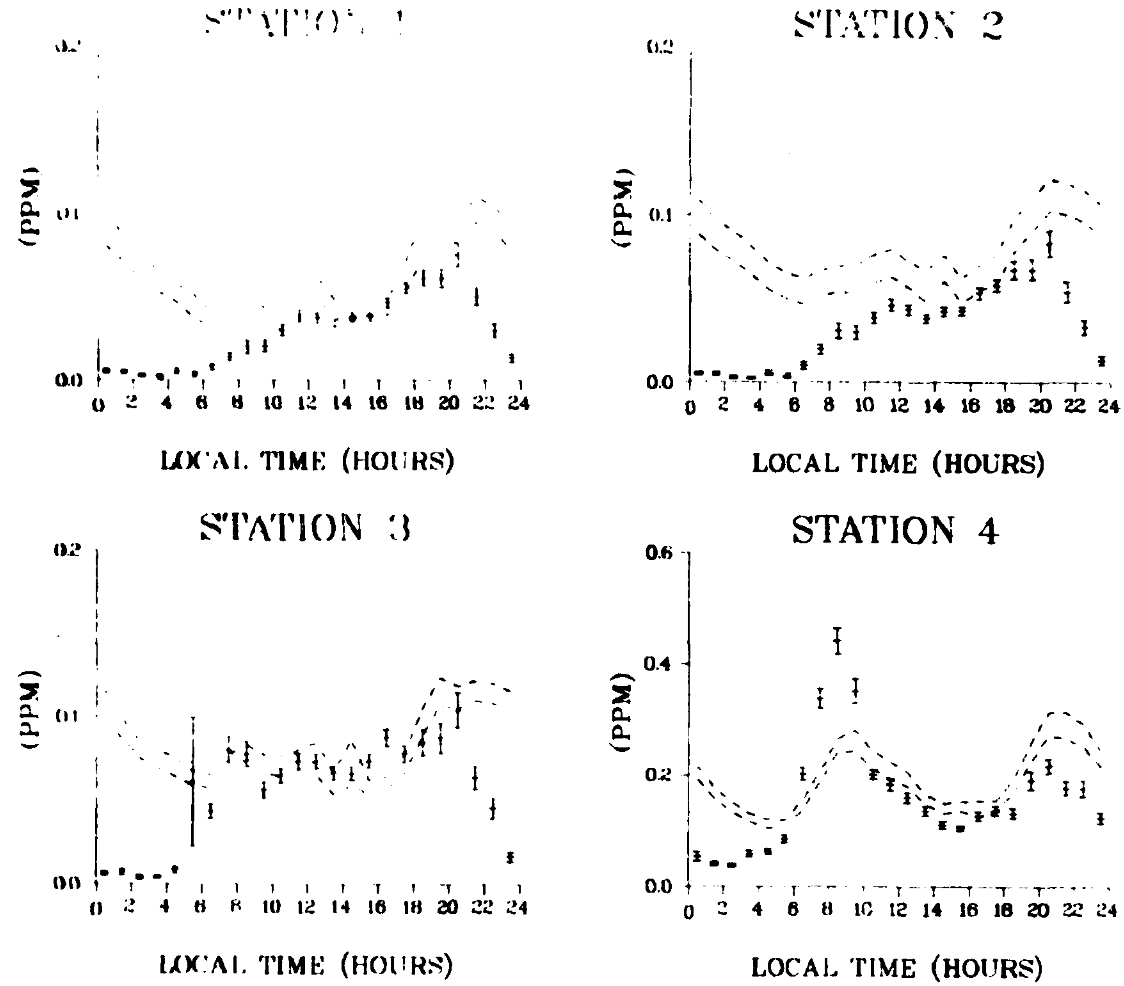


Figure 27a. Average AQAM II Predicted CO concentration at each receptor vs time of day. Error bars indicate the standard deviation of the mean. The dotted curves indicate the one standard deviation of the mean bounds for the observations. (See Fig. 17).



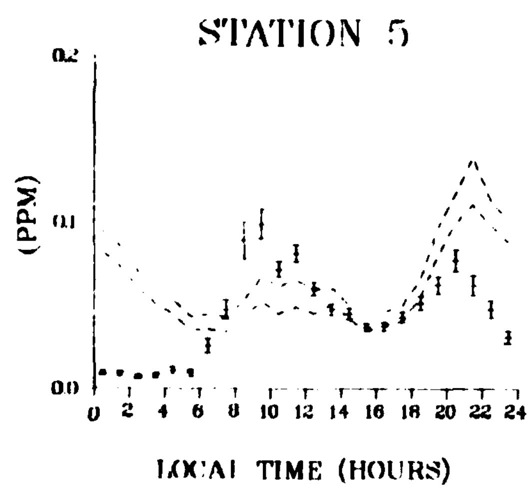


Figure 27b. Average AQAM II Predicted NMHC concentration at each receptor vs time of day. Error bars indicate the standard deviation of the mean. The dotted curves indicate the one standard deviation of the mean bounds for the observations. (See Fig. 17).

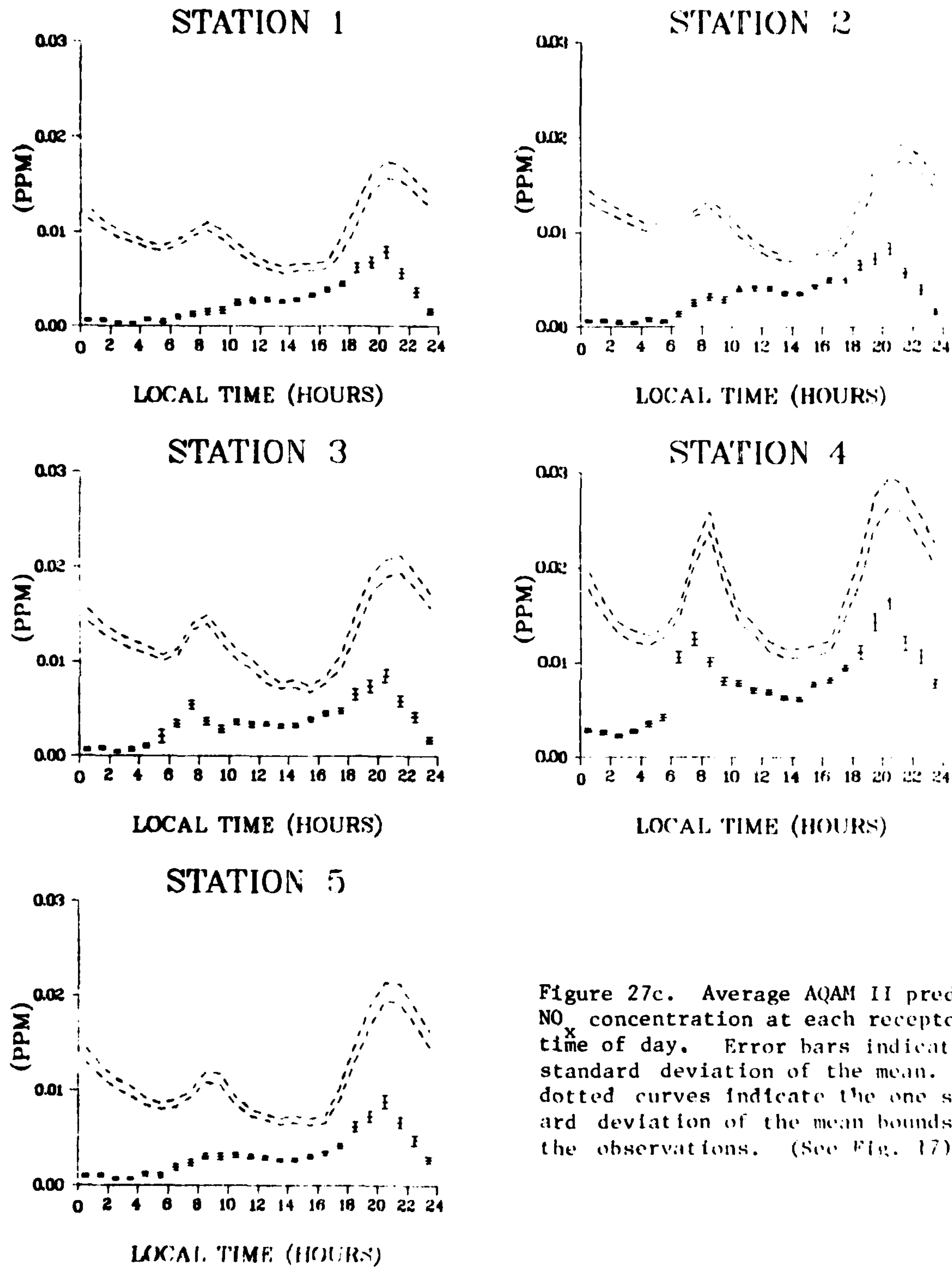


Figure 27c. Average AQAM II predicted NO_x concentration at each receptor vs time of day. Error bars indicate the standard deviation of the mean. The dotted curves indicate the one standard deviation of the mean bounds for the observations. (See Fig. 17).

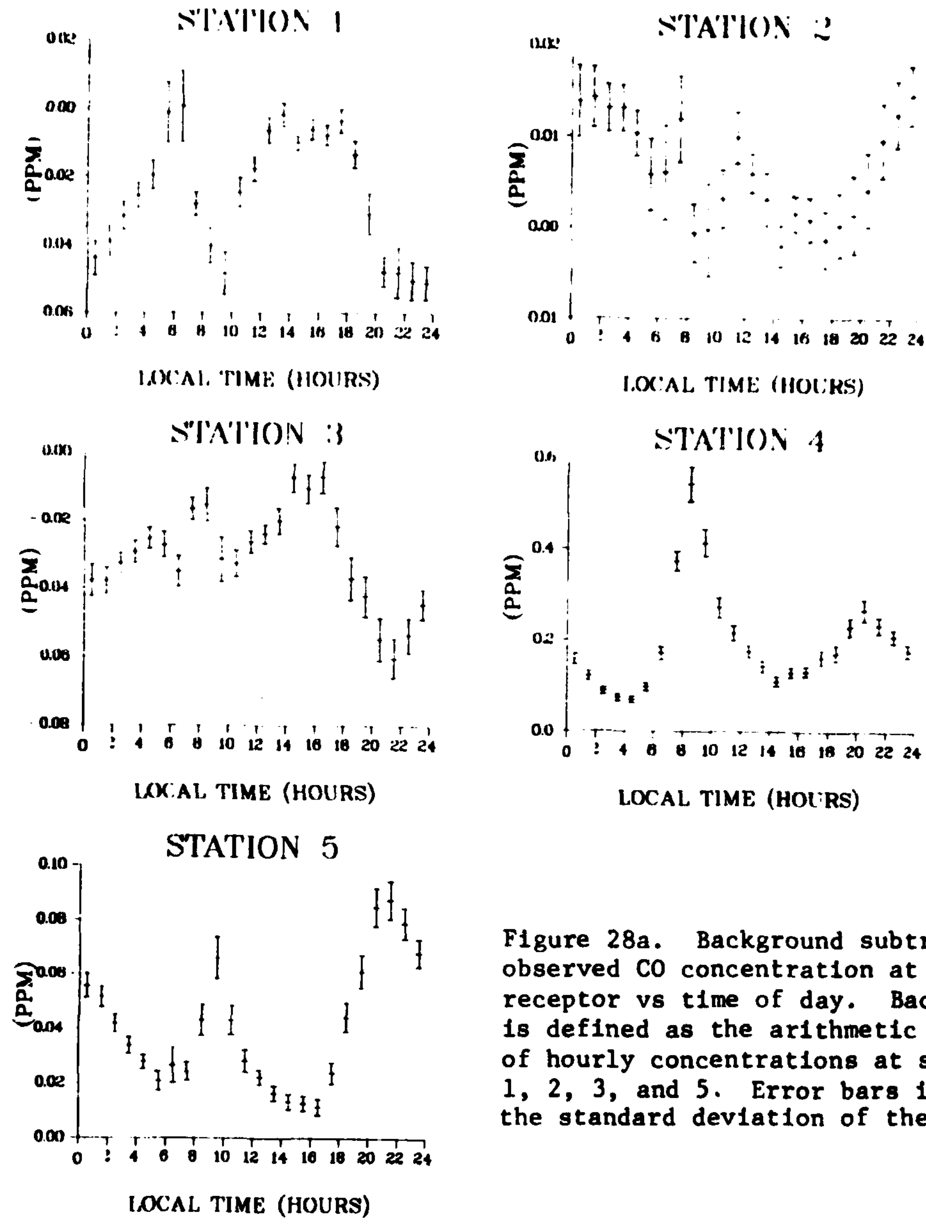
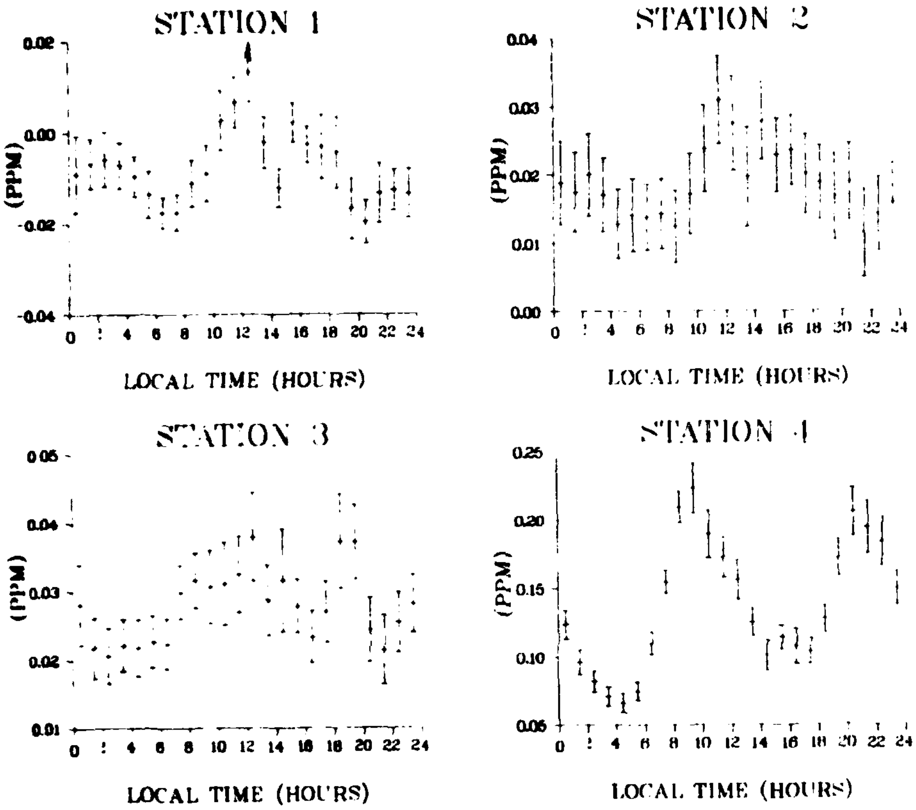


Figure 28a. Background subtracted observed CO concentration at each receptor vs time of day. Background is defined as the arithmetic mean of hourly concentrations at stations 1, 2, 3, and 5. Error bars indicate the standard deviation of the mean.



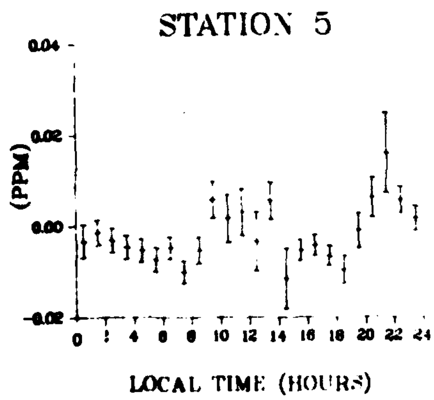


Figure 28b. Background subtracted observed NMHC concentration at each receptor vs time of day. Background is defined as the arithmetic mean of hourly concentrations at stations 1, 2, 3, and 5. Error bars indicate the standard deviation of the mean.

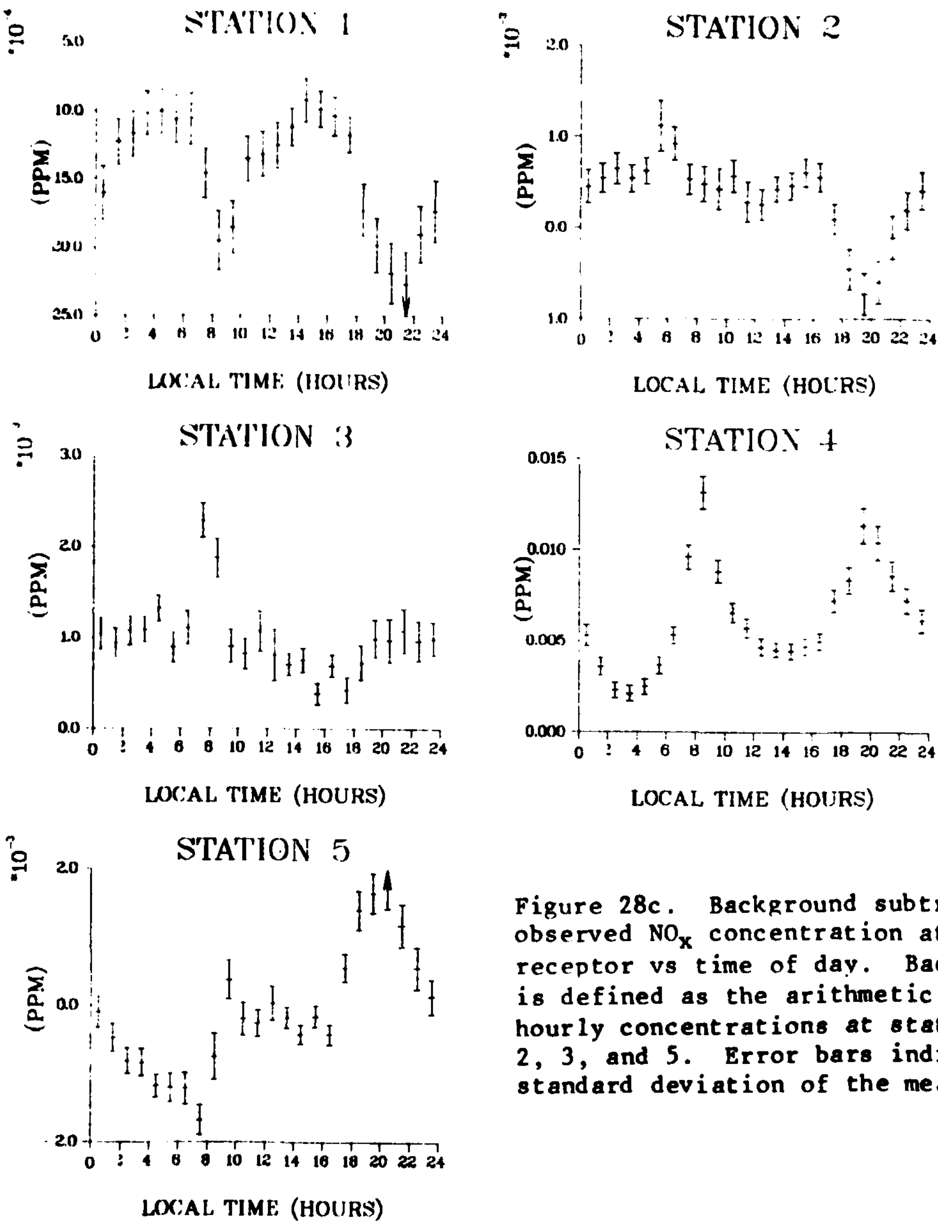
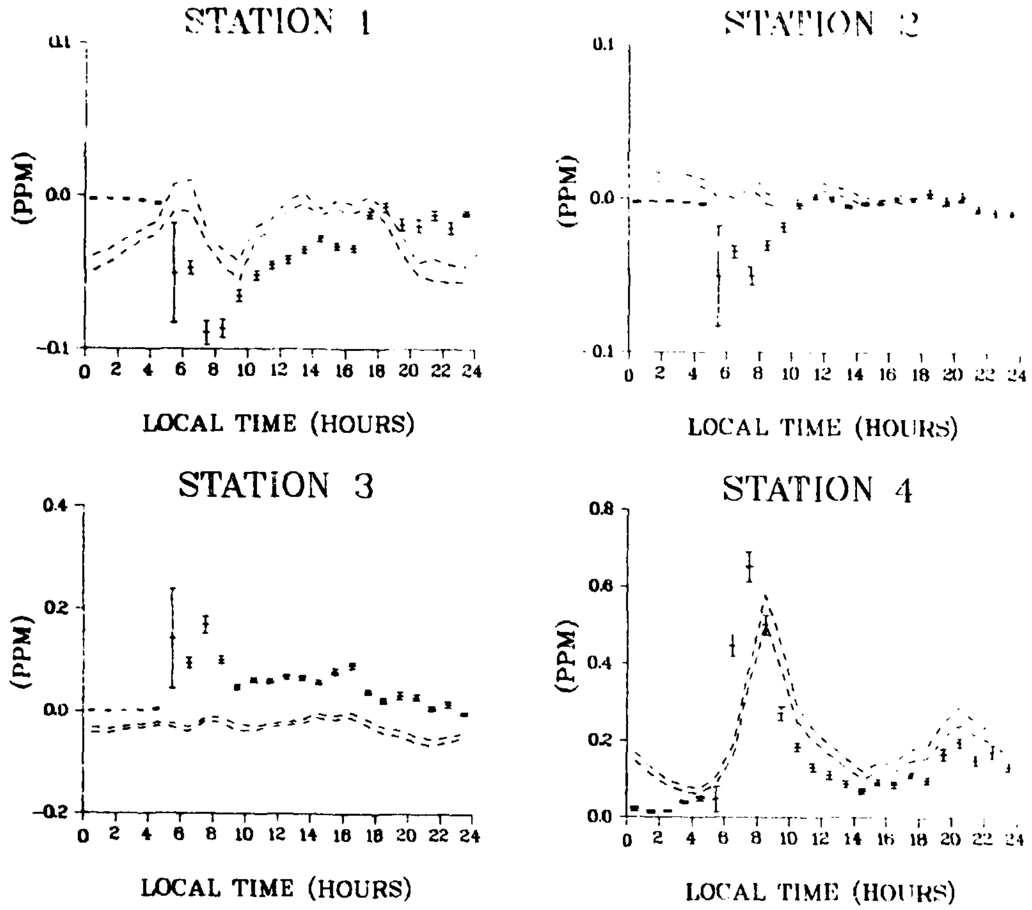


Figure 28c. Background subtracted observed NO_x concentration at each receptor vs time of day. Background is defined as the arithmetic mean of hourly concentrations at stations 1, 2, 3, and 5. Error bars indicate the standard deviation of the mean.



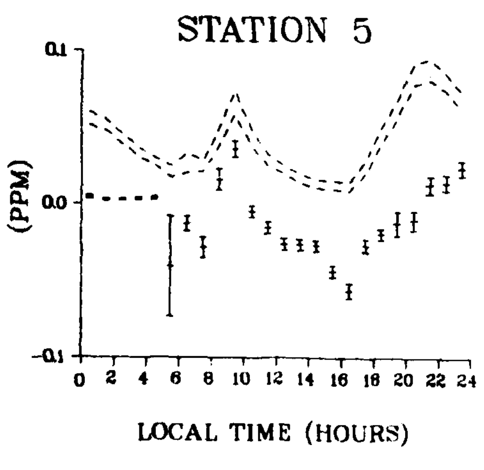
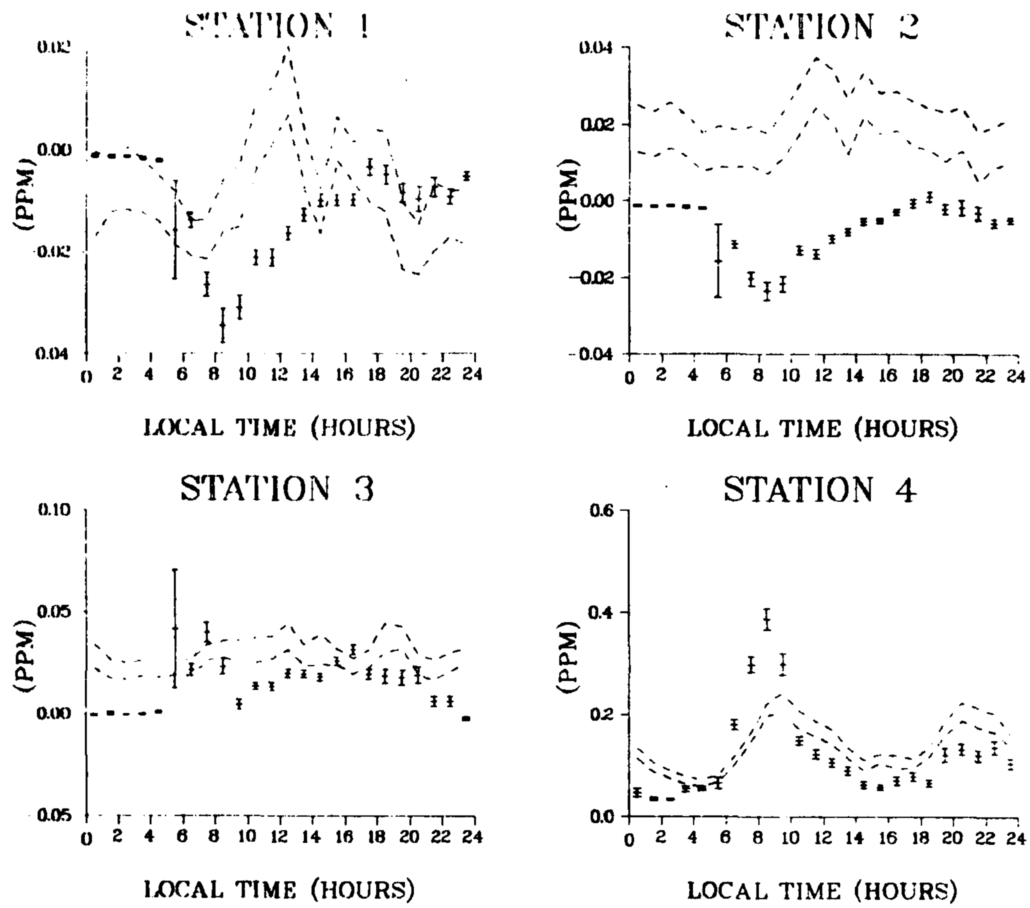


Figure 29a. Background subtracted AQAM II CO concentration at each receptor vs time of day. Background is defined as the arithmetic mean of hourly concentrations at stations 1, 2, 3, and 5. Error bars indicate the standard deviation of the mean. The dotted curves indicate the one standard deviation of the mean bounds for the observations.



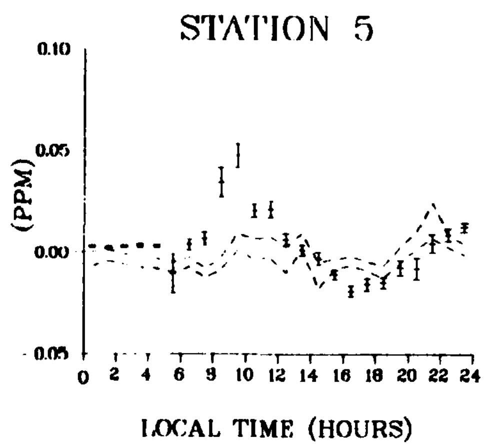


Figure 29b. Background subtracted AQAM II NMHC concentration at each receptor vs time day. Background is defined as the arithmetic mean of hourly concentrations at stations 1, 2, 3, and 5. Error bars indicate the standard deviation of the mean. The dotted curves indicate the one standard deviation of the mean bounds for the observations.

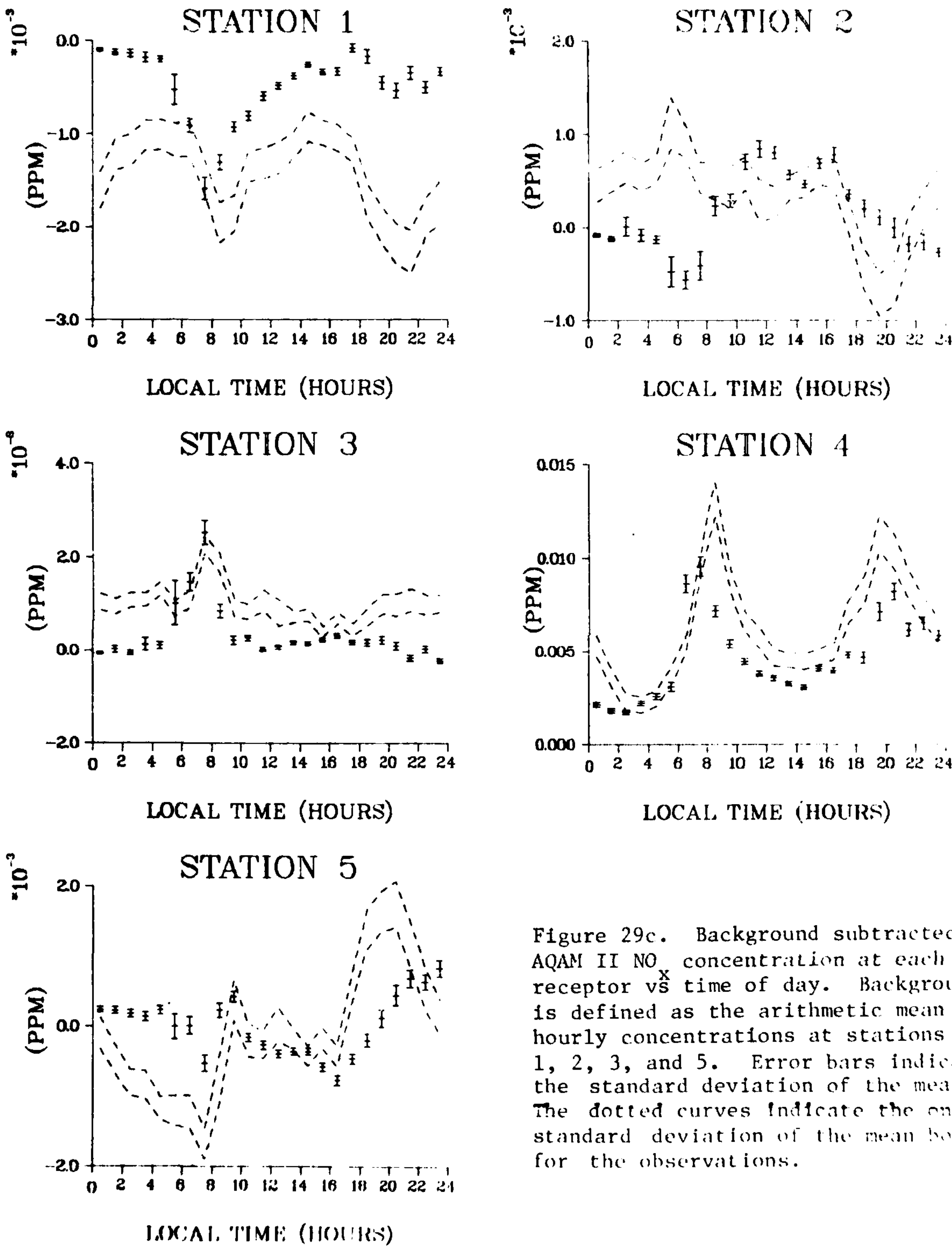


Figure 29c. Background subtracted AQAM II NO_x concentration at each receptor vs time of day. Background is defined as the arithmetic mean of hourly concentrations at stations 1, 2, 3, and 5. Error bars indicate the standard deviation of the mean. The dotted curves indicate the one standard deviation of the mean bounds for the observations.

theory/measurement comparisons. These background problems, fortunately, do not affect interstation comparisons.

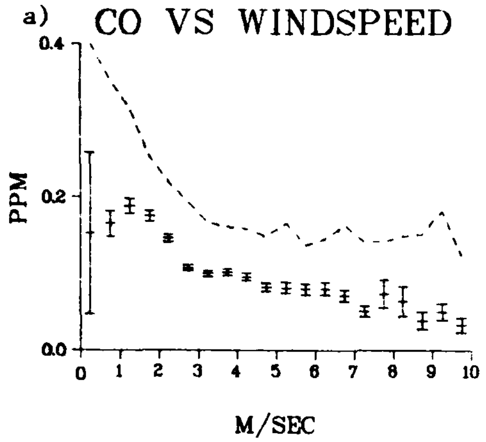
D4. The observations and predictions agree on the relative significance of the meteorological and emissions activity variables. This hypothesis can be tested by consideration of the component effects of independent variables in a multiple linear regression analysis. This is equivalent to ranking the independent variables on the magnitude of their effect and their significance. The use of bivariate spectral analysis should be considered as a means of exploring the hypothesis. More specifically, the coherence between the observations and the meteorological and aircraft activity time series can be obtained and the nature of the frequency dependent correlation explored. Results of regressions on the distributions shown in Figures 19 and 20 indicate that although dependence of CO concentration on aircraft emissions shows up in both theory and experiment, the significance of the effect is much smaller in the observed data.

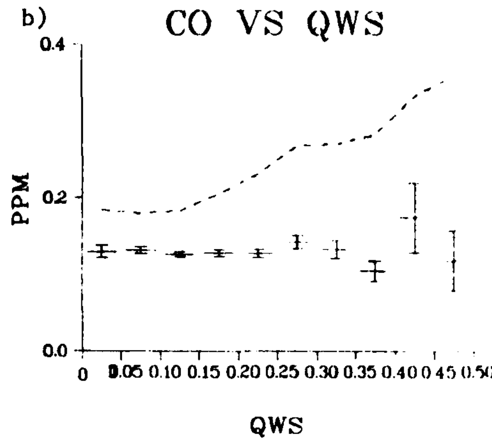
Converting the results of these regressions into percentage influence of aircraft on station 2 CO levels, one finds AQAM II predicted aircraft impacts of 63% at average emission rates and 84% at peak emission rates of 200 gms/sec, while the corresponding observed impacts are only 11% and 29% respectively. This large discrepancy between theory and observation is partially due to background levels not accounted for by AQAM, though random variables not accounted for, or averaged over, in AQAM could significantly wash out the dependence on aircraft emissions. Similar results are presented in Table 3 for other pollutants and stations. Maximum aircraft impacts are seen at station 4.

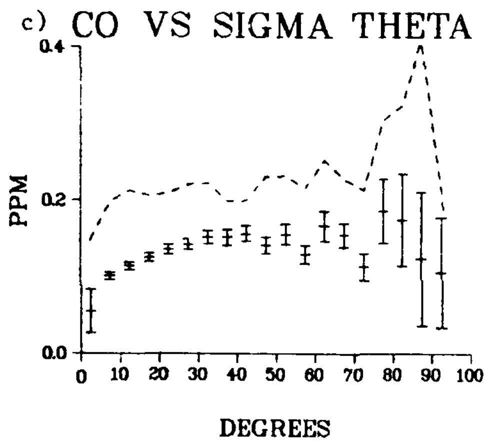
AQAM CO concentration dependences on several meteorological and aerometric quantities are presented in Figures 30 a-j and may be compared directly with measured dependences shown in Figures 26a-j. One observes directly that:

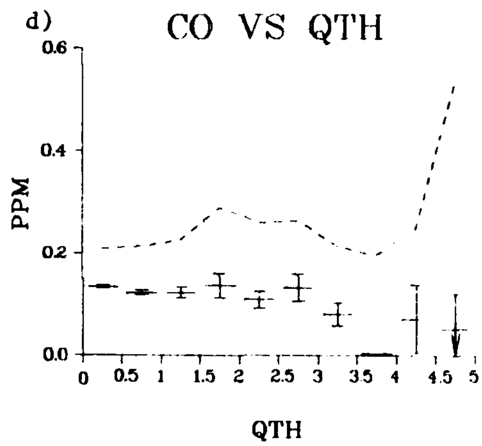
a) The windspeed dependence at low and intermediate u is similar though AQAM drops off too rapidly at high u.

b) The observed dependence on q_u is not predicted. This is not surprising since no windspeed spatial variability factor is contained in AQAM.









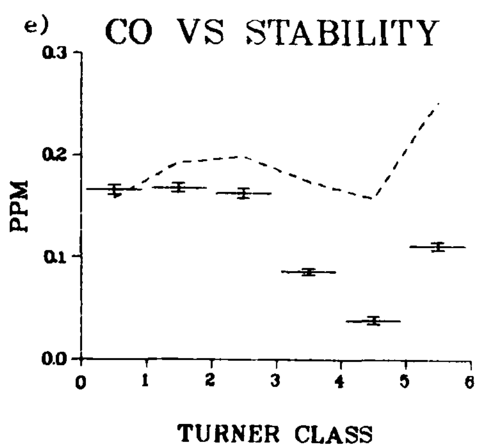


Fig. 30 a-e. Receptor Averaged AQAM II CO Concentration vs

a) u

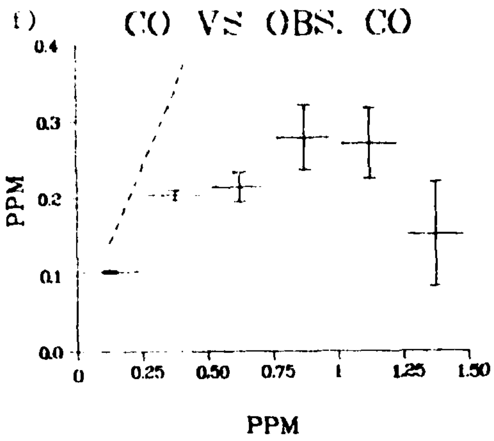
b) q_u

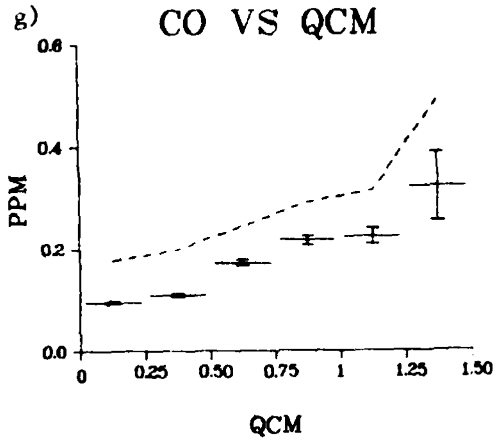
c) σ_θ

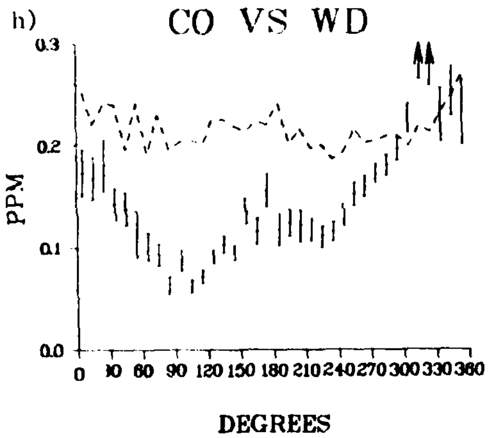
d) q

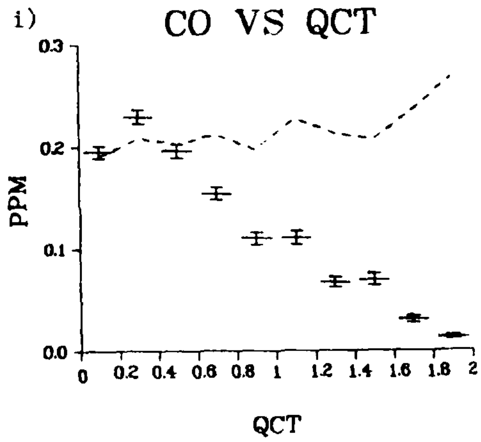
e) Turner stability class

Error bars indicate the standard deviation of the mean. The dotted curves indicate the behavior of the arithmetic mean for the observations (see Figure 26).









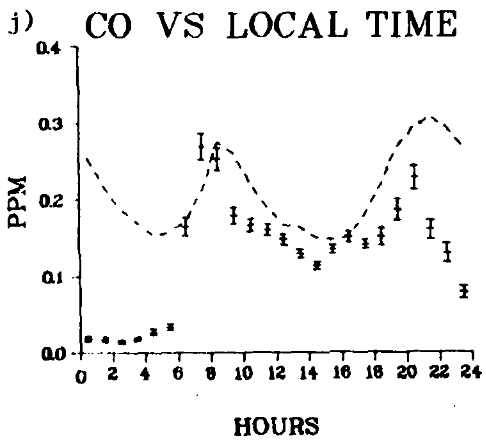


Fig. 30 f-j. Receptor Averaged AQAM II CO Concentration vs

f) $\overline{C}_M$

g) q_{CM}

h) θ

i) q_{CT}

j) local time

Error bars indicate the standard deviation of the mean. The dotted curves indicate the behavior of the arithmetic mean for the observations (see Figure 26).

c) The predicted dependence on σ_θ at low σ_θ is not observed. This probably is related to the fact that low σ_θ are related to stable, nighttime conditions which are apparently not adequately described in the model.

d) Quite different stability class dependence, again strongly coupled to time of day considerations.

e) An inability to describe the observed time of day dependence between midnight and ≈5AM. This failing manifests itself in a number of other distributions, including the rather strange non-linear dependence of AQAM concentration is observed mean concentration, and is now thought to be predominantly related to a serious underestimate (discovered after this report in press) of vehicle activity between midnight and 5AM.

D5. The correlations between levels of different pollutants at each receptor are adequately reproduced by AQAM. Bivariate spectral analysis should indicate at which frequencies the coherence between pollutants at each receptor is reproduced by the AQAM. This issue is partly considered in Appendix I for station 2 CO and NO_x. Results indicate that coherence is high at the lower frequencies, suggesting that such coherence is related to the diurnal meteorological cycle. This is also suggested by comparison of Figures 27a, b, and c with each other. Ordinary scatter diagrams with linear and robust linear regressions might also be computed.

D6. The inter-receptor correlations in the data are adequately reproduced by AQAM. These correlations may be evaluated in the frequency domain, using bivariate time series analysis. Stratification of AQAM predictions on wind direction and the comparison of frequency distributions is also recommended. The discussion concerning time dependence of theoretical and observed interstation concentration differences (Hypothesis D3) suggests that inter-receptor correlations present one of the more robust schemes for assessment of model predictive power. Also, comparison of the observed versus predicted rank ordering of stations (see Figures 4 and 5) suggests that interstation differences are better explained by the model when those differences exceed interstation resolution limits (see Figure 11); however, overall correlation coefficients of ∿0.4 indicate that AQAM only partially accounts for interstation differences.

D7. Better agreement between theory and experiment may be achieved by using the vetor mean wind speed. (This quantity was calculated from the one-minute measurements of wind speed and wind direction.) The residuals between observed air pollution concentrations and AQAM predictions with and without the vector mean wind speed can be analyzed and the hypothesis of a significant difference tested. This could be accomplished by the comparisons of the frequency distributions of residuals. AQAM model runs using the vector mean wind speed have not been performed; however, some improvement is expected as the vector mean wind speed is lower than the average wind speed and thus will yield higher predicted concentrations.

D8. <u>The residuals between observations and predictions are independent of:</u>

a. the values of the meteorological variables

b. station location

c. pollutant species

d. aircraft activity

e. time of day.

As seen from Figures 14 and 15 and as discussed previously, the residuals exhibit a number of dependences which appear to be related to the presence of backgrounds unaccounted for in the AQAM, to the decreased validity of the steady-state assumption for nighttime hours, and to an underestimate of vehicle activity between midnight and 5AM. With regard to the background alone, one can see that it would have a differing percentage impact on different predicted total concentration levels, which could then reflect into each of the above mentioned variables.

D9. <u>An examination of the residuals between observations and predictions will provide insight into the effect of factors which contribute to significant disagreements and may point to areas in the AQAM requiring improvement.</u> As mentioned above, in Section III, and as quantifed in D12 below (see also Table 2), study of the residuals enables one to discover overall model shortcomings (e.g. need for background concentrations) as well as station/pollutant inadequacies (e.g., the need for a plume rise model for the taxi mode to reconcile observed versus predicted CO concentrations at station 3).

D10. <u>Diurnal patterns in the data are succesfully reproduced by AQAM.</u> This hypothesis can be tested by measuring the coherence between observations and predictions or by examining the power density spectrum of the residuals. Hypothesis D3 and D4 also address the question of diurnal patterns, and it is clear that while daytime patterns are at least qualitatively reproduced, nighttime patterns are not reproduced. This failing may be due to the the nighttime dominance of more distant sources (and/or background levels) and the breakdown of the steady state assumption associated with such multi-hour transport of pollutants, added to the recently discovered (report in press) underestimate of vehicle activity between midnight and 5AM.

D11. The serial correlation between predictions (or observations) will break down as the data are reduced to longer averaging times. One may evaluate the autocovariance of the time series to address this hypothesis; however, it is seen to be true and yet quite trivial since

a) the covariance decreases with increasing lag time τ

b) increased averaging times imply greater spacing between adjacent time steps, thus

c) longer averaging times imply reduced covariance.

D12. The agreement beteen model and observation improves with inclusion of an appropriate background in AQAM. The distributions of $\log_{10}$ (AQAM/OBSERVED CONCENTRATION) shown in Figure 9 and summarized in Table 2 have indicated severe AQAM underprediction in the mean (i.e. a factor of ≈ 3 for CO and NMHC, and ≈ 5 for NO_x). In addition, the widths of these distributions are much wider than required to satisfy the 50% within a factor-of-two rule. Ignoring the downward shifted location of the peak, only 36% of the NO_x values (45% for CO, 42% for NMHC) fall within a factor-of-two of the distribution peak.

The highly skewed nature of these distributions, together with information gleaned from functional dependences of the residuals (see Figures 14 and 15), have indicated that a slight background added to the AQAM predictions might significantly improve the assessment of AQAM predictive power. In fact, the statement concerning 50% within a factor-of-two usually refers to calibrated (i.e., background adjusted) model performance. There are, as previously discussed, a number of ways to select a background concentration; however for this purpose we wish to determine the value of B which yields a mean value of $\log_{10}$ (AQAM + B)/OBSERVED) ≈ 0. Expanding this and retaining first order terms we obtain

$$\ln B \simeq \ln \mu_M - \frac{2}{N} \sum_i \left(\frac{\chi_{T_i}}{2B + \chi_{T_i}} \right)$$

We then approximate the second term further to obtain

$$\ln B \simeq \ln \mu_M - \frac{\mu_T}{\mu_M + \mu_T/2}$$

where μ_M and μ_T are measured and theroretical geometric means respectively. This led to assumed backgrounds of 0.09 ppm for CO, 0.035 ppm for NMHC, and 7.0 ppb for NO_x. These backgrounds proved adequate for CO and NO_x, but the NMHC background had to be increased to 0.08 ppm to bring about the desired result. Figure 31a-c shows the background modified distributions and, from the reduced widths given in Table 2c, one sees that the background term has improved the predictive power of AQAM to the point where, for both AQAM I and II, in excess of 65% of all predictions lie within a factor of two.

QUESTIONS

1. What is the best method for estimating the background component of the hourly average aerometric signals?

2. Which factors, in addition to the following should be used to stratify the data?

   Time of day

   Aircraft activity

   Wind direction

   Wind speed

   Stability category

   Signal-to-noise ratio

   Persistence of meteorological conditions

3. How will the Nephelometer measurements of b_{SCAT} be compared to AQAM predictions of particulate mass concentrations?

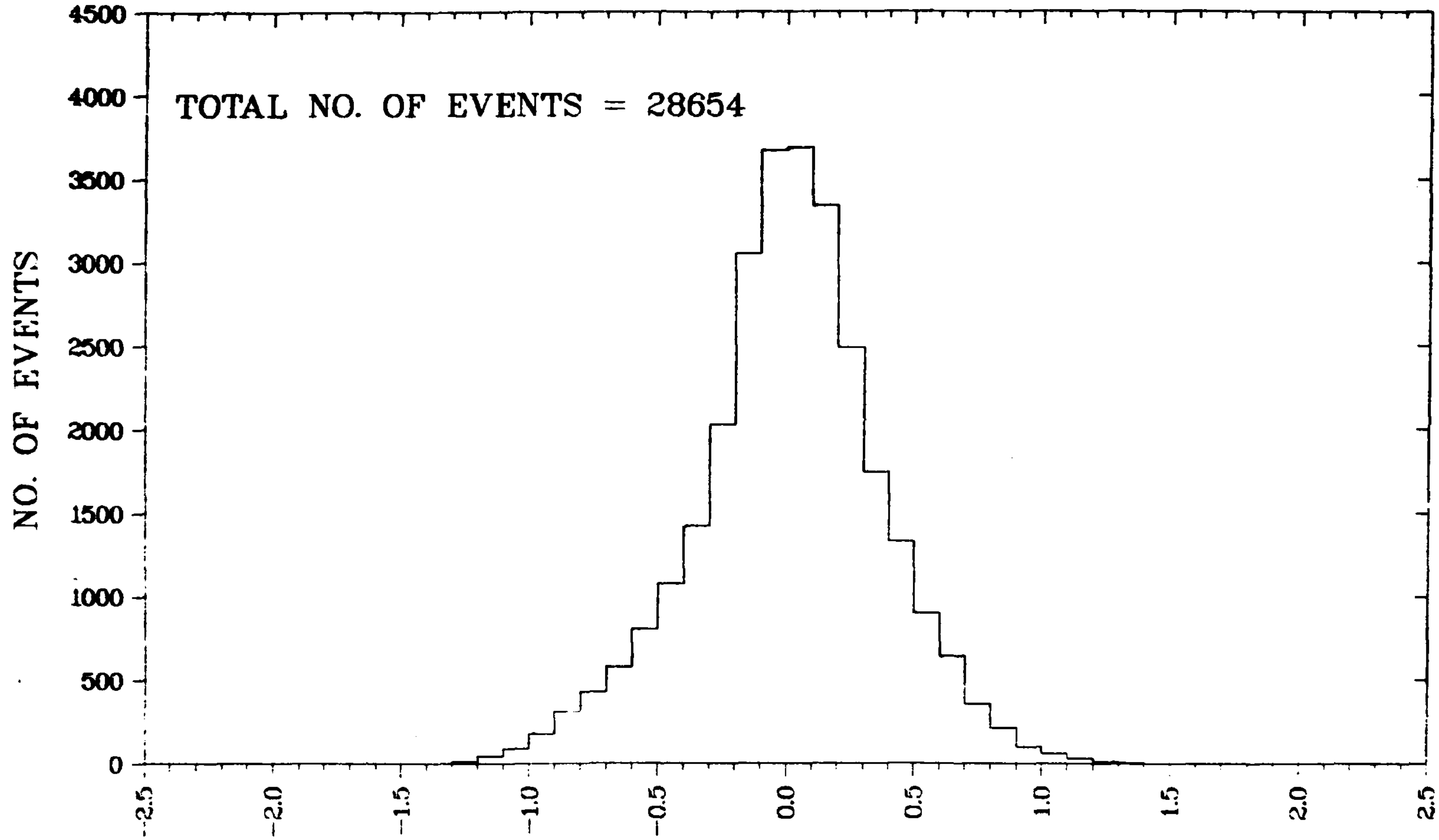


Fig. 31a. Frequency Distribution of $\log_{10}$ ((AQAM II + B)/observation) for all observed CO concentrations above threshold. Williams AFB Hourly Data.

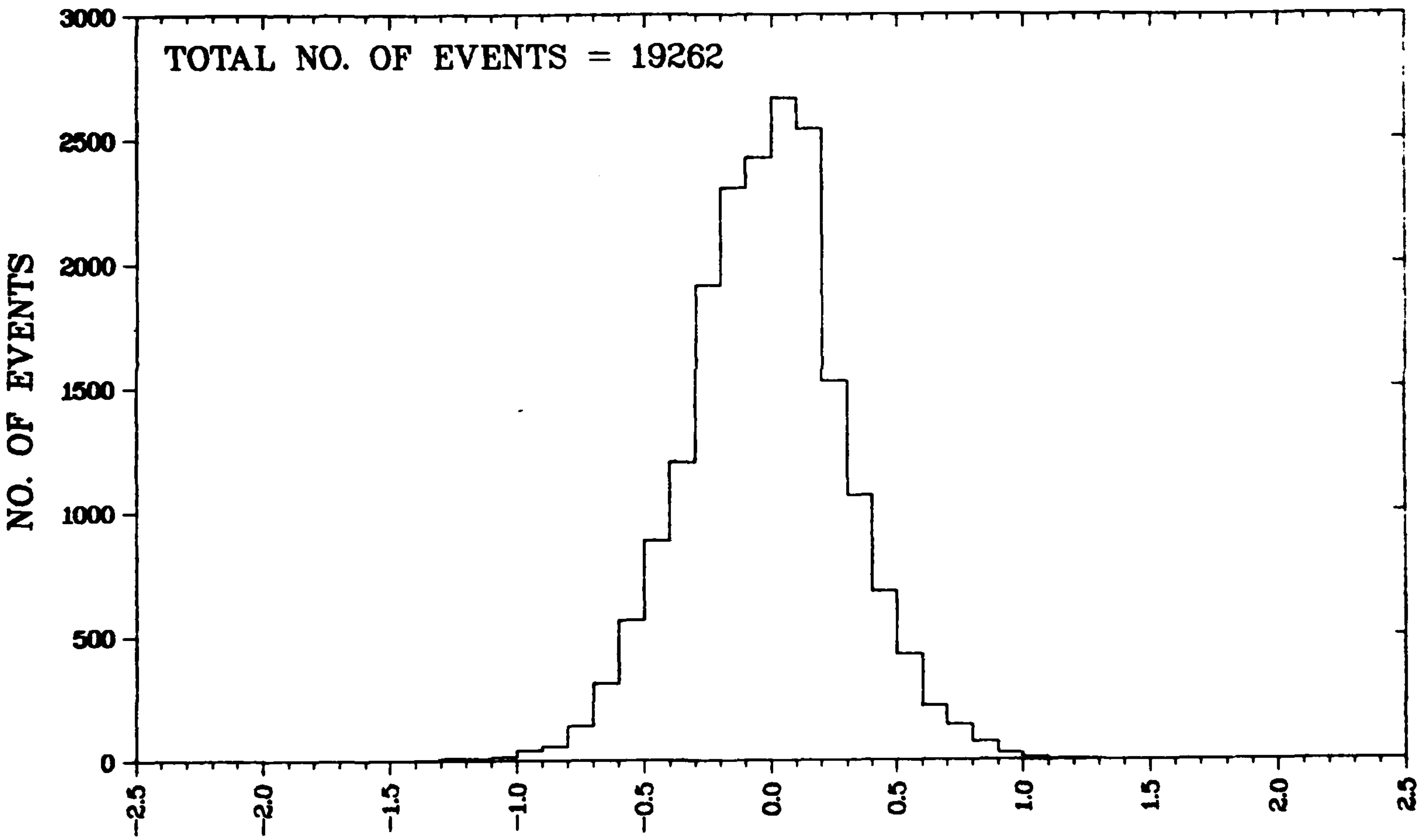


Fig. 31b. Frequency Distribution of $\log_{10}$ ((AQAM II + B)/observation) for all observed NMHC concentrations above threshold. Williams AFB Hourly Data.

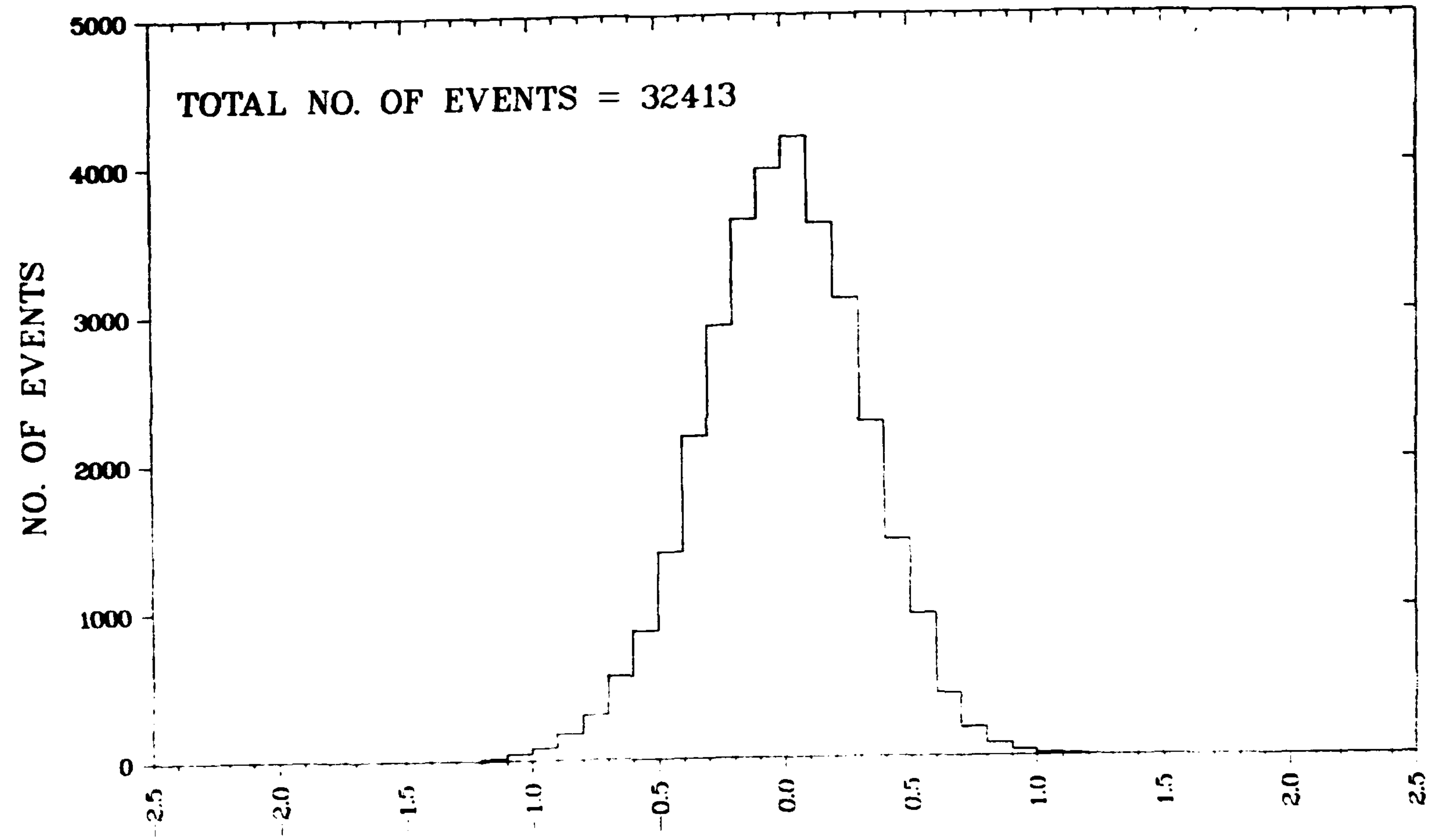


Fig. 31c. Frequency Distribution of $\log_{10}$ ((AQAM II + B)/observation) for all observed NO_x concentrations above threshold. Williams AFB Hourly Data.

SECTION V

CONCLUSIONS

An assessment of the accuracy of the AQAM based on comparison of the model results with air quality data collected during a 13 month experiment at Williams AFB suggest that:

1. The cumulative frequency distributions of AQAM predictions agree reasonably well in slope with the slope of the observed concentrations in the upper percentile range. Ignoring station 4 for the moment because of its atypical site characteristics, concentrations are observed to increase by factors of 4.3, 2.3, and 2.6 for CO, NMHC, and NO_x, respectively, between the 90 and 99 percentile values, while AQAM predictions show increase factors of 2.5, 2.9, and 3.8. Slopes at the lower percentile levels are vastly different and refelct the problem of absence of background levels in the AQAM computations.

    Estimates of the 99.99 percentile concentrations (i.e., highest hourly per year) of $\sim$3 ppm CO, 1-3 ppm NMHC, and 0.1-0.3 ppm NO_x agree surprisingly well with observed values of 2-4 ppm CO, 1-3 ppm NMHC, and 0.08-0.15 ppm NO_x if stations 1, 2, 3, and 5 are considered collectively; however, such estimates for any single station may underpredict the once per year high by as much as a factor of 1.7 for CO and NMHC and 3 for NO_x. The fact that the CFDs converge for the different stations at the upper percentiles of observed concentrations, while the individual station curves diverge slightly for the AQAM predictions, suggests that the most severe pollution episodes actually occur over a spatial domain much larger than the airbase and thus are probably not solely due to specific local sources such as aircraft.

    As for station 4, we note that both AQAM predictions and measurement agree that this station, atypical in the sense of its close proximity to buildings, trees, and automobiles, sees the highest concentrations: a factor of 2-3 higher than station 1, 2, 3, and 5 collectively in the CFD sense. The failure of AQAM to correctly reproduce the observed rank ordering among stations 1, 2, 3, and 5 is thought to be due to dynamical factors such as the neglect of aircraft plume rise (which clearly leads to overprediction of CO and NMHC at station 3).

    Finally, we include the CFDs of AQAM predictions for selected populated sites at and nearby Williams AFB. Figure 32 shows these additional computation points relative to the airbase and the actual monitoring sites. Noting that the distributions in Figures 33a-c are for

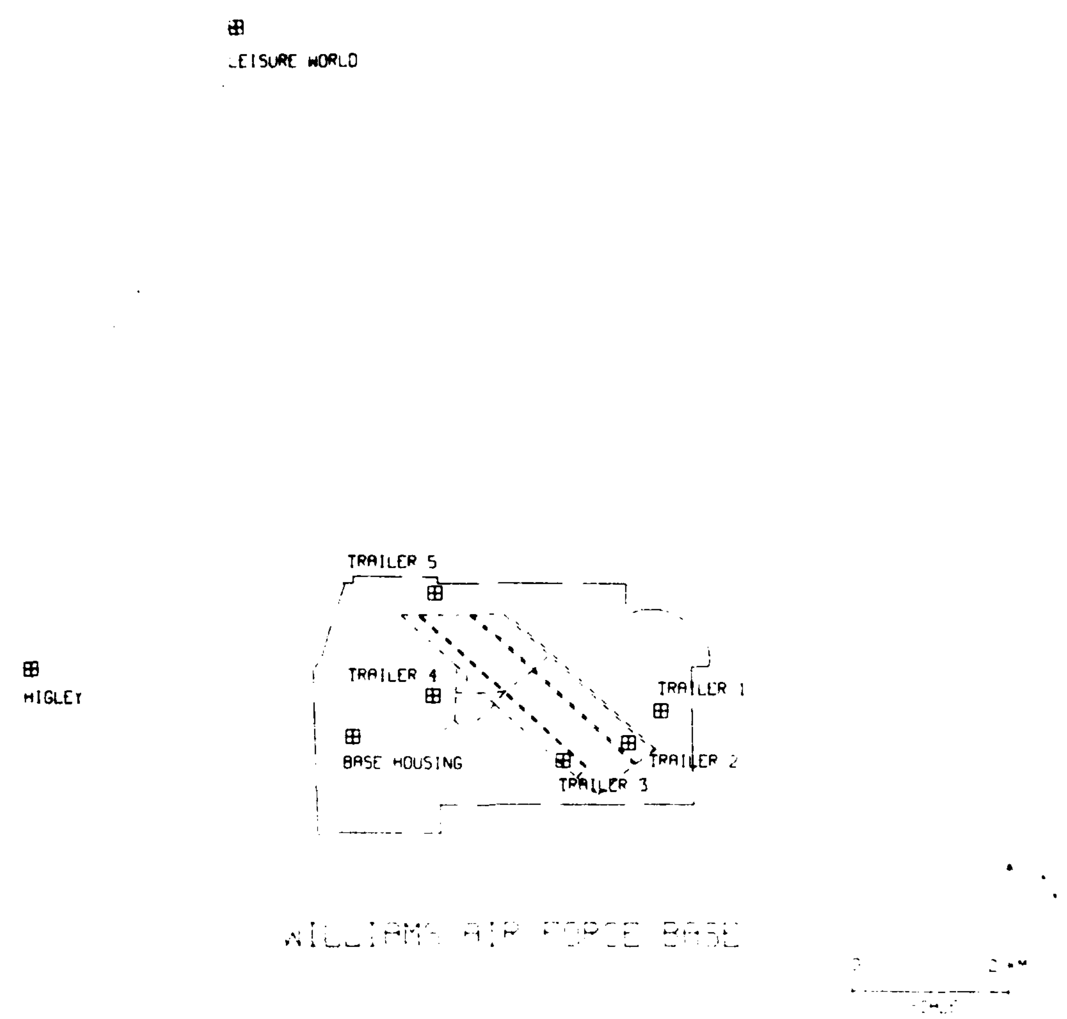


Fig. 32. Receptor Locations and Additional AQAM Computation Points Relative to Williams AFB

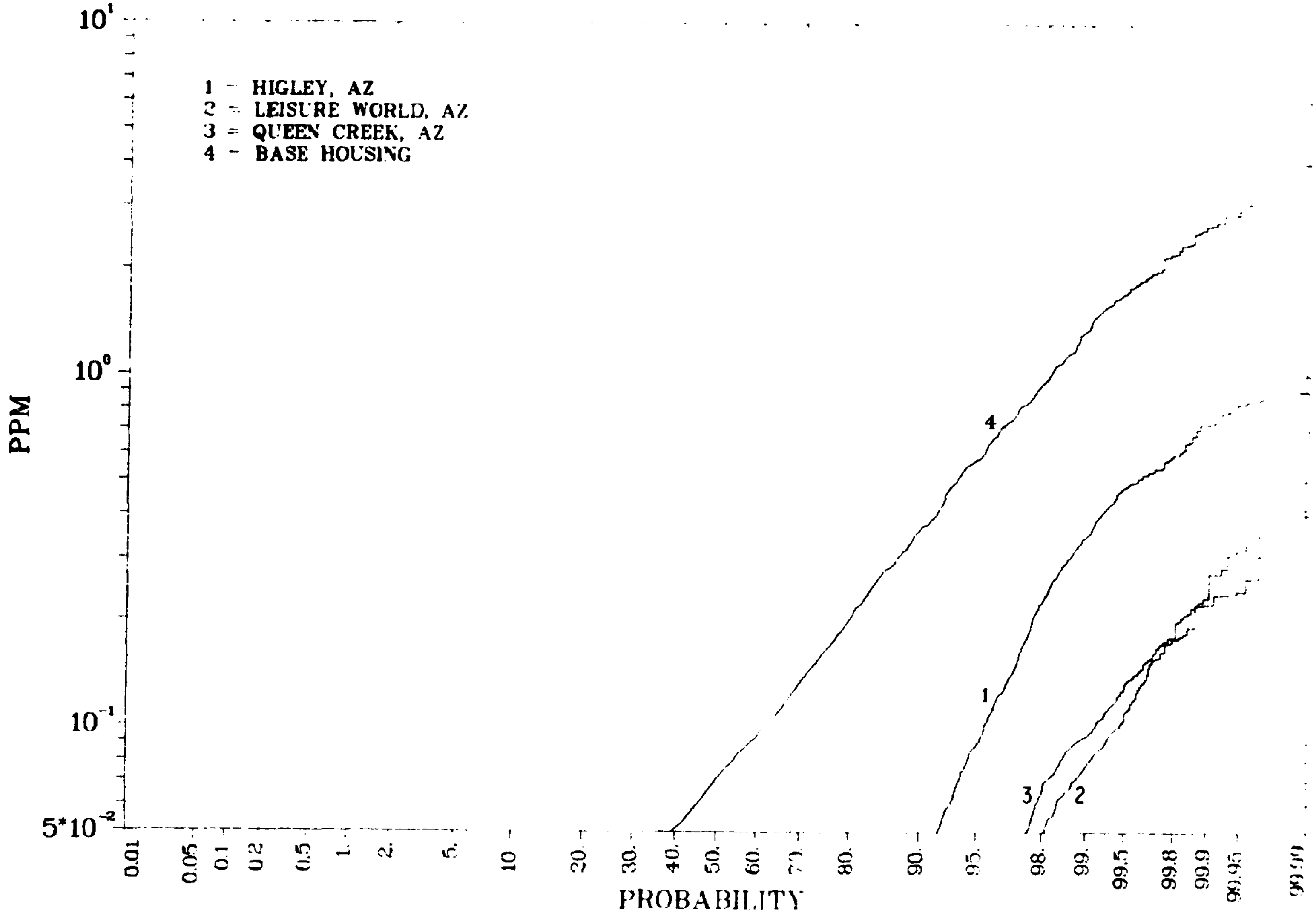


Fig. 33a. Cumulative Frequency Distribution for Hourly AQAM II Predicted CO Concentrations at Selected Sites. Only the contribution from Williams AFB, including Aircraft, is shown.

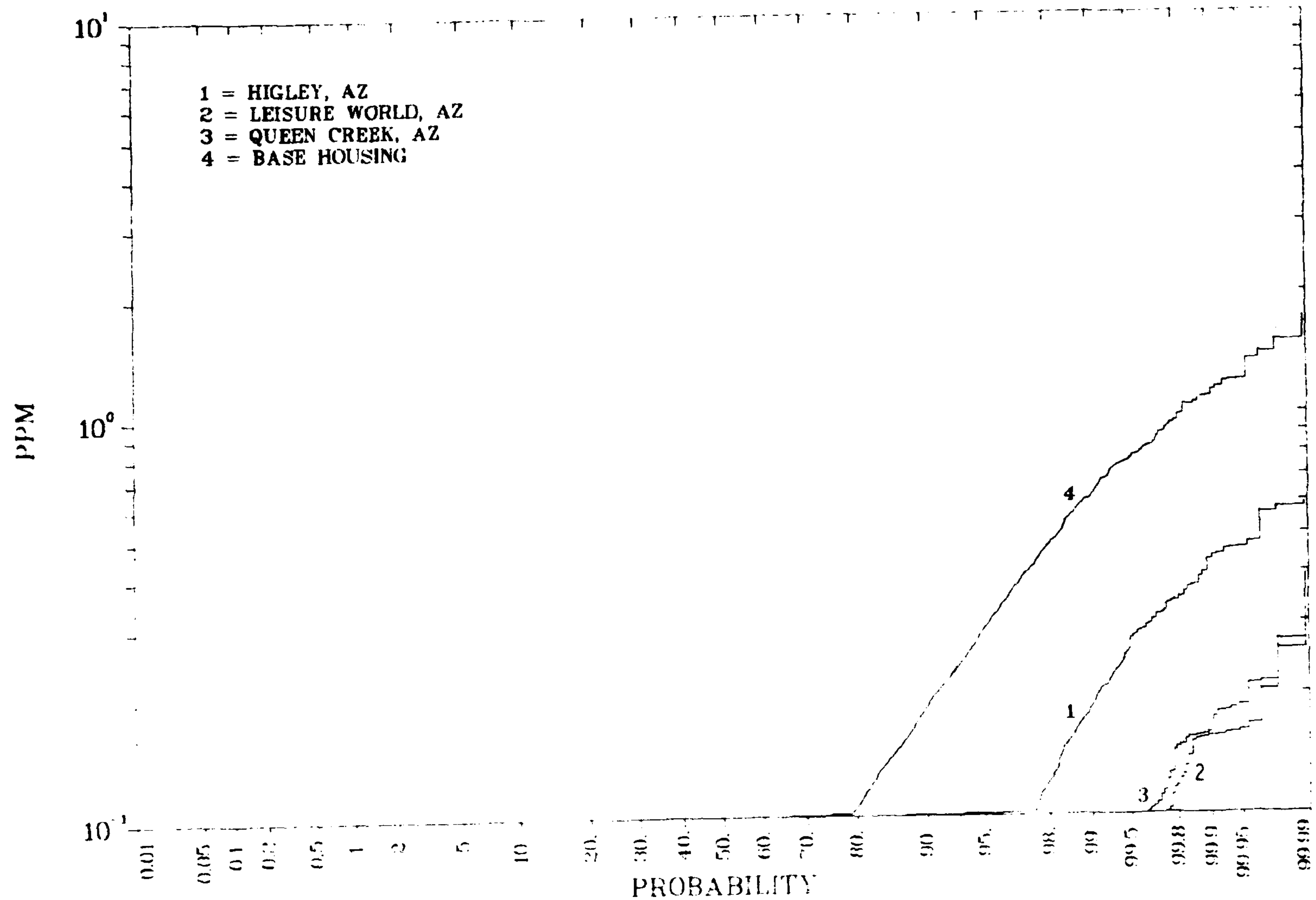


Fig. 33b. Cumulative Frequency Distribution for Hourly AQAM II Predicted NMHC Concentrations at Selected Sites. Only the contribution from Williams AFB, including Aircraft, is shown.

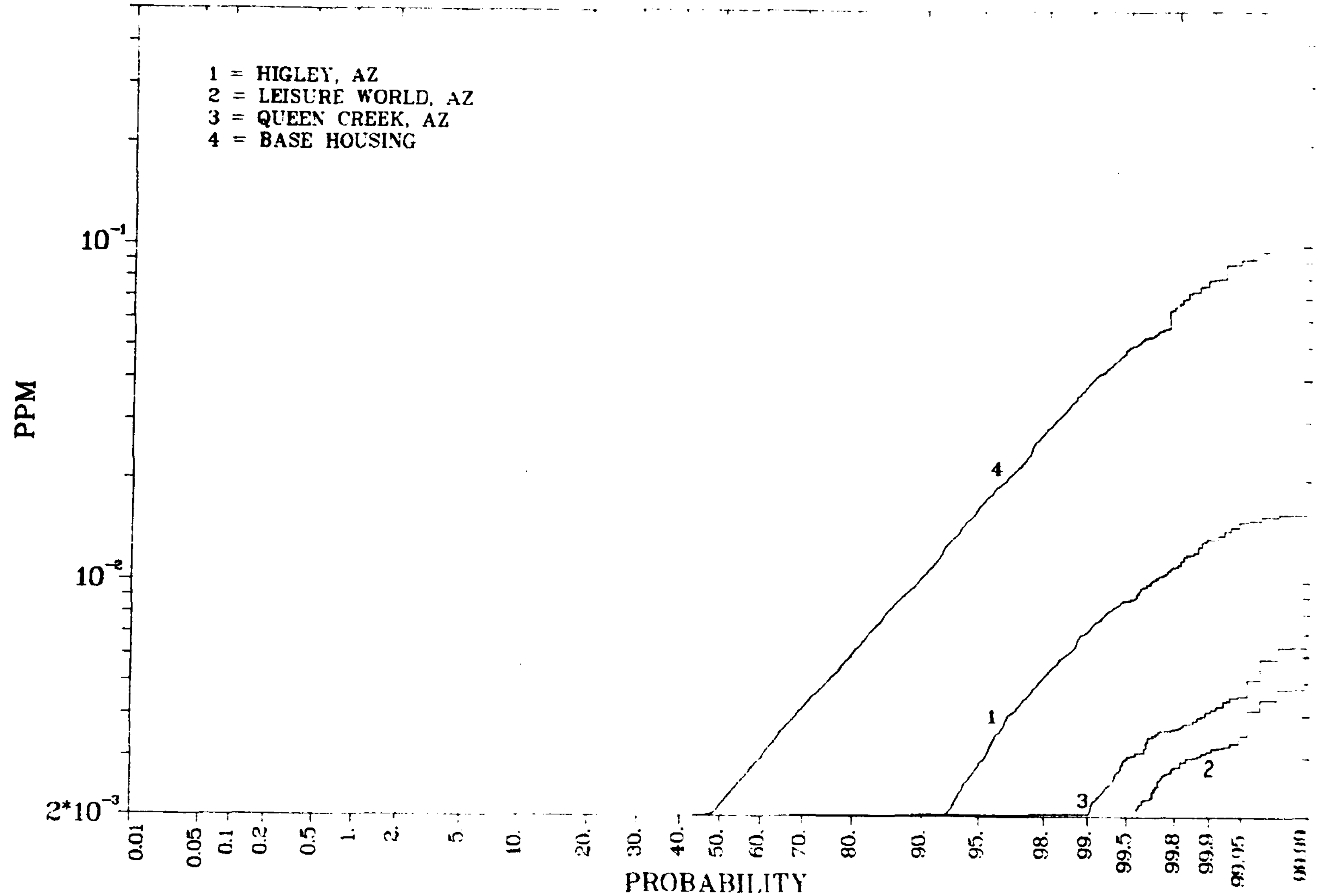


Fig. 33c. Cumulative Frequency Distribution for Hourly AQAM II Predicted NO_x Concentrations at Selected Sites. Only the contribution from Williams AFB, including Aircraft, is shown.

airbase only (including aircraft), we see that maximum concentrations predicted at Higley, Leisure World, and Queen Creek (all of which are on the order of 5 km from the base) are negligible relative to any National Ambient Air Quality Standard (NAAQS), even allowing for possible factors of 2 or 3 underestimates. The same conclusion can be reached for annual average concentrations by examining Table 4. There is, however, finite probability for violating the 6-9 AM National ambient guideline maximum NMHC concentration of 0.24 ppm at these sites, as previously concluded by Daley and Naugle.[12]

Predicted maximum concentrations at Williams base housing fall in the range of those predicted for stations 1, 2, 3, and 5. Thus, it is expected that quite good estimates of actual worst case concentrations at base housing may be obtained by comparison of AQAM and observed CFDs at the five monitoring sites.

2. Hour-by-hour comparisons of AQAM with observations (Table 2) indicate severe underprediction in the mean logarithmic sense for all three pollutants (a factor of 3 for CO and NMHC and a factor of 5 for NO_x). In addition, the standard deviations of these distributions indicate that the unadjusted model falls short of the 50-percent within a factor-of-two criteria for Gaussian models. However, addition of a modest annual mean background (0.09 ppm for CO, 0.08 ppm for NMHC and 7 ppb for NO_x) leads to a dramatic improvement in predictive power. The background adjusted model yields predictions within a factor-of-two of observation in excess of 65% of the time. Prediction errors in excess of factor-of-ten occur at a tolerable ~1% level.

3. Hour-by-hour comparisons of AQAM with observations are clearly complicated primarily by the presence of background pollutant levels, and comparison of interstation differences, where background is automatically subtracted out, appears to be a more robust means of model accuracy assessment. However, regressions on the scatter plots of mean subtracted theory vs mean subtracted observation yield correlation coefficients of less than 0.1 for all pollutants. This results from the fact that 70-90% of these deviations from the mean are instrumentally insignificant.[1] Requiring deviations from the 5-station mean to exceed 0.1 ppm for CO and NMHC (10 ppb for NO_x) one obtains correlation coefficients of 0.43 for CO and 0.34 for NMHC and accompanying regression slopes of ~0.4. Unfortunately, the greater than 10 ppb criteria for NO_x reduces this sample size by more than 90% and yet yields no significant improvement in the correlation coefficient. This poor correlation for NO_x is not so much an indictment against the model as it is a statement that the low NO_x concentration departures from the mean render NO_x

a poor candidate for a validation exercise based on inter-station differences.

4. No significant difference in predictive power between the AQAM I and AQAM II has been found, thus eliminating the need for introducing extremely detailed time histories of aircraft operations into the model.

5. Pollutant levels are found to depend significantly on aircraft emissions at several receptors (see Table 3), but the average concentration impact is small relative to NAAQS. The largest observed impact of aircraft occurs at station 4 where, on the average, aircraft account for 36% of the CO, 28% of NMHC, and 24% of the NO_x. In all cases AQAM overpredicts the percentage role of aircraft emissions but much of this is attributable to background levels not accounted for in AQAM. The fact that AQAM overpredicts the absolute role of aircraft at most stations is thought to be related to the model's neglect of plume rise and plume turbulence enhanced dispersion: two mechanisms which act to reduce concentrations nearby the aircraft.

6. Jet aircraft plume rise should be incorporated into AQAM to avoid overprediction at receptors adjacent to taxiways. (Studies at commercial airports suggest that this overprediction becomes negligible beyond a few hundered meters from the aircraft.) It is not presently known to what extent other aircraft operational modes may require additional detailed plume dynamics.

7. AQAM reproduces the major trends in daytime observed concentrations when local sources dominate but seriously underpredicts at night when more distant sources contribute. This failure, partially due to an underestimate of midnight to 5AM vehicle activity, is probably also due to a breakdown of the steady-state Gaussian plume assumption used in the model, and major revision of the model to incorporate backward trajectories would probably be required to rectify this problem. However, such a revision is perhaps of only academic interest at present since the AQAM is most successful in simulating the potential worst case airbase impact situations associated with morning, low-wind speed, stable or low inversion height conditions coincident with the commencement of high airbase emissions.

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