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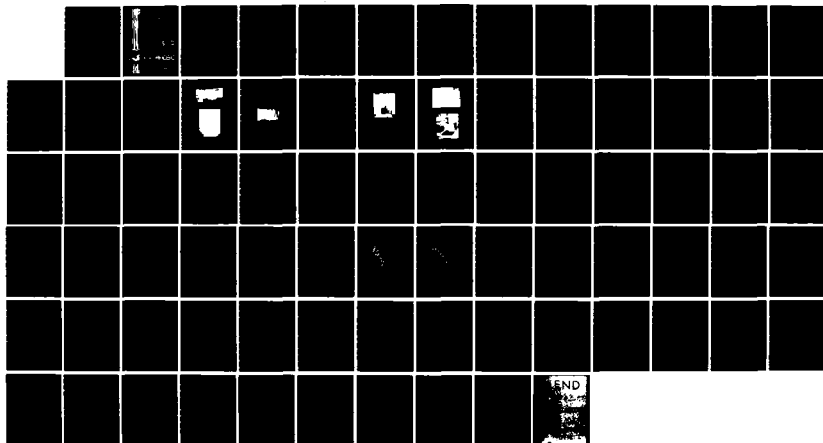
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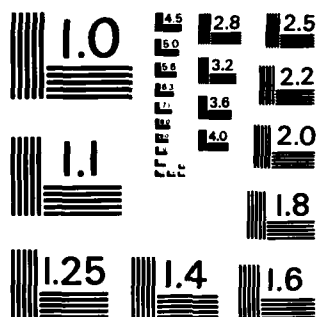
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AIR QUALITY ASSESSMENT MODEL VALIDATION IN COMPLEX TERRAIN

A.M. WACHINSKI, D.R. CROW,
J.D. DUSTIN, and G.D. SEITCHEK

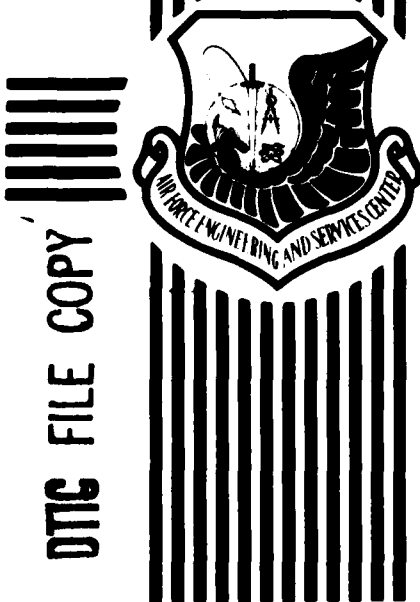
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20. ABSTRACT (Continue on reverse side if necessary and identify by block number) This research effort was conducted to validate the USAF Air Quality Assessment Model (AQAM) for use in measuring environmental impacts of coal conversion projects for Air Force heating and power plants located in a complex terrain scenario. This report documents the results of the project. The first step in the project was to conduct a tracer gas study and gather data to approximate the exhaust plume of the heating plant being studied. The tracer study methodology is discussed in depth in the report. The rationale →		

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behind the sampling network design, and the procedures used to gather the necessary meteorological data, are also covered, ~~within this section.~~

The next step ~~in the study~~ was to input the known meteorological conditions and source characteristics to both AQAM and the Environmental Protection Agency's model, COMPLEX II. Both of these models are described, ~~in the report.~~ Of particular concern are those parameters which can have a significant impact on the predicted results.

Finally, the results of the research are discussed and conclusions are drawn.

*Other topics - sampling design, and Air Pollution, Boiler
emissions, Emissions inventory, and Environmental quality.*

EXECUTIVE SUMMARY

The Air Quality Assessment Model (AQAM) is a predictive computer model developed by the Air Force in 1974 as a planning tool to assess air quality impacts from Air Force Operations; e.g., base closings, aircraft relocations, and fuel conversion projects.

This study was performed to test the validity of AQAM against experimental data gathered in complex terrain and to compare its predictive ability against a United States Environmental Protection Agency (USEPA) Model, COMPLEXII. The operational emphasis was on sulfur emissions from coal and the ability of AQAM to assess the impact of coal conversion projects. The study consisted of two tracer studies performed in the spring and fall of 1982. Sulfur hexafluoride (SF_6) was used as the tracer gas. A known amount was released from a heating plant located on the grounds of the USAF Academy. Samples were collected downwind of the heating plant and analyzed for SF_6 , using gas chromatography. Physical and chemical characteristics of the heating plant stack (source) and known meteorological conditions were input to AQAM and the model was run to predict ground-level concentrations of SF_6 . AQAM's predictions were then compared to those measured and statistically compared.

When predicting the impact on air quality of future Air Force Operations, the parameter of most importance to planners is the maximum ground-level concentrations of various pollutants. AQAM's performance in this area was determined to be considerably better than COMPLEXII. (All tests were performed in complex terrain.) AQAM was able to predict the maximum ground-level concentration within a factor of 5 of the observed, for 100 percent of the time, and within a factor of 2, for 83 percent of the time. The EPA model was able to predict the maximum ground-level concentration within a factor of 5 most of the time; however, COMPLEXII could only predict within a factor of 2, for 44 percent of the time. AQAM tended to predict a ground-level concentration value of 80 percent of that observed. COMPLEXII overpredicted the maximum observed concentration by an approximate factor of 2.

Another field study similar to this one is recommended, but with certain changes. Building wake effects had a major effect on the observed data. These effects should be documented before any definitive statements concerning the predictive performance of AQAM can be made. The performance of AQAM, compared to a data base generated under more "controlled conditions," is recommended; i.e., a flat plane with well-defined source characteristics.

AQAM offers a predictive tool for assessing the effects of Air Force boiler operations on ambient air quality. Its predictive capabilities were found to be better than the USEPA Model, COMPLEXII.

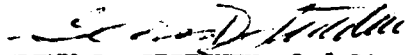
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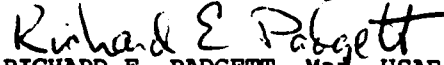
This final report was prepared by the Department of Civil Engineering, United States Air Force Academy, Colorado Springs, Colorado 80840, and covers research performed under Job Order Number 20543042, and Project Order Numbers 81-64, 82-6, and 83-23 for Air Force Engineering and Services Center, Engineering and Services Laboratory, Tyndall Air Force Base, FL 32403.

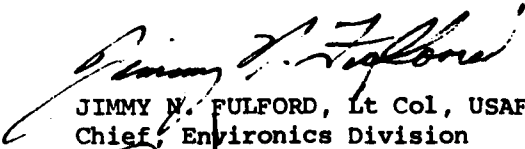
Work on this project was performed from October 1981 through September 1983. The AFESC project officers were Capt Daniel Berlinrut, 1st Lt Mario Ierardi, and 2nd Lt Glenn Seitchek. The Principal Investigators at the USAF Academy were Maj Anthony Wachinski and Maj Jacob Dustin. Mr. Dennis Crow and Mr. Gary Burris contributed significant ideas and efforts to make this research project successful.

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

This report has been reviewed and is approved for public release.


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SECTION I

INTRODUCTION

This report describes the technical approach used to validate the United States Air Force Air Quality Assessment Model (AQAM) and presents definitive conclusions concerning its accuracy. The Air Quality Assessment Model was a generalized model developed to predict the impact of Air Force operations on surrounding air quality (Reference 1). It was designed as a computational tool for preparing environmental assessments, comparing predicted pollutant concentrations to air quality standards, evaluating proposed control strategies, and rank-ordering emission sources.

The objective of this study was to determine the ability of AQAM to accurately predict impacts on air quality resulting from emissions from a stationary point source in complex terrain. The Air Quality Assessment model can analyze air quality impacts from several types of air pollutant generators, including stationary and mobile pollution sources and airborne flight operations. The model can also analyze multipollutant emissions from point, area, and line sources with a resolution of 1 hour. This study does not provide an encompassing validation of the accuracy of AQAM, but is limited to the stationary point-source algorithm in complex terrain. As such, the validation must be considered site-specific.

Secondary objectives were to compile an accurate and applicable data base, ensure that the computer models were applicable to the dispersion process described by the experimental data, and develop an objective statistical methodology to evaluate AQAM's performance.

SECTION II

TECHNICAL APPROACH

Established gaseous tracer technology (tracer release, sample acquisition, and sample analyses) was used to compile an empirical gaseous dispersion data base, against which the performance of AQAM was measured. AQAM's performance was also compared against theoretical results predicted by the United States Environmental Protection Agency's (USEPA) gaseous dispersion model -- COMPLEXII.

Tracer technology allows accurate characterization of the dispersion process. The tracer-release mechanism simulates a controlled air pollutant source. It allows the rate, time duration, and physical location of the source to be accurately controlled and measured. The chemical composition of gaseous tracers is unique, compared to other gaseous compounds in the atmosphere. As such, small concentrations of the tracer gas can be monitored without confusion with background concentrations or emissions from other sources. Finally, a comprehensive sampling network can be established downwind to the source in question. This allows an accurate spatial definition of the pollutant concentrations as they impact downwind areas from the source.

Sulfur Hexafluoride (SF_6) was selected as the tracer gas as it behaves in a manner similar to SO_2 . Conventional gas chromatographic analyses techniques were used to analyze ambient air samples. Tracer data were gathered during seven field tests performed on 3, 4, 5, and 6 May and 14, 15, and 16 September 1982. Meteorological data (windspeed and direction, temperature, atmospheric stability, and mixing-layer depth) were also collected concurrent to the field-test time intervals.

Subsequent to the field experiments, the air quality models, AQAM and COMPLEXII, were executed, using the meteorological parameters and sampler locations present during each field experiment. These predictive modeling results were compared with experimental tracer data. Selected test data were deleted from the tracer gas data base when a direct comparison to the model predictions was not possible without biasing the correlation; ie., wind shift during the test period, or inadequate spatial resolution.

SECTION III

METHODOLOGY

A. SAMPLING NETWORK DESIGN

Collection of ambient air samples was accomplished by establishing a sampling network prior to each test day. Each sampler was placed downwind of the tracer gas release point, using the relative wind direction passing across the tracer gas release point, in this case Heating Plant 2, United States Air Force Academy. Consistent test results were maintained by keeping the basic structure of the sampling network the same. This also allowed for greater accuracy in correlating field data with predictive air quality modeling results. Figure 1 shows the basic sampling network. The network consisted of 25 samplers, placed in five radial directions and downwind distances from the release point. For this network, 25 different locations could be sampled concurrently.

B. GASEOUS TRACER TECHNOLOGY

Gaseous tracer technology uses tracer release, field monitoring, and sample analyses to quantitatively trace the transport of specific airborne constituents. Established gaseous tracer materials, equipment, and instrumentation were employed during all aspects of the study.

1. Tracer Release

The tracer gas sulfur hexafluoride (SF_6), was released approximately 20 meters above ground level from an exhaust stack of the Heating Plant. (Figure 2) A standard K cylinder (Linde, 99.0 percent purity) containing 100 pounds of SF_6 was attached to a manifold system. This system, shown in Figure 3, was composed of a dual-stage regulator, a flow-metering valve, and a linear mass-flowmeter (Hastings Model AHL-5GX-215) with strip chart recorder. Tygon® tubing was used between the mass flowmeter and an in-line stainless steel stinger which was used to inject the tracer gas into the exhaust stack. (Figure 4) Release flow of the tracer gas was controlled during all testing periods. In addition, the SF_6 cylinder was weighed and the weights recorded periodically throughout each test. These differential weights were used to verify the calibration of the mass flowmeter.



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Figure 2. Heating Plant Number 2, United States Air Force Academy



Figure 3. Tracer Release System



Figure 4. Heating Plant Number 2 Exhaust Stack
Showing Stainless Steel Stinger

2. Field Sampling

Gaseous tracer samples were collected with ERCO Model DB4-B air quality samplers. (Figure 5) These samplers sequentially collected four, 1-hour, time-averaged samples using timed on-board pumps. Air samples were collected in polyethylene bags fitted with polypropylene adapters and Tygon® tubing. The accuracy of the sampler to maintain its timing interval was ± 30 seconds per hour. The samplers contained rechargeable battery packs, and could operate in remote locations for extended periods of time. During field operation, the samplers were loaded with new sample bags and deployed to designated sample locations and activated upon test initiation. Upon completion of the test, the sample bags were sealed, transported to the laboratory, and analyzed for sulfur hexafluoride within 4 hours after collection.

3. Sample Analyses

All samples were analyzed, using an ERCO four-port, discrete gas chromatograph (Figure 6). Column material was a 5-angstrom molecular sieve. The carrier gas was ultrahigh-purity nitrogen. Sulfur hexafluoride was determined using electron capture detectors (ECD, titanium tritide). Both columns and detectors were operated at ambient temperature and pressure conditions.

The ERCO Gas Chromatograph consisted of four separate ECD-gas chromatographs operated in a sequential manner, minimum detectability was 5 parts per trillion (ppt), with an accuracy of plus or minus 1 percent. The output signals were recorded on a dual-pen strip chart recorder (Soltec Model 220). Instrument calibrations were performed hourly during sample analysis periods with certified standards (Scott-Marrin Company). Calibration gas concentrations were 50.1 and 510 ppt.

D. METEOROLOGICAL MEASUREMENTS

1. Windspeed and Direction

Two temporary meteorological stations afforded acquisition of field data during the SF₆ tracer testing days. The first station was constructed by ERCO and consisted of an MRI remote meteorological monitoring system. This system was placed on a 20-foot (6.1-meter) tower and provided continuous measurements of windspeed, wind direction, and ambient temperature. This remote wind system

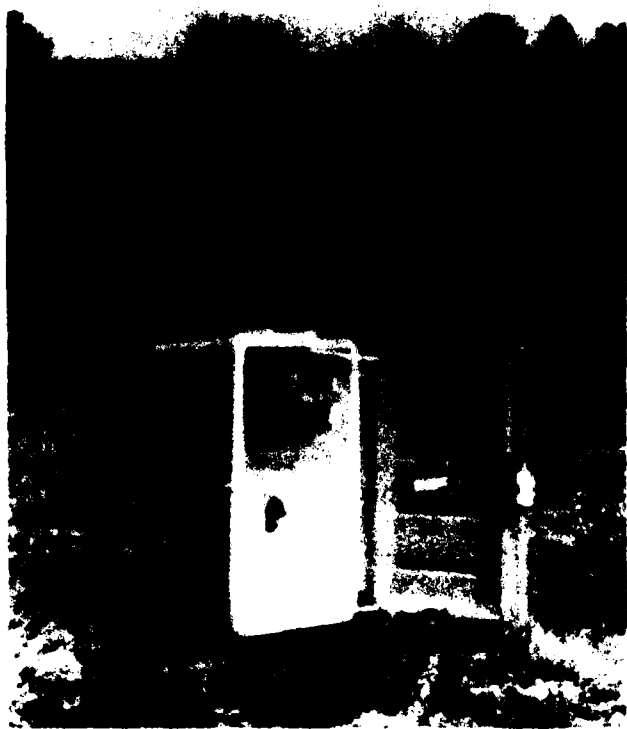


Figure 5. ERCO, Model DB4-B Air Quality Sampler

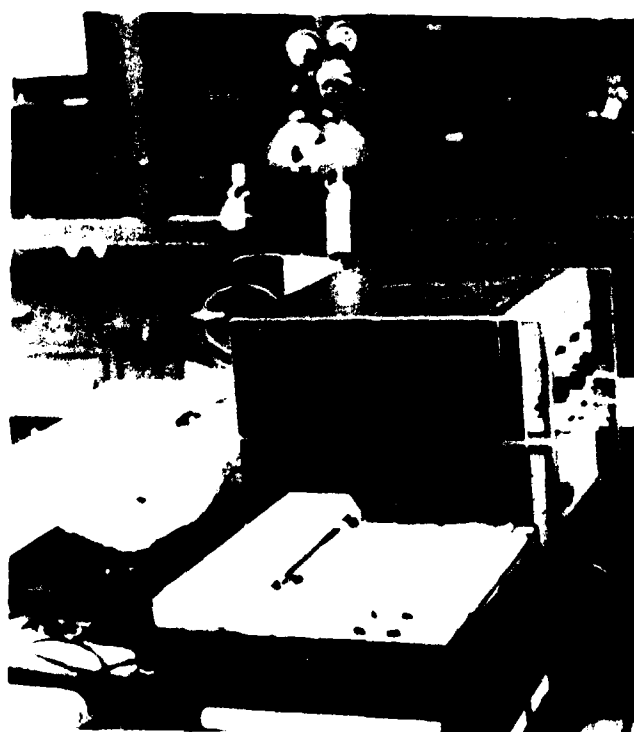


Figure 6. ERCO Gas Chromatograph

was battery-powered and provided all outputs to a strip chart recorder. The second meteorological station was established by the Civil Engineering Department of the United States Air Force Academy (USAFA). This monitoring system was also battery-powered but could not record its measurements onto a strip chart recorder. Thus, the recording of wind speed and direction was performed manually by taking several observations throughout each testing period.

2. Temperature

Temperature measurements were gathered by fixed-wing aircraft at several altitudes over the USAFA airfield. Temperature measurements were also made at ground level using calibrated thermometers. These measurements were made at Meteorological Station Number One, at ground level, when the aircraft landed. Calculations of temperature change as a function of altitude were used to determine atmospheric stability. (See Appendix A).

3. Mixing Depth Estimates

Mixing depths were estimated by using the academy airfield PIBAL wind data or Fort Carson, Colorado rawinsonde data. These data were supplied by the Staff Meteorologist, Tyndall Air Force Base, Florida. (See Appendix A).

E. QUALITY ASSURANCE CONSIDERATIONS

A predefined quality assurance plan was implemented and used during this study. The plan was directed towards the collection of SF₆ tracer data. Energy Resource Company maintained a formal quality assurance plan for use in all tracer studies. The objective of this plan was to ensure that collected data adhered to predefined requirements for completeness, precision, accuracy, representativeness, reproducibility, and comparability. The plan borrows heavily from established methodology (References 2 and 3).

During this project, many samples were reanalyzed. Typically, samples chosen for reanalysis were: (1) samples requiring analysis on a more sensitive range of the gas chromatograph; (2) questionable SF₆ concentrations that did not seem to correlate with other measured data; and (3) samples chosen at random for quality assurance purposes. All sample bags were saved until all data had been analyzed, reduced, and reviewed. Any outlying data points were identified at this point and reanalyzed with appropriate changes (if necessary) made to the data listings. All of the samples chosen at random agreed within plus or minus 5 percent of the original analysis.

Periodic calibrations of the critical testing equipment, i.e., air samplers, gas chromatographs, and the SF₆ mass flowmeter were performed either before or during testing activities. The air samplers were tested for cycling-accuracy and air-sampling flow rate prior to field testing. The accuracy of the air samplers to sequentially cycle from bag to bag was maintained within plus or minus 30 seconds per hour. The minimum acceptable air sampling flow rate was 3 cm³/min.

Gas Chromatographs were calibrated with two certified span gases. Calibrations were performed before and during each hour of sample analyses. The linear range of the gas chromatographs was 0 to 2000 ppt. All SF₆ concentrations measured during this study were less than 2000 ppt, and the data were reduced using linear interpolation techniques.

The mass flowmeter controlling the SF₆ release rate was also calibrated during each testing period. Calibration was accomplished by placing the cylinder of SF₆ on a scale and monitoring weight loss as a function of time. Appropriate corrections to the recorded release rates were performed at the conclusion of the field study.

SECTION IV

THEORETICAL MODELING APPROACH

A. MODELING RATIONALE

The primary objective of this study was to evaluate the ability of AQAM to predict short-term ambient air impacts from stationary point sources in complex terrain. The air quality predictive performance of AQAM was compared with experimentally observed results and predictive results from the USEPA Gaussian model COMPLEXII. The results from COMPLEXII are used to indicate the performance of AQAM in relationship to a standard USEPA air quality model.

Evaluation of AQAM was accomplished, using input parameters measured during each tracer release period. These parameters were input to AQAM to generate a set of point-by-point comparisons of observed and predicted concentrations.

The Parameters listed below were input to AQAM to generate ground-level concentrations of the tracer gas. These data were compared on a point-by-point basis to concentrations measured in the field.

TABLE 1. INPUT PARAMETERS USED FOR EACH RELEASE

<u>SOURCE DATA</u>	<u>METEOROLOGICAL DATA</u>	<u>RECEPTOR DATA</u>
Emission Rate	Measured Wind Direction	Receptor
Stack Exit	Measured Wind Speed	Location
Temperature	Atmospheric Stability	
Stack Exit	Ambient Temperature	
Velocity	Atmospheric Pressure	
Stack	Mixing Depth	
Diameter		
Stack Height		
Source		
Coordinates		
Stack Base		
Elevation		

COMPLEXII was executed with identical input parameters. Correlations between AQAM's predictions with the observed tracer results and COMPLEXII predictions were then ascertained.

B. MODEL DESCRIPTIONS

This section describes the efficacy of AQAM and COMPLEXII in predicting short-term ambient air impacts. Included is a brief summary of each model's characteristics and those parameters found to affect model performance.

1. AQAM

Transport and dispersion of pollutant emissions are modeled using steady-state Gaussian plume formulation, and 1-hour averaging time. AQAM can be used to model emissions from point, area, and line sources. Sources of finite initial volume are treated by a virtual source technique. Line sources are treated by an analytical integration over the length of the line, and, square-area sources are treated as pseudopoint sources located some distance upwind of the actual area source. Time-travel and travel-distance dependent dispersion coefficients are used to estimate the lateral and vertical diffusion of the plume according to stability as determined by Turner's criteria (Reference 4). Effective emission height is estimated, using the downwash rules of Briggs (Reference 5) and plume-rise equations of Holland, Moses et al., or Briggs (References 5, 6, and 7). Depth of the mixing layer can be input directly or calculated, using a model developed by the Air Force. This model utilizes surface observations and includes both mechanical and thermal contributions.

The short-term model of AQAM calculates real-time, hourly averaged pollutant concentrations over a receptor grid using conventional Gaussian plume technique which accounts for both lateral and vertical plume diffusion. AQAM uses the Pasquill-Gifford dispersion coefficients presented in Turner's Workbook of Atmospheric Dispersion Estimates, (Reference 4) which are converted from a 10- to 60-minute sampling time. The short-term model uses hourly averaged windspeed and direction, stability, and mixing depth assumed constant over the hour for which the calculation is being performed.

2. COMPLEXII

Transport and dispersion of pollutant emissions are modeled using a multiple-point-source Gaussian model with optional terrain adjustments. COMPLEXII estimates concentrations on an hour-by-hour basis for relatively inert pollutants, e.g., sulfur dioxide (SO_2). It uses Pasquill-Gifford dispersion parameters (Reference 4) and the Briggs plume rise method (Reference 5) to calculate the spread and rise of plumes. The model is most applicable for

source-receptor distances less than 10 kilometers (6.2 miles) and for locations with level or gently rolling terrain. Terrain adjustments are restricted to receptors whose elevation is no higher than the lowest stack top. Options are also available for wind-profile exponents, bouyancy-induced dispersion, gradual plume rise, stack downwash, and plume half-life.

C. MODEL PARAMETERS

Correlation of tracer data to modeled results predicted by AQAM and COMPLEXII is subject to numerous misinterpretations. Several parameters, e.g., source characteristics and meteorological conditions, can have a significant impact on the predicted results. Model accuracy and validity are, therefore, dependent upon the values of these parameters. Additionally, parameters which affect the dispersion of the SF₆ tracer which are NOT accounted for in the air quality models must be ascertained to determine why a model may or may not correctly simulate the physical environment correctly. The following directly influenced differences of modeled results to SF₆ tracer data.

1. Sampling Network Density

The density of the sampling network plays a key role in obtaining experimental data that accurately described peak plume concentration and plume widths. During unstable atmospheric conditions, a wider, less dense sampling network was required since the plume is dispersed over a wider area. During neutral or stable atmospheric conditions, however, the plume was much narrower and required a very dense sampling network to prevent it from passing between the samplers. This characteristic was evident during the tracer testing periods conducted under neutral and stable atmospheric conditions. For example, COMPLEXII predicted a peak concentration of approximately 19.7 micrograms per cubic meter ($\mu\text{g}/\text{m}^3$) for 15 Sep 82, hour 1200-1300. Changing the modeled wind direction 5 degrees resulted in a 1.86 $\mu\text{g}/\text{m}^3$ change in peak plume concentration at the same location, indicating the plume was narrower than the resolution afforded by the sampling network.

2. Plume Measurements at Low Windspeeds

Comparing modeled results to measured results during low windspeeds; i.e., less than 2 meters per second (m/s) can result in numerous errors. At times during the tracer testing period, windspeeds less than 2 m/s were recorded (near calm conditions). The wind direction under these

conditions meandered, causing the tracer plume to spread across the entire sampling network. Neither AQAM nor COMPLEXII could account for this meandering wind direction during a 1-hour sampling period, since the inputs for the models specify only one wind direction during each sampling period. Modeling under these conditions could be improved by modifying the model to accept specific wind directions as a function of time over the sampling period.

3. Complex Terrain

As AQAM was "validated" in complex terrain, any conclusions reached concerning its predictive capability must be considered site-specific. Comparing modeled results of ground-level concentrations to experimental tracer data in complex terrain resulted in many errors. For example, complex terrain added turbulence, eddies, and channeling effects to the plume at various downwind locations which could not be input to the air quality models. The mean air flow being deflected around an obstacle such as a hill would cause the centerline of the plume to change dramatically. Both AQAM and COMPLEXII cannot account for this deflection and would assume that the plume would be transported along the same path without being diverted. Additionally, as explained in the stability determination, complex terrain acts to disperse the plume more than flat terrain. These characteristics could result in poor correlation of the tracer data to modeled results.

4. Wind Measurements

Accurate measurements of windspeed and wind direction are very critical in the modeling analysis, as a difference of only 5 degrees in the wind direction could result in large differences of modeled concentrations at the same receptor location. Windspeed also has a significant effect on modeled concentrations, since deposition of ground-level pollutants is a function of windspeed. Representative windspeed must be determined to correctly characterize the values of windspeeds at all locations and times throughout the sampling network. Two wind sensors located in complex terrain are not sufficient to provide the accuracy required by the models.

5. Building Wake Effects

The tracer gas was released from the exhaust stack of the heating plant, 63 feet (20 meters) above ground level. The stack exhaust exit was only 10 feet above the building. With the stack exit located very close to the top of the building itself, building wake effects could trap the

released sulfur hexafluoride into eddies and aerodynamic wakes caused by the wind flow across the building. Huber and Snyder (Reference 8) and Huber (Reference 9) estimated that exhaust from a point source would be affected by the building wakes if the calculated plume height (the sum of the stack height and the momentum rise at a downwind distance of two building heights) is less than either two and one-half building heights or the sum of the building height and one and one-half times the building width. Both conditions were present during every hour of testing. The tracer plume was recirculated by the aerodynamic wake before being transported downwind by the mean wind flow. This recirculation process acted to alter both plume height and width.

6. Limits of Applicability of AQAM in Complex Terrain

AQAM was compared to experimental data taken during unstable atmospheric conditions. Additional data were obtained for stable atmospheric conditions. These data could not be accurately compared to AQAM's predictions because the resolution of discrete sampling points was not adequate to define the plume's signature.

Results showed that AQAM could predict ambient and quality impacts in complex terrain during unstable atmospheric conditions within acceptable accuracy. Experience has shown that improved model-experimental data correlation occurs during unstable atmospheric conditions. One reason is the ability of the plume to "flow" over complex terrain more readily during unstable conditions.

A stable air mass is not easily displaced upward and tends to "pile-up" along windward slopes. If the terrain elevation is too high, the plume will go around, rather than over the terrain. During unstable atmospheric conditions, the plume will not exhibit this tendency but will follow the contour of the terrain, resulting in less horizontal plume meander.

If sufficient experimental data were available for stable atmospheric conditions, the correlation between AQAM's predictions and experimental data would not have been as high. A specific case involves the situation where terrain height exceeds plume height, causing the plume to "flow" around, rather than over the terrain.

SECTION V

COMPARISON OF MODEL PREDICTIONS WITH OBSERVED GROUND-LEVEL CONCENTRATIONS

This section presents specific guidelines for the compilation of the data base used to summarize the tracer field experiments. Certain data were accepted, or rejected from the data base. This data base was used for direct comparison with modeled predictive results.

A. METHODOLOGY

1. Rejection of Biasing Data

Several unique physical situations occurred during data collection that AQAM and COMPLEXII were not designed to handle. Applying AQAM to a physical situation for which it was not designed affected its validity. For the following conditions, the tracer data were deleted from the data base.

- a. Wind direction shift during the sampling period
- b. Windspeeds less than 2 m/s
- c. Neutral or stable atmospheric conditions.
(Under these conditions the plume was narrower than the resolution provided by the sampling network.)
- d. Zero, near zero, and low concentration comparisons. (Taking the ratio of low concentration values with zero or near zero values results in large relative errors being associated with small differences in concentrations.) To minimize these errors, results were assumed zero when both AQAM and the tracer concentrations were near zero. The emphasis in modeling is to predict maximum concentrations; low concentrations are not as critical.

2. Wind Direction Modifications

Wind direction is a key parameter which affects the predictive performance of modeled results to measured or observed results. A relatively small shift in wind direction between two identical modeling runs can result in large changes in concentrations predicted at the receptor. The predictive performance of modeled results is highly sensitive to the choice of wind direction. Apparent model performance; i.e., correlation of observed and predicted concentrations, can be improved significantly by an

appropriate choice of wind direction since the observed plume centerline seldom coincides exactly with the measured wind direction.

For this study, the measured wind direction was modified to align the peak concentration predicted by the models with the observed peak concentration. This alignment of peak concentrations maximized model predictions at that location and biased the comparison of predicted and observed maximum concentrations. But, model validation was based on the relative error of averaged measured concentrations, rather than the single highest value.

C. Summary of Observed and Predicted Results

Tables 2 thru 13 summarize observed tracer concentrations and the predicted AQAM and COMPLEXII concentrations for each test day and hour accepted into the final data base. If both observed and predicted concentrations were zero they were omitted from these summaries. Furthermore, to allow statistics to be combined from multiple test periods, all concentrations have been normalized to remove emission rate dependence. All concentrations for combined statistics are calculated as X/Q in units of sec/m^3 .

D. Statistical Rationale

Statistics were used to identify, determine, and judge the correlation, if any, between the observed (experimental) results and those predicted by AQAM. Statistics were also used to ascertain conditions under which AQAM could provide predictions within a certain predefined tolerance. Three tolerance categories were established to define the limits in which predicted results differed from observed results. The categories were excellent agreement, moderate agreement, and no agreement. These categories were based on the ratio between observed and predicted results. Table 14 summarizes the categories.

Given these tolerances, specific statistical tests can be applied and a point-by-point comparison of observed and predicted concentrations made. These tests provide definitive and reliable indications of the performance of AQAM. These statistical tests were established to address the following three fundamental questions:

a. How effective is AQAM in predicting maximum observed concentrations?

b. How effective is AQAM in predicting all observed concentrations (both high and low)?

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TABLE 2. SF₆ SUMMARY CONCENTRATION TABLE (MICROGRAMS/M**3)

USAF SF₆ TRACER STUDY

MODELED RESULTS FOR 3 May 1982

RECEPTOR NO. NAME	EAST COORD (KM)	NORTH COORD (KM)	RECEPTOR HT ADV GRD (M)	RECEPTOR 680-LVL ELEV (FEET)	EXPERIMENTAL OBSERVED CONCENTRATIONS	ADAM PREDICTED CONCENTRATIONS	COMPLEXII PREDICTED CONCENTRATIONS
90 -25	0.31	0.00	0.6	7013.0	0.316	0.000	0.000
105-50	0.72	-0.15	0.6	6920.0	0.267	0.000	0.000
105-75	1.28	-0.33	0.6	6960.0	0.000	0.000	0.000
105-1.0	1.59	-0.41	0.6	6920.0	0.000	0.000	0.000
105-2.0	3.13	-0.77	0.6	6680.0	0.000	0.000	0.000
120-50	0.64	-0.38	0.6	6960.0	2.855	0.862	0.216
120-75	1.15	-0.67	0.6	6800.0	1.373	0.238	0.031
120-1.0	1.46	-0.82	0.6	6760.0	1.100	0.132	0.012
120-2.0	2.69	-1.56	0.6	6680.0	0.298	0.037	0.003
135-25	0.23	-0.20	0.6	7040.0	3.305	6.943	14.577
135-75	0.82	-0.87	0.6	6800.0	2.679	0.045	1.717
135-1.0	1.15	-1.21	0.6	6760.0	2.466	0.503	0.852
135-2.0	2.15	-2.28	0.6	6800.0	1.999	0.152	0.250
150-25	0.18	-0.26	0.6	7040.0	6.166	8.359	30.635
150-50	0.38	-0.69	0.6	7000.0	5.601	1.978	4.341
150-75	0.59	-1.05	0.6	6840.0	3.230	0.949	1.822
150-1.0	0.72	-1.46	0.6	6900.0	3.669	0.486	0.713
150-2.0	1.31	-2.80	0.6	6720.0	1.215	0.133	0.151

TABLE 3. SF₆ SUMMARY CONCENTRATION TABLE (MICROGRAMS/M**3)

USAF SF₆ TRACER STUDY
MODELED RESULTS FOR 6 May 1982

RECEPTOR NO. NAME	EAST COORD (KM)	NORTH COORD (KM)	RECEPTOR HT ABV GRD (M)	RECEPTOR GRD-LVL ELEV (FEET)	EXPERIMENTAL OBSERVED CONCENTRATIONS	ADAM PREDICTED CONCENTRATIONS	COMPLEXII PREDICTED CONCENTRATIONS
80 --.25	0.31	0.03	0.6	7013.0	3.627	1.558	2.308
105-.50	0.72	-0.15	0.6	6920.0	2.256	0.543	1.346
105-.75	1.28	-0.33	0.6	6960.0	0.644	0.317	0.220
105-2.0	3.13	-0.77	0.6	6680.0	0.037	0.145	0.017
130-.25	0.23	-0.13	0.6	7040.0	1.634	2.628	7.400
130-1.0	1.38	-1.13	0.6	6760.0	0.031	0.073	0.003
130-2.0	2.55	-2.15	0.6	6800.0	0.736	0.036	0.000
155-.25	0.18	-0.36	0.6	7040.0	0.000	0.004	0.000
155-.50	0.36	-0.69	0.6	7000.0	0.000	0.000	0.000
155-.75	0.54	-1.13	0.6	6840.0	0.000	0.000	0.000
155-1.0	0.67	-1.49	0.6	6900.0	0.000	0.000	0.000
155-2.0	1.31	-2.80	0.6	6720.0	0.000	0.000	0.000
180-.25	0.00	-0.32	0.6	7040.0	0.000	0.000	0.000
180-.50	-0.03	-0.75	0.6	7100.0	0.000	0.000	0.000
180-.75	0.00	-1.26	0.6	7040.0	0.000	0.000	0.000
180-1.0	0.00	-1.62	0.6	7000.0	0.000	0.000	0.000
180-2.0	0.00	-3.00	0.6	6840.0	0.000	0.000	0.000

TABLE 4. SF₆ SUMMARY CONCENTRATION TABLE (MICROGRAMS/M**3)

USAF SF₆ TRACER STUDY

MODELED RESULTS FOR 6 May 1982

HOUR	THETA (DEG)	SPEED (M/S)	MIXING HEIGHT(M)	TEMP (K)	STABILITY CLASS
11	330.00	4.00	7363.00	277.00	1

RECEPTOR NO. NAME	EAST COORD (KM)	NORTH COORD (KM)	RECEPTOR HT ABV GRD (M)	RECEPTOR GRD-LVL ELEV (FEET)	EXPERIMENTAL OBSERVED CONCENTRATIONS	ADAM PREDICTED CONCENTRATIONS	COMPLEXII PREDICTED CONCENTRATIONS
80 --25	0.31	0.08	0.6	7013.0	0.601	0.006	0.000
105-.50	0.72	-0.15	0.6	6920.0	0.097	0.019	0.000
105-.75	1.28	-0.33	0.6	6960.0	0.000	0.000	0.000
105-1.0	1.59	-0.41	0.6	6920.0	0.000	0.000	0.000
105-2.0	3.13	-0.77	0.6	6680.0	0.000	0.000	0.000
130-.25	0.23	-0.13	0.6	7040.0	5.158	1.722	1.271
130-.50	0.69	-0.51	0.6	7000.0	1.276	0.256	0.144
130-.75	1.03	-0.82	0.6	6800.0	0.693	0.187	0.048
130-1.0	1.38	-1.13	0.6	6760.0	0.255	0.140	0.018
130-2.0	2.55	-2.15	0.6	6800.0	0.061	0.079	0.003
155-.25	0.18	-0.36	0.6	7040.0	5.129	1.441	7.341
155-.50	0.36	-0.69	0.6	7000.0	1.780	0.514	1.132
155-.75	0.54	-1.13	0.6	6840.0	0.450	0.336	0.263
155-1.0	0.67	-1.49	0.6	6900.0	0.389	0.261	0.113
155-2.0	1.31	-2.80	0.6	6720.0	0.097	0.149	0.017
180-.25	0.00	-0.32	0.6	7040.0	4.520	1.201	0.936
180-.50	-0.03	-0.75	0.6	7100.0	0.073	0.246	0.039
180-.75	0.00	-1.26	0.6	7040.0	0.043	0.103	0.009
180-1.0	0.00	-1.62	0.6	7000.0	0.050	0.076	0.003
180-2.0	0.00	-3.00	0.6	6840.0	0.050	0.035	0.000

TABLE 5. SF₆ SUMMARY CONCENTRATION TABLE (MICROGRAMS/M**3)USAF SF₆ TRACER STUDY

MODELED RESULTS FOR 6 May 1982

RECEPTOR NO. NAME	EAST COORD (KM)	NORTH COORD (KM)	RECEPTOR HT ABV GRD (M)	RECEPTOR GRD-LVL ELEV (FEET)	EXPERIMENTAL OBSERVED CONCENTRATIONS	ADAM PREDICTED CONCENTRATIONS	COMPLEXII PREDICTED CONCENTRATIONS
80 -25	0.31	0.08	0.6	7013.0	1.543	0.000	0.000
105-50	0.72	-0.15	0.6	6920.0	1.440	0.027	0.000
105-75	1.28	-0.33	0.6	6960.0	0.371	0.006	0.000
105-2.0	3.13	-0.77	0.6	6680.0	0.000	0.000	0.000
130-25	0.23	-0.13	0.6	7040.0	4.435	2.547	1.802
130-50	0.69	-0.51	0.6	7000.0	1.458	0.249	0.212
130-75	1.03	-0.82	0.6	6800.0	0.559	0.085	0.070
130-2.0	2.55	-2.15	0.6	6800.0	0.109	0.029	0.004
155-25	0.18	-0.36	0.6	7040.0	5.844	2.130	10.852
155-50	0.36	-0.69	0.6	7000.0	2.163	0.510	1.674
155-75	0.54	-1.13	0.6	6840.0	0.073	0.149	0.389
155-1.0	0.67	-1.49	0.6	6900.0	0.237	0.097	0.167
155-2.0	1.31	-2.80	0.6	6720.0	0.079	0.055	0.025
180-25	0.00	-0.32	0.6	7040.0	4.556	1.776	1.383
180-50	-0.03	-0.75	0.6	7100.0	0.352	0.212	0.057
180-75	0.00	-1.26	0.6	7040.0	0.225	0.057	0.013
180-1.0	0.00	-1.62	0.6	7000.0	0.103	0.030	0.005
180-2.0	0.00	-3.00	0.6	6840.0	0.000	0.013	0.000

TABLE 6. SF₆ SUMMARY CONCENTRATION TABLE (MICROGRAMS/M**3)USAF SF₆ TRACER STUDY

MODELED RESULTS FOR 6 May 1982

RECEPTOR NO. NAME	EAST COORD (N)	NORTH COORD (N)	RECEPTOR HT ABV GRD (M)	RECEPTOR GRD-LVL ELEV (FEET)	EXPERIMENTAL OBSERVED CONCENTRATIONS	ADAM PREDICTED CONCENTRATIONS	COMPLEXII PREDICTED CONCENTRATIONS
80 -25	0.31	0.08	0.6	7013.0	0.115	0.000	0.000
105-25	0.26	-0.05	0.6	6920.0	0.073	0.313	0.001
105-50	0.72	-0.15	0.6	6920.0	0.000	0.017	0.000
105-75	1.25	-0.33	0.6	6960.0	0.000	0.006	0.000
105-2.0	3.13	-0.77	0.6	6680.0	0.000	0.000	0.000
130-25	0.23	-0.13	0.6	7040.0	2.351	1.585	1.111
130-50	0.69	-0.51	0.6	7000.0	0.395	0.155	0.132
130-75	1.03	-0.82	0.6	6800.0	0.091	0.053	0.044
130-1.0	1.38	-1.13	0.6	6760.0	0.073	0.032	0.017
130-2.0	2.55	-2.15	0.6	6800.0	0.036	0.018	0.002
155-25	0.18	-0.36	0.6	7040.0	1.652	1.325	6.738
155-50	0.36	-0.69	0.6	7000.0	1.804	0.317	1.042
155-1.0	0.67	-1.49	0.6	6900.0	0.194	0.060	0.104
155-2.0	1.31	-2.80	0.6	6720.0	0.608	0.034	0.016
180-25	0.00	-0.32	0.6	7040.0	2.473	1.105	0.856
180-50	-0.03	-0.75	0.6	7100.0	0.280	0.132	0.036
180-75	0.00	-1.26	0.6	7040.0	0.164	0.035	0.008
180-1.0	0.00	-1.62	0.6	7000.0	0.158	0.019	0.003
180-2.0	0.00	-3.00	0.6	6840.0	0.000	0.008	0.000

TABLE 7. SF₆ SUMMARY CONCENTRATION TABLE (MICROGRAMS/M**3)

USAF SF₆ TRACER STUDY
MODELED RESULTS FOR 14 SEPTEMBER 1982

RECEPTOR NO. NAME	EAST COORD (KM)	NORTH COORD (KM)	RECEPTOR ABV GRD (H)	HT (M)	RECEPTOR GRD-LVL ELEV (FEET)	EXPERIMENTAL			ADAM PREDICTED CONCENTRATIONS	COMPLEXII PREDICTED CONCENTRATIONS
						THETA (DEG)	SPEED (M/S)	MIXING HEIGHT(M)	TEMP (K)	STABILITY CLASS
30 -25	0.19	0.33	0.6	0.6	7013.0				0.000	0.000
30 -50	0.43	0.74	0.6	0.6	6960.0				0.000	0.000
30 -75	0.60	1.04	0.6	0.6	7040.0				0.000	0.000
30 -1.0	0.84	1.46	0.6	0.6	6950.0				0.000	0.000
30 -1.5	1.12	2.06	0.6	0.6	7000.0				0.000	0.000
5 -25	0.02	0.33	0.6	0.6	6960.0				2.835	0.442
5 -50	0.08	0.89	0.6	0.6	7100.0				0.237	0.026
5 -1.0	0.14	1.67	0.6	0.6	7040.0				0.099	0.004
340-25	-0.13	0.37	0.6	0.6	6980.0				7.403	19.2621
340-50	-0.25	0.69	0.6	0.6	7120.0				2.904	7.936
340-75	-0.41	1.13	0.6	0.6	7150.0				1.233	2.963
340-1.0	-0.55	1.52	0.6	0.6	7040.0				0.713	1.623
340-1.5	-0.79	2.18	0.6	0.6	7040.0				0.363	0.795
315-25	-0.30	0.30	0.6	0.6	7020.0				2.835	1.354
315-50	-0.57	0.57	0.6	0.6	7100.0				0.418	0.320
315-75	-0.81	0.81	0.6	0.6	7160.0				0.232	0.122
315-1.0	-1.08	1.08	0.6	0.6	7200.0				0.099	0.056
290-25	-0.40	0.14	0.6	0.6	7050.0				0.008	0.000
290-50	-0.75	0.27	0.6	0.6	7100.0				0.000	0.000
290-75	-1.14	0.41	0.6	0.6	7140.0				0.000	0.000
290-1.0	-1.50	0.55	0.6	0.6	7220.0				0.000	0.000

USAF SF₆ TRACER STUDY
MODELED RESULTS FOR 14 SEPTEMBER 1982

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USAF SF₆ TRACER STUDY
MODELED RESULTS FOR 14 SEPTEMBER 1982

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USAF SF₆ TRACER STUDY
MODELED RESULTS FOR 16 SEPTEMBER 1982

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TABLE 13. SF₆ SUMMARY CONCENTRATION TABLE (MICROGRAMS/M**3)

USAF SF₆ TRACER STUDY
 MODELED RESULTS FOR 16 SEPTEMBER 1982

RECEPTOR NO. NAME	EAST COORD. (KM)	NORTH COORD. (KM)	RECEPTOR ABV GRD (M)	RECEPTOR HT (M)	RECEPTOR GRD-LVL ELEV (FEET)	TEMP (K)	STABILITY CLASS	EXPERIMENTAL		ADAM		COMPLEXII	
								OBSERVED CONCENTRATIONS	PREDICTED CONCENTRATIONS	PREDICTED CONCENTRATIONS	PREDICTED CONCENTRATIONS		
1	13	140.00	4.00	9467.00	292.00	2	1						
30 -25	0.12	0.33	0.6	7013.0	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
30 -50	0.43	0.74	0.6	6960.0	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
30 -75	0.20	1.04	0.6	7040.0	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
30 -1.0	0.24	1.46	0.6	6950.0	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
30 -1.5	1.12	2.06	0.6	7000.0	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
5 -25	0.22	0.38	0.6	6960.0	0.152	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
5 -75	0.20	1.15	0.6	7080.0	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
5 -1.0	0.24	1.69	0.6	7040.0	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
5 -1.5	0.20	2.24	0.6	7060.0	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
340-25	-0.13	0.37	0.6	6980.0	7.029	0.844	0.000	0.000	0.000	0.000	0.000	0.000	0.000
340-50	-0.25	0.69	0.6	7120.0	0.844	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
340-75	-0.41	1.13	0.6	7150.0	0.407	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
340-1.0	-0.55	1.52	0.6	7040.0	0.352	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
340-1.5	-0.79	2.18	0.6	7040.0	0.103	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
315-25	-0.30	0.30	0.6	7020.0	7.685	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
315-50	-0.57	0.57	0.6	7100.0	2.703	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
315-75	-0.31	0.81	0.6	7160.0	1.397	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
315-1.0	-1.08	1.08	0.6	7200.0	0.656	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
290-25	-0.40	0.14	0.6	7050.0	1.112	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
290-50	-0.75	0.27	0.6	7100.0	0.279	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
290-75	-1.24	0.41	0.6	7140.0	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000

**TABLE 14. TOLERANCE CATEGORIES USED TO EVALUATE
RELATIVE ERROR**

DIFFERENCE IN OBSERVED VERSUS PREDICTED	TOLERANCE
$\pm (1 \text{ to } 2) \times \text{Difference}$	EXCELLENT AGREEMENT
$\pm (2 \text{ to } 5) \times \text{Difference}$	MODERATE AGREEMENT
$\pm (5 \text{ to } \infty) \times \text{Difference}$	NO AGREEMENT

c. On the average, does AQAM overpredict or underpredict observed concentrations?

To answer the first question, the top three concentrations during each test period were compared with each other. Comparing only the highest concentrations observed during each test period biased the comparison since the wind direction was aligned by matching the highest predicted concentration with the highest observed concentration. Thus, comparison of the top three concentrations during each test period would alleviate the biasing effect. Using the three maximum values to test the effectiveness of AQAM to predict maximum concentrations provided to be adequate, but the test was still somewhat biased. Averaging more points during each test period to decrease this biasing effect diminished the objectives of the first statistical test since maximum concentrations were no longer being compared. Comparing the three highest measured concentrations against AQAM's maximum predictions gave the optimum average, while still maintaining the objective of the first statistical test.

The second statistical test provided an overall evaluation of AQAM's performance to predict both high and low concentrations. All measured concentrations were compared to AQAM's predicted concentrations on a point-by-point basis. One parameter had a big effect on this test - the structure of the plume. If modeled results predict a narrower plume width than observed, the statistical test will be comparing the zero concentrations predicted by the model to nonzero observed concentrations and will tend to fall into the last tolerance category indicating no correlation. When both observed and predicted concentrations were near zero, they were omitted from the test. However, if one value was not near zero and the other one was, then this data pair was included in the test. In this case, the model could not accurately predict the plume width and this datum must be included in the statistical test.

The last statistical test determined if AQAM generally overpredicts or underpredicts the observed concentrations. A determination was made to ascertain if AQAM overpredicted or underpredicted the maximum observed concentrations (important since regulatory decisions are usually based on worst-case situations where maximum observed concentrations are analyzed). Applying this test on a point-by-point basis, indicated how lower concentrations compared with each other - an indicator of the difference in plume width and decay of the concentration downwind of the point of maximum concentration.

SECTION VI

DISCUSSION OF RESULTS

A. GENERAL

The correlation between AQAM and COMPLEXII's predictions with observed concentrations are plotted in Figures 7 and 8. These scatter plots include all data points of the final data base and illustrate the relationship of AQAM and COMPLEXII to observed data over all measured concentration levels.

Figures 7 and 8 illustrate the relative error between observed and predicted concentrations. Each figure includes a one-to-one correlation line, a factor of 2 difference line, and a factor of 5 difference line. An analysis of these figures shows:

1. Maximum concentrations predicted by AQAM tend to be slightly less than observed concentrations; maximum concentrations predicted by COMPLEXII tend to exceed observed concentrations.

2. The relative error between observed and predicted concentrations for AQAM is limited to a plus or minus factor of 5 difference; the relative error between observed and predicted concentrations for COMPLEXII tends to exceed the factor of 5 difference. One can conclude that the plume width predicted by COMPLEXII is narrower than the observed plume.

Numerical results of the statistical tests used to ascertain AQAM's performance are summarized in Table 15. Numerical results of the statistical tests used to ascertain COMPLEXII performance are summarized in Table 16. The results in Table 17 show that the AQAM and experimental data are not normally distributed, i.e., the standard deviation (σ) of both data arrays are greater than the mean (μ). The non-normal distribution can be attributed to few data points with high values and many data points with low values.

The standard deviation of AQAM is slightly lower than the standard deviation of the observed results which indicates that AQAM predicts lower concentrations than the observed results. This is also evident when the means of the top three concentrations obtained during each test period are compared. AQAM tends to underpredict the observed results by approximately 20 percent. The standard deviation of COMPLEXII is greater than both observed and AQAM results. This indicates that COMPLEXII predicts higher concentrations (larger variance) than both of these results.

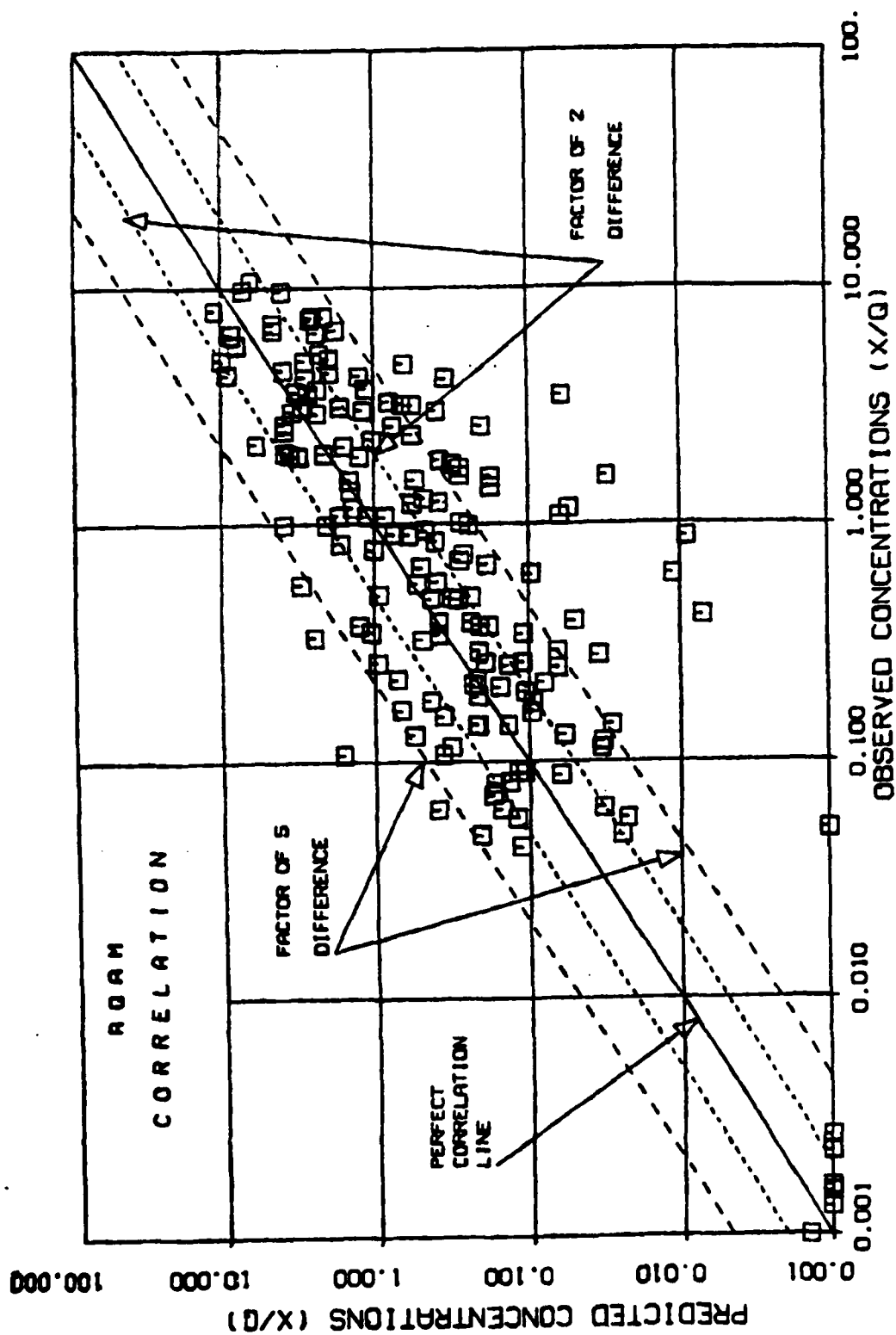


Figure 7. Predicted Concentrations Versus Observed Concentration (AQAM)

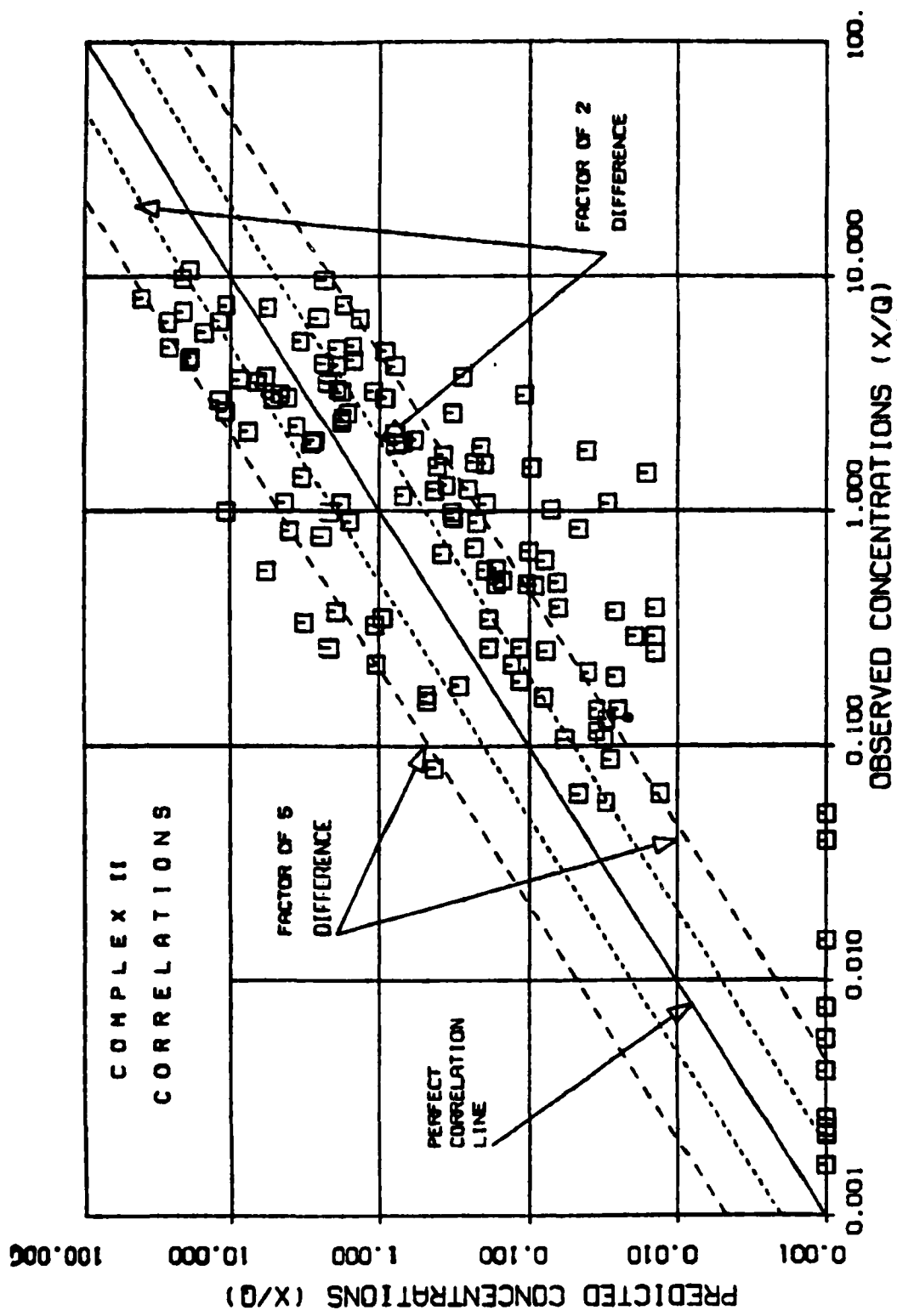


Figure 8. Predicted Concentrations Versus Observed Concentration (COMPLEX II)

TABLE 15. STATISTICAL ANALYSIS BETWEEN AQAM AND
EXPERIMENTAL TRACER DATA

Number of Tests : 12

Number of Points : 159

<u>Individual Statistics :</u>	mean conc.	std. deviation	mean of 3 highest per each test
AQAM	: 1.305	2.0054	4.094
Tracer data	: 1.810	2.2549	5.043

Comparison Statistics

Correlation coefficient : 1.4347

Regression line : slope = 0.6235
intercept = 0.1767

Distribution of Relative Error

Class interval: -infinity	-5	-2	+/-1	2	5	infinity
:	:	:	:	:	:	:
:	:	:	:	:	:	:
Percent (%)	3.1	13.8	15.7	25.2	25.2	17.0

Distribution of Relative Error
for highest 3 avg. concentrations
from each test

Class interval: -infinity	-5	-2	0	2	5	infinity
:	:	:	:	:	:	:
:	:	:	:	:	:	:
Percent	0.0	0.0	33.3	50.0	16.7	0.0

TABLE 16. STATISTICAL ANALYSIS BETWEEN COMPLEXII AND
EXPERIMENTAL TRACER DATA

Number of Tests : 12

Number of Points : 137

<u>Individual Statistics</u> :	mean conc.	std. deviation	mean of 3 highest per each test
COMPLEXII :	2.971	6.1724	10.364
Tracer data :	2.066	2.3170	5.043

Comparison Statistics

Correlation coefficient : 4.743

Regression line : slope = 1.7137
intercept = -0.5698

Distribution of Relative Error

Class interval:	-infinity	-5	-2	+/-1	2	5	infinity
Percent (%)	5.1	15.3	10.2	13.1	27.0	29.2	

Distribution of Relative Error
for highest 3 ave. concentrations
from each test

Class interval:	-infinity	-5	-2	+/-1	2	5	infinity
Percent	0.0	58.3	25.0	16.7	0.0	0.0	

TABLE 17. RELATIVE ERROR COMPARISONS: AQAM AND COMPLEXII

RELATIVE ERROR	ALL DATA	HIGHEST 3 VALUES EACH TEST		
		PERCENT DATA (AQAM)	PERCENT DATA (COMPLEXII)	PERCENT DATA (COMPLEXII)
GREATER THAN FACTOR OF 5		20.1	34.3	0.0
LESS THAN FACTOR OF 5		79.9	65.6	100.0
LESS THAN FACTOR OF 2		40.9	23.3	43.7

This characteristic is also evident when comparing the mean of the highest three concentrations obtained during each test period. COMPLEXII, on the average, tends to over-predict the observed maximum concentrations by a factor of 2.06. During each test period, the maximum concentration predicted by COMPLEXII was always greater than the observed concentrations.

A regression analysis between the observed and AQAM-predicted concentrations was performed. Fitting a first-degree polynomial equation to these concentrations resulted in a regression line with a slope of 0.6235 and intercept of 0.1767. AQAM closely parallels the observed values slightly overpredicting observed results for low concentrations and underpredicting observed results for high concentrations.

The first-degree regression analysis applied to the observed versus COMPLEXII predictions resulted in a line with a slope of 1.7137 and intercept of -0.5698. Unlike AQAM, COMPLEXII tends to underpredict the observed results for low concentrations and overpredict the observed results for high concentrations (the slope being greater than unity). Also, since the slope of this line is greater than AQAM's, COMPLEXII tends to predict a narrower plume with higher concentrations than either AQAM or the observed values.

Distribution of relative error is determined by computing the ratio at each receptor location and time of either the observed and predicted values, whichever is greater than one. If observed concentrations are greater than the predicted, then the relative error is positive. Likewise, when predicted concentrations are greater than observed, the relative error is considered negative.

B. AQAM

The distribution of the relative error results tabulated in Table 17 indicates that the observed concentrations were greater than the predicted at approximately 67.4 percent of the receptor locations. Coupled with the results in Figure 7 this indicates that AQAM generally underpredicts the observed concentrations. This conclusion is also supported by observing the results of the relative error for the average of the highest three concentrations obtained from each test period. These results indicate that the average of the maximum values predicted by AQAM are less than the observed values 66.7 percent of the time. The relative error between AQAM and the observed concentrations decreases by analyzing only the highest concentrations. Approximately

83 percent of these data fell within a factor of ± 2 , as compared to 41 percent of all the data falling within the same range. Large relative errors usually correspond to low concentrations.

C. COMPLEXII

The distribution of the relative error for COMPLEXII predictions versus observed results indicates a wide spread in the distribution. One may also conclude that COMPLEXII predict a narrower plume with higher concentrations as compared to the observed plume. A summary of the predictive performance of COMPLEXII is presented in Table 17.

SECTION VII

SUMMARY

1. AQAM predicted ground-level concentrations within a factor of 2 at 41 percent of the experimentally monitored locations for unstable conditions (Stability Categories A, B, C).
2. Insufficient data were collected to make any conclusions about AQAM's predicative performance in neutral and stable conditions (Stability Categories D, E, F)
3. COMPLEXII predicted ground-level concentrations within a factor of 2 at 23 percent of the monitored locations.
4. AQAM predicted maximum concentrations within a factor of 5, 100 percent of the time.
5. AQAM predicted maximum concentrations within a factor of 2, 83 percent of the time.
6. AQAM's predicted values were 80 percent of the observed values.
7. COMPLEXII predicted maximum concentrations within a factor of 5 for 100 percent of the time.
8. COMPLEXII's predicted maximum concentrations within a factor of 2 for 44 percent of the time.
9. COMPLEXII's predictions were 200 percent of the observed values.
10. Use of terrain correction had no effect on AQAM's predictions during unstable conditions in complex terrain.
11. Statistically, AQAM underpredicted observed concentrations.
12. Statistically, COMPLEXII overpredicted observed concentrations.
13. Building wake effects (USAFA location) caused significant discrepancies between observed and predicted concentrations.

SECTION VIII

CONCLUSIONS

1. AQAM generally underpredicts observed concentrations.
2. COMPLEXII generally predicts a narrower plume with higher concentrations than observed.
3. AQAM predicts ground-level concentrations more accurately than COMPLEXII.
4. AQAM can be used to predict the effects of future Air Force stationary sources on ambient air quality with better accuracy than COMPLEXII.

SECTION IX

REFERENCES

1. Rote, D.M. and Wangen, L.E., A Generalized Air Quality Assessment Model for Air Force Operations, AFWL-TR-74-304, Air Force Weapons Laboratory, Kirtland Air Force Base, New Mexico, February 1975.
2. United States Environmental Protection Agency, Quality Assurance Handbook for Air Pollution Measurement Systems, EPA-600/9-76-005, Research Triangle Park, North Carolina, 1976.
3. United States Environmental Protection Agency, Ambient Air Monitoring Guidelines for Prevention of Significant Deterioration (PSD), EPA-450/4-80-012, Research Triangle Park, North Carolina, 1980.
4. Turner, D.B., Workbook of Atmospheric Dispersion Estimates, PHS Publication 999-AP-26, U.S. Department of Health, Education and Welfare, National Air Pollution Control Administration, Cincinnati, Ohio, 1970.
5. Briggs, G.A., Diffusion Estimation for Small Emissions, Air Resources Atmospheric Turbulence and Diffusion Laboratory, NOAA, Oak Ridge, Tennessee, 1973.
6. Holland, J.Z., A Meteorological Survey of the Oak Ridge Area, Atomic Energy Commission Report ORO-99, Washington, D.C., 1953.
7. Moses, H., Strom, G.H., and Carson, J.E., "Effects of Meteorological and Engineering Factors on Stack Plume Rise," Nuclear Safety, 6., 1, pp 1-19, 1964.
8. Huber, A.H. and Snyder, W.H., "Building Wake Effects on Short Stack Effluents," Preprint Volume, Third Symposium on Atmospheric Diffusion and Air Quality, American Meteorological Society, Boston, Massachusetts, 1976.
9. Huber, A.H., "Incorporating Building/Terrain Wake Effects on Stack Effluents," Preprint Volume, Joint Conference on Application of Air Pollution Meteorology, American Meteorological Society, Boston, Massachusetts, 1977.

APPENDIX A

METEOROLOGICAL MEASUREMENTS

APPENDIX A

METEOROLOGICAL MEASUREMENTS

METEOROLOGICAL MEASUREMENTS

Meteorological measurements were conducted at two monitoring sites. Windspeed, wind direction, and ambient temperature were at Station 1 and windspeed and direction were monitored at Station 2. The meteorological data monitored at these locations are presented in Tables A-1, A-2, and A-3.

Mixing depths were estimated, using rawinsonde data from Fort Carson, CO or PIBAL data performed at the USAFA. Table A-8 summarizes the mixing depth estimates.

TABLE A-1. USAFA SF₆ TRACER STUDY METEOROLOGICAL DATA SUMMARY, SEPT 24, 1982

Time (MST)	Met. Station #1 (1)			Met. Station #2			Cloud Cover % Cover	Atmospheric Stability
	Wind Speed (m/s)	Wind Direction (T.N.) (2)	Temperature (°C)	Wind Speed (m/s)	Wind Direction (T.N.)			
11-12	2.9	150	13.8	2.5	155	0%		A-B
12-13	3.2	145	15.6	2.7	150	0%		B
13-14	2.0	155	17.2	1.0	160	10%		A
14-15	2.3	150	15.6	1.8	155	10%		A

(1) See Figure 1 for locations of meteorological stations

(2) Wind direction based on true north

TABLE A-2. USAFA SF₆ TRACER STUDY METEOROLOGICAL DATA SUMMARY, SEPT 15, 1982

Time (MSL)	Met. Station #1 (1)		Met. Station #2		Cloud Cover % Cover	Atmo-spheric Stability
	Wind Speed (m/s)	Wind Direction (T.N.) (2)	Temperature (°C)	Wind Speed (m/s)		
11-12	4.6	155	3	4.5	Fogged In	D
12-13	3.6	160	3	3.6	Fogged In	D
13-14	3.6	160	3	3.4	Fogged In	D
14-15	4.4	140	—	3.9	Fogged In	D

(1) See Figure 1 for locations of meteorological stations

(2) Wind direction based on true north

TABLE A-3. USAFA SF₆ TRACER STUDY METEOROLOGICAL DATA SUMMARY, SEPT 16, 1982

Time (MST)	Met. Station #1 (1)		Met. Station #2		Cloud Cover % Cover	Atmospheric Stability
	Wind Speed (m/s)	Wind Direction (T.N.) (2)	Temperature (°C)	Wind Speed (m/s)		
10-11	1.5	150	19.5	1.0	10%	A
11-12	3.1	150	22.0	2.1	5%	A-B
12-13	3.5	155	22.0	3.1	0%	B
13-14	4.0	155	22.0	3.3	5%	B

(1) See Figure 1 for locations of meteorological stations

(2) Wind direction based on true north

TABLE A-4(1). DESCRIPTION OF ATMOSPHERIC STABILITY CATEGORIES:
SOLAR RADIATION TECHNIQUE

KEY TO STABILITY CATEGORIES									
Surface Wind Speed at 40 ft. Altitude 2.24 MPH = 1.95 knots = 1 m/sec									
MPH	Knots	m/sec	Day			Night			
			Strong	Moderate	Slight	>4/8 Low Cloud	Thinly Overcast	or	Cloud
<4.5	<3.9	<2	A	A-B	B				
4.5-6.7	3.9-5.8	2-3	A-B	B	C		E		F
6.7-11.2	5.8-9.7	3-5	B	B-C	C		D		E
11.2-13.4	9.7-11.7	5-6	C	C-D	D		D		D
>13.4	>11.7	>6	C	D	D		D		D

The neutral category, D, should be assumed for overcast conditions during day or night. Night refers to a period from 1 hour before sunset to 1 hour after sunrise. For purposes of the computer program Stability Category A=1, B=2, etc.

"Strong" incoming solar radiation corresponds to a solar altitude greater than 60° with clear skies in midsummer; "slight" insolation corresponds to similar conditions in midwinter or to a solar altitude from 15° to 35° with clear skies in midsummer. Cloudiness will decrease incoming solar radiation and should be considered along with solar altitude in determining solar radiation. Incoming radiation that would be strong with clear skies can be expected to be reduced to moderate with broken (5/8 to 7/8 cloud cover) middle clouds and to slight with broken low clouds.

Caution should be used when forecasting to result in ambient concentrations with wind velocities of less than 2 meters per second (4.5 mph or 3.9 knots). At low velocities, the winds tend to meander widely. In addition, surface wind speeds at low velocities are rarely indicative of aloft velocities or of upper air stability categories.

Stability categories are reliable in open, rural areas. In urban and heavily wooded areas, the surface roughness and heat islands have an effect on the category, particularly on still nights. On calm, clear nights, stability E or F occurs in rural areas where D is likely to occur over urban areas.

(1) Extracted from: Turner, D.B. Workbook of Atmospheric Dispersion Estimates, US Department Health Education and Welfare, PHS, National Air Pollution Control Administration, Cincinnati, Ohio, 1969, p6.

TABLE A-5. ESTIMATES OF MIXING DEPTH AT USAFA
14-16 SEPTEMBER 1982

DATE	TIME	ESTIMATED MIXING DEPTH	
		MSL, ft.	AGL, ft. (USAFA Airfield)
14 Oct 82	13 Z	7500	954 (a)
	17 Z	9800	3254 (a)
15 Oct 82	12 Z	9000	2454 (b) Ft. Carson max temp. was 54°F
16 Oct 82	13 Z	9000	2454 (a)
	17 Z	10500	3954 (a)

(a) estimated using USAFA PIBAL (using wind shift as the indicator)

(b) estimated using Ft. Carson rawinsonde (using max temperature)

Note: USAFA Airfield Elevation is 6546 ft.
Cadet Area Elevation is 7250 ft.
Heating Plant elevation is 7013 ft.

Mixing Depth = (MSL mixing depth altitude) - (terrain elevation)

=====

USAFA PIBAL DATA

MSL, ft.	14 Sep 82		15 Sep 82		16 Sep 82	
	13Z	17Z	13Z	17Z	13Z	17Z
Sfc	3607	1906	PIBAL was not		0208	1406
7000	2707	1607	launched this		0706	1406
8000	2418	1206	day because		1407	1104
9000	2520	0502	ceilings were		2414	1706
10000	2617	2704	500 ft.		2607	1706
11000	2622	2412			2514	2210
12000	2526	2418			2418	2423
13000	2535	2731				2537
14000	2438	2731				2546

NOTE: MSL - Mean Sea Level
AGL - Above Ground Level

APPENDIX B

SOURCE CHARACTERISTICS

TABLE B-1. SOURCE CHARACTERISTICS - 1ST STUDY

Date: May 3, 1982

Time	Temperature (°R)(°K)	Boiler Output (10) ⁵ BTU/HR	Q m ³ /s	V m/s
16-17	855(475)	40	.82	.45
17-18	855(475)	41	.84	.46

Date: May 4, 1982

12-13	860(477)	39	.81	.44
13-14	860(477)	40	.83	.45
14-15	855(475)	38	.78	.43
15-16	860(477)	39	.81	.44

Date: May 5, 1982

10-11	850(472)	38	.78	.43
11-12	855(475)	41	.84	.46
12-13	855(475)	40	.82	.45
13-14	850(472)	38	.78	.43

Date: May 6, 1982

10-1	850(472)	35	.71	.39
11-12	845(469)	32	.65	.36
12-13	845(469)	30	.61	.33
13-14	850(472)	34	.69	.38

TABLE B-2. SOURCE CHARACTERISTICS - 2ND STUDY

Date: 9/14/82

Time	Temperature (OR)	Boiler Output (10) ⁵ BTU/HR	Q m ³ /s	V m/s
11-12	881	64	1.35	.742
12-13	875	62	1.30	.71
13-14	865	57	1.18	.65
14-15	865	57	1.18	.65

Date: 9/15/82

11-12	901	76	1.64	.90
12-13	890	74	1.58	.87
13-14	886	70	1.49	.82
14-15	884	68	1.46	.80

Date: 9/16/82

10-11	870	59	1.23	.68
11-12	865	57	1.18	.65
12-13	865	57	1.18	.65
13-14	865	57	1.18	.65

APPENDIX C

**DETERMINATION OF THE VOLUMETRIC FLOW RATE
OF THE EXHAUST GAS FROM THE HEATING PLANT**

STACK GAS VOLUMETRIC FLOW RATE CALCULATIONS

FUEL GAS ANALYSIS

<u>Component</u>	<u>Mole %</u>	<u>MW</u>
Methane, CH ₄	83.2	16
Ethane, C ₂ H ₆	5.6	30
Nitrogen, N ₂	6.0	28
Oxygen, O ₂	1.9	32
Carbon Dioxide, CO ₂	1.8	44
	<u>100%</u>	

Moles of Carbon (C) and Hydrogen (H₂) per 100 moles of fuel

	<u>C</u>	<u>H₂</u>
In CH ₄	83.2	166.4
In C ₂ H ₆	11.2	16.8
TOTALS	<u>94.4</u>	<u>183.2</u>

ASSUMPTIONS

Total Air (TA)=115% (15% excess air)

Unburned Fuel=0

Combustion Calculations - Molal Basis

Fuel, O ₂ , and Air Per Unit of Fuel				FLUE GAS COMPOSITION (Moles per Fuel Unit)			
Fuel Constituent	Moles of Fuel Constituent	O ₂ Multiplier	O ₂ Moles Req'd	CO ₂	O ₂	N ₂	H ₂ O
C to CO ₂	94.4	1	94.4	94.4			
H ₂	183.2	.5	91.6				183.2
O ₂ (Deduct)	1.9	1	-1.9				
N ₂	6.0		0			6.0	
CO ₂	1.8		0	1.8			
		SUM	184.1				
O ₂ and Air, Mole							
For Total Air - 115%							
O ₂ (Theoretical) Required			184.1				
O ₂ (Excess) = $\frac{TA-100}{100} \times O_2$			27.6		27.6		
O ₂ (Total) Supplied			211.7				
N ₂ Supplied = $\frac{79}{21} \times O_2$			796.4			796.4	
Air (DRY) Supplied = O ₂ + N ₂			1008.1				
H ₂ O in Air = Moles Dry Air X .0212			21.4				21.4
Air (Wet) Supplied			1029.5				
Flue Gas Constituents - Total				96.2	27.6	802.4	204.6
Total Moles of Fuel Gas - (Wet) <u>1130.8</u> - (DRY) <u>926.2</u>							
M.W. of Fuel = .832 (16) + .056 (30) + .06 (28) + .019 (32) + .018 (44)							
= 18.07							

$$\begin{aligned}
 \text{SPECIFIC WEIGHT OF WET FLUE GAS} &= \text{MW(Wet)}/379.5^{(1)} \\
 &= 27.65/379.5 \\
 &= .0729 \text{ lb/ft}^3
 \end{aligned}$$

$$\begin{aligned}
 \text{SPECIFIC WEIGHT OF DRY FLUE GAS} &= \text{MW(DRY)}/379.5 \\
 &= 29.78/379.5 \\
 &= .0785 \text{ lb/ft}^3
 \end{aligned}$$

(1) Volume of 1 mole of any gas at 60°F and 14.73 in HG
 = 379.5 ft³

CONVERSION FROM MOLAL TO POUND UNITS

Weight of Each Flue Gas Constituent = Flue Gas Constituent x MW

Constituent	MW	Amount of each Constituent	Weight-Per Fuel Unit (lbs)
CO ₂	44	6.2	4232.8
O ₂	32	27.6	383.2
N ₂	28	802.4	22467.2
H ₂ O	18	204.6	3682.8
Total Flue Gas Weight (WET)			31266
Total Flue Gas Weight (DRY)			27583.2

Wet Flue Gas /lb Fuel = Wet Wt. / (MW Fuel X 100)

$$= 31266 / (18.07 \times 100) = \underline{\underline{17.3 \text{ lb Wet Flue Gas}}}$$

Dry Flue Gas /lb Fuel = Dry Wt. / (MW Fuel X 100)

$$= 27583.2 / (18.07 \times 100) = \underline{\underline{15.3 \text{ lb Dry Flue Gas}}}$$

Molecular Wt. of Wet Flue Gas = Wet Weight / Wet Moles

$$= 31266 / 1130.8 = 27.65$$

Molecular Wt. of Dry Flue Gas = Dry Weight / Dry Moles

$$= 27583.2 / 926.2 = 29.78$$

CALCULATION OF VOLUMETRIC FLOW RATE

SPECIFIC GRAVITY OF FUEL = 0.6504⁽¹⁾ @ 14.73 psia & 60°F

AIR DENSITY @ 14.73 psia & 60°F:

$$\rho = \frac{P}{RT} = \frac{14.73 \text{ (144)} \frac{\text{ft}^2}{\text{ft} \text{ lb}}}{53.3 \frac{\text{ft} \text{ lb}}{\text{lbm}^\circ\text{R}} (460 + 60)} = .0765 \frac{\text{lb}}{\text{ft}^3}$$

GAS DENSITY @ 14.73 psia & 60°F:

$$\text{SF X} = .0765 \frac{\text{lb}}{\text{ft}^3} (.6504) = .0498 \frac{\text{lb}}{\text{ft}^3}$$

THE HEATING VALVE OF THE FUEL IS⁽¹⁾:

$$\text{HV} = 966.8 \frac{\text{BTU}}{\text{ft}^3} \text{ @ 14.73 psia \& 60}^\circ\text{F}$$

or, CONVERTING TO A POUND BASIS:

$$\text{HV} = \frac{966.8 \text{ BTU/ft}^3}{.0498 \frac{\text{lb}}{\text{ft}^3}} = 19413.7 \frac{\text{BTU}}{\text{lb FUEL}}$$

(1) CSPSG GAS COMPANY - NATURAL GAS ANALYSIS, 25 March 1982

ASSUME BURNING RATE OF FUEL = $77 (10)^5 \frac{\text{BTU}}{\text{HR}}$

TOTAL MASS OF FUEL CONSUMED / HR IS:

= Burning Rate / HR

$$= \frac{77(10)^5 \frac{\text{BTU}}{\text{HR}}}{19413.7 \frac{\text{BTU}}{\text{lb FUEL}}} = 396.7 \frac{\text{lb FUEL}}{\text{HR}}$$

Knowing the amount of wet Flue Gas Produced Per Pound Fuel is:

17.3 lb wet Flue Gas / lb FUEL

And solving for the amount of Wet Flue Gas Produced Per Hour:

$$\begin{aligned} \text{Wet Flue Gas/HR} &= \frac{17.3 \text{ lb Flue Gas}}{\text{lb FUEL}} \times 396.7 \frac{\text{lb FUEL}}{\text{HR}} \\ &= 6862.9 \text{ lb Wet Flue Gas/HR} \end{aligned}$$

Converting to a Volume Basis:

$$\begin{aligned} \text{Wet Flue Gas/HR} &= 6862.9 \frac{\text{lb}}{\text{HR}} \times \frac{1}{.0729 \frac{\text{lb}}{\text{Ft}^3}} \\ &= 94141 \frac{\text{Ft}^3}{\text{HR}} = (26.15 \frac{\text{Ft}^3}{\text{SEC}}) \end{aligned}$$

Correcting to an Exhaust Temperature of 900°R & Pressure = 23.05

$$\text{Wet Flue Gas/HR} = \left(\frac{26.15 \text{ FT}^3}{\text{SEC}} \right) \left(\frac{900}{520} \right) \left(\frac{29.92}{23.05} \right) = 58.75 \frac{\text{FT}^3}{\text{SEC}}$$

APPENDIX D

SF₆ SCALE CALIBRATION

USAFA SF₆ TRACER STUDY

SF₆ Scale Calibration

Date: 9/13/82

Calibration Weight (lbs)	Indicated Scale Reading (lbs)	Scale Range
35.28	35.35	0-100 lbs
70.56	70.63	0-100 lbs
105.84	107.60	100-200 lbs
211.70	211.70	100-200 lbs

NOTE: This scale was used to measure the weight loss of the SF₆ cylinder during periods of SF₆ tracer releases.

APPENDIX E

CONVERSION OF SF₆ CONCENTRATIONS IN ppt TO $\mu\text{g}/\text{m}^3$

Conversion of SF₆ Concentrations in ppt to µg/m³

$$\text{conc } (\mu\text{g}/\text{m}^3) = \frac{\text{conc (ppt)} (10)^{-12} \frac{\text{parts}}{\text{ppt}} \text{ MW SF } \frac{\text{g}}{\text{g-mole}}}{22.414 \frac{\text{l}}{\text{g-mole}} \times 10^{-3} \frac{\text{m}^3}{10^3 \text{ l}} \times \frac{T_{\text{OK}}}{T_{\text{OKstd}}}} \times \frac{10^6 \mu\text{g}}{\text{gm}}$$

$$\text{Molecular Weight of SF}_6 = 146.05 \frac{\text{g}}{\text{g-mole}}$$

$$\text{Temperature} = 293 \text{ K}$$

Thus,

$$\text{conc } (\mu\text{g}/\text{m}^3) = \frac{\text{conc (ppt)} (10)^{-12} \frac{\text{parts}}{\text{ppt}} 146.05 \frac{\text{g}}{\text{g-mole}}}{22.414 \frac{\text{l}}{\text{g-mole}} \times 10^{-3} \frac{\text{m}^3}{10^3 \text{ l}} \frac{293^{\circ}\text{K}}{273.15^{\circ}\text{K}}} \frac{10^6 \mu\text{g}}{\text{gm}}$$

$$\text{conc } (\mu\text{g}/\text{m}^3) = \text{conc (ppt)} \times 6.075 (10)^{-3}$$

Therefore, to convert conc (ppt) to conc (µg/m³) multiply SF₆ conc (ppt) x 0.006075 (conversion factor)

Reference: USEPA (1979), "Continuous Air Pollution Source Monitoring System," page E2, Research Triangle Park, NC, June.

END

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