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EVALUATION OF THE MULTIPLE SOURCE GAUSSIAN PLUME DIFFUSION MODEL - PHASE II

by

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INTRODUCTION AND SCOPE

Section 1.0

INTRODUCTION AND SCOPE

This report represents a summation, for record purposes of a variety of types and phases of work conducted under EPA Contract Number 68-02-0281, "Evaluation of the Multiple-Source Gaussian Plume Diffusion Model." Because the contract work covered an extended period of time, and because its products were documented in a number of reports, it is considered desirable to have this summation document as a matter of complete record of the work; of course, where the work has been formally reported elsewhere, this report will contain only a summary.

The scope of this report will be to briefly cover Phase I by reproducing the introduction, model description, and conclusions of the report of that work (Number EF-186). Phase II will be more definitively covered by presenting a summary of the report (Number EF-261) of the computer program and user's manual and describing the training provided EPA staff, and by accumulating the work reported elsewhere related to special aspects of the model (handling variations in emission data input, using EMSU data as meteorological input, and calculating short-term maximum concentrations). Phase I is covered in Section 2.0 of this report, the computer program, user's manual, and staff training in Section 3.0, and the special aspects in Section 4.0.

For convenience of reference, and to complete the introductory remarks, the contract scope of work is quoted in the following paragraphs.

For cross-referencing purposes, the following relationships are given relating the scope of work's paragraphs 1 and 2 (Phase I), and 3 through 7 (Phase II) with this report's sections:

	Contract Scope of Work	Report Section
Phase I	1, 2, 3 (Phase II)	2.1
	1, 2	2.2
Phase II	3	3.1
	4	3.2
	5	4.1
	6	4.2
	7	4.3

SCOPE OF WORK

Background:

This program shall be a continuation of work previously supported under Contract No. CPA 70-94, "Validity and Sensitivity of the Gaussian Plume Urban Diffusion Model." (Available from NTIS as PB 206-951).

This previous work developed a short-term, steady-state Gaussian plume model for urban diffusion and evaluated this model using three-months' data for St. Louis and one-month's data for Chicago. By proper selection of input data, this model can also be used for long-term average concentrations.

Since this model is expected to replace a currently used annual model, it is necessary to make direct comparisons with two other models with the same data base used by these two models.

It is required to completely document the model so that the dispersion modeler can completely understand its steps of operation in detail including underlying assumptions and the technical user can properly assemble required input data and interpret correctly the concentrations resulting from the model.

Abstract:

The Contractor shall conduct a research program for further evaluation and documentation of a Gaussian Plume Urban Diffusion Model.

Phase I:

1. For both St. Louis and Chicago data (as considered in the previous contract) calculate 1-hour (Chicago) and 2-hour (St. Louis) concentration frequency distributions using GEOMET (Mean Q) and using sound statistical techniques compare with the results of GEOMET (Variable Q), calculated by the previous contract and with measured concentrations.

2. Calculate concentrations for locations in the New York area for 1969 and make comparisons with measurements for the averaging times and the models indicated by the sponsor. Similar calculations will be made for particulate matter for annual averages only.

Mean annual emission rates for all point and area sources and stack characteristics for the point sources for the New York region will be furnished by EPA in the format used for IPP.

Meteorological information for the year 1969 consisting of an observation each three hours will also be furnished by EPA and will be used as the meteorological data base.

For each calculation of concentration at a receptor, a value for the concentration due to point sources will be retained as well as the calculated total concentration. All estimates of concentrations made will be stored on magnetic tape (hourly and 24-hour concentrations as time series) and delivered to EPA for possible subsequent analysis at the conclusion of the contract period.

Data on measured SO_2 concentrations will be furnished the contractor by EPA. Frequency distributions for measured concentrations and for calculated concentrations will be determined and compared by log-probability plots and by appropriate statistical techniques for each station. (There are approximately 40 locations with sufficient SO_2 measurements to obtain frequency distributions.) In consultation with the project officer, the contractor will select 10 for study of frequency distributions.

Appropriate subsets of calculations will be used to validate the usefulness of proportionate stratified sampling in obtaining frequency distributions. Resulting frequency distributions from these subsets need only be compared with the calculated frequency distribution using all data.

For each station a linear correlation coefficient, the variance (the square of the correlation coefficient), the slope and intercept of a least-squares regression line will be determined considering the calculated concentration as the independent variable and the measured concentration as the dependent variable. Considering error as the calculated value minus the measured value, the mean absolute error, the root-mean-square error, and the distribution of errors will be determined. For all but the distribution of errors, there will be a value of the above numerated statistics for each station for both 1-hour and 24-hour averaging times for each applicable model. For annual averages, the pairs of calculated and measured concentrations for all stations will be included to calculate one value of each of the above statistics for each pollutant for each model.

Phase II:

3. Considering the results of the sensitivity analysis (previous contract) and the results of the evaluation in Tasks 1 and 2, restructure the computer programs used in GEOMET (Variable Q) to minimize the digital computer execution times. One version of these programs must be compatible with the IPP. (Information on the IPP will be furnished by EPA.) If simplification will reduce computer time without significant loss of accuracy, a separate model shall be suggested and documented for annual average concentrations. Prepare a user's manual for the use of these optimized computer programs for use with or without the IPP.

4. Train 2 to 3 members of the Model Development Branch, Division of Meteorology, on the operation of the optimized models resulting from Task 3, on a computer used by NERC, North Carolina. This shall include a demonstration of the

compatibility with the IPP. (EPA personnel shall be responsible for operation of all phases of the IPP not directly connected with the dispersion model.)

5. Write procedures to be used in preparing emission data so that diurnal and seasonal variations in emissions can be used.

6. Evaluate the use of Environmental Meteorological Support Unit (EMSU) data for determination of meteorological parameter values for input to the optimized model. Enumerate procedures for the use of such data.

7. Examine the statistical portion (Larsen transform) of the AQDM and suggest alternative procedures to be utilized with the optimized dispersion model to estimate short-term (1-hour, 3-hours, and 24-hour) maxima that occur with a frequency of once per year.

Section 2.0

SUMMARY OF THE PHASE I REPORT

Section 2.0

SUMMARY OF THE PHASE I REPORT

The report of Phase I (Number EF-186) contains complete documentation of the work on the basic model, and evalution of its validation performance against monitored air quality data in comparison to other models potentially usable for similar purposes. The work is summarized here by reproducing brief descriptions of the models compared, analyses performed, and conclusions of that report.

The work accomplished during Phase I concentrated on validation of a steady-state Gaussian plume urban diffusion model which uses sampled chronological input data. The model was developed for EPA by GEOMET in previous work (Contract Number CPA 70-94). The model has been compared with three other models (using the same data base).

2.1 MODELS COMPARED

The model studies include three variations of the multiple-source, Gaussian plume, meteorological diffusion model. Two of the models, the Air Quality Display Model (AQDM) and the Climatological Dispersion Model (CDM), are primarily designed to calculate long-term mean concentrations. The third model, developed by GEOMET under previous EPA sponsorship, is designed to calculate both the long-term mean concentration and the frequency distribution of short-term concentrations using selected chronological data (SCIM). The frequency distribution is determined by concentrations calculated for a statistically selected set of short-term periods. Representative meteorological characteristics and simulated time-dependent emission characteristics are determined for each selected period. The other two models use mean emission characteristics and a specified set of combinations of meteorological characteristics (wind direction, wind speed and stability). To determine the long-term mean, the calculations for each combination of meteorological conditions are weighted by the relative frequency of occurrence of the combination.

In addition to the three Gaussian plume models, the simplified version of the Gifford-Hanna model recently described by Hanna (1971) was included. The model is

$$\chi = C \frac{Q}{u}$$

where

χ = concentration at a receptor location ($\mu g/m^3$)

Q = area source strength surrounding the receptor ($\mu g/m^2/sec$)

u = wind speed (m/sec)

C = dimensionless constant.

2.2 MODEL COMPARISONS

Calculations using the four models were compared against each other and against measured values. Each model was run in its normal mode. In addition, certain simplifications were made by averaging the inputs used for the model. The model comparisons include consideration of 10 different variations of model and inputs.

Two model comparison tasks were carried out. The first task was to compare calculations for SCIM which were obtained in a preceding program (Contract No. CPA 70-94, "Validity and Sensitivity of the Gaussian Plume

Urban Diffusion Model") with calculations made using the same model and data set, except that mean rather than time-dependent emission rates were used for all sources. These calculations involved a 3-month data period for St. Louis and a 1-month data period for Chicago, for sulfur dioxide emissions.

The second task was to compare 10 different combinations of variations in input and the four models described above with each other and with measured values using a 1-year data set for New York City. The comparisons include 3-hourly, 24-hourly, and annual concentrations of sulfur dioxide emissions, and annual concentrations of particulate matter emissions.

For the SCIM, area source emissions and the meteorological conditions of atmospheric stability and height of the mixing layer (grouped together) were treated either as varying from hour to hour or as being constant throughout the data period. Three combinations of input data conditioning were analyzed, including:

- Area source emission rates, atmospheric stability and height of the mixing layer variable
- Area source emission rates constant, but atmospheric stability and height of the mixing layer variable
- Area source emission rates, atmospheric stability and height of the mixing layer constant.

For the simplified Gifford-Hanna Model (GHM), area source emissions and wind speed were treated as both varying from hour to hour or as being constant throughout the data period. In addition, the calculated concentration at a receptor due to point sources (as estimated by SCIM with variable atmospheric stability and mixing layer height) were either added or not added to the GHM calculations. This results in four variations of this model, including:

- Constant area source emission rates and wind speed, without point sources
- Variable area source emission rates and wind speed, without point sources
- Constant area source emission rates and wind speed, with point sources
- Variable area source emission rates and wind speed, with point sources.

Calculations for CDM, which treat atmospheric stability and height of the mixing layer as either both variable or both constant, were furnished by Mr. D. B. Turner of the Division of Meteorology, EPA/NERC/RTP. Statistical results of model-to-measurement comparisons for these calculations were included for comparison with the other models. Calculations for AQDM (no variations) also were furnished by Mr. Turner and were included for comparison.

2.3 CONCLUSIONS FROM THE PHASE I REPORT

Conclusions (1-5) regarding the use of the Sampled Chronological Input Model (SCIM), a multiple-source Gaussian plume model, to estimate short-term SO_2 concentrations (e.g., 1-hour and 24-hour concentrations) are based on model-to-measurement comparisons for 1 month of Chicago, 3 months of St. Louis and 1 year of New York City (NYC) data. The model was analyzed using NYC data for three types of inputs, including: (1) variable emission rates, stability classifications and mixing heights (variable Q, S, H), (2) mean emission rates and variable stability classifications and mixing heights (mean Q, variable S, H), and (3) mean emission rates, stability classifications and mixing heights (mean Q, S, H). The model was analyzed using St. Louis and Chicago data for the first two types of input. For comparison purposes, an analysis was also made of the use of the simplified Gifford-Hanna Model (GHM).

1. Comparing the results for the three types of input to SCIM, it is concluded that:

- Use of a mean, rather than a variable, emission rate may either increase or decrease the root-mean-square error (RMSE) at a receptor but will decrease the correlation with measurements (observed at 10 of 10 St. Louis receptors for 2-hour concentrations, 5 of 8 Chicago receptors for 1-hour concentrations, and 10 of 10 NYC receptors for 1-hour and 24-hour concentrations).
- Based on comparisons using NYC data and mean emission rates, the use of a neutral stability classification and a mean mixing height will decrease the correlation with measurements but will also decrease the RMSE at a receptor (observed at 9 of 10 receptors for 1-hour concentrations and 8 of 10 receptors for 24-hour concentrations).
- Based on NYC comparisons, the combined use of a mean emission rate and mixing height and a neutral stability classification will decrease the correlation with measurements but will decrease the RMSE (observed at 10 of 10 receptors for 1-hour concentrations and 7 of 10 receptors for 24-hour concentrations).

2. In evaluating GHM, it was concluded that adding point source contributions (i.e., calculated using SCIM) to GHM calculations improved the results for this model. The RMSE was smaller at 6 of 10 NYC receptors, the correlation coefficient was higher at 6 of 10 receptors, and the standard deviation of calculated concentrations was closer to the standard deviation of measured concentrations at all 10 receptors.

3. Comparing SCIM and GHM using hourly calculations and SO_2 measurements, NYC data, SCIM produced the least annual mean error at 6 of 10 receptors, the closer agreement between standard deviations of calculated and measured concentrations at 5 of 10 receptors, the least error in estimating the maximum measured concentrations at 6 of 10 receptors, and the highest correlation coefficient at 3 of 10 receptors; GHM produced the least RMSE at all 10 receptors. Results for comparison of 24-hour SO_2 concentrations are similar but slightly more favorable to SCIM.

4. There is a need to improve the input data used with the multiple-source Gaussian plume type model, particularly atmospheric stability information, since the model is very sensitive to the rather gross changes in stability which are routinely introduced. SCIM calculations on the average, greatly overestimated concentrations associated with Turner-Pasquill stability classes 2 and 5.

5. Calculations based on a NYC emission algorithm developed in this report, particularly when applied with GHM, generally agree with diurnal and temperature dependent trends in measured SO_2 concentrations. Further improvements in this algorithm are desirable but require more detailed information.

Conclusions (6-8) regarding the use of several versions of the multiple-source Gaussian plume model and GHM to estimate long-term mean concentrations of SO_2 and particulates are based on model-to-measurement comparisons for the same data periods and locations.

6. The use of variable emission rates for SCIM and GHM are not able to demonstrate any conclusive improvement in model validity over the use of mean emission rates. It is inferred that this result is due to the failure to properly treat other causes of variance, such as those associated with atmospheric stability.

7. Based on results for NYC, the Climatological Dispersion Model (CMD) and SCIM versions of the multiple-source Gaussian plume model produce a smaller station-to-station RMSE than the Air Quality Display Model (AQDM) version (i.e., RMSE's of 52 and 59, respectively, compared to 92, with an overall mean of 135 $\mu g/m^3$ of SO_2; RMSE's 22 and 22 compared to 36 with an overall mean of 82 $\mu g/m^3$ of particulates).

8. Although the NYC validation statistics for GHM, CDM, and SCIM are similar for SO_2, GHM results for particulates have a much higher station-to-station RMSE than do CDM and SCIM (i.e., RMSE of 60 compared to 22, with an overall mean of 82 $\mu g/m^3$).

Section 3.0

PHASE II WORK REPORTED AND ACCOMPLISHED ELSEWHERE

Section 3.0

PHASE II WORK REPORTED AND ACCOMPLISHED ELSEWHERE

3.1 SCIM COMPUTER PROGRAM AND USER'S MANUAL

The treatments called for in the contract scope (Section 1.0) were performed on the SCIM computer program. The program itself and its use were documented in GEOMET Report EF-261, as briefly indicated in the excerpts from that report which follow.

The Sampled Chronological Input Model (SCIM) is an urban air pollution simulation. It is designed to provide the user with a method of estimating the air quality characteristics of a particular pollutant over a specified control area. Both the mean long-term concentration and the frequency distribution of short-term concentrations are estimated using conventional emission inventory and meteorological data.

The objective of User's Manual is to:

- Briefly describe the SCIM computer program and its intended applications
- Provide guidance and sample programs to process conventional data into the input forms required by the SCIM program
- *Describe how to set up and operate the SCIM program.*

The SCIM computer program provides the user with a tool for estimating short-term maxima of pollutant concentrations in addition to long-term means. This is done by calculating concentrations for a sample of short-term periods selected from a specified long-term period. The sample is then used to estimate the long-term mean concentration, the geometric standard deviation and the statistical frequency distribution of short-term concentrations for all specified locations. The expected annual maximum concentration may be determined from the frequency distributions or by means of the geometric standard deviation (e.g., see Larsen 1971). The calculations are made for specified receptor locations.

The calculations are made using a multiple-source Gaussian plume model. Emissions from large stationary sources are represented by elevated point sources. All other emissions are represented by an area source. Contributions from the area source to concentrations at a receptor are calculated using a numerical technique to evaluate the integral equation which must be solved. The narrow plume concept which implies that crosswind variations in emission rates may be neglected is an important assumption in the numerical technique. This assumption is valid as long as the distance between variations in the area source emission rate is large compared to the crosswind diffusion parameter (σ_y). A critical characteristic of the numerical technique is the spacing of grid points for which emission rates per unit area are determined. Model sensitivity findings show that a spacing of one-quarter mile is important in areas of high spatial variations of emissions. More generally, spacings of 1 km or more are satisfactory.

A significant feature of this program is that varying patterns of emissions are linked to a chronology of weather observations so that related variations in emission rates and in the dispersive capability of the atmosphere can be taken into account. In the emission algorithm presented here emission rates are related to ambient air temperature and to hour of the day. This algorithm is especially applicable to emissions which are related to space heating requirements. The program has been tested and found applicable to estimating sulfur dioxide and particulate air quality characteristics.

The program inputs are prepared from conveniently available data, including Implementation Planning Program (IPP) or Air Quality Display Model (AQDM) emission data and standard weather data which is available on punched cards or magnetic tape from the National Weather Records Center. The program analyzes the air quality of a region of interest by calculating a sample of hourly concentrations at specified locations. The user controls the sample size by specifying the sampling interval between successive hours for which calculations are made. The standard program outputs consist of a data file containing the concentrations calculated for each specified location for each selected hour and a printed statistical summary of the air quality characteristic of each location and of all locations combined. In addition, the user may choose to use a version of the program which will generate a Source Contribution File in the correct format to interface with IPP.

3.2 TRAINING OF EPA PERSONNEL

The final training of EPA personnel called for in the contract scope was provided at EPA by GEOMET staff in July of 1973. Ten to fifteen staff members of the Office of Air Quality Planning and Standards and of the Meteorology Laboratory were given instruction in the use of the program. This instruction was augmented by subsequent extensive interaction by phone and in person between GEOMET and EPA staff.

Section 4.0

CONSIDERATIONS OF EMISSION DATA, EMSU DATA AND SHORT-TERM MAXIMUM CONCENTRATIONS

Section 4.0

CONSIDERATIONS OF EMISSION DATA, EMSU DATA AND SHORT-TERM MAXIMUM CONCENTRATIONS

4.1 DIURNAL AND SEASONAL VARIATIONS IN EMISSIONS

The SCIM program is primarily designed to analyze air quality levels associated with emissions of stable pollutants such as sulfur dioxide, particulates and carbon monoxide. The emissions from any given source will vary with hour of the day, day of the week and season of the year. Standard emission factors have been developed for most pollutants which allow estimates of emission rates to be established as a function of fuel consumption rates or of processing rates for various industrial activities. When these fuel consumption rates and processing rates are described as functions of times, the emission rate of each pollutant is well defined.

Unfortunately, information on variations of emissions with time are not usually available. However, when emissions result from the consumption of fuel for space heating, the emissions will vary with temperature. Variations in these emissions with time can be estimated from local temperature records which are available for almost all locations. The consumption of fuel for space heating accounts for a certain percentage of the emissions of a pollutant from a particular source. A general algorithm used in SCIM which describes emissions as a function of parameters which can be related to temperature and other activity indexes is the following:

$$Q(t) = Q_A \, K(t)$$

$$K(t) = (1-F)\, A(t) + F\, [H(t) - T(t)]\, S(t), \qquad T(t) < H(t)$$

$$T(t) \geq H(t) \qquad K(t) = (f-F)\, A(t),$$

where

$Q(t)$ = emission rate at time t

Q_A = average annual emission rate

$K(t)$ = time dependent emission factor

F = fraction of emissions which result from space heating requirements

$A(t)$ = activity factor which defines activity level for time t relative to annual average activity level for activities which control emissions not related to space heating requirements

$H(t)$ = temperature threshold for space heating requirements for time t

$T(t)$ = temperature at time t

$S(t)$ = sensitivity factor which defines rate of emission per degree below temperature threshold at time t relative to annual average rate of emission per degree below temperature threshold.

In the above algorithm the parameters $A(t)$, $H(t)$ and $S(t)$ may vary with time of day, day of the week and week of the year. The information required to determine these parameters as functions of time for every point source and every square mile of an area source is far too detailed for what is normally economically feasible to collect and analyze. However, it may be useful to derive city-wide parameters which can be applied to area sources.

The ideal data for estimating the above parameters would be fuel consumption records and process operating records for a large number of sources. Lacking this, other less desirable data might be used. In the Phase I report of this project, a large set of SO_2 concentration measurements was used (12 years of almost continuous hourly observations) for New York City. Blade and Ferrand (1969) summarized these measurements by hour of the day, day of the week, and week and month of the year. The mean hourly SO_2 concentrations for each month of the year were correlated with mean hourly temperature for each month of the year for the same data period. Following the methods described in the Phase I report (Appendix A), the parameter values presented in Table 4.4-1 were developed. On the basis of this same data, it was estimated that 29 percent of the emissions are dependent on temperature variations (i.e., F = 0.29).

SCIM is programmed to use the above algorithm and the parameter values in Table 4.1-1 to estimate diurnal variations in area source emissions. There are some drawbacks to using this data. The parameter values for the emission algorithm are specifically applicable to SO_2 emissions in New York City. It is not known how applicable these are to other cities. Furthermore, since the emission rates were derived from SO_2 measurements the parameter values may contain diurnal variations which are associated with diurnal variations in meteorological conditions. The diurnal variation in activity factors shown in Table 4.1-1 does not make much sense

Table 4.1-1. Emission Parameters Developed from New York City SO_2 Data

Hour of the Day	Activity Factor, A(A)	Temperature Threshold, H(t), °F	Sensitivity Factor, S(t), $°F^{-1}$
0	1.0272	56	0.0330
1	1.0008	55	0.0280
2	0.9576	55	0.0280
3	0.9576	55	0.0293
4	1.00344	56	0.0371
5	1.1784	58	0.0717
6	1.3032	59	0.1208
7	1.3200	61	0.1437
8	1.2624	63	0.1214
9	1.1616	64	0.0977
10	1.0104	65	0.0893
11	0.9336	65	0.0841
12	0.8760	65	0.0841
13	0.8232	65	0.0852
14	0.8160	65	0.0856
15	0.8160	65	0.0886
16	0.8232	65	0.0983
17	0.8424	65	0.1060
18	0.8832	65	0.1120
19	0.9264	65	0.1142
20	0.9744	65	0.1114
21	1.0104	64	0.1024
22	1.0272	62	0.0696
23	1.0344	60	0.0416
			Mean = 0.0826

when considered in terms of normal variations in business activities. The validation analysis reported in the Phase I report showed that, when annual averages of measured and SCIM calculated concentrations were compared for different hours of the day, the SCIM calculations overestimate the measured value by the greatest amount at 7 A.M. and underestimate by the greatest amount at 1 P.M. and 4 P.M. These correspond to maximum and minimum values of A(t), respectively. These results suggest that a uniform value of A(t) = 1 may be more appropriate than the values in Table 4.1-1. It is therefore recommended that SCIM be run with A(t) = 1, rather than the values in Table 4.1-1.

The sensitivity factors shown in Table 4.1-1 have a logical basis when considered in terms of people's diurnal activities. The sensitivity factors are highest in the early morning with a peak value at 7 A.M. This is when a major portion of the population arises. Residential fuel consumption and probably certain commercial and industrial fuel consumption is increased greatly relative to other hours of the day. Therefore, the sensitivity of fuel consumption relative to the temperature deficit from the threshold space heating temperature is likely to be very great. There is a secondary maximum in the sensitivity factor in the early evening hours. This corresponds with the time that residential fuel consumption is likely to be adjusted to temperature changes (i.e., the end of the working day when people return to apartments and homes). The low sensitivity factors in the early morning hours after midnight are times of minimum residential fuel consumption and low heat replacement in commercial and institutional sources due to opening doors. Thus, there is a qualitative basis for using the sensitivity factors shown in Table 4.1-1. Although the sensitivity factors and temperature thresholds in Table 4.1-1 were developed for New York City, they are probably qualitatively applicable to other cities. If other information is not available, they are a reasonable approximation to what can be expected in other large cities.

The fractions of emissions which are temperature sensitive is likely to be variable from one city to another, depending primarily on how cold the climate is. One gross assumption which could be made is that the fraction of SO_2 emissions which are temperature sensitive is directly proportional to the climatological mean degree days which occur at a given location. However, it is recommended that estimates of the fuel use and climatological mean degree days be obtained for several different climates before attempting to define such a relationship. One other source of data is available from a study by Argonne National Laboratory (Roberts, et. al 1970). From this report it is estimated that 72 percent of SO_2 emissions in Chicago are temperature sensitive. By way of comparison, it is noted that the annual mean degree days are approximately 5000°F days and 6200°F days for New York City and Chicago, respectively. The two available estimates of 29 percent for 5000°F days and 72 percent for 6200°F days are not very consistent. Of course, other factors, such as the relative mix of industrial, commercial and residential fuel users in the area sources, affect the relationship. More data on the amount of fuel use which is related to temperature considerations is needed. For the time being, one might reasonably assume that, for large cities with normal total heating degree days (with a base of 65°F) of 5000 to 6000 degree days, SO_2 emissions from area sources are 50 percent temperature sensitive and use the temperature thresholds and sensitivity factors in Table 4.1-1.

4.2 USE OF EMSU DATA AS METEOROLOGICAL INPUT

During the late 1960's and early 1970's, Environmental Meteorological Support Units (EMSU) were established by the National Oceanic and Atmospheric Administration in roughly 20 U.S. cities. The purpose of these units was to take observations, prepare forecasts, and provide advice on the present and future meteorological conditions which affect air pollution levels. An analysis is made in this study of how data reported by EMSU's could be used to determine meteorological parameters for SCIM and how the selected values compared with values determined from conventional airport weather observations. Three meteorological parameters analyzed were mixing height, atmospheric stability and wind speed and direction.

The EMSU data consist of radiosonde observations of temperature, relative humidity and wind direction and speed from a slow rise balloon (i.e., about 65 meters per minute). The soundings are taken from urban areas and generally provide useful estimates of the temperature, moisture and wind profiles over large cities. The soundings are generally taken at times of expected minimum (near sunrise) and expected maximum (early afternoon) dispersion conditions. Additional soundings may also be available for intermediate hours.

4.2.1 Mixing Height

Mixing heights were calculated for EMSU (slow rise) radiosonde data and for standard radiosonde data using the method described in Appendix A-1. The data used included all days in August and December of 1969 for which both EMSU and standard RAOB data were available for New York City and St. Louis.

New York City represents a site at which both standard and EMSU data are available for the same city. The EMSU data are obtained from releases at Laguardia Airport which is located well within the New York Metropolitan area. The standard data are obtained from releases at Kennedy Airport which is located on the edge of the metropolitan area. Mixing heights corresponding to EMSU observation times are determined from the standard data using an interpolation scheme described in Appendix A-2. The 12Z mixing height is taken to be representative of 0600 local time and the 00Z mixing height is taken to be representative of 1400 local time. Linear interpolation with time is used between 0600 and 1400. The computed mixing heights, interpolated values and differences between mixing heights calculated using EMSU and standard RAOB data are presented in Table 4.2-1.

St. Louis represents a site at which standard RAOB data are not available, but for which EMSU data are available. The mixing height for St. Louis was estimated using an average of heights calculated for Peoria, Illinois, and Columbia, Missouri. The computed mixing heights, calculated averages, interpolated values and EMSU less standard RAOB differences are presented in Table 4.2-2.

The question of whether the EMSU data provides information about mixing heights which is significantly different from that available from standard radiosondes may be examined using the data in Tables 4.2-1 and 4.2-2. For each location and each month, the difference between mixing

Table 4.2-1. New York City Mixing Height Estimates from Standard RAOB and EMSU Data

Date (1969)	Hour	Kennedy Airport RAOB	Laguardia Airport EMSU	EMSU Minus RAOB
August 1	0600	(100)*	100	0
	0700	107		
	1100	(2446)	763	-1683
	1900	4200		
August 4	0700	107	100	-7
	1100	(2446)	125	-2321
	1900	4200		
August 5	0600	(4200)	100	-4100
	0700	4200		
	1100	(4200)	187	-4013
	1900	4200		
August 6	0600	(4200)	244	-3956
	0700	4200		
	1100	(1861)	2248	387
	1900	107		
August 7	0600	(118)	100	-18
	0700	156		
	1100	(307)	791	484
	1900	420		
August 8	0500	(628)	100	-528
	0700	567		
	1100	(325)	138	-187
	1900	143		
August 11	0600	(238)	100	-138
	0700	261		
	1100	(352)	100	-252
	1900	420		
August 12	0600	(219)	100	-119
	0700	219		
	1000	(216)	881	665
	1900	213		
August 13	0600	(119)	100	-19
	0700	138		
	1100	(214)	2770	2556
	1900	270		
August 14	0600	(100)	100	0
	0700	100		
	1100	(255)	172	-83
	1900	372		
August 15	0600	(4200)	126	-4074
	0700	4200		
	1100	(4200)	106	-4094
	1900	4200		
August 18	0600	(100)	100	0
	0700	107		
	1100	(203)	156	-47
	1900	275		
August 19	0600	(1303)	127	-1176
	0700	1172		
	1100	(647)	930	282
	1900	254		
August 20	0600	(100)	100	0
	0700	423		
	1100	(2581)	1027	-1554
	1900	4200		

* Values in parentheses are interpolated (see text).

(Continued)

Table 4.2-1. New York City Mixing Height Estimates from Standard RAOB and EMSU Data (Continued)

Date (1969)	Hour	Kennedy Airport RAOB	Laguardia Airport EMSU	EMSU Minus RAOB
August 21	0600	(292)*	100	-192
	0700	452		
	1200	(1253)	1281	28
	1900	1573		
August 22	0600	(100)	100	0
	0700	168		
	1100	(935)	1486	551
	1900	1510		
August 25	0600	(105)	100	-5
	0700	167		
	1100	(417)	671	254
	1900	605		
August 26	0600	(4200)	263	-3937
	0700	4200		
	1100	(4200)	735	-3465
	1900	4200		
August 27	0600	(642)	190	-451
	0700	643		
	1100	(649)	1194	545
	1900	653		
August 28	0600	(162)	115	-47
	0700	180		
	1100	(255)	846	592
	1900	310		
August 29	0600	(155)	192	37
	0700	149		
	1100	(125)	782	657
	1900	107		
December 1	0700	382		
	1200	(1666)	589	-1077
	1900	2179		
December 2	0700	797	561	-236
	1200	(1027)	646	-381
	1900	1119		
December 3	0700	277	403	126
	1200	(2522)	1257	-1265
	1900	3420		
December 4	0700	1057	1060	3
	1200	(1476)	1381	-95
	1900	1644		
December 5	0700	599	913	314
	1200	743	1274	530
	1900	800		
December 8	0700	481		
	0800	(449)	428	-21
	1200	(320)	453	134
	1900	255		
December 9	0700	519	544	26
	1200	(575)	673	99
	1900	597		
December 10	0700	285	351	66
	1200	(153)	352	199
	1900	100		

* Values in parentheses are interpolated (see text).

(Continued)

Table 4.2-1. New York City Mixing Height Estimates from Standard RAOB and EMSU Data (Concluded)

Date (1969)	Hour	Kennedy Airport RAOB	Laguardia Airport EMSU	EMSU Minus RAOB
December 11	0700	400	436	36
December 12	0700	117	221	105
	1200	(557)*	3638	3081
	1900	733		
December 15	0700	1172	1103	-68
	1200	(546)	1240	695
	1900	295		
December 16	0700	1154	100	-1054
	1200	(1135)	1327	192
	1900	1128		
December 17	0700	878	618	-260
	1200	(1019)	1104	85
	1900	1076		
December 18	0700	332	219	-113
	1200	(1078)	370	-709
	1900	1377		
December 19	0700	3342	2382	-960
	1200	(2653)	2644	-9
	1900	2377		
December 23	0700	448	422	-26
	1200	(547)	743	196
	1900	587		
December 24	0700	440	560	120
	1200	(332)	377	45
	1900	289		
December 29	0700	460	531	71
	1300	(506)	147	-359
	1900	514		
December 30	0700	171	224	53
	1400	451	327	-124
	1900	451		

* Values in parentheses are interpolated (see text).

Table 4.2-2. St. Louis Mixing Height Estimates from Standard RAOB and ESMU Data

Date (1969)	Hour	RAOB Peoria Sounding	RAOB Columbia Sounding	RAOB Average	St. Louis EMSU Sounding	St. Louis Minus Average RAOB
August 11	0600	227	259	243	170	-72
	1300			(2910)*	2780	-130
	1800	3269	3314	3292		
August 12	0600	236	310	273	168	-105
	1000			(1513)	1301	-212
	1400			(2753)	162	-2591
	1800	3473	2033	2753		
August 13	0600	231	294	263	211	-51
	1300			(700)	567	-133
	1800	725	800	763		
August 14	0600	260	298	279	192	-87
	1300			(2894)	2626	-268
	1800	3464	3071	3268		
August 18	0600	363	316	340	322	-18
	1100		3093	3093		
	1300			(3270)	3021	-249
	1800	3338	3230	3284		
August 19	0600	255	309	282	336	54
	1300			(2523)	2467	-57
	1800	3163	2525	2844		
August 20	0600	401	304	352	345	-7
	1300			(2191)	2345	153
	1800	3945	964	2454		
August 21	0600	443	777	610	2820	2210
	1300			(2434)	1774	-660
	1800	1333	4056	2694		
August 22	0600	250	284	267	165	-101
	1200			(1062)	154	-908
	1800	1336	1317	1326		
August 25	0600	213	276	245	155	-90
	1000			(1631)	1736	105
	1300			(2671)	1865	-806
	1400			(3018)	251	-2767
	1800	2223	3813	3018		
August 26	0600	217	280	249	157	-92
	1000			(1571)	1926	355
	1300			(2563)	2005	-559
	1800	2214	3574	2894		
August 27	0600	228	310	269	178	-91
	1000			(1244)	2018	773
	1400			(2220)	2002	-218
	1800	426	4014	2220		
August 28	0600	225	291	258	170	-87
	1000			(1908)	3050	1142
	1400			(3558)	2013	-1545
	1800	3412	3704	3558		
August 29	0600	233	284	258	173	-89
	1300			(1072)	3080	2008
	1800	812	1565	1189		

* Values in parentheses are interpolated (see text).

(Continued)

Table 4.2-2. St. Louis Mixing Height Estimates from Standard RAOB and EMSU Data (Concluded)

Date (1969)	Hour	RAOB Peoria Sounding	RAOB Columbia Sounding	RAOB Average	St. Louis EMSU Sounding	St. Louis Minus Average RAOB
December 4	0600	299	285	292	216	-75
	1300			(604)*	928	324
	1800	284	1014	649		
December 5	0600	302	544	423	455	32
	1300			(651)	897	246
	1800	557	809	683		
December 8	0600	492	307	400	942	543
	1300			(307)	1313	1006
	1800	246	341	293		
December 9	0600	301	375	338	257	-81
	1300			(816)	1074	258
	1800	1414	355	885		
December 11	0600	733	821	777	1737	960
	1200			(1098)	717	-381
	1800	1214	1196	1205		
December 12	0600	559	902	730	1098	368
	1300			(624)	1003	380
	1800	805	412	608		
December 15	0600	344	988	666	921	255
	1300			(799)	1109	310
	1800	566	1070	818		
December 16	0600	231	379	305	426	121
	1200			(474)	802	327
	1800	396	663	530		
December 17	0600	841	799	820	318	-502
	1300			(621)	786	164
	1800	712	472	592		
December 18	0600	580	826	703	1085	381
	1300			(648)	914	266
	1800	920	444	682		
December 19	0600	483	293	388	345	-43
	1300			(1055)	1794	740
	1800	1238	1062	1150		
December 22	0600	529	998	764	1175	412
	1200			(822)	965	143
	1800	639	1044	841		
December 23	0600	902	1398	1150	1207	57
	1200			(1356)	1851	495
	1800	1552	1297	1425		
December 24	0600	294	912	603	305	-297
	1200			(607)	753	146
	1800	612	603	608		

* Values in parentheses are interpolated (see text).

heights estimated from EMSU and standard RAOB data is summarized in Table 4.2-3 for sunrise and for mid-day observation times. Overall these comparisons show that the mean differences (-205m) is about 20 percent of mean mixing height (1044m). However, there is a large amount of variability for individual comparisons as demonstrated by the large root mean square difference of 1146m. These results suggest that for the overall climatological average, the EMSU information may not be important. However, for day to day variations, there is important information available in the EMSU data. Mixing height is most important in determining dispersion conditions during the day. It is less important near sunrise when stable or neutral stability conditions prevail. An examination of the data in Tables 4.2-1 and 4.2-2 shows that in 46 percent (18 comparisons) for New York City and 47 percent (16 comparisons) for St. Louis, the EMSU mixing height estimate differs from that derived with standard RAOB data by over 50 percent of the standard RAOB estimate. As a result, it is concluded that, when EMSU data is available, it should be used in place of or to supplement the standard data.

The following procedures are suggested for using the EMSU data. Use the interpolation scheme described in Appendix A-1 as a model of diurnal variation in mixing height. The following steps may be followed.

1. If a sunrise EMSU sounding is available, use the mixing height from it for the period from Midnight to 6 a.m. If not, use an estiamte from standard RAOB data.

Table 4.2-3. Statistics of Difference Between EMSU and Standard RAOB Mixing Height Estimates

Location	Month (1969)	Time of Day	Number of Comparisons	EMSU Less Standard RAOB Mixing Height (m)			Mean Mixing Height (m)	
				Range	Mean Difference	Root Mean Square Difference	Standard	EMSU
New York City	August	Sunrise	21	-4074 to 37	-892	1776	1018	127
New York City	August	Mid-Day	21	-4094 to 2556	-509		1337	828
St. Louis	August	Sunrise	14	-105 to 2210	98	944	299	397
St. Louis	August	Mid-Day	20	-2767 to 2008	-328		2185	1857
New York City	December	Sunrise	18	-1054 to 314	-107	673	710	603
New York City	December	Mid-Day	18	-1265 to 3081	69		961	1030
St. Louis	December	Sunrise	14	-502 to 960	152	413	597	747
St. Louis	December	Mid-Day	14	-381 to 1006	316		749	1065
TOTAL			140	-4094 to 3081	-205	1146	1044	839

2. If one or more mid-day EMSU soundings are available, obtain mixing heights from each. Use linear interpolation with time to estimate mixing heights for hours between EMSU soundings.

3. If more than one EMSU sounding is available these may be linearly extrapolated with time to estimate mixing heights over the period from 6 a.m. to 2 p.m.

4. If only one EMSU sounding is available, compute the mixing height for other hours in the period from 6 a.m. to 2 p.m. by substituting the hourly surface temperature for the surface temperature in the sounding and computing the mixing for the revised sounding.

4.2.2 Stability Class

Since EMSU sounding data is obtained from a slow rise balloon, it should be useful in characterizing the temperature and wind profiles of the lowest layers of the atmosphere, which determine dispersion conditions. Several ways of characterizing the stability of the atmosphere using EMSU data are compared with the Pasquill stability classes determined by a method suggested by Turner using surface weather observations of cloud cover and wind speed. The extent to which the EMSU data suggest stability classifications different from the Turner-Pasquill categories is discussed. In conclusion a method of integrating the two types of data is proposed.

Bulk Richardson number, calculated over three different heights, was used to characterize stability. The three heights were from the lowest height in the EMSU sounding with both wind and temperature data to (1) the top of the mixing layer, (2) 140 meters, as used by McElroy (1969) to classify measurements of σ_y and σ_z, and (3) the next lowest height with wind and temperature data. The wind speed data within the mixing layer were fitted to a power law profile by the method of least squares. This too was used to characterize the atmospheric stability. These estimates were obtained from St. Louis EMSU soundings for August and December 1969. The three bulk Richardson numbers, the wind speed profile power law and the mean mixing layer wind speed and direction, for each EMSU sounding with reasonably complete data, are listed in Table 4.2-4. For comparison the Pasquill stability class and surface wind determined from the closest (in time) three-hour surface weather observation are also listed.

In order to compare the sounding stability characteristics with the Pasquill stability classes, the correspondence shown in Table 4.2-5 was assumed. The correspondence in Table 4.2-5 is hypothetical and was selected to be reasonably consistent both with the data shown in Table 4.2.4 and with information reported by other investigators. Using these correspondences, the best agreement between EMSU stability data and the Pasquill stability classes (listed in Table 4.2-4) is obtained using the bulk Richardson number over 140 meters. This gives 19 hours out of 38 in agreement. The next best was the bulk Richardson number over the lowest 2 heights, which gives 18 hours of agreement out of 44 comparisons.

Since 50 percent of the compared hours differ between EMSU and surface data stability classifications, there is probably a significant amount of additional information available in the EMSU data. However, it is difficult to see how to use the EMSU data, except to modify the single hour for which EMSU stability classifications are obtained. The stability changes so rapidly from hour to hour during the periods over

Table 4.2-4. Stability and Wind Characteristics for St. Louis

Date (1969)	Hour	Bulk Richardson Number			Pasquill Stability Class	Wind Speed Profile Power Law	Wind Direction/ Speed (m/sec)	
		Over Mixing Layer	Over 140 m Layer	Lowest Two Sounding Heights			Mixing Layer Mean	Surface
Aug. 25	1000	1.690	0.072	0.009	B	-0.06	47/4	10/3
Aug. 25	1200	-0.550	-	0.015	C	0.06	65/5	10/4
Aug. 25	2000	0.036	0.044	0.003	E	0.28	59/6	30/3
Aug. 26	0500	0.146	0.101	0.149	E	0.22	48/5	calm
Aug. 26	0900	0.136	0.131	-0.069	C	0.15	70/6	350/3
Aug. 26	1200	-0.632	-0.038	-0.079	A	-0.01	62/5	70/2
Aug. 27	0500	0.851	1.028	0.307	E	0.08	133/2	calm
Aug. 27	1000	4.620	-0.134	-0.156	B	-0.06	169/3	160/5
Aug. 27	1300	1.125	-0.019	-0.103	A	0.14	162/7	190/2
Aug. 28	0500	0.119	0.109	0.073	D	0.34	203/6	calm
Aug. 28	1000	7.968	-0.007	-0.016	D	-0.04	228/8	160/5
Aug. 28	1400	0.200	0.003	-0.040	B	0.06	179/9	180/2
Aug. 29	0500	0.090	0.097	0.058	E	0.28	223/8	150/2
Aug. 29	1300	0.389	0.029	-0.043	D	0.03	210/6	200/4
Dec. 4	0500	0.027	0.033	0.017	E	0.05	32/12	30/3
Dec. 4	1200	0.016	-0.070	-0.060	C	0.04	42/7	40/4
Dec. 5	0500	0.031	0.009	-0.002	D	0.15	157/14	130/6
Dec. 5	1200	0.051	0.005	-0.004	D	0.08	155/11	130/6
Dec. 8	0500	0.271	0.038	0.021	D	0.17	269/13	240/4
Dec. 8	1200	0.051	0.010	-0.007	C	0.14	254/13	230/5
Dec. 9	0500	0.026	0.030	0.026	D	0.33	190/11	160/4
Dec. 9	1200	0.294	0.016	0.007	D	0.17	200/16	170/7
Dec. 10	1200	0.238	-0.004	-0.083	D	0.32	69/10	30/3
Dec. 11	1200	-0.044	-0.007	-0.001	D	0.05	298/14	290/7
Dec. 12	0500	0.138	0.010	0.007	D	0.08	272/5	260/4
Dec. 12	1200	-0.012	-0.060	-0.077	D	0.16	301/7	310/4
Dec. 15	0500	0.168	0.004	-0.002	E	0.06	13/19	10/3
Dec. 15	1200	0.039	-	-0.038	D	0.07	355/10	350/6
Dec. 16	0500	0.322	0.177	0.094	E	0.19	85/4	60/1
Dec. 16	1200	-0.007	-0.180	-0.138	C	0.02	180/8	160/3
Dec. 17	0500	0.030	0.034	0.030	E	0.38	355/9	260/3
Dec. 17	1200	-0.795	-0.057	-0.165	D	0.01	175/6	130/3
Dec. 18	0500	0.020	-0.264	0.002	D	0.33	253/15	250/5
Dec. 18	1200	-0.035	-0.220	-0.008	D	0.08	324/13	280/6
Dec. 19	0500	-0.022	0.091	-0.012	E	0.17	318/11	230/3
Dec. 19	1200	0.094	-	-0.063	D	0.28	313/21	300/4
Dec. 22	0500	-0.538	0.330	0.170	D	0.10	356/10	300/5
Dec. 22	1200	0.065	0.670	0.330	D	0.15	158/8	100/4
Dec. 24	0500	0.226	-	0.167	D	0.82	90/3	100/4
Dec. 24	1200	0.069	-	-0.066	D	0.26	184/11	140/5
Dec. 30	0500	0.308	0.233	0.184	D	0.04	7/14	320/5
Dec. 30	1200	-0.544	0.112	0.035	D	0.02	352/13	320/5
Dec. 31	0500	-1.904	0.226	-0.005	D	0.08	315/10	260/5
Dec. 31	1200	-5.829	-	-0.315	D	0.18	271/4	280/4

which EMSU data is available that the surface data is much better that an extrapoliation of EMSU data. The EMSU data has limited use. The data would be more useful if soundings were available every three hours.

Table 4.2-5. Proposed Correspondence Between Three Types of Stability Classifications

Time of Day	Pasquill Class	Bulk Richardson Number	Wind Speed Profile Power Law
Day	A	< -0.05	< 0.05
Day	B	-0.05 to -0.031	0.05 to 0.12
Day	C	-0.03 to -0.011	0.13 to 0.17
Day	D	> -0.01	> 0.17
Night	D	≤ 0.01	≤ 0.22
Night	E	> 0.01	> 0.22

Another uncertainty with stability data related to vertical temperature and wind profiles is that the relation of this data to the commonly used Pasquill dispersion parameters is not well established. In the light of the above considerations, it is recommended that EMSU data not be used to determine stability characteristics.

4.2.3 Wind Direction and Speed

The data given in Table 4.2-4 shows comparisons between the surface wind speed and direction and the vector mean wind speed and direction for the mixing layer. It is clear from these comparisons that the EMSU data provides significant additional information on the wind profile. Of particular interest is the frequent occurrence of a noticeable turning of the wind with height. This can have a significant effect on model calculations. The need for a detailed study of how to use wind profile data in estimating the wind direction and speed used in model calculations is clearly indicated by this data. No attempt has been made to develop general techniques from the limited data presented in Table 4.2-4. However, the data does suggest some possible ways of using EMSU data to improve the wind direction and speed estimates used in modeling. During some periods the vertical wind shear remains nearly fixed from one EMSU sounding to the next. This suggests that an average shear could be derived and applied to all surface wind observations between the EMSU observation times. Another possibility is to develop diurnal patterns of wind shear from other data sources (e.g., St. Louis micromet tower data of 1964) and use the EMSU data to identify and scale the patterns. The turning of the wind with height should be taken into account in dispersion models.

For the present it is suggested that the following tentative procedure be used to account for turning of the wind.

1. Determine the mean wind direction for the mixing layer for each EMSU sounding. If the sources being modeled are mostly elevated sources, use this as the wind direction; if the sources are mostly ground sources, use the surface wind direction.

2. If the succeeding EMSU sounding is less than 24-hours away and the mixing layer mean wind direction has changed by less than 90°, estimate the wind direction for intervening hours by linear interpolation. Use these wind directions in place of the surface wind direction if mostly elevated sources are being modeled. If the wind direction has shifted by 90° or more or ground sources are being modeled use the reported surface wind directions for intervening hours. If the time period between soundings exceeds 24 hours, use the reported surface wind directions for intervening hours.

4.3 PROCEDURE FOR CALCULATING ANNUAL SHORT-TERM MAXIMUM CONCENTRATIONS

4.3.1 Introduction

The operational implementation of the Gaussian plume model of this study for purposes of evaluating proposed air quality strategies could impose a severe computational burden. The model might be used to calculate all hourly concentrations within a long-term period, e.g., one year, for which both emission and meteorological data are available. This is repeated for each of a number of stations in each of many control regions for each of several proposed air quality control strategies. A statistical sampling procedure was devised to reduce the amount of computations and was tested on 10 stations in New York City. the procedure consists of reducing the number of hourly concentrations calculated; the number of stations, air quality regions, and control strategies do not change. The reduction is achieved by selecting a sample of the variable hours in a systematic manner and using the sample to calculate the parameters required for evaluating air quality strategies (e.g., mean annual concentration, daily value exceeded only once a year, etc.).

The test on the 10 stations consisted of choosing samples of various sizes and determining the loss in accuracy is given by the difference between a parameter value calculated from all available hours and the value of this same parameter calculated from a sample. Six air quality control parameters were chosen for analyses, and differences were obtained for each of 29 sample sizes. Tables and graphs of a function of these differences, are presented in a fashion to provide information on the tradeoff between reduction of computations and loss in accuracy. These furnish guidance for choosing a sample size, and thereby reducing computations, in any operational implementation of the model for evaluating air quality strategies.

The test procedure, and the results of the test are described below including: method of calculating the six air quality control parameters, the sampling scheme, and development of the function of the differences which serves as an overall measure of accuracy.

4.3.2 Test Procedure

4.3.2.1 Air Quality Parameters

In current EPA practice, it is generally assumed that air pollution concentration values follow the log-normal distribution. This assumption was adopted in this study. Although other distributions have been advanced, and may in fact eventually replace the log-normal assumption, it is our opinion that results obtained here would not be changed substantially. For any set of hourly concentrations (e.g., all 2920 third hours in a year or a sample thereof), the log-normal distribution was fitted by calculating the mean, $\overline{Y}$, and the standard deviation, s_Y, of the logarithms of the concentrations. Three air quality values were then derived as follows:

$$\text{Mean} = \exp\left(\overline{Y} + 0.5\, s_Y^2\right)$$

$$\text{Value exceeded once in 1000 hours} = \exp\left(\overline{Y} + 3.091\, s_Y\right)$$

$$\text{Value exceeded once in 2920 hours} = \exp\left(\overline{Y} + 3.396\, s_Y\right)$$

Three additional values were calculated in a similar manner from daily mean concentrations, i.e., the arithmetic mean of the eight hourly concentrations for the day. The log-normal distribution was fitted to these means; the parameters are:

Mean = exp $(\bar{Z} + 0.5\ s_Z^{\ 2})$

Daily value exceeded once in a 100 day = exp $(\bar{Z} + 2.33\ s_Z)$

Daily value exceeded once in a year = exp $(\bar{Z} + 2.776\ s_Z)$

Where $\bar{Z}$ and s_Z are, respectively, the mean and standard deviation of the logarithms of the daily values.

4.3.2.2 Sampling Procedure

The sampling procedure for the daily values (average of 8 three-hourly values) is presented first because it is simpler. Two terms require definition: a sampling interval is the number of values from one selected value to the next (e.g., a sampling interval of two means that every other day is included in the sample); the initial time indicates the starting day of the sample. Twenty-nine sampling intervals were chosen, each value from 2 through 30. For each interval, from 2 to 8 different samples were selected by varying the initial time. Thus, for a sampling interval of 2, two samples were drawn: the first consisted of days 1, 3, 5, ..., 365 and the second of days 2, 4, 6, ..., 364. The number of samples for a sampling interval is given by the maximum of [sampling interval or eight]. Thus, for sampling intervals up to eight the number of samples is equal to the sampling interval; for sampling intervals beyond eight exactly eight samples were drawn from the 365 days by varying the initial time from 1 through 8. The value of eight has no significance; it simply reduces the amount of computation.

When the sampling procedure is applied to the 3-hourly data some unequal sampling intervals may result, e.g., for interval two every other value <u>within</u> one day is selected, but from the last value of one day to the first value of the next, the interval is either 1 or 3. However, it was deemed more important to ensure equal representation of each of the eight hours of the day than to maintain a consistent sampling interval. Again, 29 sampling intervals were used but this time they do not proceed by steps of one but range from 2 to 249. They are listed in Table 4.3-1. As before, for each interval from two through eight the number of samples equals the sampling interval and beyond eight exactly eight samples were selected.

4.3.2.3 Measure of Accuracy

At each of the 10 stations, three air quality parameters were calculated using all 2920 hourly concentrations and an additional three using the 365 daily mean concentrations. For each sample selected from the 2920 hourly values, three air quality parameters were calculated and differences were taken between them and the corresponding parameter values using all 2920 hours. The same procedure was followed for samples drawn from the 365 daily concentrations. The differences were combined to obtain a measure of accuracy for each sampling interval for each air quality parameter.

Table 4.3-1. Measures of Accuracy - Hourly Concentrations

Sampling Interval	Average No. of Cases in Sample	Proportion of Cases in Sample	Measures of Accuracy for		
			Mean	1/1000	1/2920
2	1460	0.500	0.011	0.020	0.023
3	973	0.333	0.015	0.024	0.026
4	730	0.250	0.032	0.082	0.097
5	584	0.200	0.045	0.102	0.113
6	487	0.167	0.033	0.077	0.085
7	417	0.143	0.056	0.166	0.195
9	325	0.111	0.050	0.097	0.109
11	266	0.091	0.057	0.144	0.165
13	225	0.077	0.056	0.149	0.175
15	195	0.067	0.125	0.323	0.376
17	172	0.059	0.101	0.287	0.336
19	154	0.053	0.077	0.218	0.254
21	139	0.048	0.113	0.257	0.290
23	127	0.043	0.109	0.380	0.457
25	117	0.040	0.080	0.216	0.246
27	108	0.037	0.115	0.261	0.291
29	101	0.034	0.122	0.258	0.290
31	95	0.032	0.106	0.257	0.295
39	75	0.026	0.127	0.312	0.362
47	63	0.021	0.189	0.406	0.457
55	54	0.018	0.232	0.812	0.997
63	47	0.016	0.157	0.408	0.481
71	42	0.014	0.173	0.535	0.615
79	37	0.013	0.260	0.491	0.530
95	31	0.011	0.201	0.476	0.524
119	25	0.008	0.336	0.810	0.910
159	19	0.006	0.234	0.615	0.693
199	15	0.005	0.336	0.976	1.105
249	12	0.004	0.403	0.842	0.982

Let A_{jk} denote the measure of accuracy for air quality parameter j (j = 1, 2, ..., 6) for sampling interval k (k = 2, 3, ..., 29). Then,

$$A_{jk} = \left\{ \frac{1}{10} \cdot \frac{1}{N_k} \sum_{m=1}^{10} \sum_{n=1}^{N_k} \left(X_{jkmn} - X_{j1mn} \right)^2 \right\}^{1/2} \Bigg/ \frac{1}{10} \sum_{m=1}^{10} X_{j1mn} \qquad (4\text{-}1)$$

Where

X_{jkmn} = the value of air quality parameter j for sampling interval k at station m for sample n

X_{j1mn} = same as above with sampling interval of one (i.e., using all available data)

N_k = number of samples for sampling interval k.

The numerator in Equation 4-1 is the root-mean-square of the differences between air quality parameters calculated from a sample and the corresponding air quality parameters calculated using all available data. The denominator is the mean over the 10 stations of the parameter calculated by using all available data. The measure of accuracy, A_{jk}, is similar to the coefficient of variation (standard deviation/mean) except that the numerator is a root-mean-square rather than a standard deviation.

4.3.3 RESULTS

Table 4.3-1 gives values of A_{jk} for the hourly concentrations and Table 4.3-2 contains results for the daily concentrations. Both tables indicate considerable savings in computational effort with reasonably small losses in accuracy. In Table 4.3-1, the loss in accuracy, as defined by A_{jk}, is below 20 percent for all three air quality parameters for sampling intervals up to 13 (i.e., sample size only 0.056 as large as all available 2920 hours). The loss in accuracy is less for the mean than it is for the two exceedance values. This is consistent with statistical theory which indicates greater accuracy in estimating the mean of a distribution than the tails. In Table 4.3-2, the loss in accuracy for the daily concentrations is greater than for the hourly concentrations for the same proportion of cases in the sample. But even here, the loss is below 31 percent for sampling intervals up to 10 days. Again the loss is less for the mean than for the two exceedance levels.

To facilitate use of the results, the measures of accuracy were plotted against proportion of total cases in the sample, and lines were fitted by least squares. Figure 4.3-1 contains the measures from the hourly concentrations and Figure 4.3-2 the measures calculated from the daily concentrations. Only the first several values are plotted because, as can be seen in Tables 4.3-1 and 4.3-2, the measures show large fluctuations for small proportions of cases. In an operational problem, these graphs can be entered with an hypothesized proportion of cases to estimate what loss in accuracy would occur. It must be cautioned, however, that the graphs are based on SO_2 at 10 stations in New York City. It is our subjective

Table 4.3-2. Measures of Accuracy - Daily Concentrations

Sampling Interval	Average No. of Cases in Sample	Proportions of Cases in Sample	Measures of Accuracy for		
			Mean	1/100	1/365
2	183	0.501	0.047	0.088	0.100
3	122	0.334	0.081	0.190	0.228
4	91	0.249	0.094	0.191	0.230
5	73	0.200	0.100	0.181	0.205
6	61	0.167	0.122	0.256	0.305
7	52	0.142	0.090	0.202	0.244
8	46	0.126	0.124	0.234	0.276
9	41	0.112	0.096	0.218	0.262
10	37	0.101	0.149	0.270	0.309
11	33	0.090	0.127	0.202	0.230
12	31	0.085	0.235	0.472	0.576
13	28	0.077	0.245	0.515	0.629
14	26	0.071	0.192	0.407	0.488
15	25	0.068	0.275	0.514	0.616
16	23	0.063	0.162	0.283	0.333
17	22	0.060	0.125	0.250	0.291
18	21	0.058	0.125	0.279	0.328
19	20	0.055	0.233	0.488	0.596
20	19	0.052	0.208	0.371	0.453
21	18	0.049	0.271	0.602	0.748
22	17	0.047	0.228	0.366	0.411
23	16	0.044	0.313	0.704	0.903
24	16	0.044	0.257	0.328	0.363
25	15	0.041	0.227	0.516	0.673
26	14	0.038	0.229	0.379	0.432
27	14	0.038	0.221	0.360	0.405
28	13	0.036	0.225	0.376	0.422
29	13	0.036	0.283	0.585	0.754
30	13	0.036	0.427	0.916	1.173

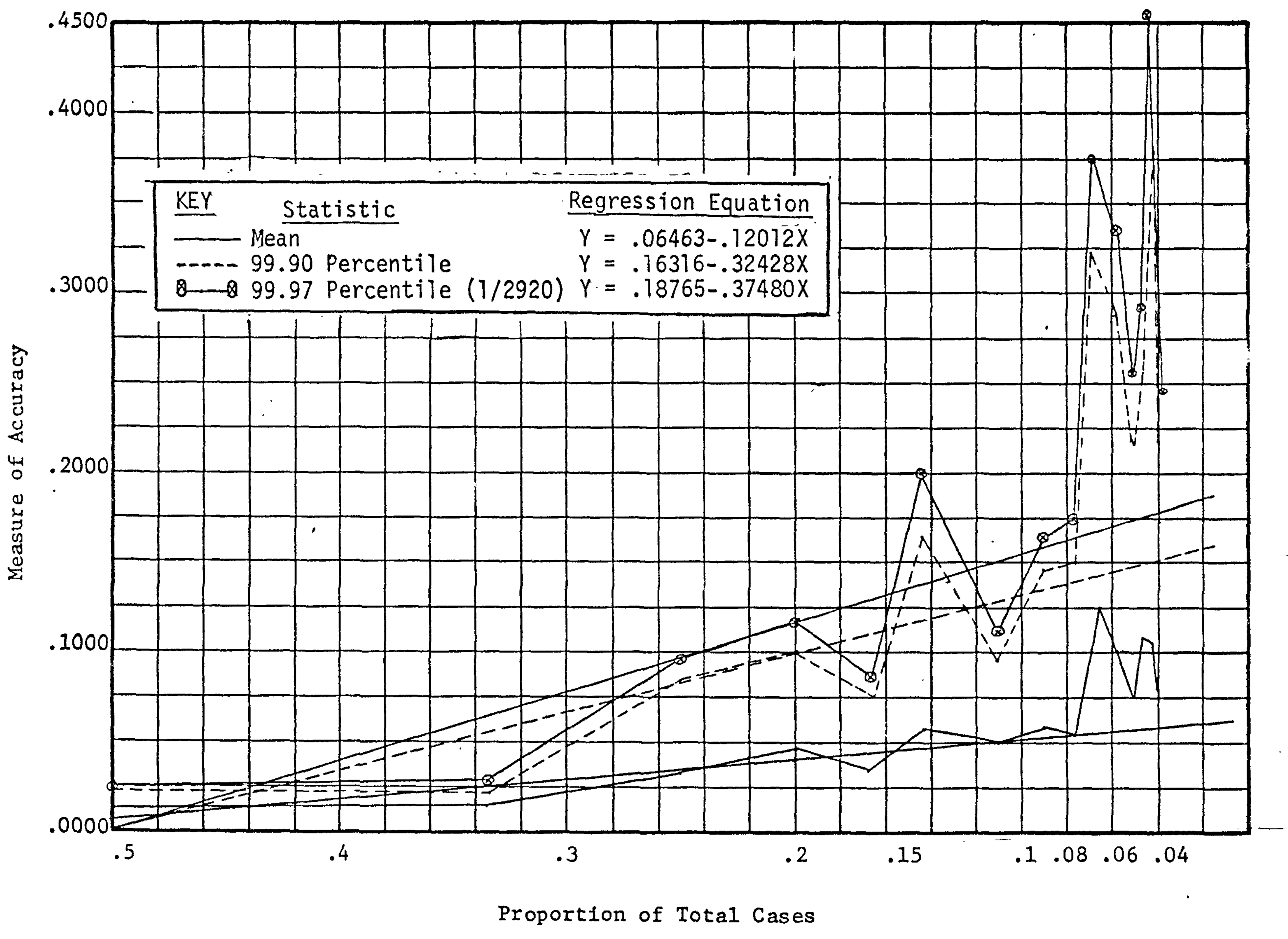

Figure 4.3-1. Accuracy as a Function of Sample Size for Hourly Concentrations

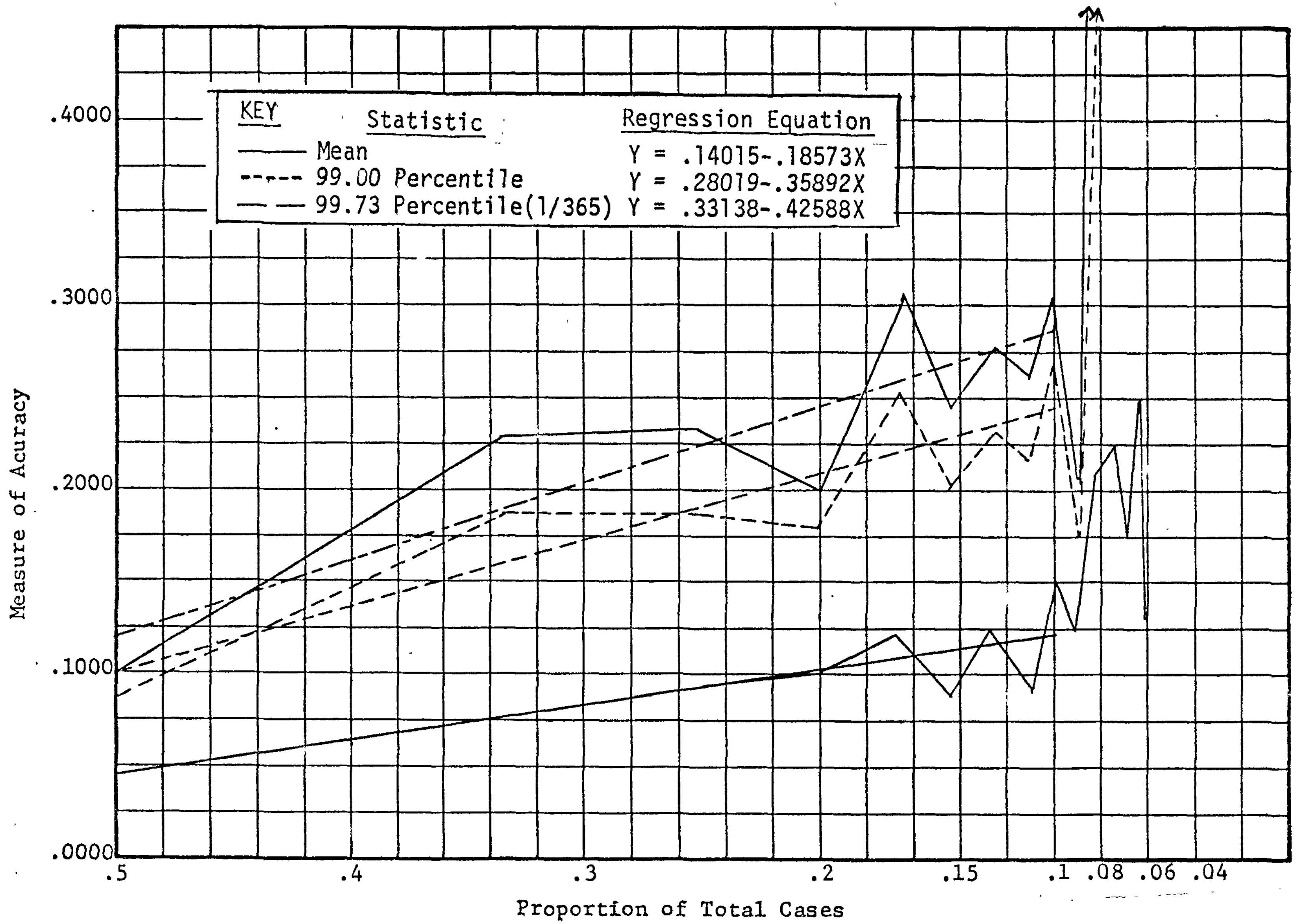

Figure 4.3-2. Accuracy as a Function of Sample Size for 24-Hour Concentrations

judgement that they are applicable to other pollutants and other sites, but this remains to be proven.

Section 5.0

REFERENCES

Section 5.0

REFERENCES

Blade, E. and E.F. Ferrand. 1969. Sulfur Dioxide Air Pollution on New York City: Statistical Analysis of Twelve Years. Journal of the Air Pollution Control Association, Volume 19, Number 11, pp. 873-878.

Davidson, B. 1967. "A Summary of the New York Urban Air Pollution Dynamics Research Program." Journal of Air Pollution Control Association, 17, pp. 154-158.

Haltiner, G.J. and F.L. Martin. 1957. Dynamical and Physical Meteorology. McGraw-Hill, New York.

Hanna, S.R. 1971. A Simple Method of Calculating Dispersion from Urba Area Sources. Journal of the Air Pollution Control Association, Volume 21, Number 12, pp. 774-777.

Larsen, R.I. 1971. A Mathematical Model for Relating Air Quality Measurements to Air Quality Standards. Environmental Protection Agency, Office of Air Programs, Research Triangle Park, N.C. 1971.

Ludwig, F.L., W.B. Johnson, et al. 1970. A Practical Multipurpose Urban Diffusion Model for Carbon Monoxide. Contracts CAPA-3-68 and CPA 22-69-64. Menlo Park, California: Standford Research Institute.

McCaldin, R.O. and R.S. Sholtes. 1970. Mixing Height Determinations by Means of an Instrumented Aircraft. Contract No. CPA 22-69-76. Gainesville, Florida: University of Florida.

McElroy, J.L. 1969. A Comparative Study of Urban and Rural Dispersion. Journal Applied Meteorology 8, pp. 19-31.

Roberts, J.J. et al. 1970. Chicago Air Pollution Systems Analysis Program: A Multiple-Source Urban Atmospheric Dispersion Model, ANL/ES-CC-007, Argonne National Laboratory, Argonne, Illinois.

Saucier, W.J. 1955. Principles of Meteorological Analysis. The University of Chicago Press, Chicago, Illinois.

APPENDICES

Appendix A-1

METHOD OF ESTIMATING THE HEIGHT OF THE MIXING LAYER

Appendix A-2

MIXING HEIGHT INTERPOLATION

Appendix A-1

METHOD OF ESTIMATING THE HEIGHT OF THE MIXING LAYER

Mixing heights may be estimated using either standard or EMSU radiosonde data. The data may be obtained from the NOAA National Weather Records Center in Asheville, North Carolina on magnetic tapes. The method outlined here consists of determining the mixing height by a parcel displacement method. The temperature and mositure content of a representative parcel are defined for ground level. The reported surface temperature may be used, or a more representative temperature from a nearby urban location, or another time may be selected. The moisture content is defined by the maximum mixing ratio in the vertical profile. The temperature change which will occur if the parcel is displaced upward is traced until the parcel temperature is 1°C less than the sounding temperature. The temperature change is assumed to be adiabatic between the ground surface and the mixing condensation level, and pseudo-adiabatic above the mixing condensation level. The following seven steps are used to determine the mixing layer height for each observation time.

1. Read and store the height, pressure, temperature, and relative humidity of each data level.

2. Convert all relative humidities to mixing ratios using the following equations (Saucier 1955):

$$M = 0.01\ U\ S \qquad \text{(A-1)}$$

$$S = \frac{0.62197\ f\ E}{P - f\ E} \approx 0.622\ \frac{E}{P} \qquad \text{(A-2)}$$

$$E = 6.11\,(10)^{\frac{7.5\,T}{T + 237.3}} \tag{A-3}$$

where

M = mixing ratio

U = reported relative humidity (percent)

S = saturation mixing ratio

$f \approx 1$ = correction factor for departure from ideal gas laws

E = saturation vapor pressure of water (mb)

P = reported pressure (mb)

T = reported temperature (°C).

3. Find the maximum mixing ratio for the observation time (M_x).

4. Find the mixing condensation level by the following equations (Saucier 1955):

$$Z_c = \frac{1000}{8.2}\,(T_o - D_o) \tag{A-4}$$

where

Z_c = mixing condensation level (m)

T_o = ground level temperature (°C)

D_o = ground level dewpoint (°C).

In order to account for evaporation of dew during the early morning, it is assumed that the mixed atmosphere will contain moisture equal to that indicated by M_x. D_o is determined from M_x by means of Equations A-2 and A-3 using $S = M_x$ and $T = D_o$:

$$D_o = \frac{237.3\,\log_{10}\left[\dfrac{M_x\,P_o}{6.11\,(0.622)}\right]}{7.5 - \log_{10}\left[\dfrac{M_x\,P_o}{6.11\,(0.622)}\right]} \tag{A-5}$$

where

P_o = ground level pressure.

5. Using the reported data levels to define layers, find the layer (Z_{i-1} to Z_i) containing the top of the mixing layer. The top of the mixing layer is identified by the parcel method. When the reported vertical temperature profile exceeds the temperature of a parcel lifted from the surface by 1°C, this is assumed to be the top of the mixing layer (Z_m). The layer containing the mixing layer height is identified by testing if

$$T_i \geq T_i' + 1 \qquad \text{(A-6)}$$

where

T_i = temperature of ith level (°C)

T_i' = temperature of parcel lifted to ith level (°C).

The parcel temperature is calculated as follows:

$$T_i' = T_{i-1}' + \gamma' (Z_i - Z_{i-1}) \qquad \text{(A-6)}$$

$$\gamma' = \begin{cases} -0.0098, & Z_i \leq Z_c \\ -0.0098 \dfrac{1 + \dfrac{L\, S_{i-1}'}{R_d\,(T_{i-1}' + 273)}}{1 + \dfrac{L^2\, S_{i-1}'}{c_p\, R_v\,(T_{i-1}' + 273)^2}}, & Z_i > Z_c \end{cases} \qquad \text{(A-7)}$$

where

γ' = temperature lapse rate (°C/m, Haltiner and Martin 1957)

L = 2500 = latent heat of vaporization (joules/g)

S_{i-1}' = saturation mixing ratio of parcel lifted to (i-1)th level, estimated from Equations A-2 and A-3 using P_{i-1} and T_{i-1}'

R_d = 0.287 = gas constant for dry air (joule/g/°C)

c_p = 1.003 = specific heat of dry air at constant pressure (joule/g/°C)

R_v = 0.461 = gas constant for water vapor (joule/g/°C).

6. Estimate the height of the mixing layer by linear interpolation as follows:

$$Z_m = Z_{i-1} + \frac{[1 - (T_{i-1} - T_{i-1}')]\,(Z_i - Z_{i-1})}{(T_i - T_i') - (T_{i-1} - T_{i-1}')} - H_s \qquad \text{(A-8)}$$

where

H_s = Station height (m., above sea level)

7. If Z_m is less than 100m, set it equal to 100m. If Z_m is above the 600mb level, set it equal to 5000m.

8. Enter Z_m on the output data file.

Appendix A-2

MIXING HEIGHT INTERPOLATION

The vertical mixing ceiling is defined as that height above ground level at which there is a marked reduction in vertical diffusion. Such barriers are observed as a sharp drop in the concentration observed in a vertical sounding (e.g., Davidson, 1967). It may be observed as a delineation between the smoke-filled layer and cleaner air aloft over many cities in the early morning. Much higher ceilings typical of afternoon hours are clearly visible to air travelers climbing to or descending from cruising altitudes. The ceiling may vary from 100 meters at night to over 1500 meters during the day. Hourly estimates of the ceiling are required for use in the model.

Unfortunately, this mixing ceiling is not always visibly discernible and no routine systems for taking vertical soundings of pollutant materials are in operation. Therefore, the ceiling is generally inferred from temperature soundings which are routinely observed twice daily at certain airports by the National Oceanic and Atmospheric Administration (NOAA). These observing locations are separated by about 200 km on the average and are usually located outside the urban area. The mixing layer is generally characterized by a near adiabatic lapse rate extending from the ground to some latitude at which a deep, (several kilometers) more stable lapse rate exists. However, the vertical temperature structure of the atmosphere is frequently not this well defined. As a result, considerable judgement may be required to define where, in a vertical temperature profile, an effective mixing ceiling exists.

Unfortunately very little data have been collected on the relationship between vertical pollution and temperature profiles which could be used to develop and substantiate rules for defining the mixing ceiling over an urban region.

The procedure which is generally used to define the mixing ceiling is the following: Determine the general rural vertical temperature profile from the nearest appropriate (same air mass) radiosonde, or by interpolation of two or more nearby radiosondes. Estimate minimum morning and maximum afternoon air temperatures which are representative of the urban area. The afternoon temperature may be obtained directly from airport observations or other available data. In most cases the morning urban temperature will exceed the rural temperature. The following equation (Ludwig, et al., 1970) may be used to estimate morning urban temperatures (T_u) from rural temperatures (T_r) using the urban population Φ and the radiosonde temperature lapse rate (dT/dp) as parameters:

$$T_u = T_r + \Phi^{0.25}(0.0633 - 0.298 \frac{dT}{dp}) \quad \text{(A-8)}$$

Construct adiabatic temperature profiles from the urban temperatures which intersect the rural temperature profile. The height of these intersections are assumed to be the minimum and maximum mixing ceilings.

A method of interpolating between these values to give hourly estimates is to:

1. Use the morning minimum from midnight to 6 a.m.

2. Linearly interpolate between the minimum and the maximum between 6 a.m. and 2 p.m.

3. Use the afternoon maximum between 2 p.m. and midnight.

This pattern of diurnal variations is illustrated in Figure A.2-1.

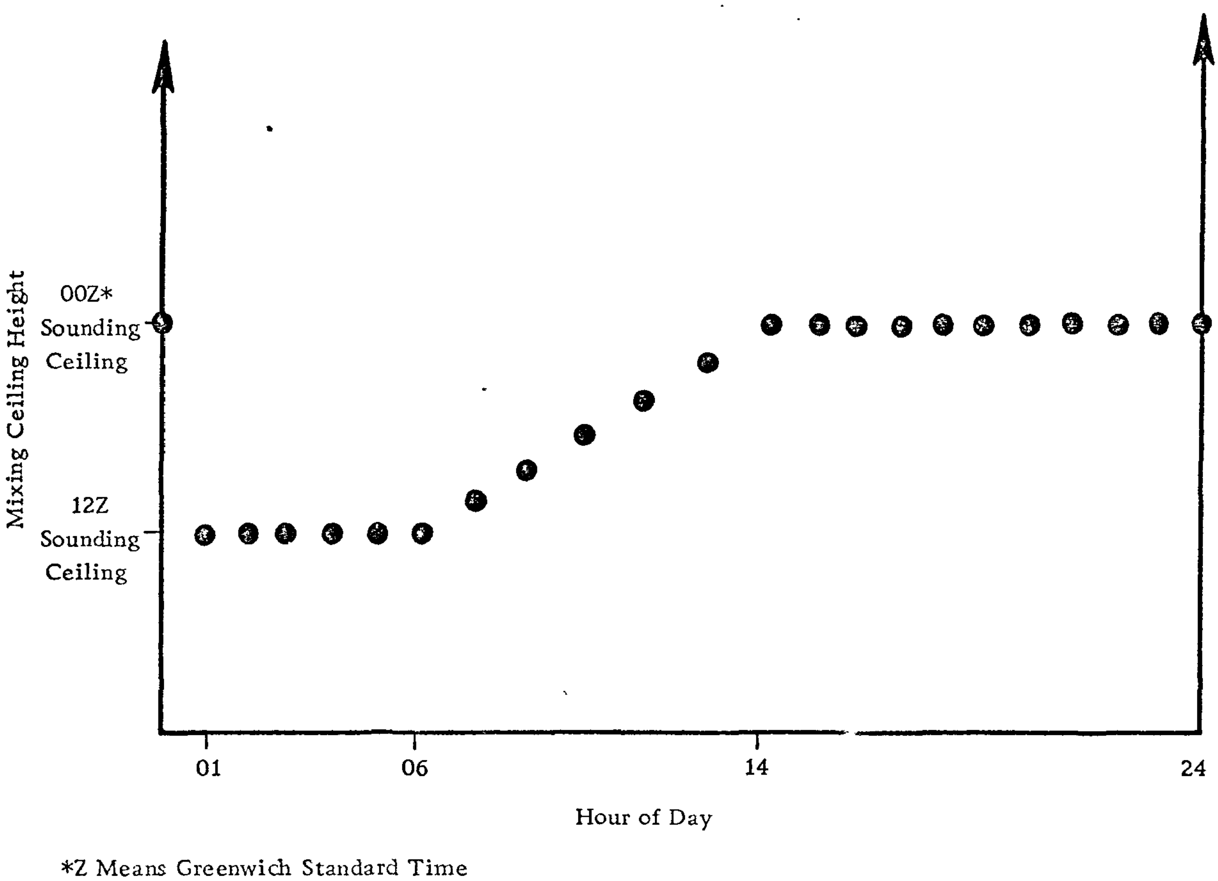

Figure A.2-1. Graphical Model of Procedure Used to Interpolate in Time Between Mixing Ceiling Estimates Obtained for Standard Radiosonde Observing Times

Limited simultaneous observations of temperature and SO_2 or particle concentration profiles reported by Davidson (1967), Roberts, et. al (1970) and McCaldin and Sholtes (1970) attest to the general validity of this approach.

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(Please read Instructions on the reverse before completing)

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		6. PERFORMING ORGANIZATION CODE
7. AUTHOR(S) Robert C. Koch, Scott D. Thayer		8. PERFORMING ORGANIZATION REPORT NO. GEOMET Report No. EF-467
9. PERFORMING ORGANIZATION NAME AND ADDRESS GEOMET, Incorporated, 15 Firstfield Road, Gaithersburg, Maryland 20760		10. PROGRAM ELEMENT NO. 1AA009
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16. ABSTRACT

This report summarizes work done to compare a computer model for estimating air pollution concentrations from multiple sources with measured SO_2 and particulate concentrations and with other model calculations. The model is capable of estimating short-term and long-term concentrations, and produces results which are equivalent in validity to results produced with other models. Since the model represents hourly variations in both emissions and meteorological conditions, this report considers available sources of data and how these can best be used to estimate parameters for the model. Use of temperature and industrial and commercial activity indexes to estimate seasonal and diurnal variations in emissions is discussed. Use of slow-rise balloon soundings taken in urban areas is discussed as a possible supplement to conventional weather data. Finally, the applicability of using sampled calculations when estimating short-term maximum concentrations is evaluated.

17. KEY WORDS AND DOCUMENT ANALYSIS

a. DESCRIPTORS	b. IDENTIFIERS/OPEN ENDED TERMS	c. COSATI Field/Group
Air Pollution	Air Quality Model	1302
Urban Areas		0401
Atmospheric Diffusion		
Diurnal Variation		
Emission		
Sequential Sampling		

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