DP-1597

Proceedings of the
FIRST SRL MODEL VALIDATION WORKSHOP
(November 19-21, 1980
at Hilton Head, South Carolina)

E. I. du Pont de Nemours & Co.
Savannah River Laboratory
Aiken, SC 29808

PREPARED FOR THE U. S. DEPARTMENT OF ENERGY UNDER CONTRACT DE-AC09-76SR00001

Printed in the United States of America

Available from

National Technical Information Service
U. S. Department of Commerce
5285 Port Royal Road
Springfield, Virginia 22161

Price: Printed Copy A07; Microfiche A01

726933

DP-1597
Distribution Category UC-11

Proceedings of the FIRST SRL MODEL VALIDATION WORKSHOP (November 19-21, 1980 at Hilton Head, South Carolina)

MELVIN R. BUCKNER, COMPILER

Sponsored by the Office of Health and Environmental Research
of the U.S. Department of Energy

Approved by

T. V. Crawford, Research Manager
Environmental Sciences Division

Publication Date: October 1981

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ABSTRACT

The "Clean Air Act" and its amendments have added importance to knowing the accuracy of mathematical models used to assess transport and diffusion of environmental pollutants. These models are the link between air quality standards and emissions. To test the accuracy of a number of these models, a Model Validation Workshop, sponsored by the Department of Energy and hosted by the Savannah River Laboratory, was held November 19-21, 1980. The meteorological, source-term, and Kr-85 concentration data bases for emissions from the separations areas of the Savannah River Plant during 1975-1977 were used to compare calculations from various atmospheric dispersion models. Participants included representatives from nine DOE-funded laboratories. Observers from several government agencies and private organizations were also present.

The results of statistical evaluation of the models show a degradation in the ability to predict pollutant concentrations as the time span over which the calculations are made is reduced. Forecasts for annual time periods were reasonably accurate. Weighted-average squared correlation coefficients (R^2) were 0.74 for annual, 0.28 for monthly, 0.21 for weekly, and 0.18 for twice-daily predictions. Model performance varied within each of these four categories; however, the results indicate that the more complex, three-dimensional models provide only marginal increases in accuracy. The increased costs of running these codes is not warranted for long-term releases or for conditions of relatively simple terrain and meteorology.

The overriding factor in the calculational accuracy is the accurate description of the wind field. Further improvements of the numerical accuracy of the complex models is not nearly as important as accurate calculations of the meteorological transport conditions.

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ACKNOWLEDGMENT

This meeting was sponsored by the U.S. Department of Energy (DOE), Office of Health and Environmental Research (OHER). In particular, Mr. D. S. Ballentine, DOE-OHER, was instrumental in securing sponsorship for the meeting and in coordinating activities with other laboratories. The meeting was hosted by the Savannah River Laboratory (SRL). Individual responsibilities and duties for coordinating the various technical aspects of the meeting were as follows:

T. V. Crawford,
Workshop Organizer,
Observers' Model Validation Programs
D. W. Pepper,
Workshop Coordinator, 3-D Models
C. E. Bailey,
Workshop Data Base,
Wind Field Graphics, Gaussian Statistical Models
A. H. Weber,
Statistical Analysis
A. J. Garrett,
Wind-Rose Models, Wind Analysis
M. M. Pendergast,
Gaussian Trajectory/2-D Models, Wind Analysis
R. E. Cooper,
3-D Models

In addition, D. D. Hoel provided technical assistance in the planning and operation of the workshop. J. L. Mitchell of SRL was responsible for much of the physical planning for the meeting and also for the social activities during the workshop. J. H. Weber of the Savannah River Plant (SRP) provided technical assistance in the statistical analysis of data and the interpretation of results, and participated in many technical discussions during the workshop.

The workshop committee wishes to express its appreciation to the participants and observers who attended the workshop. The quality of discussion during the meeting was excellent. The exchange of information and ideas during the workshop is expected to help focus research and development in the area of atmospheric transport modeling and mesoscale wind analysis for the next several years.

PROCEEDINGS OF THE FIRST SRL MODEL VALIDATION WORKSHOP

I. INTRODUCTION

In the last 25 years, numerous atmospheric transport and diffusion models have been developed to address the country's problems on air pollution and other related questions. The development of many of these models was funded by the Department of Energy and its predecessors. With time, the use of models for preparing environmental assessments has become widespread; it has become required by some legislation. Because environmental quality criteria have been set, the accuracy of the models becomes very important when used to establish particular emission requirements. In September 1977, the Department of Energy sponsored a workshop[1] on the evaluation of models used for the environmental assessment of radionuclide releases. Atmospheric models were a part of that assessment. The American Meteorological Society (AMS) subsequently published a statement on the accuracy of models.[2] In both cases a strong requirement was stated for testing models against real data. At the 72nd Annual Meeting of the Air Pollution Control Association, an in-depth critical review of present state-of-the-art methods of atmospheric dispersion modeling was given.[3] Considerable emphasis was placed upon model validation and testing against a well-suited data base by nearly all of the attendees.

Recent trends in model development are shifting from the classical models used by regulatory authorities to more sophisticated models for use in complex terrain. These complex models should be tested against measurements made in relatively level terrain and their limitations understood before beginning studies involving complex terrain. Success in modeling dispersion under complex conditions is possible only when a more thorough understanding of the processes under less complex conditions is obtained.

A unique data base which is well-suited for testing mesoscale models in relatively level terrain was obtained during the Savannah River Experiment (SRE) at the Savannah River Plant from 1975-1977.[4] An inert radioactive gas, Kr-85, which is routinely emitted from the chemical separations facilities at SRP, was measured at 13 sites located between 25 and 150 km from the SRP release site over a 2-1/2-year period. In addition, meteorological data were also obtained from the SRP tower network, plus surrounding tower data from six power plant sites and National

Weather Service stations in Georgia and South Carolina. The emission source was well-defined, semi-continuous, and adequate for valid measurements out to the distances of interest. The terrain was moderately flat. In all, the field study was as nearly ideal as possible for verifying a model under simple, but realistic, conditions.

To evaluate existing and newly developed models used at DOE-funded laboratories, the Savannah River Laboratory (SRL) hosted, with sponsorship from the Office of Health and Environmental Research of DOE, a model validation workshop which used the Kr-85 measurements as a basis for comparison of various transport models. Nine DOE laboratories participated in the year-long effort which culminated in a workshop meeting on November 19-21, 1980 at Hilton Head, SC. (See Appendix A for the workshop agenda and a list of participants and observers.) The following laboratories participated:

Air Resources Laboratory (ARL)
Argonne National Laboratory (ANL)
Atmospheric Turbulence & Diffusion Laboratory (ATDL)
Battelle-Pacific Northwest Laboratory (PNL)
Brookhaven National Laboratory (BNL)
Lawrence Livermore National Laboratory (LLNL)
Los Alamos National Laboratory (LANL)
Oak Ridge National Laboratory (ORNL)
Savannah River Laboratory (SRL).

Representatives from the following government and private organizations concerned with model validation also attended the workshop:

Air Pollution Control Association (APCA)
American Meteorological Society (AMS)
  Committee on Turbulence & Diffusion
Atomic Industrial Forum (AIF)
Electrical Power Research Institute (EPRI)
Environmental Protection Agency (EPA)
Nuclear Regulatory Commission (NRC)
U. S. Air Force
Weather Service Nuclear Support Office.

A brief description of current efforts in model validation by several of these organizations is presented in Appendix B.

This report describes the data base, the models tested, statistical analysis of results, and presents general conclusions and recommendations drawn from analysis of the model comparisons.

II. DESCRIPTION OF DATA BASE (C. E. Bailey)

From 1975-1977, the Air Resources Laboratory (ARL) of the National Oceanic and Atmospheric Administration (NOAA), the Argonne National Laboratory (ANL), and SRL measured weekly and twice-daily Kr-85 surface air concentrations within 150 km of SRP. The objectives of this program were:[4]

1) "Provide weekly average air concentrations for model verification at distances from about 25 km to 150 km from a quasi-continuous point source."

2) "Provide verification of estimates of long-term air concentrations and dose-to-man from routine Savannah River Plant (SRP) emissions."

3) "Conduct several periods of intensive short-term sampling (twice-daily) to provide more detailed data for model development and verification."

4) "Test the adequacy of standard stability-wind rose techniques for estimating monthly, seasonal, and annual air concentrations out to 150 km from a continuous source."

The Kr-85 air concentration measurements were obtained using 13 cryogenic air samplers previously used by ARL in a 1974 dispersion experiment.[5] The location of the 13 samplers is shown in Figure II-1. The experimental details of the sample collection program are given in Reference 4.

Data collected in this program during the two-year period from August 1, 1975 to July 31, 1977 were used for the workshop studies. These data consisted of three major categories: meteorological data, measured Kr-85 average surface air concentrations for time periods of 10 hours and 1 week, and hourly releases of Kr-85 from the Savannah River Plant.

The data used in the workshop studies are available on magnetic tape from the National Climatic Center in Asheville, North Carolina. A complete description of the data, the format of the data on the tapes, and instructions for ordering the tapes are given in References 4 and 5. Thus, only a summary of the data is presented below.

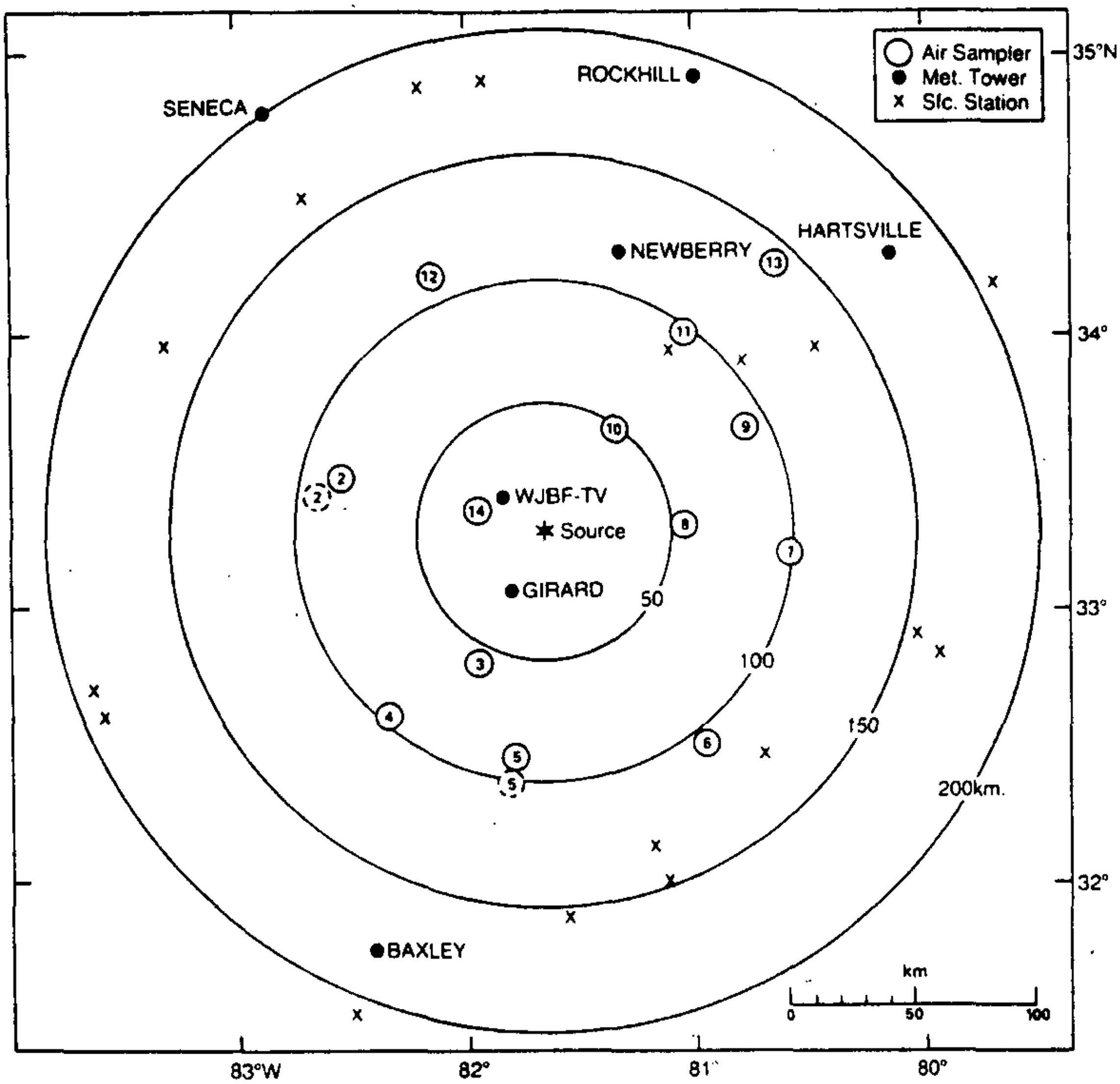

FIGURE II-1. Krypton-85 Cryogenic Air Sampling Stations, Meteorological Towers and Surface Weather Stations Within 200 km of the SRP Source. Dashed circles indicate earlier sampling location.

Meteorological Data

The meteorology data consist of five types:

- National Weather Service surface weather observations
- National Weather Service rawinsonde observations
- Meteorological tower observations
- Wind-rose statistics
- Mixed depths from acoustic sounder observations.

Hourly data from approximately 60 surface weather stations lying between 86°W and 77°W, 37°N and 30°N are included. The direction and speed, along with other information, are reported hourly for each surface station.

Twice-daily observations of wind speed and direction and temperature at various heights as reported by four NWS rawinsonde stations are included for the 24-month period. The rawinsonde station locations are Waycross and Athens, Georgia; Greensboro, North Carolina; and Charleston, South Carolina.

Data are included from three types of towers. Local utility companies (Carolina Power and Light Company, Duke Power Company, Georgia Power Company, and South Carolina Electric and Gas Company) provided meteorological data from seven power plant sites in the vicinity of SRP (locations of six of these towers are shown in Figure II-1). These measurements usually included wind speed, direction and directional range at one to three levels, along with other information. The second type of tower data was obtained from turbulence quality wind sensors and temperature sensors at heights of 10, 91, and 243 meters on the WJBF-TV tower, located 21 km from the Kr-85 emission point. Data obtained at 5-sec intervals were averaged to obtain hourly mean values and standard deviations of the wind speed and direction for use in calculations. The third kind of tower data is an hourly space-averaged wind speed and direction, along with standard deviations obtained from 7 towers on the SRP site. The data were recorded at 62 meters (the same as the stack heights in the separations areas).

Monthly wind-rose statistics were derived from the hourly arithmetic average 62-m wind obtained from the seven 62-m towers on the SRP site. The statistics provide the joint frequency distribution for direction (16 sectors), speed (6 classes), and stability (7 categories).

Hourly estimates of mixing depths, obtained from subjective analysis of data from an acoustic sounder at SRP, are provided, along with a characterization of the acoustic record into one of 17 categories.

Measured Kr-85 Surface Air Concentrations

The cryogenic air samplers used in the Kr-85 measurement programs are described in detail in Reference 4. Each sampler used approximately 20 liters of liquid nitrogen per day to liquefy a constant flow of incoming air. After liquefaction, the more volatile components were allowed to boil off, which concentrated krypton from approximately 1 ppm to about one part per hundred. Cylinders of the concentrate were shipped to Argonne National Laboratory for analysis.

During the 24 months from August 1975 through July 1977, weekly samples were collected for 20 months; twice-daily (10-hour) samples were collected for 4 months (November 1976 and February, April, and July 1977). The distance of the samplers from the source ranged from 28 to 144 km (see Figure II-1).

The background level of Kr-85 in air was approximately 15 pCi/SCM (piçocuries per standard cubic meter of air), and was due almost entirely to atomic energy activities over the last 40 years. A few of the air samples collected exceeded 1000 pCi/SCM of Kr-85; however, most ranged from background level up to a few hundred pCi/SCM. About 1100 samples were collected during the 20 months when weekly samples were collected; about 1800 twice-daily samples were collected.

As noted in the report presenting the krypton air sampling data,[4] the actual collection rate of the cryogenic samplers was often lower than the programmed rate, and the volumes collected sometimes varied in an erratic manner from one sampling period to the next. This behavior could have a significant effect on values determined from individual measurements, but should have a relatively small effect on seasonal and annual averages derived from the individual measurements.

As described in detail in Reference 4, in an effort to determine the validity of the sampler measurements, two cryogenic air samplers were operated side by side 10 km from the source from October 10, 1977 through January 20, 1978. Twice-daily samples were collected for the first two weeks and the last two weeks of the sampling period. Weekly samples were collected for a period of eleven weeks. The samplers were not routinely maintained in a deliberate attempt to induce erratic behavior.

The results of the intercomparisons were encouraging. Erratic collection volumes were noted on occasion, but no serious discrepancies were detected in the measured concentrations in eight such cases. The following conclusions are taken from Reference 4.

1. Measured concentrations above background definitely indicate that a plume was present at some time during the sampling period.

2. It is possible that a small number of measured values may greatly overestimate or underestimate the true average concentration during the sampling period, due to fluctuations in the collection rate. However, the measured concentration must have existed in the ambient air at some time during the sampling period.

3. The great majority of measured concentrations are within ±10% of the true average ambient air concentration during the sampling period.

4. Long-term mean concentrations (e.g., seasonal or annual) obtained from these data are believed to provide reliable estimates of the true long-term averages.

Kr-85 Source Term

Kr-85 is released from each of the separations areas in a semicontinuous, periodic manner. The releases from the two separations areas were assumed to occur at a point midway between the separations areas which are separated by approximately 4 km. Because the sampler locations ranged from 28 to 144 km from the separations areas, little error is introduced by this assumption.

The rate of release of Kr-85 from the separations plant stacks was not measured directly. The release rate of Kr-85 was calculated using a mathematical model based on studies of the the separations areas. The mathematical model was based on studies of the reaction kinetics of the dissolving process and actual stack measurements during typical dissolutions.[6] Data for each dissolving cycle, obtained from operator's log books, provided the input for the release rate calculations.

Figure II-2 shows the Kr-85 release rate for February and March of 1976, typical of the 24-month period. The average monthly release of Kr-85 was approximately 55,000 Ci during the 24-month period for which data were provided. During this time, Kr-85 was being released 55% of the time. The average rate of release over the 24 months was approximately 75 Ci/hr; the average release rate for the 55% of the time that Kr-85 is actually being released was approximately 135 Ci/hr. The quantity of Kr-85 released during each hour of the 24-month period was calculated to provide the source term for the calculations.

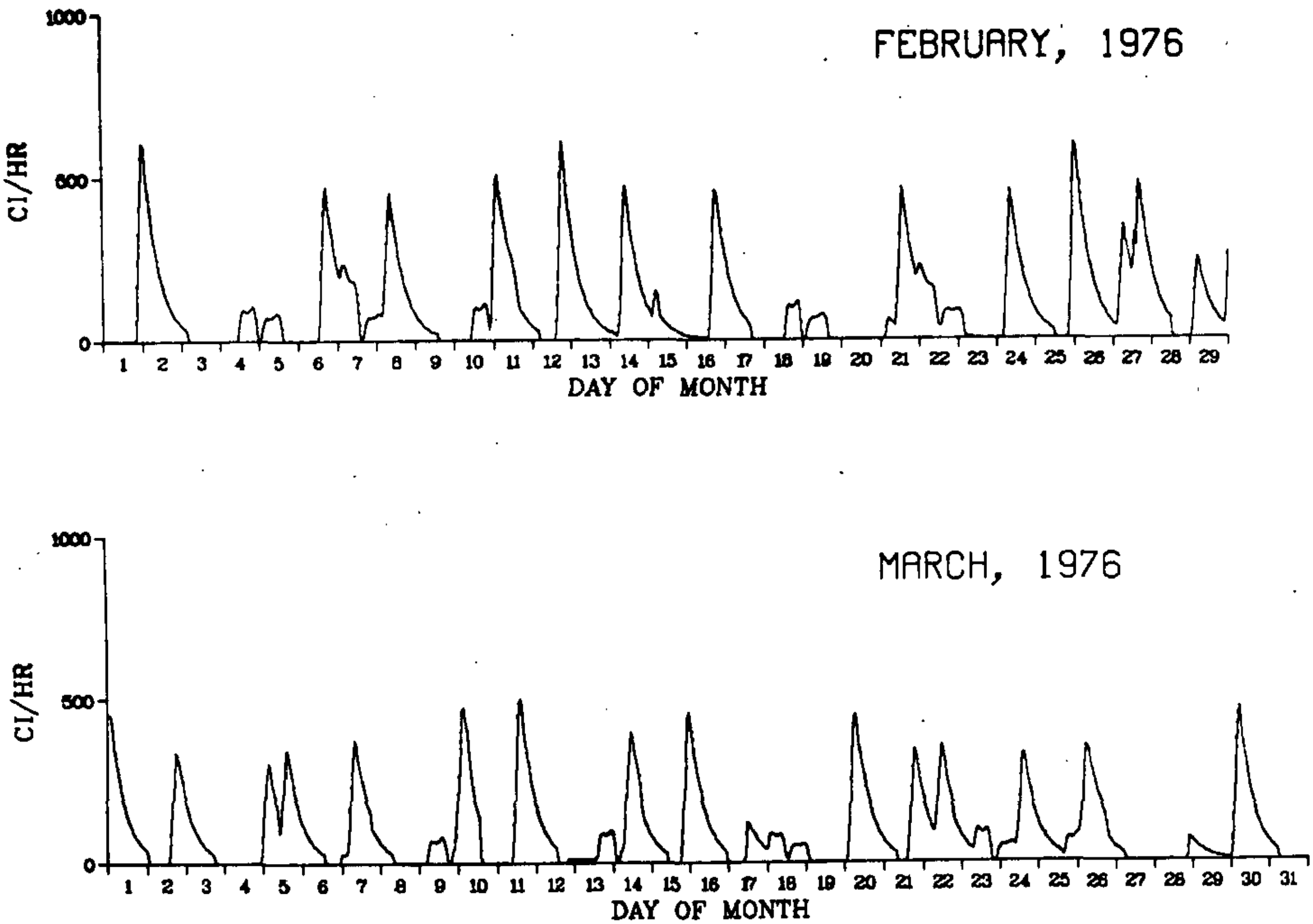

FIGURE II-2. Krypton-85 Release Rate for February and March, 1976

III. STATISTICAL ANALYSIS (A. H. Weber)

A number of statistical parameters[7] were used to evaluate how well the predictive model fit the measured data. As recommended by the recent American Meteorological Society (AMS) Workshop,[8] two general measures of performance were used: (1) measures of difference and (2) measures of correlation. The measures of difference include the bias, the noise, and the gross variability or root mean squared error (RMSE).

The measures of correlation were paired in space and time. The AMS workshop also suggested computing correlations lagged in time and separated in space. A few lagged and spatially separated correlations were computed, but these added statistics did not significantly increase the ability to assess model performance and are not included in these proceedings.

In the analysis, M refers to measured concentration and P refers to predicted concentration

$$\text{Mean } \bar{P} = \frac{1}{N} \sum_{i=1}^{N} P_i \; ; \quad \bar{M} = \frac{1}{N} \sum_{i=1}^{N} M_i ,$$

where N is the total number of measurements.* Both M and P refer to concentration above background so a background of 14 pCi/m^3 was subtracted out.

Measures of Difference

Difference	$D_i = M_i - P_i$
Bias	$\bar{D} = \bar{M} - \bar{P}$
Variance (Noise)	$S_d^2 = \frac{1}{N-1} \sum (D_i - \bar{D})^2$
RMSE	$\text{RMSE} = \left[\frac{(N-1)}{N} S_d^2 + \bar{D}^2\right]^{1/2}$

---

* The limits on the summation $\sum_{i=1}^{N}$ will be dropped from this point on for convenience.

Measures of Correlation

Pearson's R:

$$R = \frac{\Sigma(M_i - \bar{M})(P_i - \bar{P})}{[\Sigma(M_i - \bar{M})^2 \Sigma(P_i - \bar{P})^2]^{1/2}}$$

This parameter is used for quantifying the relationship between M and P.

Spearman's ρ:

If the measured and predicted concentrations are ranked, Spearman's ρ is simply the Pearson correlation between the ranks of measured and predicted concentration. The value of ρ is between -1 and 1. Points near the origin (PNOs)* can have significant effects on Spearman's ρ because the ranking is significantly influenced depending on whether PNOs are included or deleted in the analysis. The advantage of Spearman's ρ in the present application is that it is not sensitive to one or two outliers.**

Kendall's τ:

Kendall's τ is a measure of correlation which uses the ranks of the measured and predicted values rather than the values themselves. To compute Kendall's τ, put the measured values in order of their ranks and in an adjoining column put the rank of the corresponding predicted value. Take each rank of the predicted value in turn and count how many of the ranks above it are larger and add these counts. If the counts total is Q, then Kendall's τ is

$$\tau = 1 - 4Q/N(N-1).$$

Like the previous two correlation coefficients, τ lies between -1 and 1. The same comments about outliers and PNOs will apply as before for Spearman's ρ.

---

* PNOs is a term for points which have both measured and predicted values very close to zero. There seems to be no accepted term in statistics which is used to describe these points so an acronym is used.

** Outliers refer to points on a graph of measured vs. predicted concentration which are separated from the bulk of the data by large distances.

Distribution Statistics of the Differences

Skewness: The third moment about the mean of the distribution of the bias or the skewness (Sk) is defined as

$$Sk = \frac{\sum (D_i - \overline{D})^3 / N}{\sigma^3}$$

, where σ is the standard deviation of the distribution. The skewness is the third moment about the mean of the distribution of the bias divided by the standard deviation cubed. If low values of D are bunched close to the mean, but high values are far above the mean, the skewness will be positive. If the sample comes from a normal population, the skewness is zero and its standard deviation is $\sqrt{6/N}$.

Kurtosis: Kurtosis is a measure of the curvature of the distribution. Gaussian distributions have a fourth moment equal to three. If the ratio exceeds three, there is an excess of values near the mean and a depletion of values in the flanks of the distribution. A value less than three means an excess of values in the flanks of the distribution. The kurtosis (κ) is defined as

$$\kappa = \frac{\sum (D_i - \overline{D})^4 / N}{\sigma^4} - 3$$

The value three is subtracted from the fourth moment in these definitions so that normal distribution will have kurtosis equal to zero.

Tests for Normality

A goal in the statistical evaluation of the models was to have the predicted concentration equal to the measured concentrations plus a random error. If the distribution of the predicted concentration was the same as the distribution of the measured values, then a reasonable assumption would be that the differences were normally distributed with mean zero and a constant variance. The Shapiro-Wilk or the Kolmogorov-D statistics were used to determine that none of the differences were normally distributed. The fact that the differences were not normally distributed does not invalidate the statistics themselves. Statistical statements about the values of the parameters being significant at some probability level are affected by a non-normal distribution. However, for the tables in this report, probability statements are only used in a small number of cases, and the statements are not expected to be strongly affected by the fact that the distributions are not normal.

Scatter Diagrams

Scatter diagrams were plotted of measured versus the predicted values. These diagrams are drawn on a uniform set of axes for each problem category; annual, monthly, weekly, and twice-daily. The scatter diagrams are shown in Appendix C.

To evaluate the accuracy of the models, it was desired to make an arithmetical statement of the form

$$P = M \pm KM \tag{1}$$

where K is some fraction or integer value such that the two bands contain 95% of the predicted values. K x 100 represents the percentage of the measured value by which P overestimates or underestimates the measured concentration. Since the difference D is defined as

$$D = M-P \tag{2}$$

then Equation 1 can be expressed as

$$M-D = M \pm KM \tag{3}$$

or $$D = \pm KM \tag{4}$$

Thus, on a plot of D versus M, two straight lines of slope ± K would define the region (see Figure III-1) where values satisfying Equation 4 would be contained. The bands, K, were allowed to take on values 0.5, 0.75, 1.0, 2.0, 3.0, 5.0 and 10.0.

Some modelers felt that by imposing Equation 4, too high a penalty was given for "near misses," i.e., when M was zero and P was any value, the point was outside the bands. This was solved by arbitrarily adding a value to Equation 4:

$$|D| < KM + C_0 \tag{5}$$

where C_0 = 15 pCi/m^3 for twice-daily and C_0 = 5 pCi/m^3 for weekly model categories. The lower value for weekly models was chosen because the scatter of points near the origin was less than for twice-daily models. The region defined by Equation 5 is shown in Figure III-2.

Linear regression lines were derived and the slope (β), intercept, and R^2 value determined. This was done to allow modelers to either improve their models or to help determine the physical and mathematical reasons for the slope of the regression line being different from the desired one.

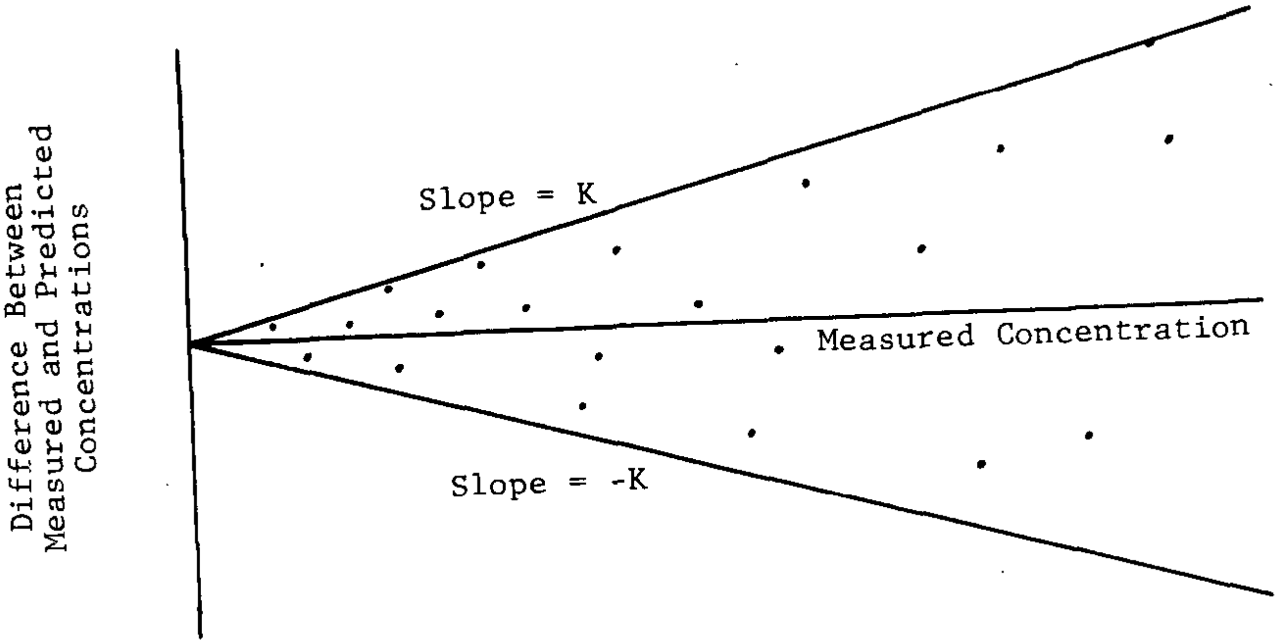

FIGURE III-1. Bandwidth for Model Predictions

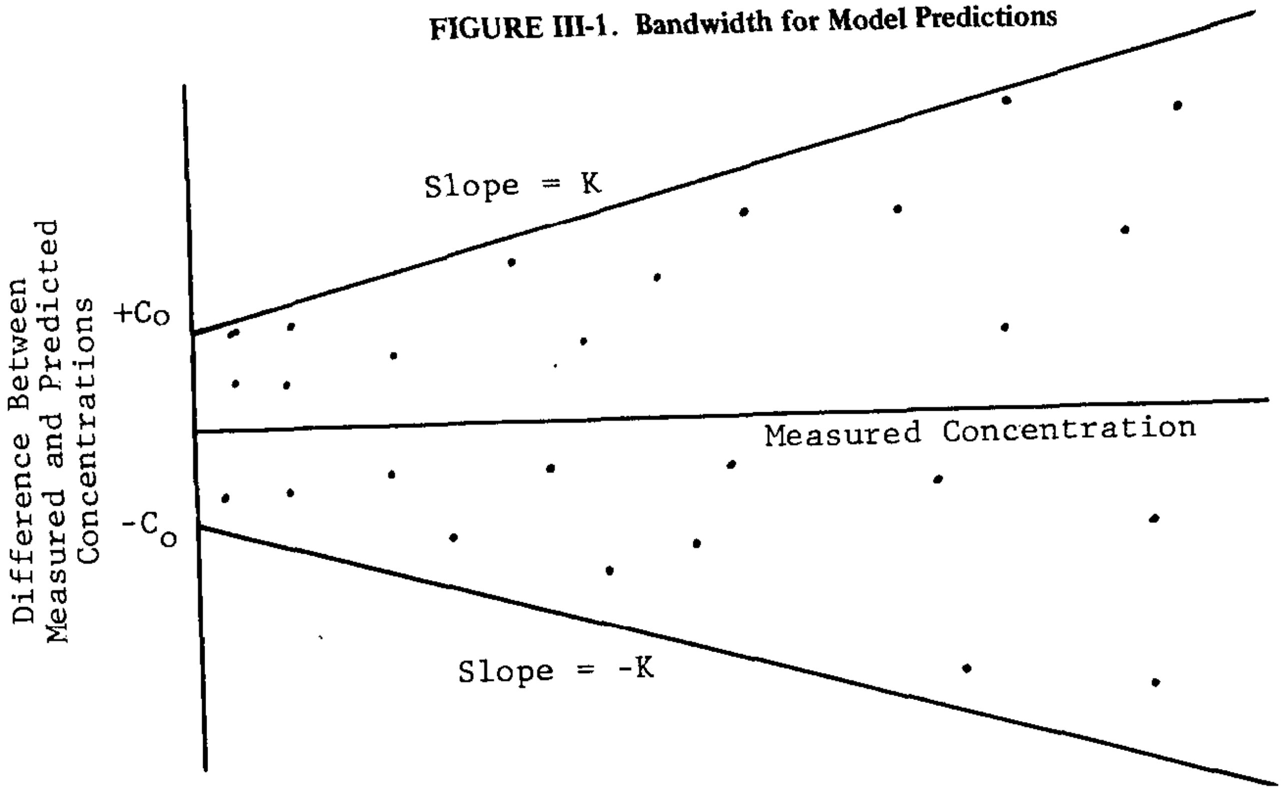

FIGURE III-2. Modified Bandwidth for Model Predictions

In regression analysis the dependent variable can be partitioned into three parts as illustrated in Figure III-3.

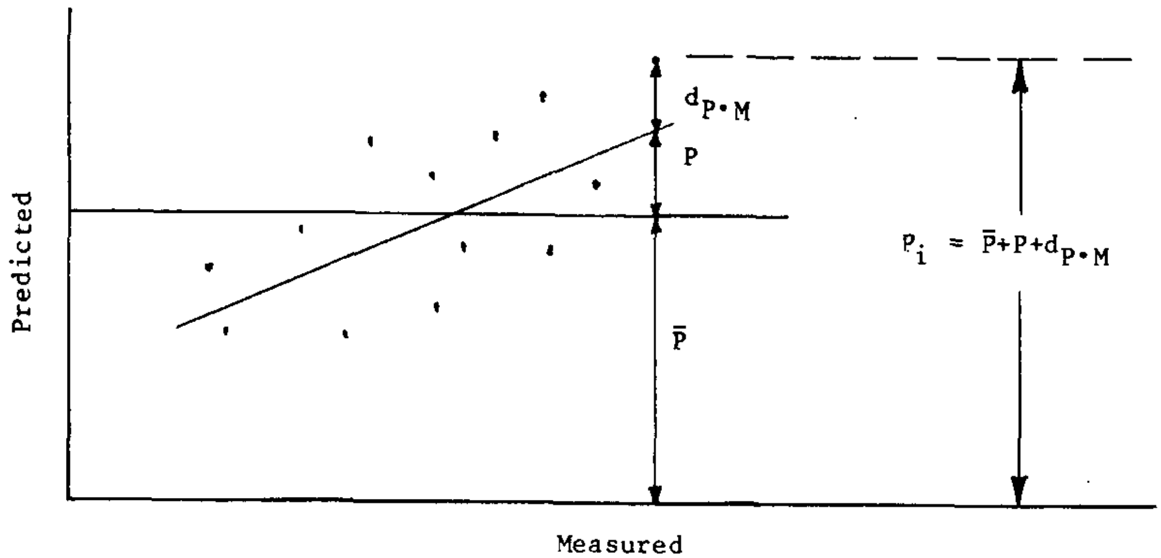

FIGURE III-3. Representative Predicted vs. Measured Concentrations

The dependent variable P_i can be written

$$P_i = \bar{P} + P + d_{p\cdot M}$$

where $\bar{P}$ is the mean of the predicted value, P is the difference between $\bar{P}$ and the regression line, and $d_{P\cdot M}$ is the difference between P_i and P. The sum of the squared values of the dependent variable P_i from its mean value $\bar{P}$ is called the corrected total sum of squares. This quantity can be broken down into two parts called the sum of squares due to error and the sum of squares due to regression. The following relationship holds:

Corrected total sum of squares =

Sum of squares due to regression (SSR) +

Sum of squares due to error (SSE)

An important measure of how well the regression line fits the data is the R^2 value. R^2 is the ratio of the sum of squares caused by regression to the corrected total sum of squares.

IV. MODEL DESCRIPTIONS

Statistical Models (A. J. Garrett and C. E. Bailey)

General Description

Statistical air pollution models were defined for the purposes of this workshop to be those models which use sector-averaged meteorological data as input to their calculations. Because all models use data that are averaged to some extent, this criterion is not exact. However, the statistical models considered here primarily predict monthly, seasonal, and annual concentrations.

Despite their simplicity, the statistical models varied considerably in structure. In addition to differences in averaging periods for winds and emission rates, there were variations in the methods of treatment of mixing depths, lateral and vertical diffusion, and special situations, such as calms. For example, the model AIRDOS-EPA, which was tested by ORNL personnel, averages the emission rate over the entire period of calculation, whereas the SRL SHEAR-ROSE model and the ARL DRAX1 use hourly emissions data. The SRL and ARL models differ in their treatment of some meteorological parameters, such as mixing depth. The ARL model includes diurnal variations, whereas the SRL model uses a constant value.

Model Descriptions

Statistical models utilized by the Workshop participants are briefly described in this section.*

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* These forms were completed by the participants prior to, or at the meeting.

MODEL DESCRIPTION FORM

Laboratory: Oak Ridge National Laboratory

Division/Group: Technology Assessments Section, Health and Safety Research Division

Model Type: Gaussian Plume **Model Name:** AIRDOS-EPA

Short Description: The AIRDOS-EPA computer code is a methodology that estimates radionuclide concentrations in air; rates of deposition on ground surfaces; ground surface concentrations; intake rates via inhalation of air and ingestion of meat, milk, and fresh vegetables; and radiation doses to man from airborne releases of radionuclides. The code may be run to estimate highest annual individual dose in the area or annual population dose.

Basic Equation Solved: A modified Gaussian plume equation is used to estimate both horizontal and vertical dispersion of as many as 36 radionuclides released from one to six stacks or area sources. Diffusion coefficients used are those recommended by Briggs. Average mixing height for time period considered is input to the code.

Input Requirements:

a) **Wind fields:** Joint frequency distribution of wind direction and stability with average wind speed
b) **Source terms/background:** Annual average release rate, or its equivalent
c) **Mesh/grids:** Either a square (20 x 20) polar (20-r x 16-θ) grid option

Error Estimates: Annual average concentrations could be within a factor of 2-4 within 80 km of source; the error goes up as the averaging time goes down

Applicability: Chronic and acute radionuclide releases from stacks and uniform area sources

Time periods used for workshop: Monthly, quarterly, and annual averages, September 1975 through August 1976

Available? Yes **Documented?** Yes

Computer Type: IBM 360/IBM 3033

Core Size: 650K **Running time (SRP data)** 35 sec/time period

Reference: R. E. Moore, C. F. Baes, III, L. M. McDowell-Boyer, A. P. Watson, F. O. Hoffman, J. C. Pleasant, and C. W. Miller. AIRDOS-EPA: A Computerized Methodology for Estimating Environmental Concentrations and Dose to Man from Airborne Releases of Radionuclides. ORNL-5532 (June 1979).

MODEL DESCRIPTION FORM

Laboratory: Savannah River Laboratory

Division/Group: Environmental Sciences Division

Model Type: WIND Rose **Model Name:** SHEAR-ROSE

Short Description: Basically a Gaussian plume model using wind rose statistics with the addition of an adjustment to the horizontal plume spread using the formulation of Pasquill.

Basic Equation Solved: A modified Gaussian plume equation. The code compiles wind rose statistics for 22.5-deg sectors centered on azimuth of interest. The code uses the Briggs open country equations and an average mixing height for each stability and wind direction class.

Input Requirements:

a) **Wind fields:** Joint frequency distribution of wind direction, stability and in 22.5-deg sectors centered on azimuth of receptor.
b) **Source terms/background:** Hourly release rate.
c) **Mesh/grids:** Polar grid.

Error Estimates: Annual average concentrations within a factor of 2-4.

Applicability: Chronic releases from stacks.

Time periods used for workshop: Average of 40 weeks in 1976.

Available? No **Documented?** No **Computer type:** IBM 360

Core size: 300K **Running time (SRP data)** 2 min/month (mostly input/output)

Developed by: M. M. Pendergast

Reference: None

MODEL DESCRIPTION FORM

Laboratory: Air Resources Laboratory (NOAA)

Division/Group: Silver Spring, Md.

Model Type: Gaussian/Sector Average **Model Name:** DRAX1

Short Description: A long-term sector average Gaussian dispersion model that incorporates temporal vertical stability variations, estimated wind speed at release height, a method to account for calm winds, and day-night mixing depths is developed from meteorological data at a single surface station.

Basic Equation Solved:

$C = (2/\pi)^{1/2} (Q/\theta X_r U \sigma_z)$
C - ground level air concentration
Q - emission rate
θ - sector size
X_r - receptor distance
U - wind speed
σ_z - vertical dispersion

Horizontal diffusion is assumed to be uniform in 30 sectors. Vertical diffusion is calculated from the relation $(2\sum_i kDt_i)^{1/2}$, where the diffusivity, k, is specified for each hourly interval (i) along the trajectory. The mixing height is determined from Holzworth's published climatological values for each season.

Input Requirements:

a) **Wind fields:** Single surface station and Pasquill stability
b) **Source terms/background:** Hourly source term, 15 pCi/m^3 background
c) **Mesh/grids:** None

Error Estimates: 95% of 2-year average values within a factor of 7

Applicability: Receptors at about 100 km downwind

Time periods used for workshop: Two years of weekly sampling periods

Available: Yes **Documented?** Yes **Computer type:** IBM 360

Core size: 80K bytes **Running time (SRP data)** 2 min/year

Developed by: R. Draxler

Reference: R. Draxler. "An Improved Gaussian Model for Long-Term Average Air Concentration Estimates" Atm. Environ. 14, 597 (1980).

MODEL DESCRIPTION FORM

Laboratory: Pacific Northwest Laboratory

Division/Group: Atmospheric Sciences

Model Type: Gaussian/deposition with source depletion

Model Name: ANDEP

Short Description: ANDEP is a deposition model applicable to monthly, seasonal, annual or longer-term assessments of the effects of a single source on a region extending out to 50 km (or farther with minor adjustment). Basic input consists of joint frequency distribution of winds and if available, a precipitation distribution. Dry deposition is calculated from ground level air concentration using a deposition velocity approach.

Basic Equation Solved: Sector averaged form of bivariate-normal plume equation with source-depletion correction for deposition.

Input Requirements:

a) **Wind fields:** Wind rose - joint frequency using 16 direction, 6 wind speed classes, 7 stability classes.
b) **Source terms/background:** Source term may be specified in any convenient units, or may be set to 1 for X/Q estimates - no background.
c) **Mesh/grids:** Original model calculates concentrations and deposition at 6 distances between 1 and 50 km for each of 16 radical sectors around source. Modified for these tests to extend to greater distances.

Error Estimates: Not Available.

Applicability: Region within 50 km of source; may be easily modified to extend this region.

Time periods used for workshop: "Monthly" periods corresponding to those defining the wind rose data periods.

Available? Yes **Documented?** Being developed
Computer type: PDP 11/70 **Core size:** Minimal

Running Time (SRP data) 3-1/2 minutes for 27 data periods

Developed by: C. E. Hane, W. F. Sandusky, and D. R. Drewes

Reference: B. E. Vaughn, et al. Review of Potential Impact on Health and Environmental Quality from Metals Entering the Environment as a Result of Coal Utilization. Battelle Energy Program Report, Battelle-Northwest, Richland, Washington (1975).

MODEL DESCRIPTION FORM

Laboratory: Savannah River Laboratory

Division/Group: Environmental Sciences Division

Model Type: Gaussian Plume **Model Name:** XOQDOQ

Short Description: XOQDOQ is a computer code used by the U.S. Regulatory Commission in its meteorological evaluation for routine releases from commercial nuclear power reactors.

Using a "straight-line" airflow model, this code implements the assumptions outlined in Section C (excluding C1a and C1b) of Regulatory Guide 1.111, Methods for Estimating Atmospheric Transport and Dispersion of Gaseous Effluents in Routine Releases from Light-Water Cooled Reactors. For routine plant releases, it calculates average relative effluent concentrations (X/Q's) and average relative deposition values (D/Q's) at locations specified by the user, and at standard radial distances and segments for downwind sectors. It also calculates these values at the specified locations for intermittent releases.

Basic Equation Solved: A modified Gaussian plume equation is used to estimate both horizontal and vertical dispersion. Horizontal diffusion is assumed uniform over 16 sectors. Vertical diffusion is based on Pasquill-Gifford curves fitted with polynomials. The mixing height is set to 1000 m.

Input Requirements:

a) **Wind fields:** Joint frequency distribution of wind direction and stability.
b) **Source terms/background:** Monthly average release rate
c) **Mesh/grids:** Polar

Error Estimates: Annual average concentrations could be within a factor of 2-4 within 80 km of source.

Applicability: Chronic releases from stacks.

Time periods used for workshop: Monthly and annual averages, Sept. 75 - Aug. 76 and Dec. 76 - Aug. 77.

Available? Yes **Documented?** Yes **Computer type:** IBM 360

Core size: 500K with plotting **Running time (SRP data)** 20 sec/time period

Developed by: Sagendorf & Goll

Reference: J. F. Sagendorf and J. T. Goll. NUREG-0324, Sept. 77, NRC, Washington, D.C. (1977).

MODEL DESCRIPTION FORM

Laboratory: Oak Ridge National Laboratory

Division/Group: Union Carbide Corporation

Model Type: Gaussian Sector Model **Model Name:** ATM

Short Description: ATM is a Gaussian sector model for either gaseous or particulate pollutants. The code treats either point, line, area, or resuspension sources. Output consists of average ground level concentrations and ground deposition at user-specified points for periods of interest.

Basic Equation Solved: A Gaussian plume model modified to calculate particle deposition. The model uses either the Briggs, Pasquill-Gifford, or Smith diffusion coefficients. The model employs a variable, user-specified mixing height.

Input Requirements:

a) **Wind fields:** Uses STAR or similar data
b) **Source terms/background** Monthly averaged release rate
c) **Mesh/grids** Polar, user-specified

Error Estimates: Based on SRL data, 50% within a factor of two and most with a factor of 10.

Applicability: Chronic releases from multiple sources.

Time periods used for workshop: "Monthly" periods corresponding to those defining the wind rose periods.

Available? Argonne Code Center **Documented?** Yes

Computer type: IBM

Core size: - 320K **Running time (SRP data)** - 40 seconds for 26 time periods

Developed by: W. M. Culkowski and M. R. Patterson

Reference: W. M. Culkowski and M. R. Patterson, <u>Comprehensive Atmospheric Transport and Diffusion Model</u>. ORNL/NSF/EATC-17 (April 1976).

Gaussian Trajectory Models (M. M. Pendergast)

General Description

Gaussian trajectory models have been developed to make air pollution assessments at travel distances where a single wind at the source may no longer be representative of the "true" transport of the pollutants. The most important aspect of these models is the calculation of pollutant trajectories. On the other hand, the diffusion of the pollutant is handled in a manner similar to that used in the wind-rose models. (This can be contrasted with the more complex 3-D models where transport and diffusion are computed by complex numerical algorithms.) This simple treatment of diffusion is justified for three reasons: (1) for transport beyond 20 km, the plume is well-mixed in the vertical so diffusion is scaled with the mixing depth, (2) diffusion in the horizontal, σ_y, has not been satisfactorily specified for use in Eulerian numerical models, and (3) the inherent errors in wind fields derived from observations are translated to errors in calculating the trajectories. These errors have a pronounced effect on the calculation of air concentrations at a single point located downwind from a source. Often these errors can overwhelm the error attributed to the modeling of the diffusion rate. For these reasons, the success of the Gaussian trajectory models will largely depend on the manner that (1) wind fields, (2) mixing depths, and (3) diffusion are modeled.

The laboratories providing a significant number of calculations were ARL, ANL, SRL and ATDL. Although similar in basic principles, the models varied significantly in operation. Upper air data were used in the ATAD (WJBF-TV tower data also) and ASTRAP models; one model used surface data only, DRAGON; and two models used a combination of upper air and surface data, DRAX2 and ADPLUM. The methods used to incorporate mixing depth varied for all models. Varying mixing depths were used in the ADPLUM, DRAX2, and ATAD models, while daily maximum mixing depths were used in the DRAGON models. ASTRAP used an average diurnal pattern of stability profiles for each month. Vertical diffusion was limited to the mixing depth in all models although methods varied for the specification of σ_z. ASTRAP specified profiles of K_z based upon observed climatology and field studies. Horizontal diffusion was assumed to be directly related to travel distance in the ATAD and DRAX2 models; whereas, ASTRAP computed horizontal dispersion statistics from the distribution of simulated trajectory endpoints as a function of plume age. The other models used the familiar BNL and Briggs specifications.

Computer requirements varied considerably between models (2 min to 36 hours CPU time to do calculations for annual comparisons) although intercomparisons are not comparable unless computing speeds are taken into account for different computers.

Model Descriptions

Gaussian trajectory models utilized by the Workshop participants are briefly described in this section.

MODEL DESCRIPTION FORM

Laboratory: Atmospheric Turbulence and Diffusion Laboratory (NOAA)

Division/Group: Oak Ridge, Tennessee

Model Type: Trajectory Puff **Model Name:** DRAGON

Short Description: DRAGON is a trajectory-puff model for pollutant releases from multiple elevated or point sources. Output consists of time-integrated concentrations over a 33 x 33 grid and at 13 selected stations.

Basic Equation Solved:

1) DRAGON GP: Gaussian Puff with σ_z = 0.8H, H = mixing depth, and $\sigma_x = \sigma_y$ from Briggs' dispersion curves.
2) DRAGON TH: same as (1) but top hat distribution of material and plume segments instead of circular puffs.
3) DRAGON THP: Same as (2) except σ_z is a function of travel distance.

Input Requirements:

a) **Wind fields:** Hourly values
b) **Source terms/background:** Hourly values
c) **Mesh/grids:** 5 km grid spacing

Error Estimates: Factor of 4 overprediction for Gaussian Puff; factor of 2 overprediction for top hat.

Applicability: Uniform terrain

Time periods used for workshop: Period 1 to 5 (see Appendix D)

Available? No **Documented?** No **Computer type:** IBM-3033

Core size: **Running time (SRP data)** Gaussian 60 min/month
Top Hat 10 min/month

Developed by: Nappo-Snodgrass

Reference: None available

MODEL DESCRIPTION FORM

Laboratory: Air Resources Laboratory (NOAA)

Division/Group: Silver Spring, Md.

Model Type: Trajectory **Model Name:** DRAX2

Short Description: A mesoscale Lagrangian trajectory transport and diffusion model has been developed which takes into account stability changes along the trajectory. The required input data for trajectory computations are hourly surface meteorological observations and standard upper air observations. The vertical mixing coefficient is based on the Pasquill stability category each hour. Dry deposition and washout are calculated if required.

Basic Equation Solved: $ds/dt = V(x,y,t)$
ds/dt = trajectory, V = wind velocity field given hourly

Horizontal diffusion is assumed to be linear with time about each trajectory. However, trajectory variability over averaging periods of greater than one hour contributes much more to the horizontal diffusion. Vertical diffusion is computed from a Gaussian or finite-difference solution of the diffusion equation. Vertical diffusivities are specified hourly. The mixing height each day is determined from the intersection of the maximum surface temperature with the morning temperature sounding. Diffusivities above this height are set to a very small value.

Input Requirements:
a) **Wind fields:** Hourly surface and 12-hour soundings
b) **Source terms/background:** Hourly
c) **Mesh/grids:** None

Error Estimates: 95% within a factor of:
- 16 for 12-hour average samples
- 6 for 2-year average samples

Applicability: One hour to several days travel time and any averaging time.

Time periods used for workshop: All twice-daily and weekly sampling periods.

Available? Yes **Documented?** Yes **Computer type:** IBM 360

Core size: 300K bytes **Running time (SRP data)** 2 min/month

Developed by: R. Draxler

Reference: R. Draxler. "Modeling the Results of Two Recent Mesoscale Dispersion Experiments." Atm. Environ., 13, 1523 (1979).

MODEL DESCRIPTION FORM

Laboratory: Air Resources Laboratory (NOAA)

Division/Group: Silver Spring, MD

Model Type: Lagrangian **Model Name:** Atmospheric Transport & Dispersion Model (ATAD)

Short Description: The Air Resources Laboratories Atmospheric Transport and Dispersion Model (ATAD) is oriented toward practical application for pollution studies. ATAD calculates trajectories of 5 days duration from any number of origins, starting every 6 hours during any selected period (e.g., a day, month or season), moving either forward or backward in time. Each trajectory is calculated using transport winds averaged in a vertical layer. Dispersion calculations are made for the forward trajectories. Standard model output includes tables of transport layer depth, maximum vertical wind shear in the transport layer, and trajectory positions. Optional output includes trajectory plots and map of time-averaged surface air concentrations and deposition amounts.

Basic Equation Solved:

A Gaussian plume model combined with an objective analysis scheme for calculating plume trajectories. Horizontal diffusion, σ_H (meters) = 0.5 t (seconds), is used in ATAD.

The mixing height is determined from a variable transport layer depth (TLD) calculated by the model for transport during nighttime and daytime. The nighttime TLD = $2(2K_z t)^{1/2}$ where K_z = 1 m^2/sec. The daytime TLD is determined by converting a temperature sounding at a rawinsonde station to potential temperature (θ) and locating the lowest critical inversion satisfying the criteria:

a) $\Delta\theta/\Delta Z > .005\ ^\circ K/m$

b) $\theta_{TOP} - \theta_{BASE} \geq 2^\circ K$

A constant TLD can also be specified by the user if desired.

Input Requirements:

a) **Wind fields:** Upper-air wind and temperature observations from tapes archived at NCC
b) **Source terms/background:** Average or measured
c) **Mesh/grids:** None

Error Estimates: 95% within a factor of 3 for weekly predictions

Applicability: Mesoscale to continental scale, short and long term measurements from multiple sources of constant or variable emission rates.

Time periods used for workshop: All designated in worksheet

Available? Yes **Documented?** Yes **Computer type:** IBM 360

Core size: 256K **Running Time (SRP data)** 20 min.

Developed by: J. L. Heffter

Reference: J. L. Heffter. Air Resources Laboratories Atmospheric Transport and Dispersion Model (ARL-ATAD). NOAA Tech Memo ERL ARL-81, Air Resources Laboratories, Silver Spring, Maryland, 20910 (1980).

MODEL DESCRIPTION FORM

Laboratory: Argonne National Laboratory

Division/Group: RER

Model type: Statistical Trajectory **Model Name:** ASTRAP

ASTRAP is composed of three subprograms. ASTRAP develops horizontal dispersion statistics by releasing simulated tracers at each source or source region and transporting the tracers in 2-D wind fields. From the ensemble of trajectories from each source, the mean position and the spread about the mean position are calculated as a function of plume age (time since release). A series of 2-D Gaussian puffs can then be used to describe transport and horizontal diffusion. When the model is used to simulate dispersion of pollutants subject to wet deposition, such as SO_2/SO_4, wet removal statistics are gathered by removing portions of tracers according to the half-power of the (typically) 6-hour prediction amount. Similar mean and standard deviations are then gathered for both dry (airborne) and wet (deposited) tracers, along with the number of trajectories contributing to each statistic, as a function of plume age.

Basic Equation Solved: 1-D diffusion in vertical.

Horizontal dispersion statistics are produced by fitting Gaussian puffs to simulated tracer ensemble trajectory endpoints as a function of plume age (time since release); vertical dispersion is calculated separately in a 1-D numerical model, with a diurnal variation (repeated) of the K_z profile. Concentrations are calculated by combining the above statistics with the emission rate.

Input Requirements:

a) **Wind fields:** Normally a grid of mean winds through 1500 m or so, as analyzed from radiosonde obs; mean tower winds were used in this application to save time and effort.
b) **Source terms/background:** Monthly average if no finer resolution is available/no background term used.
c) **Mesh/grids:** Arbitrary 20 x 20 concentration grid, spacing 0.1 NMC, plus concentrations at observation sites.

Error Estimates: Factor of 2?

Applicability: Monthly, seasonal, or annual (combination of monthly or seasonal results).

Time periods used for workshop: 23 monthly periods from Oct. 75 through Aug. 77.

Available? Not yet **Documented?** In part

Computer type: IBM 360/195

Core size: 3 subprograms* **Running Time:** 3 subprograms*
* trajectory program 104 K 60 s
vertical integration 116 K 108 s
concentrations 104 K 21 s
(times are for the combined 23 monthly simulations)

Developed by: Jack Shannon

Reference: J. D. Shannon. "A Model of Regional Long-Term Average Sulfur Atmospheric Pollution, Surface Removal, and Net Horizontal Flux." Atm. Environ. 15, 689 (1981).

MODEL DESCRIPTION FORM

Laboratory: Savannah River Laboratory

Division/Group: Environmental Sciences Division

Model Type: Gaussian Segmented Plume **Model Name:** ADPLUM

Short Description: To simulate atmospheric transport and diffusion for use in dose calculations the SRL has developed a computational framework called JEREMIAH. The simplest model in the JEREMIAH system is the segmented plume model coded ADPLUM. The model is capable of providing air concentration estimates at numerous receptor locations from multiple release points.

Basic Equation Solved: A modified Gaussian Plume Model (using a 2-D wind field). The main features of the model include segmented plumes and displaced effective source terms, reflective upper and lower boundaries, formulations including the effects of time varying meteorology and well-mixed layer. Diffusion coefficients are derived from the BNL formulations based on measured values of σ_θ and σ_ϕ. (For workshop calculations neutral stability was assumed for all cases.)

Input Requirements:

a) **Wind fields:** Hourly input from NWS surface and upper air and meteorological towers.
b) **Source terms/background:** Hourly release rate.
c) **Mesh/grids:** 33 x 33 square grid

Error Estimates: 10-hour average values 90% within factor of 2; 98% within factor of 10.

Applicability: Releases from stacks and uniform area sources.

Time periods used for workshop: Weekly samples during first 5 months of 1976.

Available? No **Documented?** No **Computer type:** IBM 360

Core size: 700K **Running time (SRP data)** 3 hours/month

Developed by: Environmental Sciences Division Staff Members C. D. Kern, M. R. Buckner, M. M. Pendergast, C. E. Bailey, and J. C. Huang).

Reference: J. C. Huang. "Evaluation of Modified Gaussian Plume Model for Travel Distances 25-150 km." Second Joint Conference on Applications of Air Pollution Meteorology, March 24-27, 1980. New Orleans, LA (1980).

MODEL DESCRIPTION FORM

Laboratory: Brookhaven National Laboratory

Division/Group: Atmospheric Sciences

Model Type: *Gaussian* **Model Name:** DISTHEATCENT

Short Description: The model tested is a standard EPA Gaussian dispersion model modified in application by the addition of a mixing height preprocessor that accounts for momentum effects in defining the nocturnal boundary layer and also modified to allow hourly variations in emission strength.

Basic Equation Solved: Gaussian form for elevated point sources.

Input Requirements:

a) **Wind fields:** Hourly surface winds
b) **Source terms/background:** Hourly emission values
c) **Mesh/grids:** Grid is arbitrary

Error Estimates: The error estimates for the Standard Gaussian equations are given by D. B. Turner in Workbook for Atmospheric Dispersion Estimates.

Applicability: The model as modified has been applied only to a conceptual study of a district heating plant. If the preprocessor modification demonstrates a significant advantage, wider application is likely.

Time periods used for workshop: Ten-hour periods: calculational order 1-4 (letter, C. E. Bailey, 12 June 1980 - see Appendix D).

Available? Yes **Documented?** Incomplete

Computer Type: CDC 7600

Core size: 11,234 (octal length) **Running time (SRP data)** 1.5 sec for 24 hours.

Developed by: EPA model developed by D. B. Turner. Preprocessors developed by T. Carney, J. Tichler, K. Johnson, and others at BNL.

Reference: Mixing Depth Estimation for the District Heating Study. Keith W. Johnson (unpublished).

D. B. Turner. Workbook of Atmospheric Dispersion Estimates. USDHEW, PHS Pub. No. 995-AP-26, 84 pp (1969).

3-D Models (D. W. Pepper and R. E. Cooper)

General Description

Three laboratories tested their three-dimensional models against several days of data. LLNL used the ADPIC and PATRIC particle-in-cell dispersion models to calculate an 18-hour sample period for the first day of the priority periods. Wind fields for the ADPIC calculation were generated with the wind field analysis code MATHEW. LANL used a finite difference model along with the terrain following wind field code, ATMOS1, to model the same 18-hour sampling period. LANL also ran the three additional sampling periods modeled by SRL for a total of almost 9 days. Four different 3-D models were used by SRL in the validation studies. These models consisted of (1) second moment, (2) chapeau (linear finite element), (3) particle-in-cell, and (4) pseudospectral. The first three models were run against ten days of data; the pseudospectral technique was used for only two days of data, due principally to excessive core and running time constraints. The one-day sample period calculated by LLNL was not sufficient to adequately analyze statistically. The calculations performed by SRL and LANL proved to be moderately sufficient, but not sufficiently adequate to make all inclusive conclusions as to their general usefulness. Each model analyzed had its relative assets and limitations. Basic characteristics of the models and their requirements are discussed in this section. All three laboratories have successfully tested their codes in previous numerical and analytical validation tests, as well as with actual field data of limited extent.

The basic physics inherent in all the models analyzed were similar, i.e., solution of the 3-dimensional advection-diffusion equation; gridded wind fields were obtained by objective analysis (interpolation from known data points), followed by mass consistence ensurance through solution of the Euler-Lagrange Poisson equation for the Lagrangian multipliers. The wind field analysis section (page 52) describes the wind field analysis in more detail. Closure of the equation was kept simple, i.e., the eddy diffusivities were related to the empirical expression based on Pasquill-Gifford approximations used in the more commonly used Gaussian models. Attempts to use more sophisticated closure schemes were felt by all the participants to be too difficult to address within the time frame of the workshop. Some models were capable of including topography. However, topography was not considered significant since the terrain surrounding SRP consists of gently rolling hills with little variation, i.e., relatively flat for the distances considered in the validation studies. The models run by SRL and LANL assumed "flat plate" lower boundaries. The upper boundaries were assumed to be perfect reflectors, and were set at predetermined heights by each laboratory (usually 1000 m).

Model Descriptions

Three-dimensional models utilized by the Workshop participants are briefly described in this section.

MODEL DESCRIPTION FORM

Laboratory: Los Alamos National Laboratory

Division/Group: Group X-5 MS G-8

Model Type: 3-D Diagnostic Codes **Model Name:** ATMOS1/ATMOS2

Short Description: A mesoscale system of wind field and particle transport codes developed mainly for problems associated with drainage flow in complex terrain. (ATMOS1 and ATMOS2).

Basic Equation Solved: Continuity Equation, assuming $\nabla \cdot u = 0.0$ for the wind fields; Advection-Diffusion Equations in 3D for particle transport, all in Sigma coordinates.

Input Requirements:

a) **Wind fields:** Ground level, tower, and rawinsonde for instance.
b) **Source terms/background:** Volume emission near surface.
c) **Mesh/grids:** 33 x 33 x 9 $\Delta x = \Delta y = 5$ km Δz variable

Error Estimates: 97% < factor 10; 80% factor 2

Applicability: Mesoscale transport.

Time periods used for workshop:

1800	10/5/76	→	1600	10/6/76	23 hours
1800	2/16/77	→	800	2/19/77	63 hours
2200	4/5/77	→	800	4/9/77	46 hours
2200	7/10/77	→	1900	7/12/77	46 hours

Available? Not yet **Documented?** Not yet **Computer type:** 7600 CDC
Core size: ATMOS1(140K) ATMOS2(210K) **Running time (SRP data)**
Wind fields ~90 sec/hour; Transport run 1.5 min/problem

Developed by: Still being developed

References: M. H. Dickerson, Ed. A Collection of Papers Based on Drainage Wind Studies in the Geysers Area of Northern California. USDOE Report ASCOT-80-7, Lawrence Livermore National Laboratory, Livermore, CA (1980).

C. G. Davis and B. E. Freeman. Modeling Drainage Flow with SEGMET. USDOE Report ASCOT-81-1, Los Alamos National Laboratory, Los Alamos, NM (1981).

MODEL DESCRIPTION FORM

Laboratory: Lawrence Livermore National Laboratory

Division/Group: G

Model Type: Transport & Diffusion **Model Name:** MATHEW

Short Description: MATHEW is a regional three-dimensional diagnostic wind field model which uses a variational analysis technique to determine a three-component non-divergent velocity field. It was specifically designed to provide advection velocities to the ADPIC (Particle-In-Cell) code. MATHEW incorporates terrain explicitly, is site independent, and uses available meteorological measurements in developing initial values of the wind components within the volume of interest.

Basic Equation Solved:

$$E(\bar{U};\lambda) = \int_V \left[(\bar{U} - \bar{U}_o) \cdot \underline{\underline{D}} \cdot (\bar{U} - \bar{U}_o) + \lambda \Delta \cdot \bar{U}\right] dV,$$

where E is the functional being minimized, $\bar{U}$ are the velocity components to be minimized, $\bar{U}_o$ are the corresponding initial values, λ is a Lagrange multiplier, and $\underline{\underline{D}}$ is a tensor of second rank containing Gauss precision moduli weights.

Input requirements:

a) **Wind fields:** MATHEW receives reference level (6 m) winds, grid top winds and profile information from an ancillary code with which it constructs a full three-dimensional field.
b) **Source terms/background:** N/A
c) **Mesh/grids:** The standard grid has 51x51x15 points in the x, y, and z directions.

Error Estimates: Errors cited under the ADPIC model description refer to the combined errors from MATHEW and ADPIC.

Applicability: The regions of interest have horizontal distances of 10 to 200 km and extend less than 2 km above topography.

Time periods used for workshop: Calculations were made over a 22-hour period surrounding the twice-daily sample on 5 Oct 76.

Available? Yes **Documented?** Yes **Computer type:** CDC 7600

Core size: 340000 dec **Running time (SRP data)** 33 CPU min

Developed by: Christine Sherman

Reference: C. S. Sherman. "MATHEW: A Mass-Consistent Wind Field Model." Ph.D. Thesis, Lawrence Livermore National Laboratory Report UCRL-52479 (1978).

MODEL DESCRIPTION FORM

Laboratory: Lawrence Livermore National Laboratory

Division/Group: G

Model Type: Transport & Diffusion **Model Name:** ADPIC

Short Description: ADPIC is a hybrid Lagrangian-Eulerian transport and diffusion code to calculate the three-dimensional distribution of atmospheric pollutants in transient flow fields. The code employs the particle-in-cell method in diffusing Lagrangian marker particles in hourly varying mean flow fields which are given to ADPIC in mass conservative form. Modeling capabilities include: inert or radioactive pollutants, multiple sources, deposition, particle size distribution, washout and topography.

Basic Equation Solved:

$$\partial\chi/\partial t + \nabla \cdot \left[\chi(\bar{U}_A - (K/\chi)\nabla\chi)\right] = \partial\chi/\partial t + \nabla \cdot \left(\chi \bar{U}_p\right) = 0,$$

where χ is a scalar concentration, $-K\ \nabla\chi/\chi$ is a diffusivity velocity, $\bar{U}_A$ is an advection velocity, and $\bar{U}_p \equiv \bar{U}_A - K\ \nabla\chi/\chi$ is a "pseudo-transport" velocity.

Input Requirements:

a) Wind fields: MATHEW supplies three-dimensional, mass-consistent fields of advection velocities.
b) Source terms/background: ADPIC can simulate up to five point and/or area sources.
c) Mesh/grids: The standard mesh consists of 41x41x15 points.

Error Estimates: ADPIC agreed within 5% of selected analytic solutions to the transport-diffusion equation and, in a series of tracer studies, agreed within a factor of 2 of field data 60% of the time.

Applicability: ADPIC is typically used for short-term assessments in situations of complex meteorology and terrain with modeling done on a regional scale in the range of 10 to 200 km.

Time periods used for workshop: Calculations were made over a 22-hour period surrounding the twice-daily PM sample on 5 Oct 76.

Available? Yes **Documented?** Yes **Computer type:** CDC 7600

Core size: 273000 dec **Running time (SRP data)** 18 CPU min

Developed by: Rolf Lange

Reference: R. Lange. "ADPIC -- A Three-Dimensional Model for the Dispersal of Atmospheric Pollutants and Its Validation Against Regional Tracer Studies." J. Appl. Meteor. 17, 320 (1978).

MODEL DESCRIPTION FORM

Laboratory: Lawrence Livermore National Laboratory

Division/Group: G

Model Type: Transport & Diffusion **Model Name:** PATRIC

Short Description: PATRIC is a hybrid Lagrangian-Eulerian transport and diffusion code to calculate the three-dimensional distribution of atmospheric pollutants in transient flow fields over a flat terrain. The code employs the particle-in-cell method and the diffusivities are based on a Gaussian distribution. Its capabilities include: inert or radioactive pollutants, multiple sources, deposition, particle size distribution and washout.

Basic Equation Solved:

$$\partial\chi/\partial t + \nabla \cdot [\chi(\bar{U}_A - K/\chi \; \nabla\chi)] = \partial\chi/\partial t + \nabla \cdot (\chi\bar{U}_P) = 0,$$

where χ is a scalar concentration, $-K/\chi \; \nabla\chi$ is a diffusivity velocity, $\bar{U}_A$ is an advection velocity, and $\bar{U}_P \equiv \bar{U}_A - K/\chi \; \nabla\chi$ is a "pseudo-transport" velocity.

Input Requirements:

a) **Wind fields:** The hourly varying mean flow fields are computed in PATRIC from interpolated meteorological station data. No vertical winds are permitted, but speed and directional shear are modeled by permitting vertical variation of horizontal winds.
b) **Source terms/background:** PATRIC allows up to five point and/or area sources.
c) **Mesh/grids:** Transport velocities are interpolated and extrapolated to an 11x11x7 point grid. Imbedded within this matrix are 40x40x12 diffusion cells.

Error Estimates: PATRIC has been shown to give results to within 5% of selected analytic solutions to the transport-diffusion equation.

Applicability: PATRIC is designed for monthly, seasonal and annual assessments on a regional scale (10 to 200 km). This code is applicable to short-term assessments when the terrain within the target area is reasonably flat.

Time periods used for workshop: Calculations were made over a 22-hour period surrounding the twice-daily PM sample on 5 Oct 76.

Available? Yes **Documented?** Yes **Computer type:** CDC 7600

Core size: 200000 dec **Running time (SRP data)** 2 CPU min

Developed by: Rolf Lange

Reference: R. Lange. **PATRIC -- A Three-Dimensional Particle-In-Cell Sequential Puff Code for Modeling the Transport and Diffusion of Atmospheric Pollutants.** Lawrence Livermore National Laboratory Report UCID-17701 (1978).

MODEL DESCRIPTION FORM

Laboratory: Savannah River Laboratory

Division/Group: Environmental Sciences Division

Model Type: 3-D Linear Finite Elements **Model Name:** CHAPEAU

Short Description: CHAPEAU is a 3-D time-split chapeau function (linear finite element) code. The one-dimensional advection-diffusion equation is solved successively for each dimension.

Basic Equation Solved:

$$\partial c/\partial t + U\ (X_i)\ \partial c/\partial t = \partial/\partial X_i\ \left(K\ (X_i)\ \partial c/\partial X_i\right) + S + Q$$

Vertical eddy diffusivity K_z was calculated by using fitted curves to F. B. Smith's (1973) profiles for stable, neutral, and unstable conditions. Smith's curves are based on Taylor's statistical theory and empirical data applied as

$$K \simeq \frac{1}{15}\ \varepsilon^{1/3} \lambda_m^{\ 4/3}$$

where ε is the rate of energy dissipation and λ_m is the wavelength corresponding to maximum energy in the vertical turbulence spectrum.

The horizontal eddy diffusivity was calculated for Pasquill's (1976) recommended form

$$\frac{\sigma_y}{x} = \sigma_A\ f(x)$$

and corrected for sampling time, according to Doran, Horst, and Nickola.

The mixing height was limited to a maximum of 700 meters to limit computer storage requirements and to afford a direct comparison with other SRL 3-D Models.

Input Requirements:

a) **Wind fields:** Mass consistent winds are generated for 33x33 mesh at 8 levels. No vertical winds.
b) **Source terms/background:** Hourly emission rates.
c) **Mesh/grids:** 33x33x8 grids. 5 km spacing on X and Y. 100 m spacing on Z.

Error Estimates:

Applicability:

Time periods used for workshop:
1600 10/05/76 → 1700 10/06/76; 300 02/16/77 → 1700 02/19/77;
1200 04/05/77 → 1300 04/09/77; 2000 07/10/77 → 500 07/03/77.

Available? No **Documented?** No **Computer type:** IBM 360/195

Core size: 500K **Running time (SRP data)** 0.57 sec/iteration

Developed by: D. W. Pepper and R. E. Cooper

References: D. W. Pepper and A. J. Baker. "A Simple One-Dimensional Finite Element Algorithm With Multi-Dimensional Capabilities." Num. Heat Transfer 2, 81 (1979).

P. E. Long and D. W. Pepper. "An Examination of Some Simple Numerical Schemes for Calculating Scalar Advection." J. Appl. Meteor. 20, 146 (1981).

F. B. Smith. A Scheme for Estimating the Vertical Dispersion of a Plume from a Source Near Ground Level (Unpublished British Meteorology Society Note) (1973).

F. Pasquill. Atmospheric Diffusion. 2nd ed., John Wiley and Sons, New York (1974).

J. C. Doran, T. W. Horst, and P. W. Nickola. "Variations in Measured Values of Lateral Diffusion Parameters." J. Appl. Meteor. 17, 825 (1978).

MODEL DESCRIPTION FORM

Laboratory: Savannah River Laboratory

Division/Group: Environmental Sciences Division

Model Type: 3-D Moments **Model Name:** MOMENTS

Short Description: Zeroth, first and second moments of concentration distribution are conserved within cell boundaries to allow advection free of numerical dispersion. Diffusion is effected by a combination of central differencing and cubic splines.

Basic Equation Solved:

$$\partial c/\partial t + U(X_i)\ \partial c/\partial X_i = \partial/\partial X_i \left[K(X_i)\ \partial c/\partial X_i\right] + S$$

Diffusion coefficients and the mixing height are treated as described for the CHAPEAU model.

Input Requirements:

a) **Wind Fields:** Mass consistent wind fields are generated for a 33x33 mesh at 8 levels. No vertical wind components.
b) **Source terms/background:** Hourly emission rates
c) **Mesh/grids:** 33x33x8 grids. 5 km spacing on X and Y. 100 m spacing on Z.

Error Estimates:

Applicability:

Time periods used for workshop:
1600 10/05/76 → 1700 10/06/76; 300 02/16/77 → 1700 02/19/77;
1200 04/05/77 → 1300 04/09/77; 2000 07/10/77 → 500 07/13/77.

Available? No **Documented?** No **Computer type:** IBM 360/195

Core size: 1100K **Running time (SRP data)** 0.51 sec/iteration

Developed by: D. W. Pepper

Reference: B. A. Egan and J. R. Mahoney. "Numerical Modeling of Advection and Diffusion of Urban Area Source Pollutants." J. Appl. Meteor. 11, 312 (1972).

L. B. Pedersen and L. P. Prahm. "A Method for Numerical Solution of the Advection Equation." Tellus 26, 594 (1974).

MODEL DESCRIPTION FORM

Laboratory: Savannah River Laboratory

Division/Group: Environmental Sciences Division

Model Type: 3-D Pseudospectral **Model Name:** FOURIER

Short Description: A fast Fourier Transform method is used to accurately evaluate spatial derivatives for advection and diffusion.

Basic Equation Solved:

$$\partial c/\partial t = -\bar{\nabla} \cdot (\bar{V} \cdot c) + \bar{\nabla} \cdot (D\,\bar{\nabla} c) + Q - S$$

Diffusion coefficients and the mixing height are treated as described for the CHAPEAU model.

Input Requirements:

a) **Wind fields:** Mass consistent winds are generated for 33x33 mesh at 8 levels. No vertical wind components.
b) **Source terms/background:** Used SRL Kr-85 data.
c) **Mesh/grids:** 33x33x8 grids. 5 km spacing on X and Y. 100 m spacing on Z.

Error Estimates:

Applicability:

Time periods used for workshop:
2100 07/10/77 → 1400 07/11/77; 1600 10/05/76 → 1700 10/06/76.

Available? No **Documented?** No **Computer type:** IBM 360/195

Core size: 1500K **Running time (SRP data)** 10 sec/iteration

Developed by: R. E. Cooper

Reference: O. Christensen and L. P. Prahm. "A Pseudospectral Model for Dispersion of Atmospheric Pollutants." J. Appl. Meteor. 15, 1284 (1976).

MODEL DESCRIPTION FORM

Laboratory: Savannah River Laboratory

Division/Group: Environmental Sciences Division

Model Type: 3-D Particle-In-Cell **Model Name:** PIC

Short Description: A Eulerian-Lagrangian Method using discrete particles to represent concentration. A pseudo-velocity is computed as the sum of the wind field velocity and a computed fictitious diffusion velocity to advect the particles.

Basic Equation Solved:

$$\partial c/\partial t = - \bar{\nabla} \cdot (\bar{V} \cdot c) + \bar{\nabla} \cdot (D\, \bar{\nabla}\, c) + Q - S$$

Diffusion coefficients and the mixing height are treated as described for the CHAPEAU model.

Input Requirements:

a) **Wind fields:** Mass consistent winds are generated for a 33x33 mesh at 8 levels. No vertical wind components.
b) **Source terms/background:** Hourly emission rates.
c) **Mesh/grids:** SRL Kr-85 source data
33x33x8 grids. 5 km spacing on X and Y. 100 m spacing on Z.

Error Estimates:

Applicability:

Time periods used for workshop:
1600 10/05/76 → 1700 10/06/76; 300 02/16/77 → 1700 02/19/77;
1200 04/05/77 → 1300 04/09/77; 2000 07/10/77 → 500 07/13/77.

Available? No **Documented?** No **Computer type:** IBM 360/195

Core size: 1100K **Running time (SRP data)** 0.35 sec/iteration

Developed by: R. E. Cooper

Reference: R. H. Sklarew, A. J. Fabrick, and J. E. Prager. "A Particle-In-Cell Method for Numerical Solution of the Atmospheric Diffusion Equation, and Applications to Air Pollution Problems." Systems, Science, and Software Report 35R-844, La Jolla, CA (1971).

SRL Wind Field Analysis (A. J. Garrett)

The basic philosophy of the SRL wind field analysis codes was twofold: (1) keep the mathematics of the analysis simple, and (2) make as few assumptions about atmospheric structure as possible. The procedure that was finally developed is summarized by the flow chart in Figure IV-1. The three sources of raw wind data were National Weather Service (NWS) surface and rawinsonde stations, and a variety of privately owned meteorological towers. The towers and their locations, and the NWS stations are described in detail by Telegadas, et al.[4]

The sparse upper-air stations forced considerable interpolation in time and space in order to generate three-dimensional winds. First, the rawinsonde winds were linearly interpolated in time to provide hourly wind data, in accordance with the surface stations and towers. These hourly data were then interpolated in space to each tower or surface station location. The weighting function (W) used for the space interpolation is defined by:

$$W = EXP\ [-(R/D)^2] \qquad (1)$$

Where R is the distance between a rawinsonde and a surface station and D is mean station spacing (250 km).

Barnes[9] first used Equation 1 in objective analyses of mesoscale and synoptic scale winds and pressure fields. The interpolated variable (V) at a surface station (i) is thus

$$V\ (i) = \sum_{k=1}^{K} W\ (k) \times V\ (k) / \sum_{k=1}^{K} W\ (k) \qquad (2)$$

where k refers to one of a total of K rawinsonde stations.

After these artificial soundings were built at each surface station and tower location, vertically interpolating polynomials of the form

$$V\ (h) = bh + ch^2 + \frac{d}{h} + \frac{e}{h^2} \qquad (3)$$

were fitted to the wind data. In Equation 3, h is the natural logarithm of height above the surface, and b, c, d, and e are constants which are determined by a least squares fit. The decision to use Equation 3 for vertical interpolation of winds was based on two considerations: (1) some continuity was forced on the wind profiles, and (2) interpolating vertically from observed points to grid points was simpler.

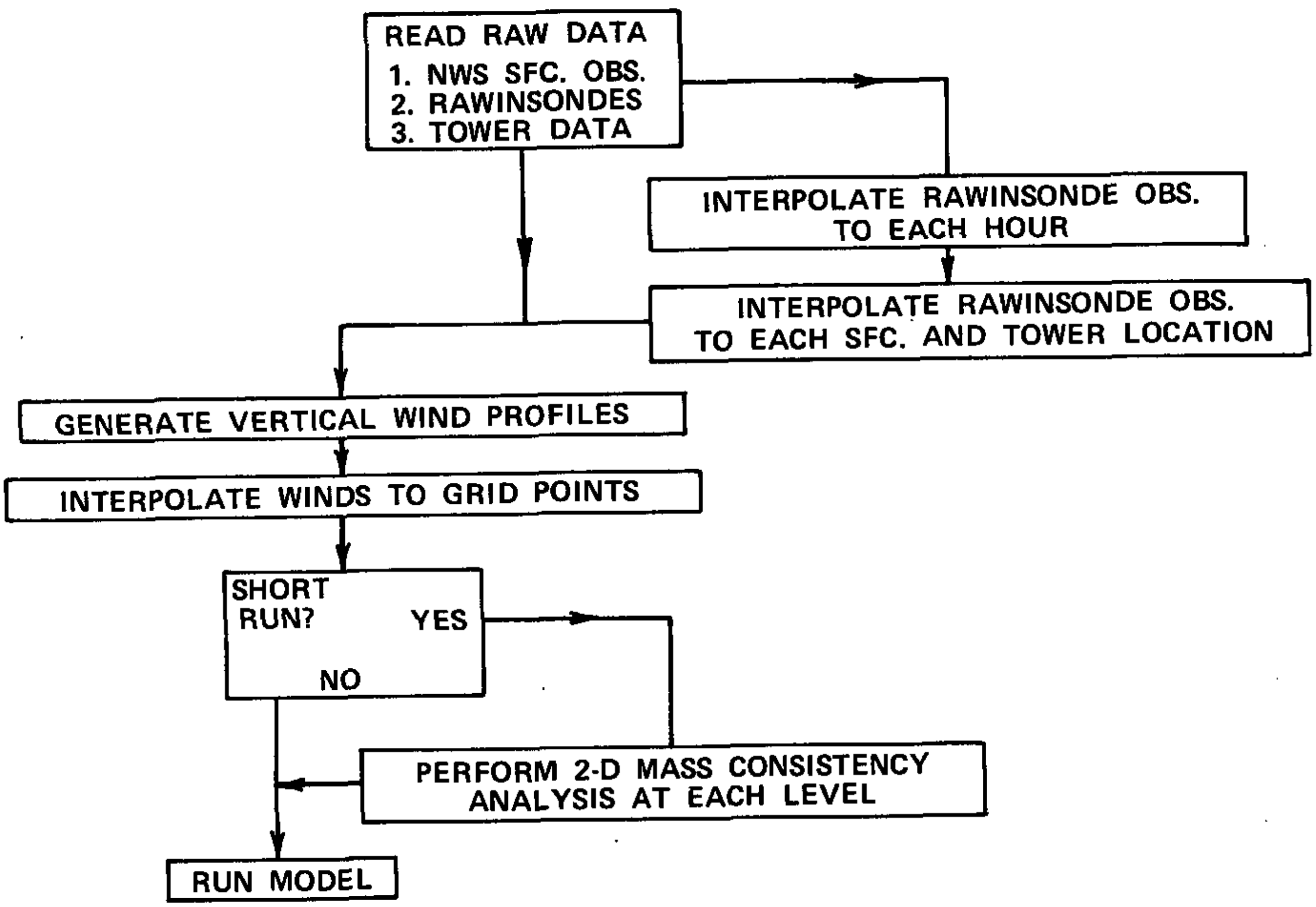

FIGURE IV-1. Flow Chart for SRL Wind Field Analysis Method

Final steps of the wind field analysis were model-dependent. Simpler models, such as the Gaussian Model ADPLUM, used a procedure almost identical to Equations 1 and 2 to interpolate from station locations to grid points (see Reference 10 for details). The three-dimensional models used Equations 1 and 2 to interpolate to grid points. In addition, the horizontal winds were constrained to be non-divergent at each grid level, i.e.:

$$\frac{\partial u}{\partial x} + \frac{\partial u}{\partial y} = 0 \qquad (4)$$

The variational method used to apply the constraint in Equation 4 to the winds is described by Sasaki.[11,12]

V. RESULTS AND STATISTICAL ANALYSIS (A. H. Weber)

Basis for Model Comparisons

Models have been categorized in terms of the time period over which the results are averaged:

- Annual
- Monthly
- Weekly
- Twice-daily

The models were evaluated subjectively by examining statistical parameters in the following order:

- Number of predictions (N)
- R, ρ, and/or τ
- Bias and/or RMSE
- Band (K)

The slope estimate and regression statistics based on the logarithms of predicted and measured concentrations were calculated but were not found to change the conclusions about model performance. Thus, those statistics are not presented in the discussions that follow.

Provided a sufficient number of predictions were available, Pearson's R was considered to be the most important statistic of the group because it is the most sensitive to changes in values of predicted and measured quantities; however, R is sensitive to outliers. Spearman's ρ and Kendall's τ were allowed to change the relative evaluation if analysis of other statistical parameters indicated that a high R was simply fortuitous. A regression line slope of one is desirable because that indicates that predicted concentration is equal to measured plus a constant bias. When the slope is not equal to one, the relation between M and P can still be strong, but the prediction model can no longer be corrected by subtracting the bias. When R is small, there is no relationship between measured and predicted concentration, i.e., one could do as well by drawing a predicted value at random and using it. This is true no matter what regression line is fit through the data.

The treatment of outliers and PNOs was also considered in the comparison of the statistical results. Outliers usually occur as a single value or a pair of values which appear to have little or no relationship to the bulk of the data or to another outlier. They are unfortunate results of limited sample size at the higher values in the data set. The major objection to outliers is that they can completely dominate the regression line parameters such as slope, intercept, and R^2 value. These outliers prevent using the slope and intercept for feedback to improve the models. Two things can be done with outliers depending on one's point of view: they can be retained or thrown out. If one is interested in the second highest predicted or measured value (as per EPA guidelines), then outliers need to be retained. For the purpose of these model evaluations, almost all outliers were eliminated. (In a few cases, the decision as to whether or not a point qualified as an outlier was difficult, and in those cases the points were retained.) By removing outliers, a representative regression line could be determined which can be used to improve model performance. The confidence in the Pearson correlation coefficient which was used as a primary evaluation statistic was also improved. Robust statistics such as Spearman's ρ and Kendall's τ tend to be insensitive to outliers.

PNOs may also strongly bias the statistical results without demonstrating the accuracy of a model. In the lifetime of a sampling station, the interception of the plume is a relatively rare event so that for shorter sampling times zero is a good, safe prediction. In evaluating the short-term prediction models, model performance could be tested more stringently by eliminating PNOs. Therefore, for weekly and twice-daily models, both sets of statistics are presented, i.e., with PNOs retained and deleted. Pearson's R was found to be rather insensitive to PNOs; whereas, the robust parameters ρ and τ were changed considerably.

In the sections that follow, statistical results are presented for the model comparisons with the Kr-85 data. As stated earlier, the comparisons are for the four basic sampling periods considered (annual, monthly, weekly, and twice-daily). In several cases, participants were able to provide predictions for only a very few time periods; thus, statistically significant comparisons were not possible. These included the results for the DISTHEATCENT models, as well as the 3-dimensional models except for the SRL CHAPEAU, MOMENTS, and PIC models and the LANL ATMOS model. The last section presents a comparison of several models for a common data base.

Annual Predictions

The group of annual prediction models tend to have significant correlation between the predicted and the measured concentrations. A large fraction of the variation can be explained by a linear model. The statistical parameters for the models are listed in Table V-1.

TABLE V-1

Statistical Results for Annual Predictions

Model	N	R	R^2	Avg. Bias, pCi/m^3	RMSE, pCi/m^3	K	Slope
AIRDOS-EPA	13	0.98	0.97	-29	31	1	1.7
XOQDOQ	13	0.89	0.80	-31	35	2	1.4
Shear-Rose	13	0.68	0.46	-12	26	3	0.9

All models in this group have a negative average bias. The slope of the linear regression lines for two of the models tend to have a slope greater than one indicating an overprediction. The average R^2 for this group was 0.74 so about three-fourths of the variation in this group was explained by a linear model.

Based on the statistical results, the AIRDOS-EPA model was superior to the other models used for annual predictions. The superiority of the AIRDOS-EPA model can perhaps be attributed to better estimates of mixed-layer depth. AIRDOS-EPA used averaged mixed-layer depths taken from acoustic sounder records. XOQDOQ used a constant mixed-layer depth of 1000 m.

The relatively poor performance of SHEAR-ROSE could be caused by its attempt to use hourly emissions and wind data to calculate a more accurate source term for each sector. Another possibility is that the horizontal diffusivities used by SHEAR-ROSE are sensitive to errors in the wind field analysis. Another factor influencing the SHEAR-ROSE model is that sectors can "spill" unaccounted pollutant from one sector to another. This could cause the relatively lower bias and slope for the SHEAR-ROSE results.

In conclusion, the annual models appear to need only annual average emissions and meteorological data to give a good fit to measurements. Overprediction by annual models is probably caused by underestimation of the effective mixed-layer depth which includes the effects of convective clouds and large scale convective motions.

Monthly Predictions

The group of monthly prediction models had representatives from most of the participating laboratories. Table V-2 shows the range of values of the statistics. The models are listed in

Table V-2 based on the Pearson R statistic. The ASTRAP and AIRDOS-EPA models had the highest R values for this group. Examination of Spearman's ρ and Kendall's τ shows that the models do not differ greatly except for DRAX1 and ANDEP.

TABLE V-2

Statistical Results for Monthly Predictions

Model	N	R	ρ	τ	Bias, pCi/m^3	RMSE, pCi/m^3	K	Slope	R^2
ASTRAP	295	0.75	0.69	0.51	0.2	18	0.75	0.59	0.56
AIRDOS-EPA	155	0.65	0.72	0.54	-30	53	10	1.22	0.43
XOQDOQ	309	0.56	0.65	0.47	-36	62	10	1.20	0.31
ATM	335	0.43	0.60	0.43	-39	70	10	1.02	0.18
DRAX1	193	0.42	0.51	0.36	5	28	1	0.43	0.18
ANDEP	348	0.31	0.33	0.22	6	32	2	0.31	0.10

The average bias is negative, but half the group had a small positive bias. For three of the models the estimate of regression line slope was less than one indicating an underprediction. The other three had estimates of slope greater than one for an overprediction. The ATM model results had a slope closest to the desired value of one; however, the bias for this model was the largest, indicating an overprediction over the range of measurements. The ASTRAP, DRAX1, and ANDEP models had small positive biases and their RMSE errors were also the smallest.

The ASTRAP model had the smallest bandwidth which included 95% of its predictions. While the slope of the regression line did not approach the desired value of one, the model did predict the measured concentrations with reasonable success.

The ASTRAP model with its diurnally varying K_z seems to have the most physically correct representation of the processes so it is gratifying to see that it was at the top of the group. The bandwidth of the three middle-ranked models is larger than would have been expected.

As a group the monthly models are less accurate than the annual models. The weighted average* R^2 for this group is 0.28 compared to 0.74 for the annual models.

Using the slope criterion the XOQDOQ and ATM models perform best, but they had large absolute values of bias and large bandwidths were necessary to include 95% of the data.

Table V-2 shows that each laboratory made predictions for a different number of cases. It is difficult to make meaningful comparisons of statistical parameters under those circumstances. In order to make direct comparisons of the models a merged data set was formed. This merged data set had only those time periods which were common to a particular group of laboratories. The statistical results for the merged data sets are summarized in the Comparison Section (page 66).

Weekly Predictions

Weekly prediction models show a degradation in the predictions compared with monthly models. The weighted average correlation coefficient (R^2) is 0.21 compared with 0.28 for monthly and 0.74 for annual models. Results are shown in Table V-3.

---

* Weighted by the number of observations; e.g., if N_i is the number of observations and X_i is the value of the statistic for the i^{th} model, then

$$\text{weighted average } \bar{x} = \sum_{i=1}^{m} N_i X_i \Big/ \sum_{i=1}^{m} N_i$$

where m is total number of models for a particular category.

TABLE V-3

Statistical Results for Weekly Predictions (PNOs Included)

Model	N	R	ρ	τ	Bias, pCi/m^3	RMSE, pCi/m^3	K	Slope	R^2
ATAD	497	0.48	0.68	0.52	2	62	3	0.58	0.23
DRAX2	419	0.48	0.72	0.54	-8	90	5	0.75	0.23
ADPLUM	258	0.36	0.50	0.35	19	47	1	0.09	0.13
DRAGONGP*	66	0.51	0.43	0.29	-429	900	>10	8.7	0.26
DRAGONTH*	66	0.39	0.38	0.27	-128	292	>10	2.1	0.16
DRAGONTHP*	66	0.39	0.39	0.29	-158	362	>10	2.5	0.16

* See model description.

The DRAX2 model has a provision for changing atmospheric stability along the plume trajectory. Surface and upper air wind observations are used. The ATAD model uses transport winds averaged over a vertical layer. These two models performed best of the group of models used for weekly predictions. Statistically significant differences between the two were hard to distinguish.

Model performance of the remaining four models was fairly uniform. There seemed to be no significant statistic to recommend one model over the other. The segmented Gaussian plume model (ADPLUM) had a rather restricted range of prediction although a total of 258 cases were considered. The DRAGON models considered 66 cases, but the range of prediction was comparable with ATAD and DRAX2. The DRAGON models use a trajectory-puff concept similar to ADPLUM and, thus, it is not surprising that model performance is similar.

There is very little difference in R values between the ATAD or DRAX2 models and the DRAGONGP model (see Table V-3), but there was in the Spearman ρ and Kendall's τ correlations. Again there was little difference between ATAD and DRAX2. The difference between these two models is the bandwidth necessary to include 95% of the values and in the smaller root mean square error for the ATAD model. On this basis, the ATAD model is listed first and DRAX2 is listed second. The ADPLUM model is listed ahead of the DRAGONGP model on the basis of a larger Spearman's ρ and Kendall's τ, plus a smaller bias and root mean square error and smaller bandwidth. The only criterion for which DRAGONGP would rank above

ADPLUM is using the Pearson R, but since the difference between the R values did not seem as important as the difference in the other variables, the rankings were not changed. There is little difference between the last two models, DRAGONTH and DRAGONTHP, for any of the parameters.

In order to evaluate the effect of PNOs, statistics were calculated for the results with values less than 5 pCi/m^3 for both measured and predicted concentrations excluded. As shown in Table V-4, the same two models displayed the best predictive capability. However, the non-parametric correlations are significantly smaller. The bias, RMSE, bandwidth, and slope do not change significantly.

TABLE V-4

Statistical Results for Weekly Predictions (PNOs Excluded)

Model	N	R	ρ	τ	Bias, pCi/m^3	RMSE, pCi/m^3	K	Slope	R^2
ATAD	349	0.41	0.44	0.30	3	74	3	0.51	0.17
DRAX2	304	0.43	0.49	0.34	-12	106	5	0.68	0.18
ADPLUM	180	0.25	0.13*	0.08*	27	56	1	0.07	0.06
DRAGONGP**	63	0.50	0.39	0.26	-450	921	>10	8.6	0.25
DRAGONTH**	58	0.37	0.29	0.21	-139	304	>10	2.0	0.14
DRAGONTHP**	60	0.38	0.34	0.24	-166	370	>10	2.4	0.14

* Not statistically significant from zero at the 95% level.

** See model description.

For ADPLUM, the correlation coefficients, especially Spearman's ρ and Kendall's τ, are significantly decreased, which puts ADPLUM at the bottom of the list based on the correlation coefficients. The bias, RMSE, bandwidth, and slope do not change much. The three DRAGON models were less affected by PNOs (probably because they had fewer of them).

Again, direct comparison of the models is difficult unless a common data set is available. This was done, and the results are discussed in the Comparison Section (page 69).

Twice-Daily Predictions

As with the weekly data sets, statistics for the twice-daily data were run twice: including and then excluding PNOs. PNOs in this case were defined as values for which the measured and computed values were simultaneously below 10 pCi/m^3. The latter case resulted in including only the data that were significantly above background. The two sets of results are shown in Tables V-5 and V-6. With PNOs included, the Pearson's R value is statistically different from zero at the 95% level for all seven models listed. With PNOs excluded, only three of the seven have statistically significant R values. ATMOS and DRAX2 are the only models with both ρ and τ values statistically different from zero at the 95% level. Root mean square error was uniformly highest for this group averaging about 240 pCi/m^3. ATMOS and ADPLUM were the only models with a bandwidth less than a factor of 10 that contained 95% of the data.

TABLE V-5

Statistical Results for Twice-Daily Predictions (PNOs Included)

Model	N	R	ρ	τ	Bias, pCi/m^3	RMSE, pCi/m^3	K	Slope	R^2
DRAX2	381	0.49	0.61	0.47	-0.5	201	>10	0.73	0.24
ATMOS	93	0.80	0.67	0.53	-2	87	2	1.05	0.63
CHAPEAU	103	0.64	0.47	0.40	-41	167	>10	1.28	0.41
MOMENTS	103	0.35	0.61	0.54	-18	154	>10	0.52	0.12
PIC	103	0.25	0.63	0.54	-15	163	>10	0.37	0.06
ATAD	341	0.21	0.50	0.41	23	229	>10	0.11	0.04
ADPLUM	273	0.34	0.29	0.23	7	46	.75	0.11	0.12

TABLE V-6

Statistical Results for Twice-Daily Predictions (PNOs Excluded)

Model	N	R	ρ	τ	Bias, pCi/m^3	RMSE, pCi/m^3	K	Slope	R^2
DRAX2	159	0.43	0.19	0.13	0.3	310	>10	0.39	0.19
ATMOS	38	0.75	0.52	0.38	-7	137	2	1.05	0.57
CHAPEAU	54	0.60	0.24*	0.16*	-77	230	>10	1.2	0.35
MOMENTS	36	0.14*	0.18*	0.13*	-52	260	>10	0.03	0.02
PIC	39	0.05*	0.19*	0.10*	-41	265	>10	0.07	0.00
ATAD	136	0.10*	-10*	-0.06*	56	363	>10	0.05	0.01
ADPLUM	41	0.11*	-0.16	-0.09	38	117	>10	0.03	0.01

* Not statistically significant at the 0.05 level.

Statistical analyses of results for the ATMOS and SRL 3-D models are less meaningful, in a statistical sense, than for the other models because of the small amount of data processed. The amount of data processed by the 3-dimensional models was limited in most cases because of the amount of computer time required to process the meteorological data was prohibitive. Because of the varying numbers of points in the data sets, a ranking of these models is not appropriate.

Because most of the models in this group were outside the bands, an alternate criterion was set up for K. If only 80% of the data is required to be within the bands, then the results for twice-daily predictions are given in Table V-7.

TABLE V-7

K Values Determined by Allowing 80% of the Data Within the Bands

Model	K*	K**
ATMOS	1.0	0.5
DRAX2	>10	0.75
ATAD	10	1.0
ADPLUM	1.0	0.5
MOMENTS	10	0.5
PIC	>10	0.75
CHAPEAU	>10	10

* PNOs excluded

** PNOs included

Comparison of measurements and computed results for the SRL 3-D models are shown in Table V-8 where measurements or estimates were significant. Differences between measurements and estimates are attributed to be due to the errors of the following type:

1. Kr-85 measurement.
2. Meteorology measurement.
3. Modeling physics.
4. Numerical computation.
5. Boundary treatment.
6. Source term specifications.

It is presently impossible to quantify these errors on an absolute basis. However, it is obvious that the wind field ascribed to the computational domain is crucial for isolated field positions. The SRL models all used the same hourly computed mass consistent wind fields which were derived from analyzing essentially instantaneously measured data. The results of Table V-8 show a high correlation between the SRL codes. This indicates that erroneous advective transport direction may be a large factor in differences between measurement and calculation.

TABLE V-8

Measured and Calculated Integral Concentrations for SRL 3-D Models

Day	Hour	Sta*	Integral Ground-Level Concentration, pCi				
			Meas	CHP	FFT	MOM	PIC
100576	2200	12	0	0	6	0	0
100576	2200	14	660	1595	1595	410	673
40677	1000	7	184	189	-	242	106
40677	1000	8	616	2	-	134	125
40677	2200	7	128	215	-	59	260
40677	2200	8	157	186	-	107	178
40777	2200	10	147	348	-	347	240
40777	2200	11	-	151	-	168	357
71077	2100	8	-	390	0	159	184
		9	-	98	73	68	106
		10	-	121	79	9	0
		11	0	0	12	0	0
71177	900	7	3	174	-	4	162
		8	15	6	-	0	0
		9	111	16	-	40	6
		10	27	0	-	0	0
71277	900	8	0	640	-	722	426
		9	10	536	-	347	291
		10	146	531	-	739	864
		11	59	598	-	616	874
		12	-	168	-	266	202
		13	95	111	-	109	154

* Station number as shown in Figure 1.

Comparison of Monthly, Weekly, and Twice-Daily Predictions Over a Common Data Base

As mentioned previously, statistical results for the various model classes are difficult to compare unless a common data set exists. Initially the participants sent in results representing a wide range of prediction times. Using the data management features of the SAS statistical package, common data sets were formed for monthly, weekly, and twice-daily categories to evaluate models on a more equal basis. Also, the common data set could be used to correlate model predictions with the others in each category. The results of these comparisons are shown in Table V-9 through V-17 for several different groupings. The groupings were varied to maximize the number of predicted concentrations and to include as many models as possible in the comparisons.

Tables V-9, V-10, and V-11 show that comparing the models over a common data set tends to reduce the variability between models. When compared over a common data set, there is little difference among AIRDOS-EPA, XOQDOQ, and ATM. Using the robust parameters ρ and τ, ASTRAP, AIRDOS-EPA, XOQDOQ, and ATM are very similar; however, ASTRAP consistently had the smallest bias, RMSE, and bandwidth.

TABLE V-9

Statistical Results for Monthly Prediction Models with a Common Data Base (N=142)

Model	N	R	ρ	τ	Bias, pCi/m^3	RMSE, pCi/m^3	K	Slope	R
ASTRAP	142	0.78	0.73	0.55	3	18	0.75	0.62	0.60
ATM	142	0.70	0.71	0.52	-33	51	10	1.31	0.49
AIRDOSE-EPA	142	0.69	0.70	0.53	-34	55	10	1.38	0.47
XOQDOQ	142	0.68	0.69	0.50	-35	57	10	1.40	0.46
ANDEP	142	0.22	0.25	0.17	9	36	1	0.21	0.05

TABLE V-10

Statistical Results for Monthly Prediction Models with a Common Data Base (N=140)

Model	N	R	ρ	τ	Bias, pCi/m^3	RMSE, pCi/m^3	K	Slope	R^2
ASTRAP	140	0.67	0.67	0.49	0.3	19	1	0.56	0.45
ATM	140	0.62	0.68	0.50	-33	49	10	1.19	0.38
XOQDOQ	140	0.59	0.67	0.48	-32	53	10	1.25	0.35
DRAX1	140	0.46	0.55	0.39	4.1	28	1	0.53	0.21
ANDEP	140	0.27	0.29	0.20	4	31	1	0.30	0.07

TABLE V-11

Statistical Results for Monthly Prediction Models with a Common Data Base (N=64)

Model	N	R	ρ	τ	Bias, pCi/m^3	RMSE, pCi/m^3	K	Slope	R^2
ASTRAP	64	0.68	0.68	0.50	4	22	1	0.58	0.46
AIRDOS-EPA	64	0.62	0.64	0.48	-39	56	10	1.13	0.38
ATM	64	0.59	0.70	0.51	-37	58	10	1.16	0.35
XOQDOQ	64	0.57	0.70	0.51	-34	60	10	1.23	0.33
DRAX1	64	0.42	0.47	0.32	8	35	0.75	0.50	0.17
ANDEP	64	0.38	0.27	0.20	10	30	0.75	0.31	0.14

Tables V-12, V-13, and V-14 present correlations between models for the monthly predictions using common data sets. A very high correlation of ~0.98 exists between XOQDOQ and ATM. ATM, XOQDOQ, and AIRDOS-EPA are also well correlated with ASTRAP with a value of about 0.80 for each.

TABLE V-12

Range of Pearson Correlation Coefficients Among Monthly Models for Predicted Concentration for Three Different Groupings of Data (N = 64, 140, and 142)

	ASTRAP	AIRDOS-EPA	ATM	XOQDOQ	DRAX1	ANDEP	Measured Concentrations
ASTRAP	1.00	0.81-0.82	0.73-0.80	0.76-0.81	0.72	0.37-0.68	0.65-0.78
AIRDOS-EPA	0.81-0.82	1.00	0.55-0.70	0.57-0.69	0.56	0.16-0.59	0.62-0.69
ATM	0.73-0.80	0.55-0.70	1.00	0.98-0.99	0.42-0.48	0.15-0.47	0.59-0.70
XOQDOQ	0.76-0.81	0.57-0.69	0.98-0.99	1.00	0.46-0.50	0.19-0.51	0.57-0.68
DRAX1	0.72	0.56	0.42-0.48	0.46-0.50	1.00	0.47-0.85	0.42-0.46
ANDEP	0.37-0.68	0.16-0.59	0.15-0.47	0.19-0.51	0.47-0.85	1.00	0.22-0.38
Measured Concentrations	0.67-0.78	0.62-0.69	0.59-0.70	0.57-0.68	0.42-0.46	0.22-0.38	1.00

TABLE V-13

Range of Spearman Correlation Coefficients Among Monthly Models for Predicted Concentration for Three Different Groupings of Data (N = 64, 140, and 142)

	ASTRAP	AIRDOS-EPA	ATM	XOQDOQ	DRAX1	ANDEP	Measured Concentrations
ASTRAP	1.00	0.74-0.77	0.73-0.75	0.70-0.77	0.66-0.68	0.25-0.35	0.67-0.73
AIRDOS-EPA	0.74-0.77	1.00	0.79-0.82	0.71-0.81	0.56	0.16-0.34	0.64-0.70
ATM	0.73-0.75	0.79-0.82	1.00	0.96-0.99	0.55-0.56	0.15-0.34	0.68-0.71
XOQDOQ	0.70-0.77	0.71-0.81	0.96-0.99	1.00	0.57-0.61	0.15-0.39	0.67-0.70
DRAX1	0.66-0.68	0.56	0.55-0.56	0.57-0.61	1.00	0.27-0.31	0.47-0.55
ANDEP	0.25-0.35	0.16-0.34	0.15-0.34	0.15-0.39	0.27-0.31	1.00	0.25-0.29
Measured Concentrations	0.67-0.73	0.64-0.70	0.68-0.71	0.67-0.70	0.47-0.55	0.25-0.29	1.00

TABLE V-14

Range of Kendall Correlation Coefficients Among Monthly Models for Predicted Concentration for Three Different Groupings of Data (N=64, 140, and 142)

	ASTRAP	AIRDOS-EPA	ATM	XOQDOQ	DRAX1	ANDEP	Measured Concentrations
ASTRAP	1.00	0.56-0.59	0.55-0.57	0.53-0.59	0.51	0.17-0.23	0.49-0.55
AIRDOS-EPA	0.56-0.59	1.00	0.59-0.62	0.52-0.62	0.41	0.11-0.24	0.48-0.53
ATM	0.55-0.57	0.59-0.62	1.00	0.85-0.93	0.38-0.40	0.10-0.23	0.50-0.52
XOQDOQ	0.53-0.59	0.52-0.62	0.85-0.93	1.00	0.42	0.10-0.27	0.48-0.51
DRAX1	0.51	0.41	0.38-0.40	0.42	1.00	0.19-0.22	0.32-0.39
ANDEP	0.17-0.23	0.11-0.24	0.10-0.23	0.10-0.27	0.19-0.22	1.00	0.17-0.20
Measured Concentrations	0.49-0.55	0.48-0.53	0.50-0.52	0.48-0.51	0.32-0.39	0.17-0.20	1.00

A similar procedure was followed to form a common data set for weekly prediction values. Tables V-15 through V-19 show the results. DRAX2 seems to stand above others for the first grouping (N=61). The coefficients for ATAD are comparable with the DRAGON models, but the bias and RMSE are considerably less. For the second grouping (N=125, Table V-16), ATAD performs as good as, or slightly better than, DRAX2. The three DRAGON models are highly correlated with one another, as seen in Tables V-17 through V-19, but others in the group are only moderately correlated.

TABLE V-15

Statistical Results for Weekly Prediction Models with a Common Data Base (N=61) PNOs Included

Model	N	R	ρ	τ	Bias, pCi/m^3	RMSE, pCi/m^3	K	Slope	R^2
DRAX2	61	0.50	0.58	0.42	-3	51	5	0.57	0.25
ATAD	61	0.32	0.43	0.30	-3	70	>10	0.44	0.10
DRAGONGP	61	0.47	0.43	0.29	-425	877	>10	7.67	0.22
DRAGONTHP	61	0.39	0.36	0.26	-142	338	>10	2.62	0.15
DRAGONTH	61	0.38	0.34	0.25	-118	283	>10	2.14	0.14
ADPLUM*	-	-	-	-	-	-	-	-	-

* ADPLUM had no cases in common with DRAGON models

TABLE V-16

Statistical Results for Weekly Prediction Models with a Common Data Base (N=125 PNOs Included)

Model	N	R	ρ	τ	Bias, pCi/m^3	RMSE pCi/m^3	K	Slope	R^2
DRAX2	125	0.38	0.71	0.52	-17	109	10	0.84	0.15
ATAD	125	0.54	0.72	0.53	6	55	3	0.61	0.30
ADPLUM	125	0.34	0.42	0.29	28	57	1	0.10	0.12
DRAGONGP*	-	-	-	-	-	-	-	-	-
DRAGONTHP*	-	-	-	-	-	-	-	-	-
DRAGONTH*	-	-	-	-	-	-	-	-	-

* ADPLUM had no cases in common with DRAGON models.

TABLE V-17

Range of Pearson Correlation Coefficients Among Weekly Models For Predicted Concentrations for Two Different Groupings of Data (N = 61 and 125; PNOs Included)

	DRAGONGP	DRAGONTHP	DRAGONTH	DRAX2	ATAD	ADPLUM	Measured Concentrations
DRAGONGP	1.00	0.87	0.86	0.50	0.27	-	0.47
DRAGONTHP	0.87	1.00	0.98	0.58	0.25	-	0.39
DRAGONTH	0.86	0.98	1.00	0.53	0.27	-	0.38
DRAX2	0.50	0.58	0.53	1.00	0.31-0.48	0.49	0.38-0.50
ATAD	0.27	0.25	0.27	0.31-0.48	1.00	0.34	0.32-0.54
ADPLUM	-	-	-	0.49	0.34	1.00	0.34
Measured Concentrations	0.47	0.39	0.38	0.38-0.50	0.32-0.54	0.34	1.00

TABLE V-18

Range of Spearman Correlation Coefficients Among Weekly Models for Predicted Concentration for Two Different Groupings of Data (N = 61 and 125; PNOs Included)

	DRAGONGP	DRAGONTHP	DRAGONTH	DRAX2	ATAD	ADPLUM	Measured Concentrations
DRAGONGP	1.00	0.89	0.87	0.34	0.29	-	0.43
DRAGONTHP	0.89	1.00	0.99	0.37	0.28	-	0.36
DRAGONTH	0.87	0.99	1.00	0.35	0.26	-	0.34
DRAX2	0.34	0.37	0.35	1.00	0.63-0.80	0.42	0.58-0.71
ATAD	0.29	0.28	0.26	0.63-0.80	1.00	0.35	0.43-0.72
ADPLUM	-	-	-	0.42	0.35	1.00	0.42
Measured Concentrations	0.43	0.36	0.34	0.58-0.71	0.43-0.72	0.42	1.00

TABLE V-19

Range of Kendall Correlation Coefficients Among Weekly Models for Predicted Concentration for Two Different Groupings of data (N = 61 and 125; PNOs Included)

	DRAGONGP	DRAGONTHP	DRAGONTH	DRAX2	ATAD	ADPLUM	Measured Concentrations
DRAGONGP	1.00	0.72	0.68	0.25	0.20	-	0.29
DRAGONTHP	0.72	1.00	0.95	0.28	0.19	-	0.26
DRAGONTH	0.68	0.95	1.00	0.26	0.18	-	0.25
DRAX2	0.25	0.28	0.26	1.00	0.46-0.62	0.31	0.42-0.52
ATAD	0.20	0.19	0.18	0.46-0.62	1.00	0.25	0.30-0.53
ADPLUM	-	-	-	0.31	0.25	1.00	0.29
Measured Concentrations	0.29	0.26	0.25	0.42-0.52	0.30-0.53	0.29	1.00

Table V-20 shows the statistics for twice-daily models using a common data base. The large value of R^2 for ATMOS is a result of outliers (see Figure C-30)* because the nonparametric statistics ρ and τ are almost identical to those of DRAX2. These statistics yield similar conclusions and relative evaluations of the models.

TABLE V-20

Statistical Results for Twice-Daily Prediction Models with a Common Data Base (N=64; PNOs Included)

Model	N	R	ρ	τ	Bias, pCi/m^3	RMSE, pCi/m^3	K	Slope	R^2
ATMOS	64	0.81	0.68	0.56	7	83	1	1.13	0.65
DRAX2	64	0.53	0.68	0.55	1	93	2	0.51	0.28
CHAPEAU	64	0.50	0.32	0.24	-13	107	>10	0.57	0.25
MOMENTS	64	0.35	0.58	0.48	3	96	2	0.41	0.12
PIC	64	0.36	0.60	0.48	3	119	2	0.40	0.13
ATAD	64	0.24	0.48	0.39	35	35	1	0.06	0.06
ADPLUM*	-	-	-	-	-	-	-	-	-

* ADPLUM had only 4 cases in common with the other models.

The high degree of correlation shown between the SRL three dimensional models is evident in Table V-21. Tables V-22 and V-23 show high correlations between PIC and MOMENTS which is not too surprising. The values of ρ and τ for SRL three-dimensional models was expected to be higher.

In conclusion, the statistics in this section have resulted in conclusions similar to those in earlier sections. The models within a given group correlate better with each other than with the measured concentration.

* Two points which could have been classed as outliers were retained as a result of a discussion with the LANL participants. The CHAPEAU model was also allowed a single outlier after a similar discussion with SRL modelers. These are the only two conscious exceptions to the general policy of omitting outliers.

TABLE V-21

Pearson Correlation Coefficients Among Twice-Daily Models for Predicted Concentrations for a Single Grouping of Data (N = 64; PNOs Included)

	ATMOS	DRAX2	CHAPEAU	MOMENTS	PIC	ATAD	ADPLUM*	Measured Concentrations
ATMOS	1.00	0.53	0.64	0.48	0.47	0.14	-	0.81
DRAX2	0.53	1.00	0.62	0.68	0.74	0.13	-	0.53
CHAPEAU	0.64	0.62	1.00	0.88	0.91	0.17	-	0.50
MOMENTS	0.48	0.68	0.88	1.00	0.94	0.25	-	0.35
PIC	0.47	0.74	0.91	0.94	1.00	0.15	-	0.36
ATAD	0.14	0.13	0.17	0.25	0.15	1.00	-	0.24
ADPLUM*	-	-	-	-	-	-	-	-
Measured Concentrations	0.81	0.53	0.50	0.35	0.36	0.24	-	1.00

* ADPLUM had only four cases in common with the other models.

TABLE V-22

Spearman Correlation Coefficients Among Twice-Daily Models for Predicted Concentrations for a Single Grouping of Data (N = 64; PNOs Included)

	ATMOS	DRAX2	CHAPEAU	MOMENTS	PIC	ATAD	ADPLUM*	Measured Concentrations
ATMOS	1.00	0.66	0.53	0.71	0.76	0.42	-	0.68
DRAX2	0.66	1.00	0.49	0.72	0.75	0.35	-	0.68
CHAPEAU	0.53	0.49	1.00	0.64	0.62	0.15	-	0.32
MOMENTS	0.71	0.72	0.64	1.00	0.94	0.34	-	0.58
PIC	0.76	0.75	0.62	0.94	1.00	0.32	-	0.60
ATAD	0.42	0.35	0.15	0.34	0.32	1.00	-	0.48
ADPLUM*	-	-	-	-	-	-	-	-
Measured Concentrations	0.68	0.68	0.32	0.58	0.60	0.48	-	1.00

* ADPLUM had only four cases in common with the other models.

TABLE V-23

Kendall Correlation Coefficients Among Twice-Daily Models for Predicted Concentrations for a Single Grouping of Data (N = 64; PNOs Included)

	ATMOS	DRAX2	CHAPEAU	MOMENTS	PIC	ATAD	ADPLUM*	Measured Concentrations
ATMOS	1.00	0.58	0.46	0.65	0.71	0.39	-	0.56
DRAX2	0.58	1.00	0.41	0.63	0.66	0.30	-	0.55
CHAPEAU	0.46	0.41	1.00	0.57	0.54	0.12	-	0.24
MOMENTS	0.65	0.63	0.57	1.00	0.89	0.31	-	0.48
PIC	0.71	0.66	0.54	0.89	1.00	0.29	-	0.48
ATAD	0.39	0.30	0.12	0.31	0.29	1.00	-	0.39
ADPLUM*	-	-	-	-	-	-	-	-
Measured Concentrations	0.56	0.55	0.24	0.48	0.48	0.39	-	1.00

* ADPLUM had only four cases in common with the other models.

VI. GENERAL CONCLUSIONS AND RECOMMENDATIONS

The general purpose of the workshop was to test new and existing atmospheric transport models in use at DOE laboratories with a common measurement and meteorological data base. Although this very ambitious undertaking was not completely fulfilled, the workshop does represent a first step in this process. Further steps in the process will include detailed study and analysis of the workshop results, further comparisons of models with the SRL Kr-85 data base, and perhaps other workshops in which this data base is used as a standard for comparison of different models.

The principal benefits of the workshop were:

- Evaluation of mesoscale models based on an actual 2-1/2 year set of dispersion measurements and meteorology out to distances of 150 km from the source.
- Quantification of the relative accuracy achievable for different predictive time scales.
- Better understanding of research needs in the areas of mesoscale modeling and wind analysis.
- Development and use of statistical evaluation tests to analyze the validity of the model and data set.

Many participants and observers felt that a second workshop should be conducted, with participation open to private and foreign industry, as well as to government-sponsored agencies. Considerable effort has gone into obtaining and formalizing the data base, which is one of the most extensive data sets available for evaluating mesoscale dispersion. Because considerable effort was devoted to ensuring the quality of the data during the measurement program, the data base provides a unique data base for testing models under realistic conditions over long measurement periods.

Several disappointments in the operation of the workshop that limited the overall success included:

- Lack of time for the laboratories to run their models over longer periods of time; thus, consistent comparisons were not possible for all sampling periods.
- Lack of more extensive calculations with the 3-D models; thus, only limited evaluations are possible for these models.

- Less emphasis on critically examining the important meteorological parameters in dispersion modeling, i.e., the effectiveness of incorporation of variable mixing height, terrain, or different forms of eddy diffusivities (or standard deviations); thus, only limited insight is possible as to the effect of various approximations for these meteorological parameters.

The relative benefits discussed above, however, far overshadow these disappointments.

General Conclusions

Based on the results of the workshop, the weighted average statistics for each model category are shown in Table VI-1. The statistics for the leading model in each category are shown in Table VI-2.

In general, the results of the model comparisons indicate that the simple windrose models are adequate for annual assessments and provide accuracy comparable to that obtainable with Gaussian trajectory models for monthly predictions. For hourly to daily time scales, the Gaussian trajectory models are as good as the three-dimensional models for the cases calculated at SRL. The reason for this is primarily the lack of resolution of the available meteorological data and fairly simple situation (no large topographic or sea breeze influence). Further improvement of the numerical accuracy of these models is not nearly as important as accurate calculation of transport winds. Under conditions of complex terrain, the higher computer costs required for the three-dimensional models may be warranted; however, the accurate calculation of the wind fields becomes even more important in these cases.

TABLE VI-1

Statistical Results for Models Using a Weighted Average

	N	R	ρ	τ	Average Bias, pCi/m^3	RMSE, pCi/m^3	K	Slope	R^2
Annual	13	0.85	-	-	-24	31	2	1.33	0.74
Monthly	273	0.51	0.57	0.41	-16	44	6	0.78	0.28
Weekly	229	0.45	0.62	0.46	-33	134	4	1.10	0.21
Weekly*	169	0.39	0.38	0.26	-44	164	4	1.18	0.15
Twice-Daily	200	0.40	0.52	0.42	1	161	8	0.48	0.18
Twice-Daily*	72	0.31	0.11	0.08	3	280	9	0.35	0.15

* PNOs excluded.

TABLE VI-2

Statistical Results for "Best" Models

Model	Frequency	N	R	ρ	τ	R^2	Average Bias, pCi/m^3	RMSE, pCi/m^3	K	Slope
AIRDOS-EPA	Annual	13	0.98	–	–	0.97	–29	31	1	1.7
ASTRAP	Monthly	295	0.75	0.69	0.51	0.56	0.2	18	1	0.59
ATAD	Weekly	497	0.48	0.68	0.52	0.23	2	62	3	0.58
ATAD*	Weekly	349	0.41	0.44	0.30	0.17	3	74	3	0.51
ATMOS†	Twice-Daily	93	0.80	0.67	0.53	0.63	–2	87	2	1.05
ATMOS*†	Twice-Daily	38	0.75	0.52	0.38	0.57	–7	137	2	1.05
DRAX2	Twice-Daily	381	0.49	0.61	0.47	0.24	–0.5	201	>10	0.73
DRAX2*	Twice-Daily	159	0.43	0.19	0.13	0.19	0.3	310	>10	0.39

* PNOs excluded.

*† Sample size for ATMOS was about 25% that of DRAX2, therefore, the statistics are not as reliable as for DRAX2. When ATMOS and DRAX2 are evaluated using a common data base, the values of ρ and τ for the two models are almost identical.

A point of concern that was raised during the workshop is the adequacy of the data base for testing models over short measurement periods. As pointed out in Section II, the long-term measurements (e.g., seasonal or annual) are believed to be reliable estimates of the true long-term averages. Although an intensive quality control program was conducted during the experiment, human errors and instrument malfunctions and errors tend to limit the confidence in the measurements for some of the short-term periods (in particular, twice-daily). Thus, some care must be exercised in interpreting model comparisons for these time periods. Unfortunately, suspect data or data derived from other nearby instruments during equipment outages are not easily identified in the data set; thus, it is not possible to account for these effects.

A primary conclusion of the workshop is that more effort should be directed toward improving the analyses of the wind fields that drive the models. To do this efficiently, two questions must be answered. First, what is the best way to improve the analysis? Second, as a practical matter, how much can the analysis be improved, given the resources available? Some perspective on the problems involved can be found through inspection of Table VI-3 The meteorological systems included in Table VI-3 are responsible for much of the uncertainty in wind field analysis and day-to-day weather forecasting as well. It is generally accepted that for scales below the lower mesoscale, statistical methods can describe the time and space variability of the winds in terms of diffusion parameters. However, in complex terrain even this assumption is not valid. Above the synoptic scale, there are the planetary waves, with wavelengths on the order of 10,000 km and time scales of weeks or more. Planetary waves are well resolved by the present synoptic network over most land masses.

TABLE VI-3

Space and Time Scales for Mesoscale and Synoptic Scale Atmospheric Systems

System	Space Scale	Time Scale	Examples
Synoptic	~1000 km	3-5 days	Rossby Waves
Upper Mesoscale	~100 km	6-12 hours	Seabreeze, Squall Line, Mountain-Valley Circulations
Lower Mesoscale	~10 km	1 hour	Thunderstorm Downdraft, Lee Waves

Over the eastern U. S., the National Weather Service surface station network has an average spacing of about 100 km. Commercially operated meteorological towers add some information, but it is apparent from Table VI-3 that upper mesoscale systems cannot be resolved accurately even at the surface; because upper-air stations are about 500 km apart, which is barely adequate for synoptic scale systems. Dupuis and Scoggins[13] show that mesoscale systems slip through the synoptic rawinsonde network, thus causing bad results when the 12-hour rawinsonde data are interpolated linearly between observations to generate hourly data.

The following conclusions are drawn from the preceding discussion:

1. The ten-hour average ^{85}Kr concentrations reflected variability due to passage of upper mesoscale systems; however, the wind observing network resolves only synoptic scale systems with any accuracy. Furthermore, upper mesoscale systems such as Lee side troughs, squall lines and occasional seabreezes affect the winds over South Carolina. Unless wind field analysis schemes are developed to resolve these mesoscale systems, improvements in the accurate prediction of short-term measurements are not likely.

2. The longer averaging periods used to validate the simpler models improved their performance, because the errors introduced by the poorly resolved mesoscale systems tended to average out. However, many of these models tended to show persistent overprediction, at least partly because the additional dispersion due to mesoscale system is not treated statistically in the standard formulas for σ_y and σ_z.

Recommendations

Based on discussions at the workshop and subsequent analysis and study of the results, the following courses of action are recommended to improve the accuracy of mesoscale transport modeling:

1. Objective analysis methods that contain dynamic as well as mass constraints should be developed. This is expected to produce more realistic wind fields by including pressure observations and the effects of stability on friction, both of which are not considered in the mass consistency analysis. Sasaki[12,13] and Fankhauser[14] have formulated methods to perform the combined dynamic and mass constraint analysis.

2. Agree on the scale of motion where the method of analysis should change from resolving the detailed structure of an individual system to treating the combined effects of a number of small systems collectively, such as turbulent eddies. At present, diffusion formulas have been validated only out to about 10 km. Thus the scales of motion from around 10 km to somewhere between 100 and 1000 km are not observed or treated statistically in diffusion models at present. This "mesoscale gap" needs to be closed at the high end through more complete and realistic analysis of available data (as described above), and possibly the use of other data sources, such as satellites. In areas where mesoscale circulations are strongly forced by topography, numerical boundary layer models might contribute useful wind information. The "mesoscale gap" also should be shortened from the low end through focused research on the nature and dispersive abilities of lower mesoscale turbulent eddies. These systems cannot be resolved by our operational observation system, so they must be treated statistically.

3. Validation experiments focused on short time scales (i.e., few hours) in relatively flat terrain should be performed with meteorological data on a similar time and space scale to test models, in particular the 3-D models. The validation results would improve with increasing data and with space and time resolution. Thus, the greater detail in the wind field description would be expected to increase the precision of the concentration calculations correspondingly. Techniques should be developed to describe this changing precision with changing resolution in the input data.

4. Then, mesoscale three-dimensional advection-diffusion models should be tested in regions where local topography generates mesoscale wind systems that overwhelm other systems. In such locations, repeatable experiments with the models are possible. Tests of mesoscale wind-field analysis schemes should

also be performed in such areas, or in areas where dense, permanent observational networks exist, such as the National Severe Storms Laboratory (NSSL) near Norman, Okalahoma.

5. For models used in emergency response support, the time concentration history at a specific point is not so important as a general direction and concentration levels of pollutants. Statistical techniques need to be developed to assess models against the emergency response application in which general patterns and concentration levels are more important than specific values at a specific location.

6. In measurement programs such as that used to develop the Kr-85 data base, additional emphasis should be placed on quality assurance of the measurements for short time periods. This would include redundant samplers at many locations, dense spacing of samplers in some sectors, and the discarding or flagging of any suspect data or data derived from other measurements.

7. A second workshop, open to the general meteorological community, should be held in which the Kr-85 data base is used to test transport models for the various sampling periods, with particular emphasis on weekly and twice-daily measurements. The number of cases should be limited so that modelers can calculate all cases with a reasonable expense of time and effort. Additional quality assurance of the meteorological and Kr-85 data should be performed to insure the reliability of the data for testing models. As good experimental data (see 3 and 4 above) becomes available, similar workshops should be held that use these data bases for comparison and improvement of atmospheric transport models.

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APPENDIX A. WORKSHOP AGENDA AND LIST OF ATTENDEES

Agenda

Tuesday, November 18

7:30 p.m. - 10:30 p.m. - Hospitality

Wednesday, November 19

8:00 a.m.	- Welcome (D. W. Pepper/D. S. Ballentine)
8:10	- Announcements (J. L. Mitchell)
8:15	- Introduction (T. V. Crawford)
8:30	- Workshop data base (C. E. Bailey)
9:00	- Statistical tests (A. H. Weber)
9:30	- Break
9:45	- I. Wind Rose Models (A. J. Garrett) ORNL SRL (M. M. Pendergast)
10:00	- Wives' Coffee (J. L. Mitchell)
10.35	- Statistical Results (A. H. Weber) Discussion
11:15	- II. Gaussian Models (C. E. Bailey)
12:00	- Lunch
1:00 p.m.	ARL ORNL SRL (M. M. Pendergast)
2:30	- Break
2:45	PNL
3:10	- Statistical Results (A. H. Weber) Discussion
4:00	- Observers' Model Validation Programs (T. V. Crawford) AMS NRC AIF EPA APCA EPRI
6:30	- Cocktail hour
7:30	- Dinner (D. W. Pepper)

Thursday, November 20

8:00 a.m.	- III. Gaussian-trajectory/2-D Models (M. M. Pendergast)	
	ARL SRL BNL	
9:30	- Break	
9:45	- (cont'd)	
	ATDL ANL	
10:45	- Statistical Results (A. H. Weber) Discussions	
12:00	- Lunch, followed by afternoon recreation	
5:30 p.m.	- IV. 3-D Models (D. W. Pepper)	
	SRL LLNL LANL	
7:00	- Statistical Results (A. H. Weber) Discussions	
7:30	- Adjourn	

Friday, November 21

8:00 a.m.	- Wind Field Analysis (A. J. Garrett)
9:00	- Break
9:15	- Draft Session Conclusions In Four sub groups
10:45	- Plenary Session (T. V. Crawford) Conclusions from four sub groups (10 min. ea) General Conclusions Future recommendations/plans
12:00	- Adjourn Workshop

List of Attendees

Participants

ANL (Argonne National Laboratory)	J. D. Shannon
ARL (Air Resources Laboratory)	J. L. Heffter R. Draxler
ATDL (Atmospheric Turbulence & Diffusion Laboratory)	W. M. Culkowski C. J. Nappo H. Snodgrass
B-PNL (Battelle - Pacific Northwest Laboratory)	R. C. Easter
BNL (Brookhaven National Laboratory)	A. Carney P. Michaels
DOE (Department of Energy)	D. S. Ballentine J. C. Tseng
LANL (Los Alamos National Laboratory)	S. S. Bunker W. E. Clements C. G. Davis C. F. Keller
LLNL (Lawrence Livermore National Laboratory)	M. Dickerson D. Rodriguez
ORNL (Oak Ridge National Laboratory)	B. D. Murphy C. W. Miller
SRL (Savannah River Laboratory)	T. V. Crawford D. W. Pepper C. E. Bailey M. M. Pendergast J. H. Weber A. H. Weber A. J. Garrett R. E. Cooper

Observers

AIF (Atomic Industrial Forum)	F. J. Mogolesko
AMS (American Meteorological Society)	F. D. White D. G. Fox B. A. Egan
APCA (Air Pollution Control Association)	R. C. Sklarew
EPA (Environmental Protection Agency)	J. Homolya W. Peterson
EPRI (Electric Power Research Institute)	D. H. Minott
NRC (Nuclear Regulatory Commission)	R. F. Abbey, Jr. S. Lewellen
USAF (U. S. Air Force)	S. O. Ouzts
WSNSO (Weather Service Nuclear Support Office and the AMS)	D. Randerson

APPENDIX B. OTHER VALIDATION PROGRAMS

Observers from non-Department of Energy (DOE) organizations attended the meeting because of the high interest in model validation by other government and professional organizations. These observers participated in all discussions and were asked to make short presentations on model validation programs which the group they represented was funding or performing. Short summaries of these presentations are included in this appendix.

Nuclear Regulatory Commission (NRC) - R. F. Abbey

The NRC is vitally interested in validated models for use in assessments and use in response to accidental releases. There is an increased interest in the accuracy of models for use in real-time following accidental releases.

The NRC and its predecessors have funded diffusion tests using SF_6, freons, and perfluorocarbons at the Nuclear Reactor Test Site (NRTS) in Idaho, in Tennessee, and in Utah. Field work has largely been done by the National Oceanographic and Atmospheric Administration (NOAA) Meteorology Group at the NRTS. Sampler distances are typically less than 2 km although there were two tests at NRTS out to 80 km. Sample times are typically 1 hour. The above data and some results have been published. NRC is currently funding efforts to identify further sources of tracer data out to 80 km and is planning dispersion experiments around the Indian Point Reactor Site, New York. These tests will be performed by NOAA personnel from NRTS assisted by subcontracted help from the Stanford Research Institute (SRI), Menlo Park, California. NRC is also interested in the developing of criteria against which models can be judged.

Environmental Protection Agency (EPA) - W. B. Peterson

The EPA is concerned about the accuracy of models used for assessment purposes under the Clean Air Act and used by various local air pollution agencies. EPA funded the collection of an extensive data set around St. Louis, Missouri (the RAPS program), for use in validation of urban air pollution models. SRI is completing an analysis of these data versus their RAM model. Another subcontractor has collected two years of SO_2 data 2 to 8 km from three different coal burning power plants in Indiana. The EPA assessment model, CRESTER, will be tested against these data.

Electric Power Research Institute (EPRI) - D. H. Minott

The EPRI is sponsoring a program to obtain quality assured statistically significant data to validate models for calculating dispersion from tall stacks. Extensive data will be collected around a power plant in a plains site (the Kincaid Power Plant in Illinois), a moderately complex site, and a mountainous site. Concentrations of SO_2 and of tracers will be measured at distances of up to 50 km and with averaging times of 1, 3, and 24 hours. Surface and aircraft measurements of the atmospheric boundary layer structure will be made during intensive sampling periods. The data will be published so that it is generally available for model validation by the meteorological community.

Plains site data were obtained from March to August 1980 and will be published in March 1981. A number of EPA Models will be tested statistically against these data as well as first and second order closure models being developed by EPRI subcontractors. Detailed descriptions of this EPRI program was published in the Proceedings of the American Meteorological Society 5th Symposium on Atmospheric Turbulence and Diffusion to be conducted in Atlanta, Georgia, March 1981.

American Meteorological Society (AMS) - D. G. Fox

The AMS and the EPA have entered into an agreement whereby the AMS would aid in the scientific development and application of atmospheric dispersion models. The AMS convened a small group of experts in September 1980 to discuss current practices in model evaluation, recommend model performance evaluation measures and methods, and, if possible, to set model performance standards. A proceedings of this workshop is in preparation and a review was published in the Proceedings of the American Meteorological Society 5th Symposium on Atmospheric Turbulence and Diffusion being held in Atlanta, Georgia, March 1981. There are no new field data being developed by the AMS.

Atomic Industrial Forum (AIF) - F. J. Mogolesko

The AIF is very concerned about the accuracy of models and the modeling requirements being imposed on the utility industry in support of emergency response by NUREG/FEMA 0654. The AIF has no model validation programs of its own but follows closely the effort of others and the applicability of these models to the utility industry's problems.

Air Pollution Control Association (APCA) - R. C. Sklarew

The APCA has no current model validation programs but follows workshops of the kind held by SRL very closely. It may consider sponsoring a specialty conference on model validation.

U.S. Air Force (USAF) - S. O. Ouzts

The USAF has no current model validation programs but follows workshops of the kind held by SRL very closely.

APPENDIX C. SCATTER DIAGRAMS FOR MODEL COMPARISONS

Scatter diagrams for each of the model comparisons are provided in this section in the order that they were discussed in Section V. Points are plotted using alphabetic characters to represent multiple occurrences of the same points; i.e., A-1 occurrence, B-2 occurrences, ..., Z-26 or more occurrences. The number of hidden points is indicated on each plot.

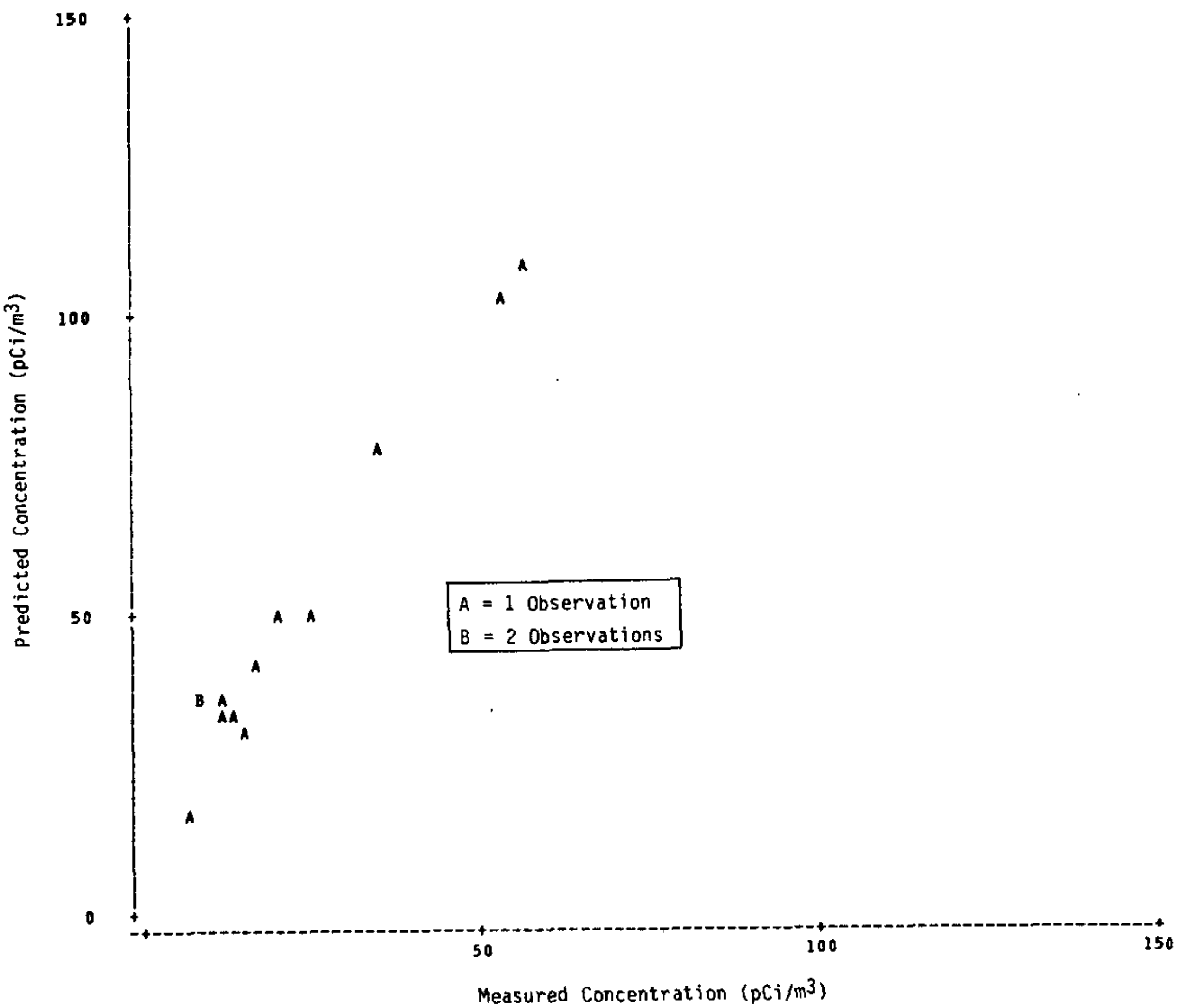

FIGURE C-1. Annual Predictions for the AIRDOS-EPA Model

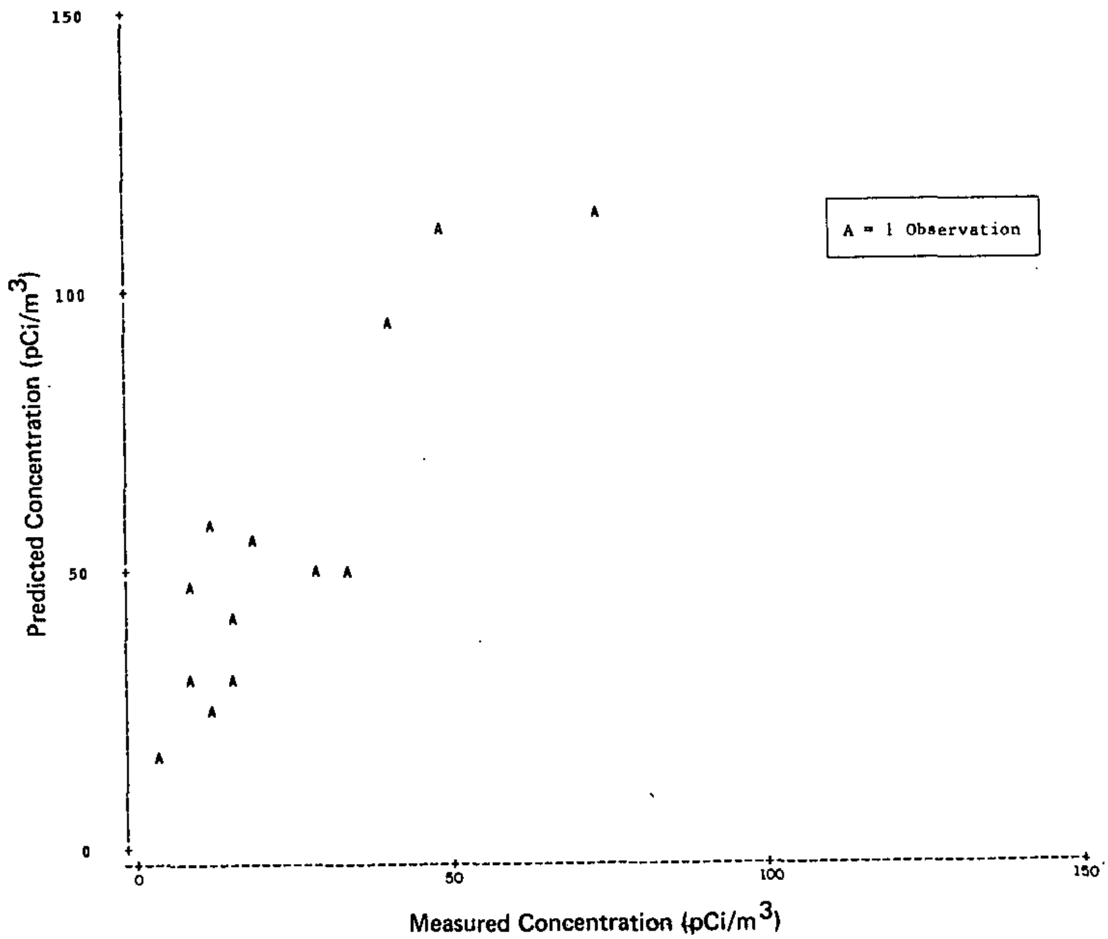

FIGURE C-2. Annual Predictions for the XOQDOQ Model

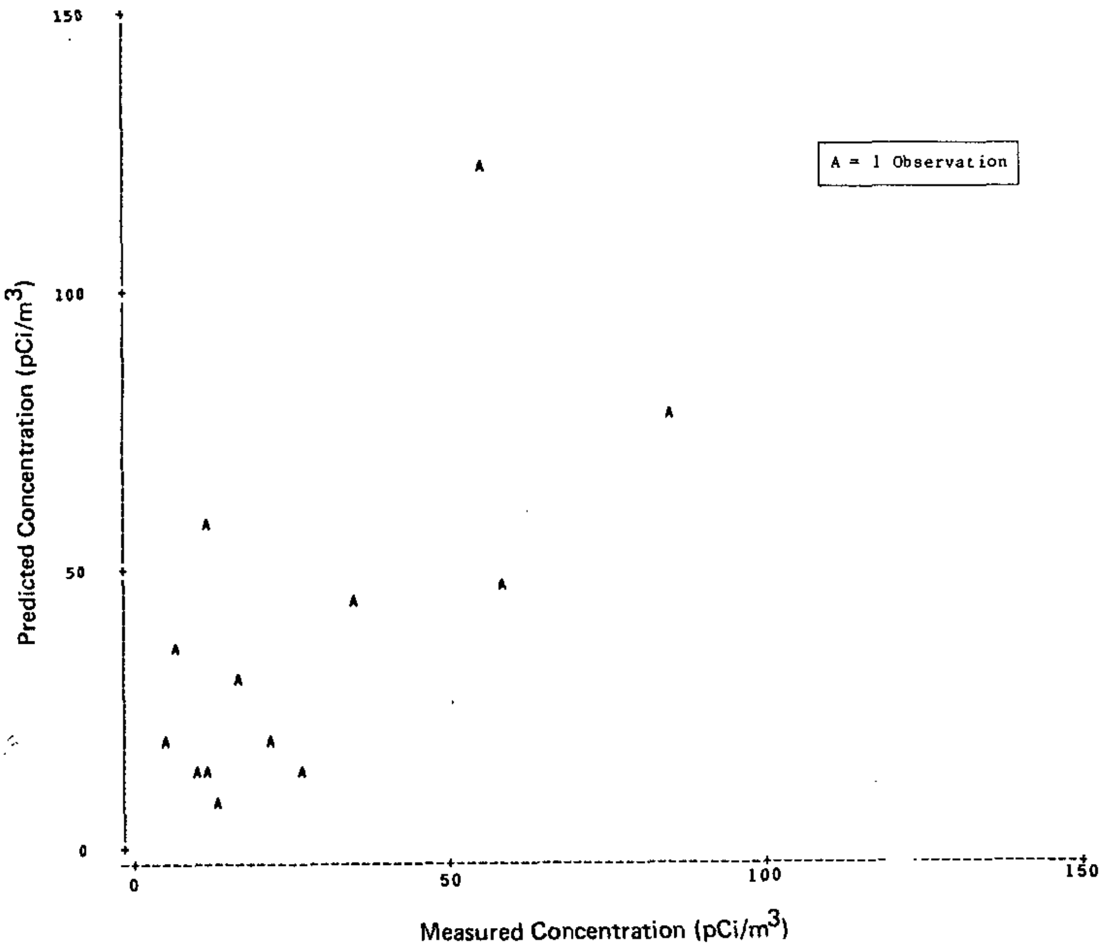

FIGURE C-3. Annual Predictions for the SHEAR-ROSE Model

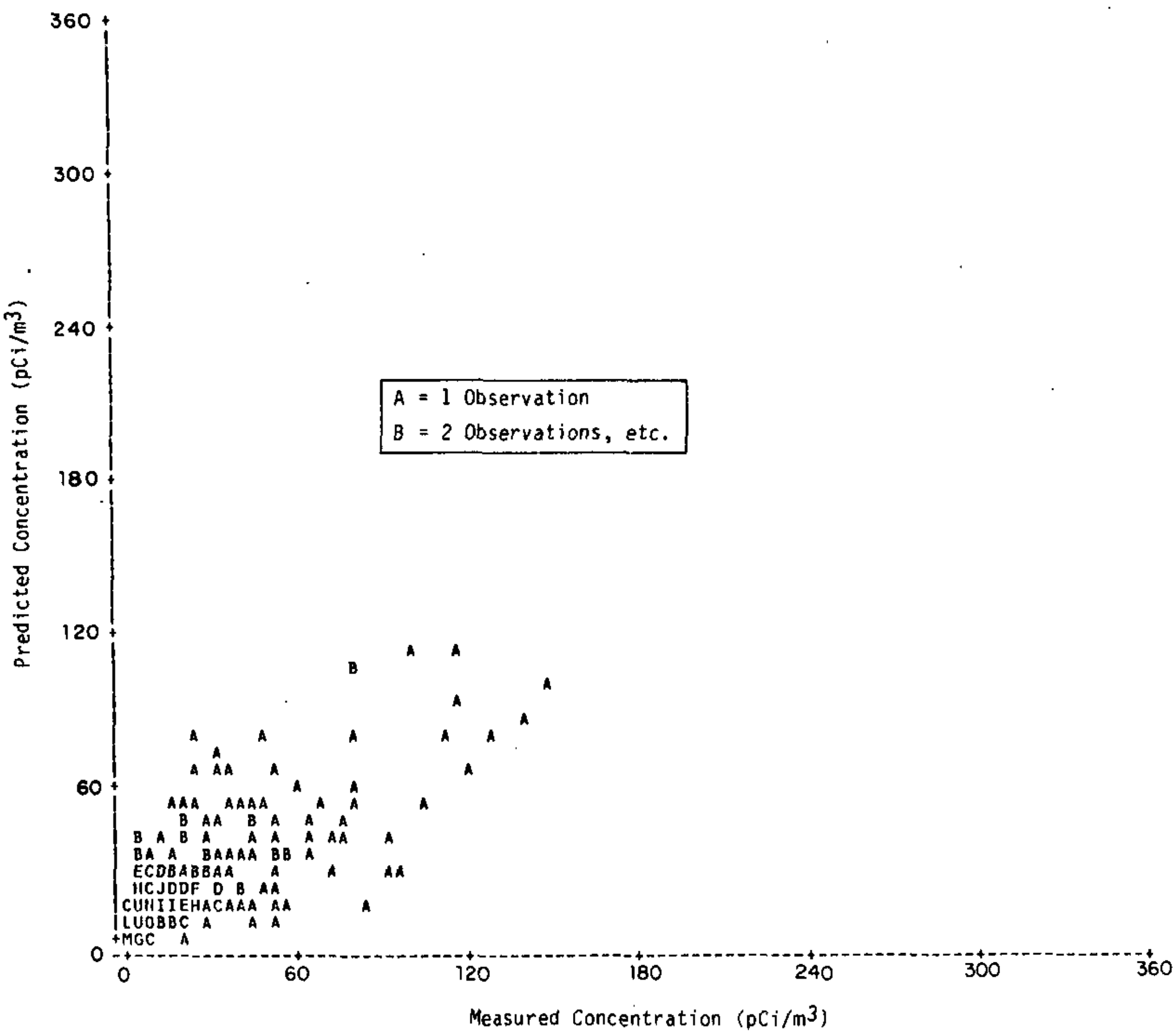

FIGURE C-4. Monthly Predictions for the ASTRAP Model

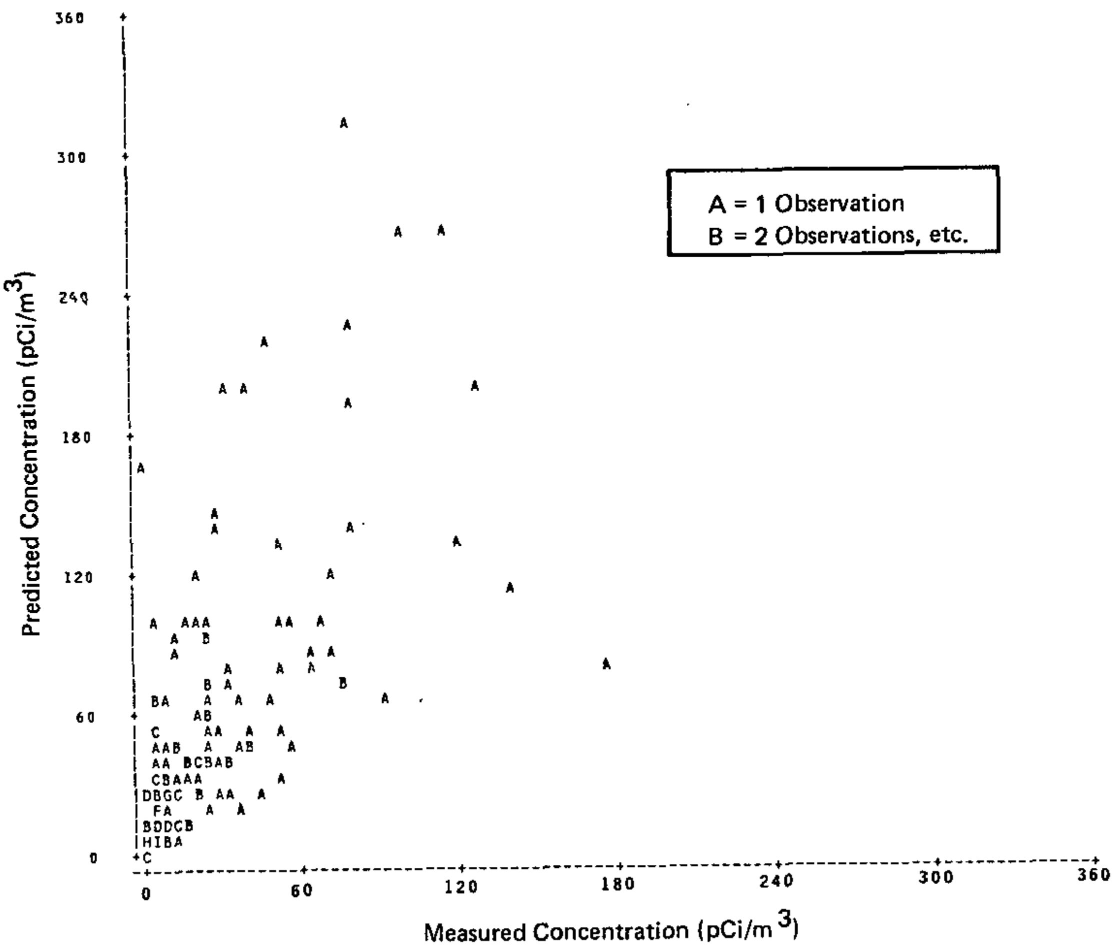

FIGURE C-5. Monthly Predictions for the AIRDOS-EPA Model

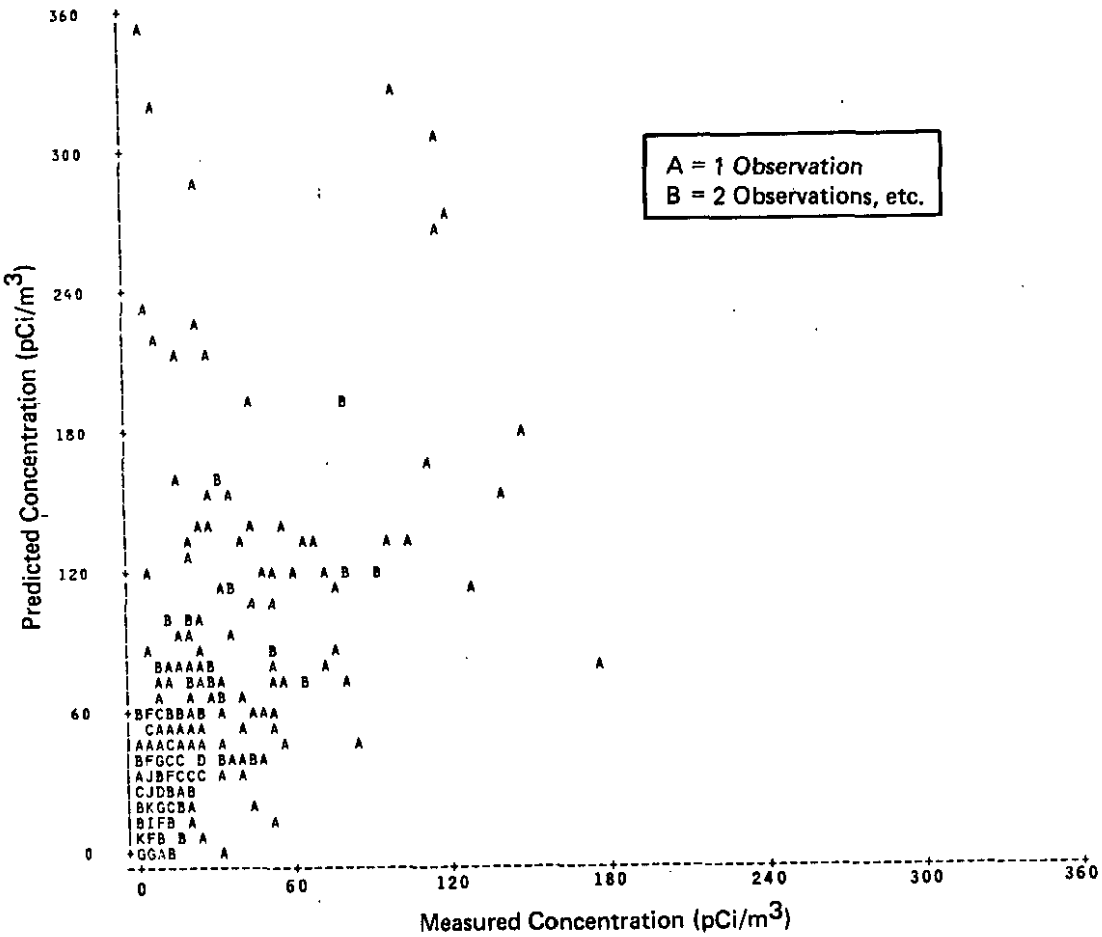

FIGURE C-6. Monthly Predictions for the XOQDOQ Model

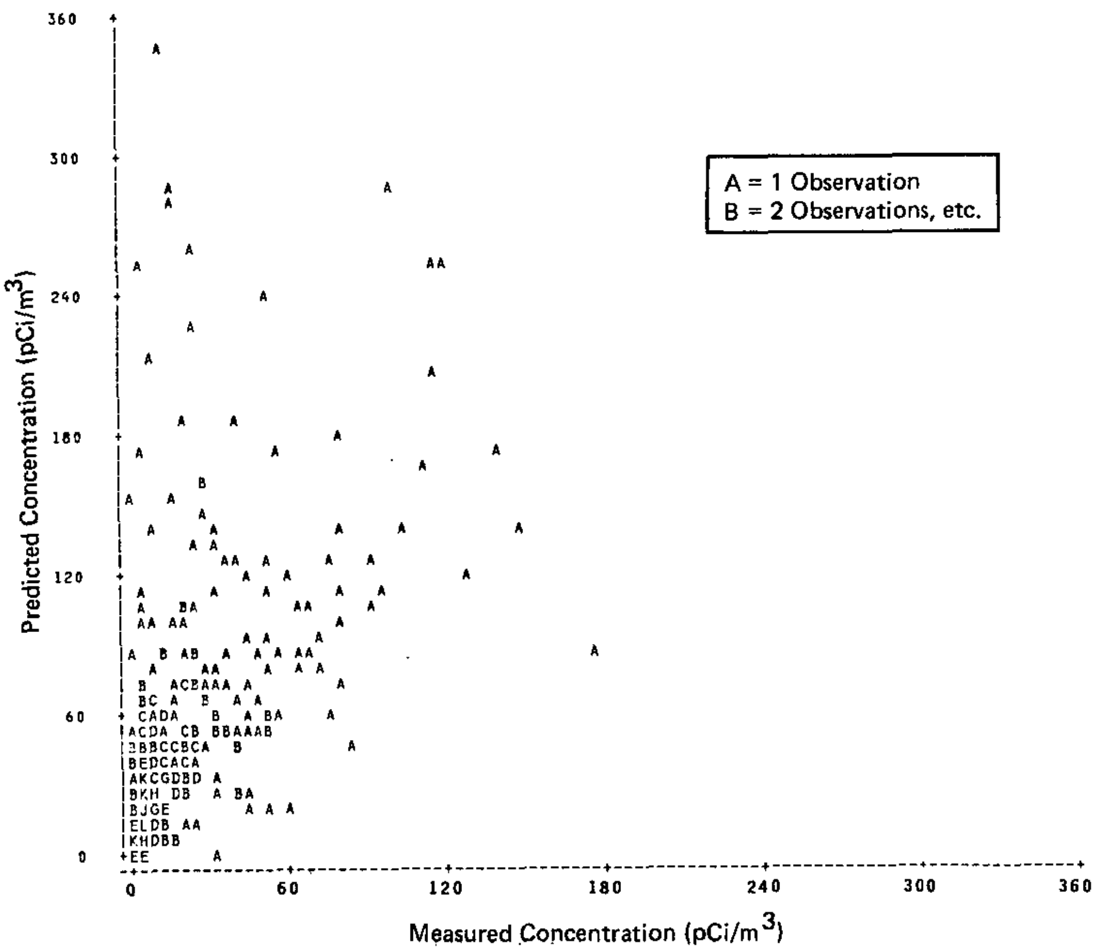

FIGURE C-7. Monthly Predictions for the ATM Model

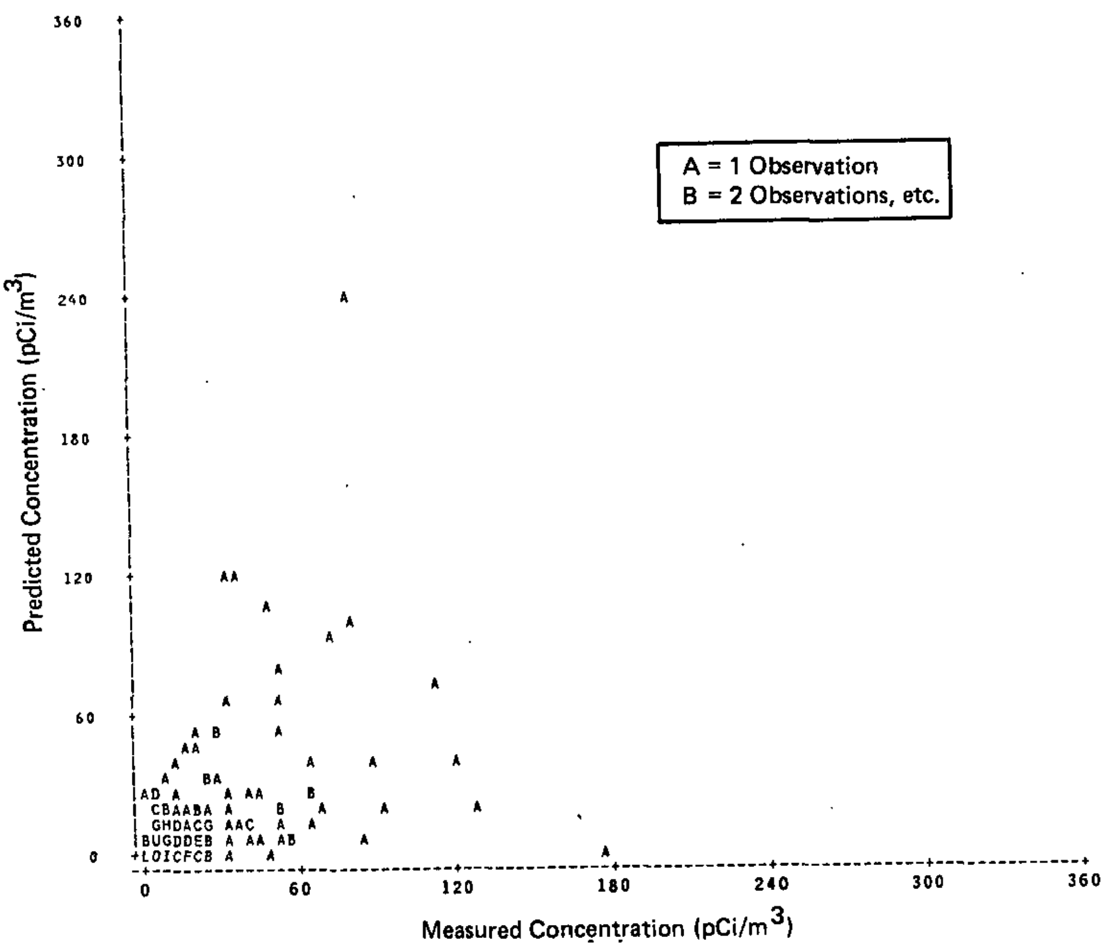

FIGURE C-8. Monthly Predictions for the DRAX1 Model

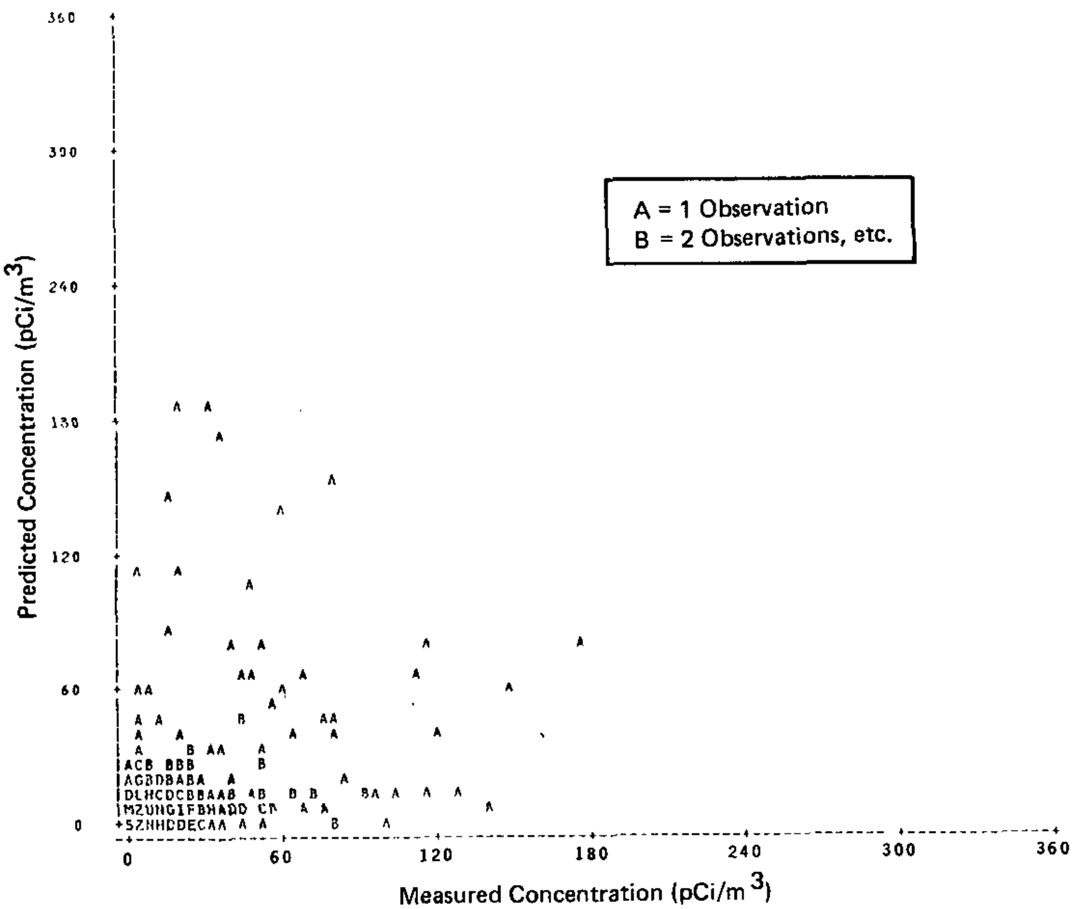

FIGURE C-9. Monthly Predictions for the ANDEP Model

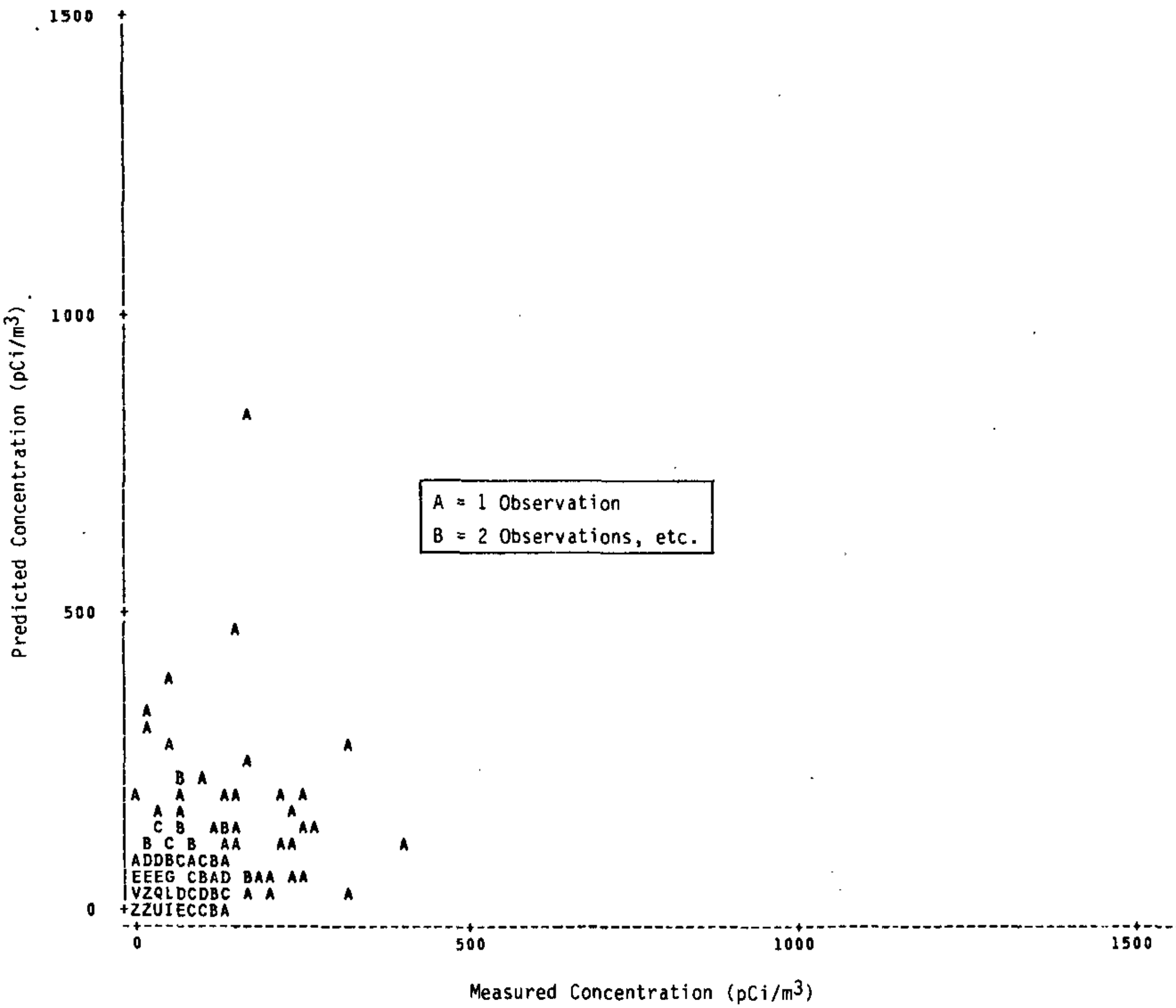

FIGURE C-10. Weekly Predictions for the ATAD Model (All Points Included)

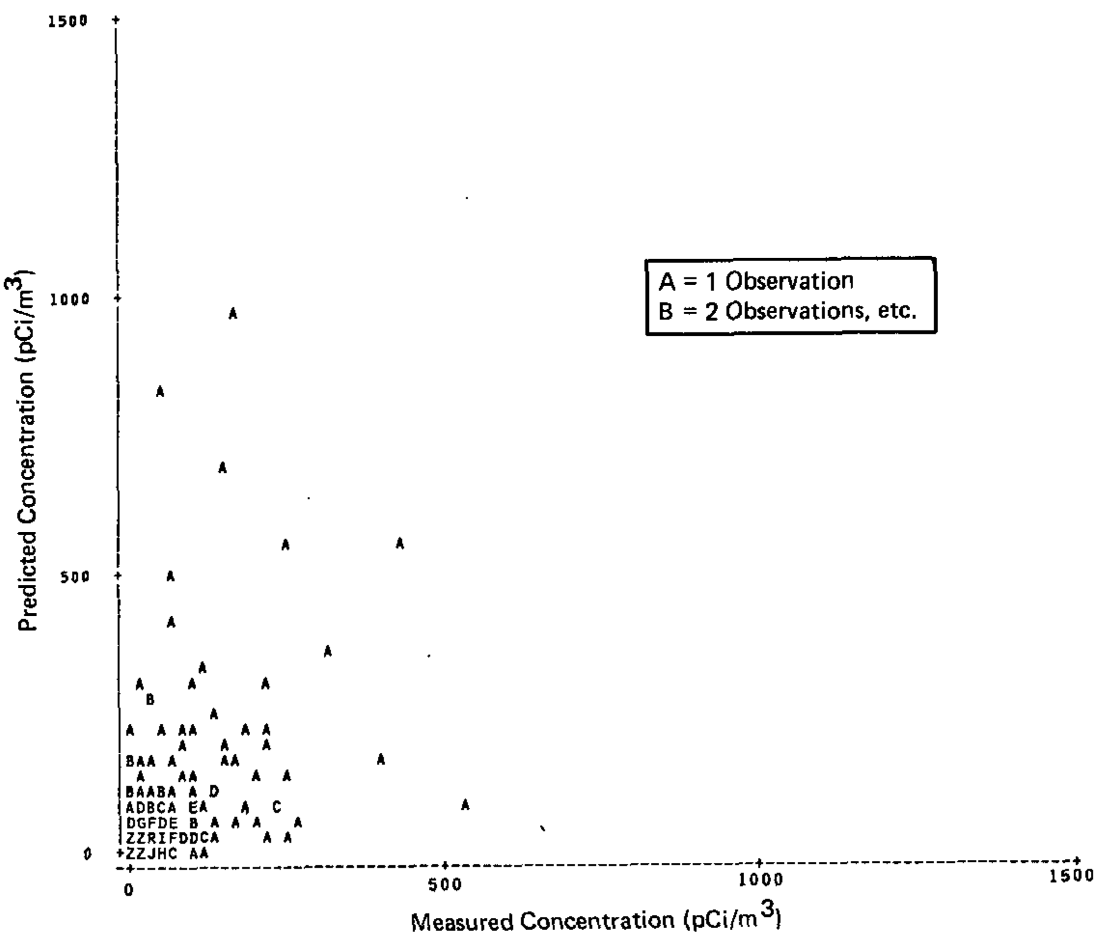

FIGURE C-11. Weekly Predictions for the DRAX2 Model (All Points Included)

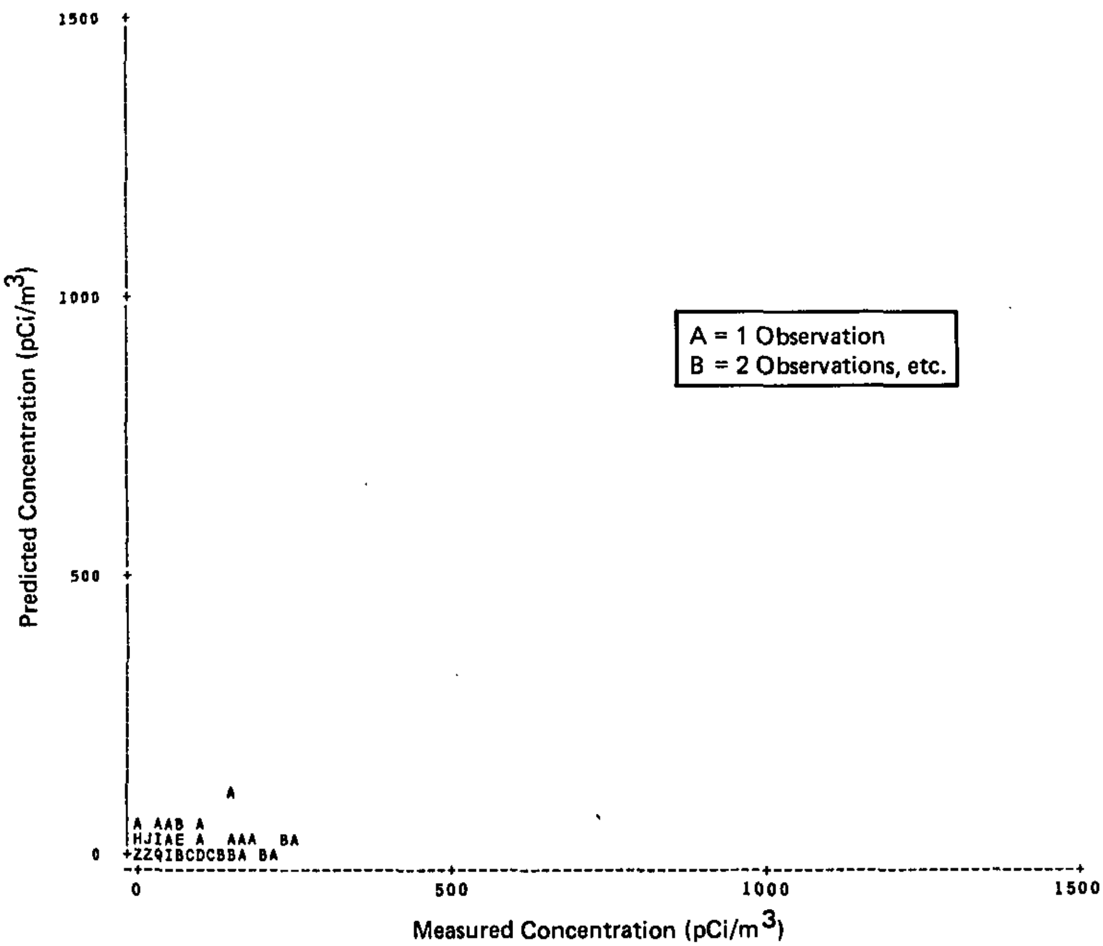

FIGURE C-12. Weekly Predictions for the ADPLUM Model (All Points Included)

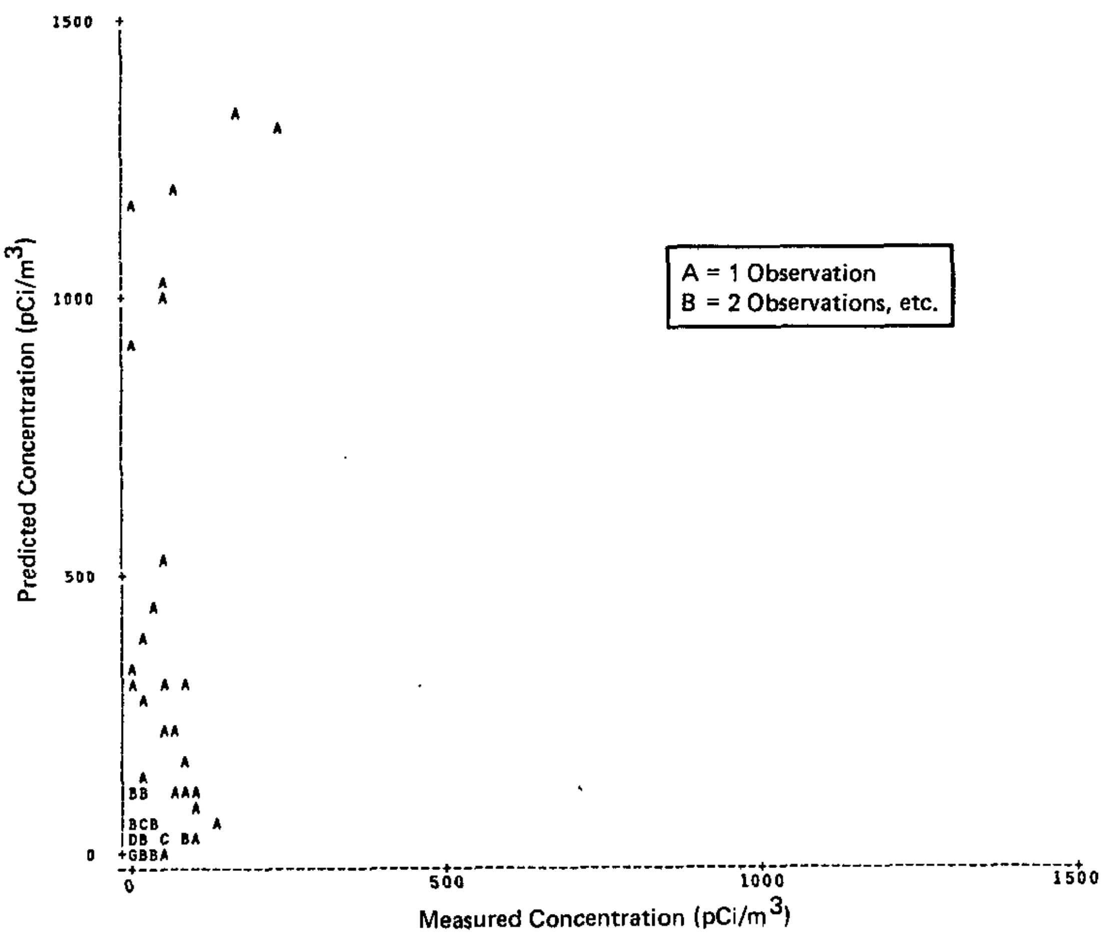

FIGURE C-13. Weekly Predictions for the DRAGONGP Model (All Points Included)

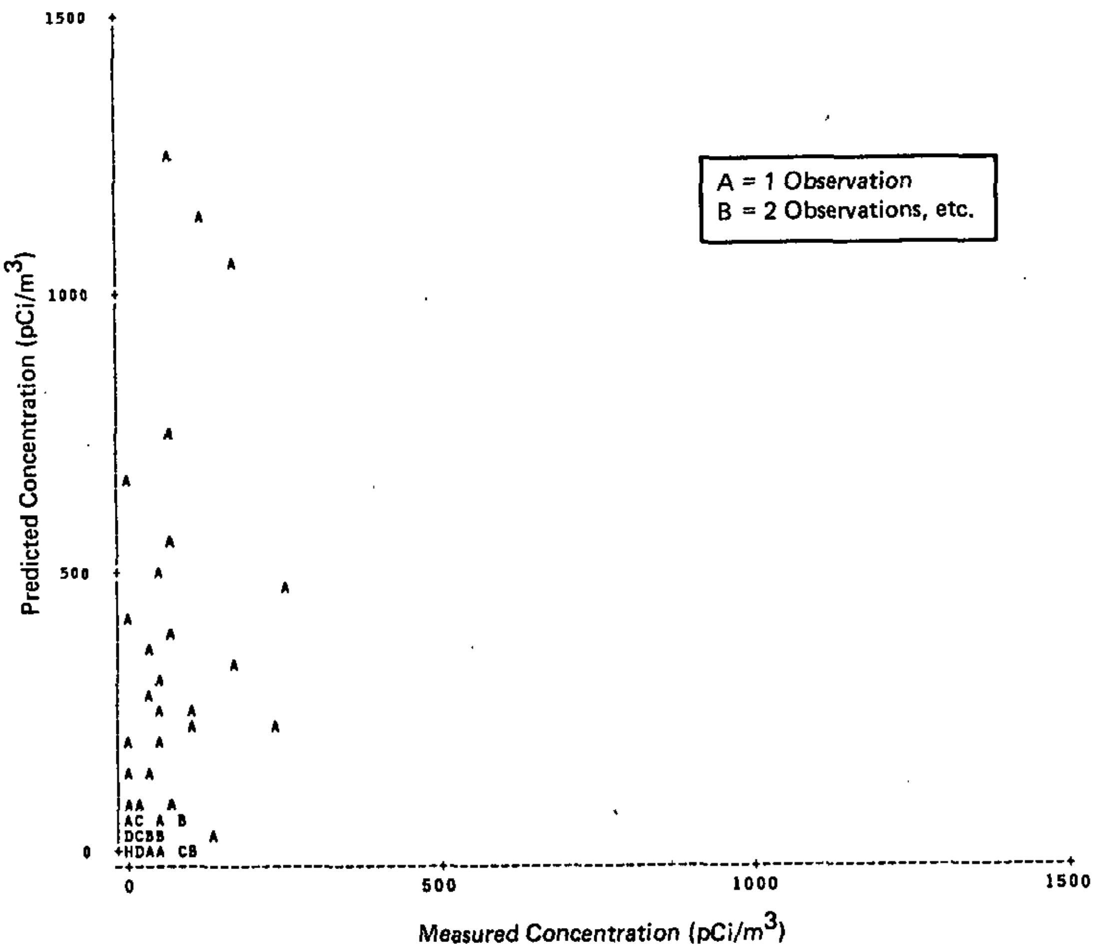

FIGURE C-14. Weekly Predictions for the DRAGONTH Model (All Points Included)

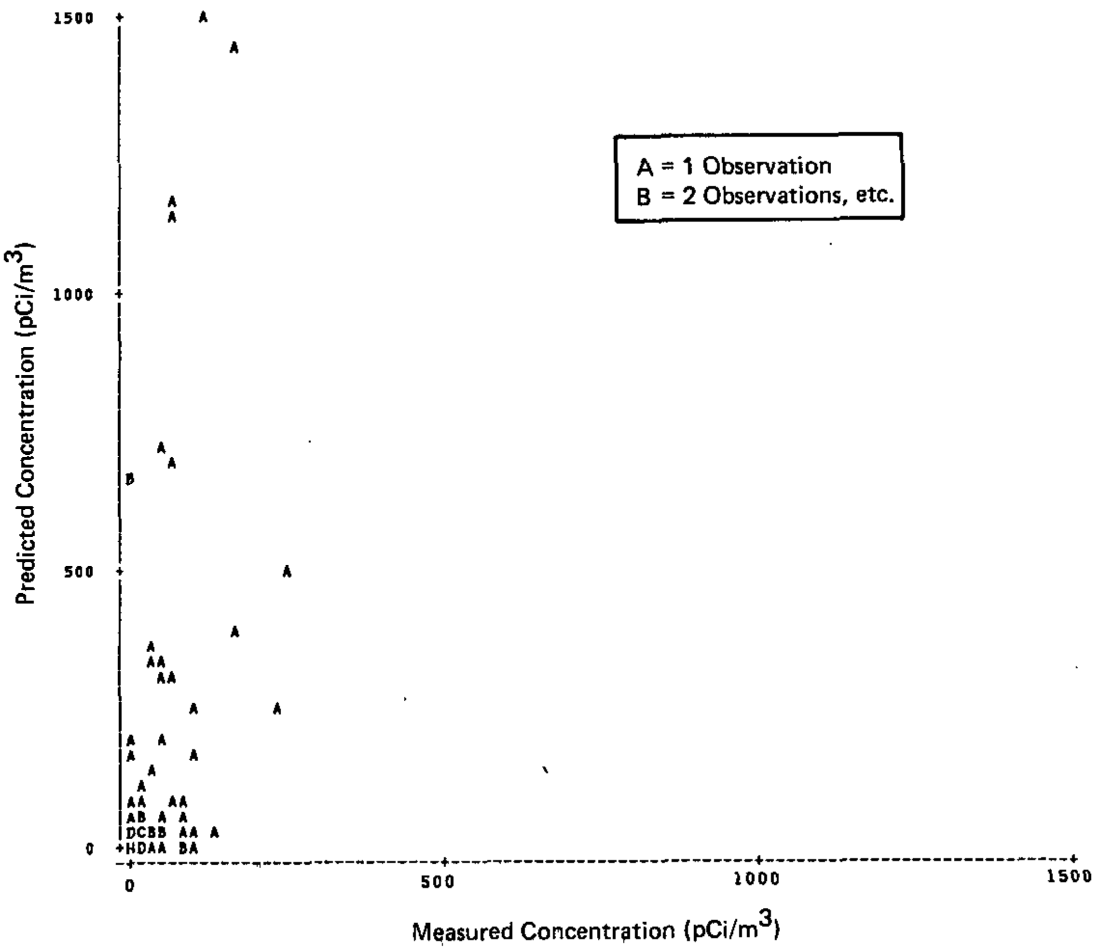

FIGURE C-15. Weekly Predictions for the DRAGONTHP Model (All Points Included)

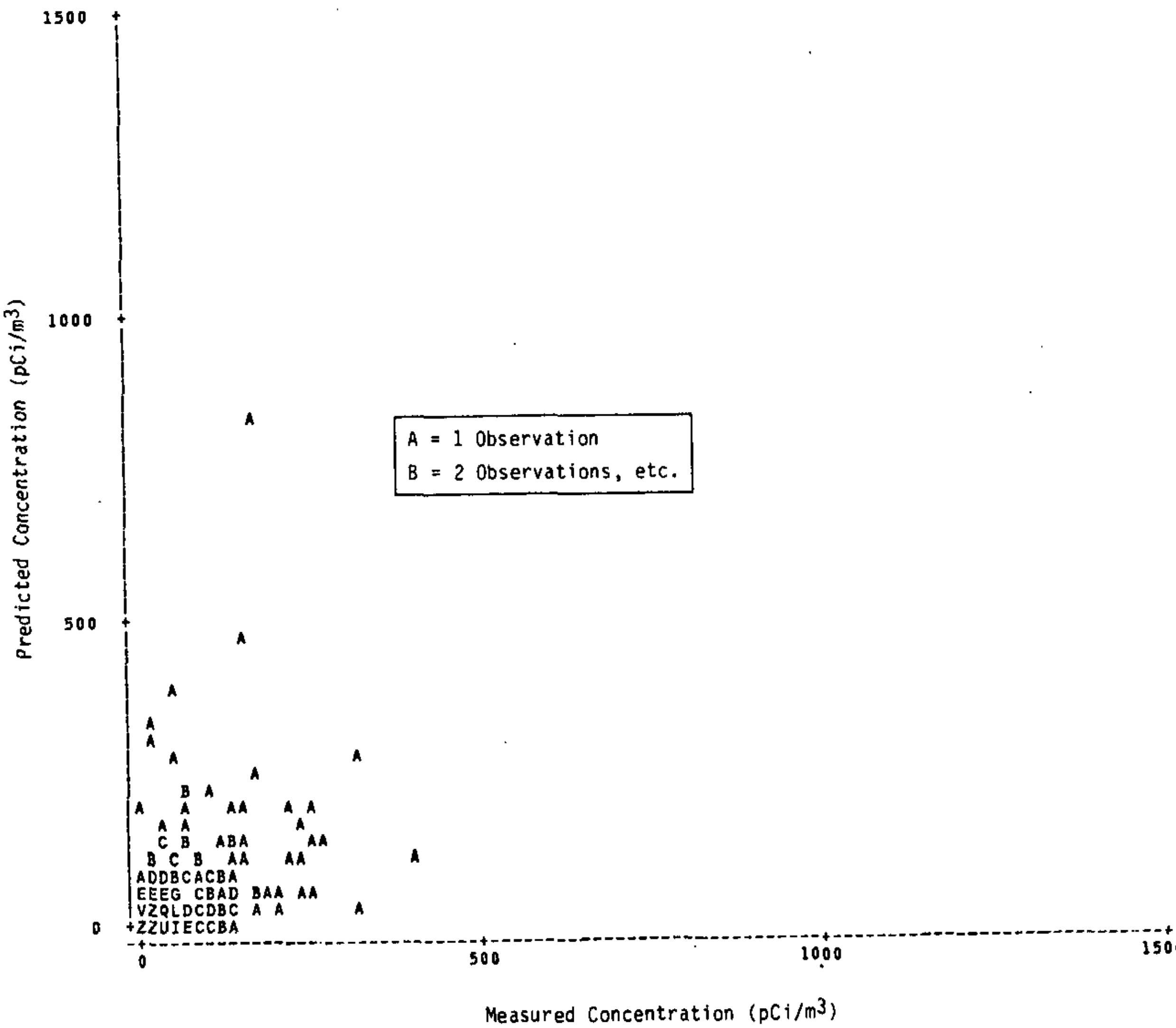

FIGURE C-16. Weekly Predictions for the ATAD Model (PNOs Excluded)

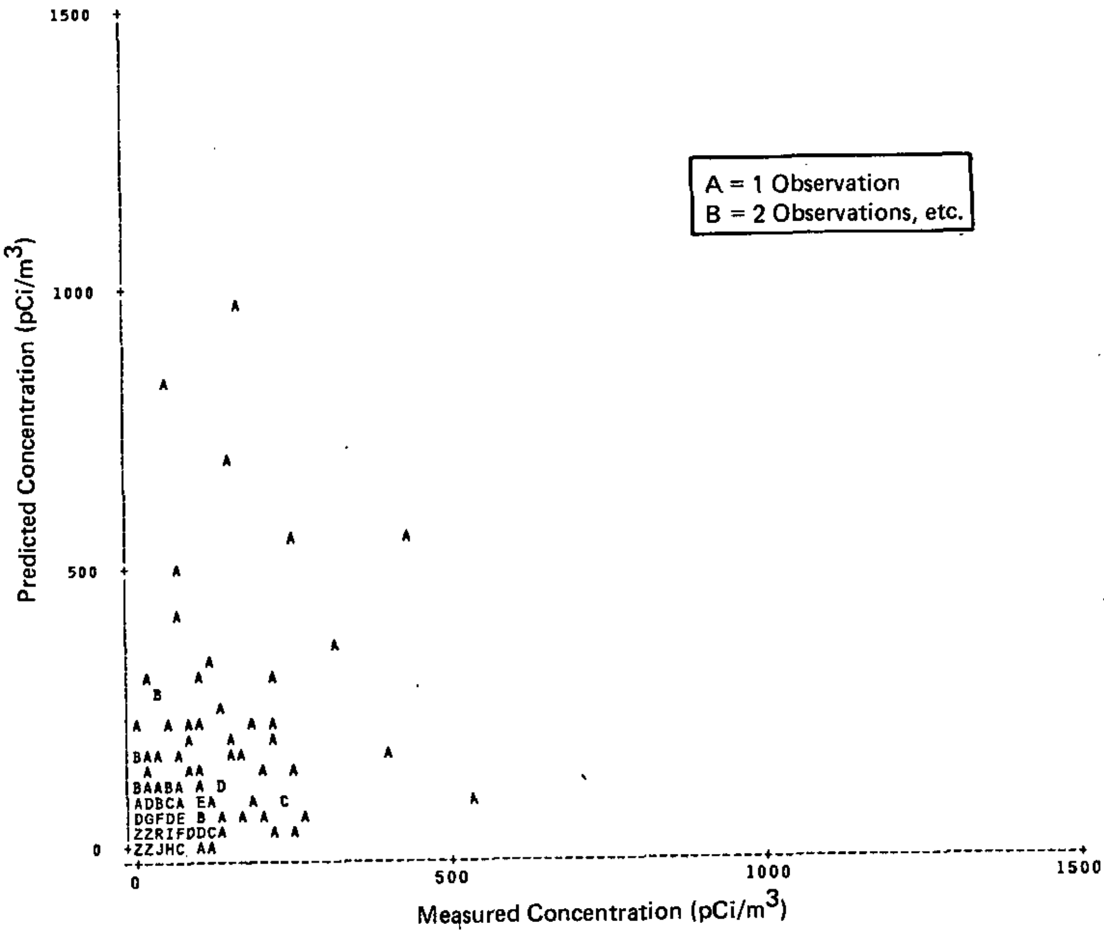

FIGURE C-17. Weekly Predictions for the DRAX2 Model (PNOs Excluded)

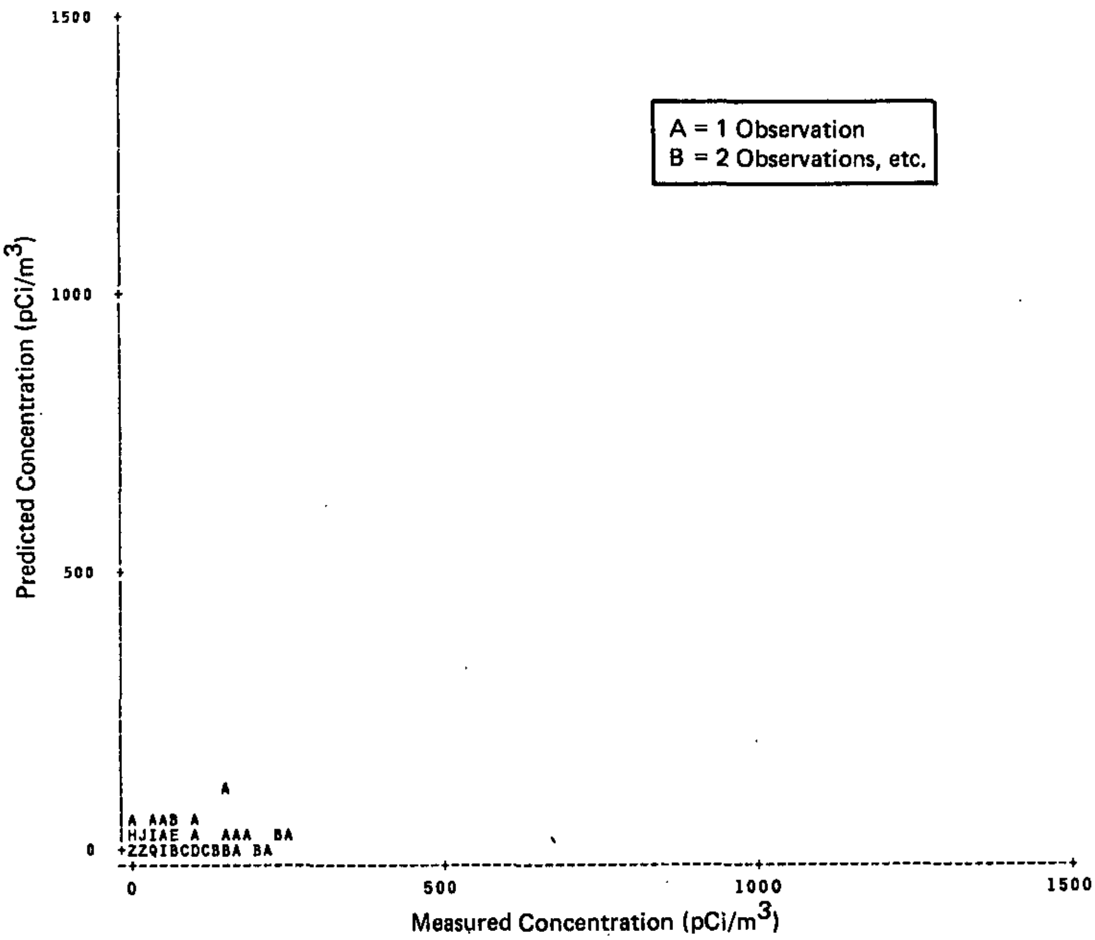

FIGURE C-18. Weekly Predictions for the ADPLUM Model (PNOs Excluded)

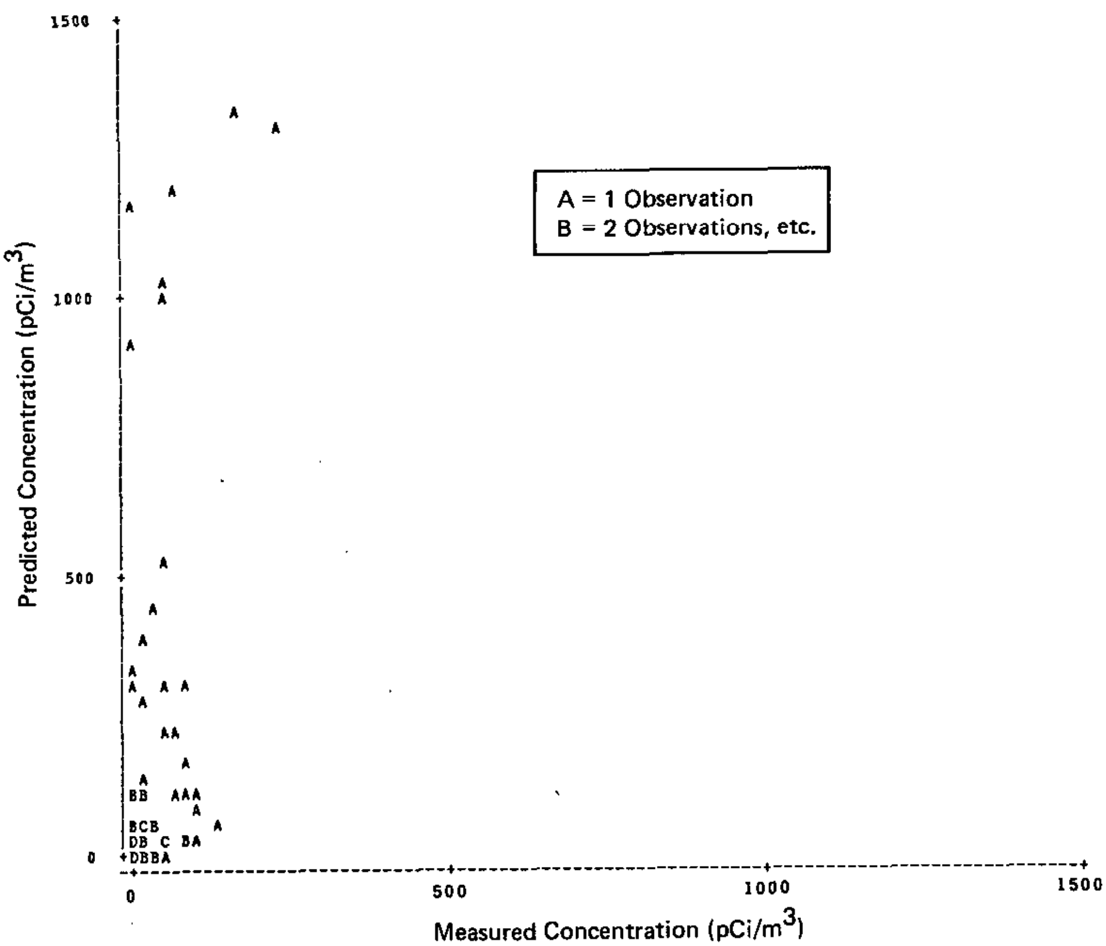

FIGURE C-19. Weekly Predictions for the DRAGONGP Model (PNOs Excluded)

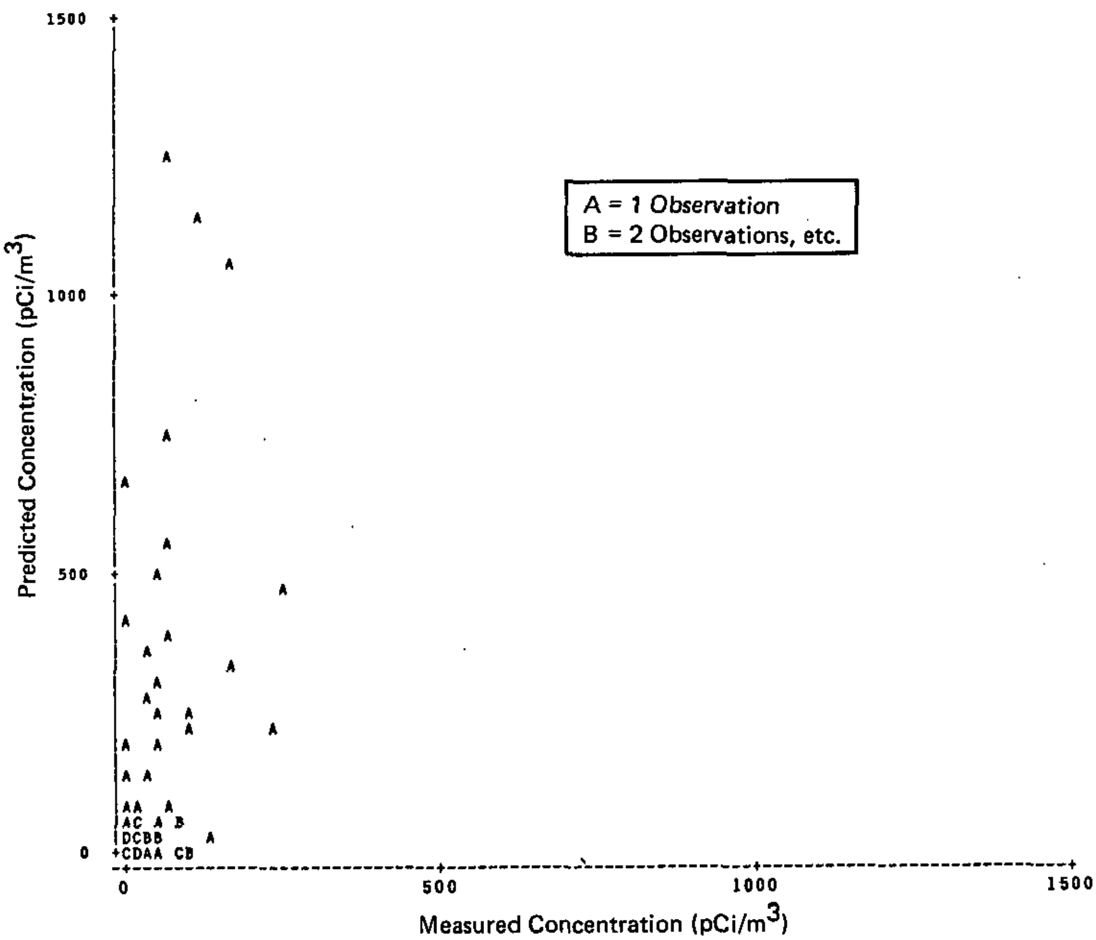

FIGURE C-20. Weekly Predictions for the DRAGONTH Model (PNOs Excluded)

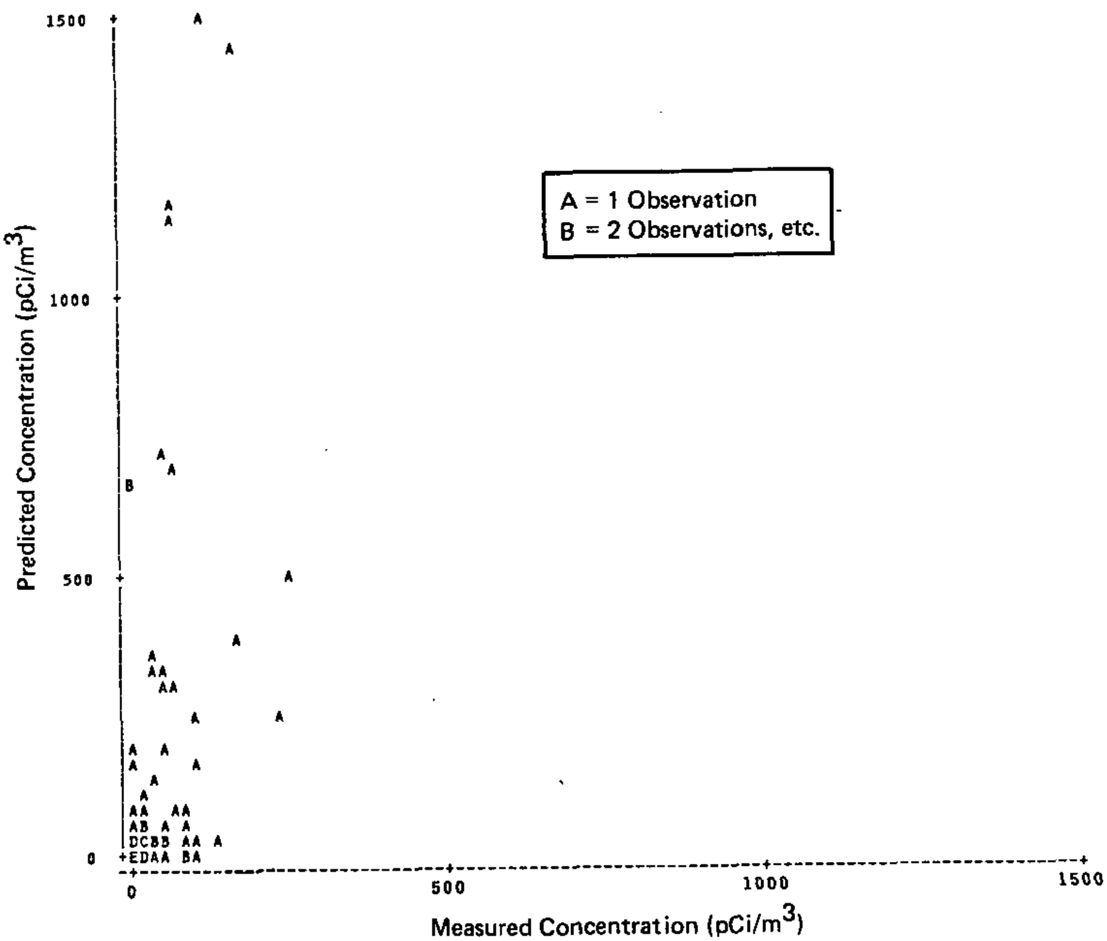

FIGURE C-21. Weekly Predictions for the DRAGONTHP Model (PNOs Excluded)

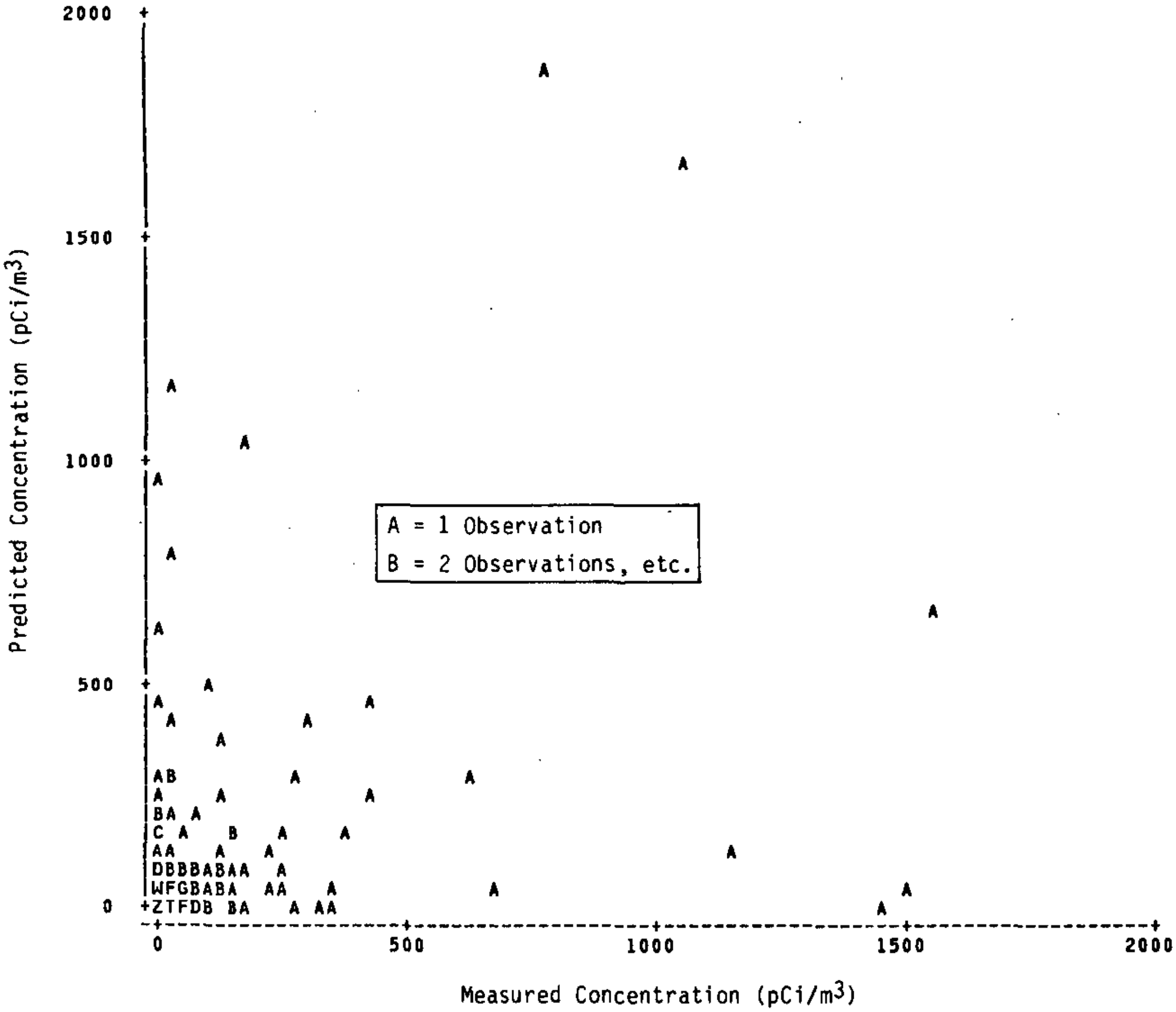

FIGURE C-22. Twice-Daily Predictions for DRAX2 Model (All Points Included)

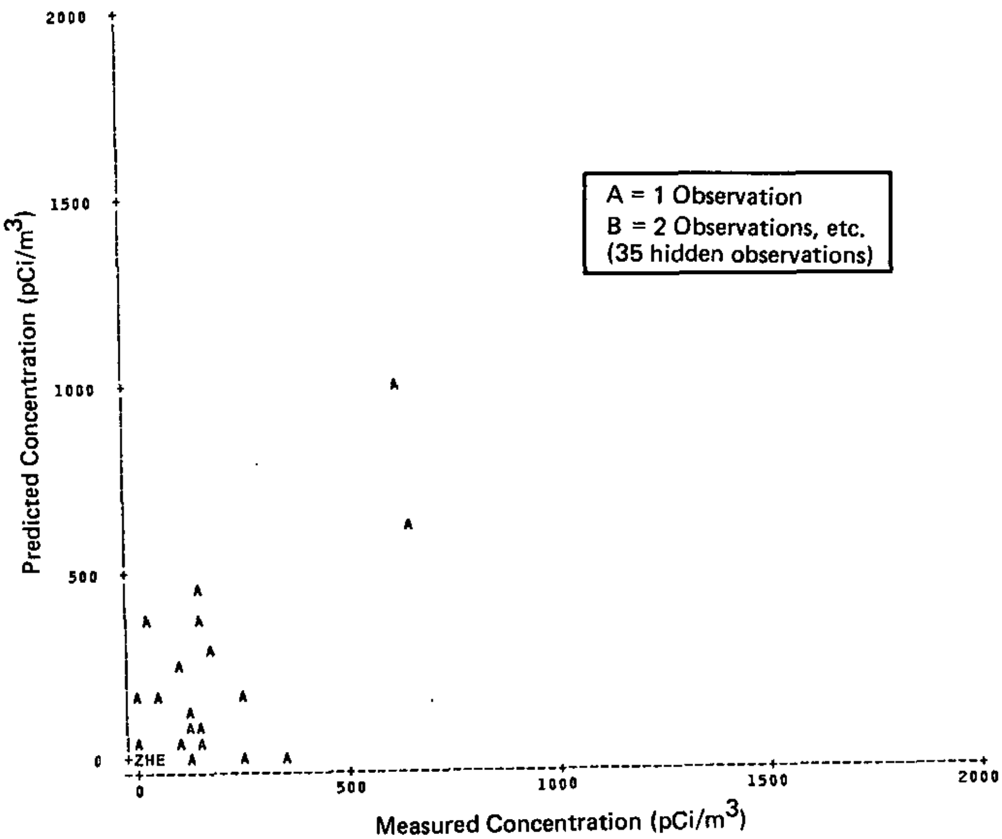

FIGURE C-23. Twice-Daily Predictions for ATMOS Model (All Points Included)

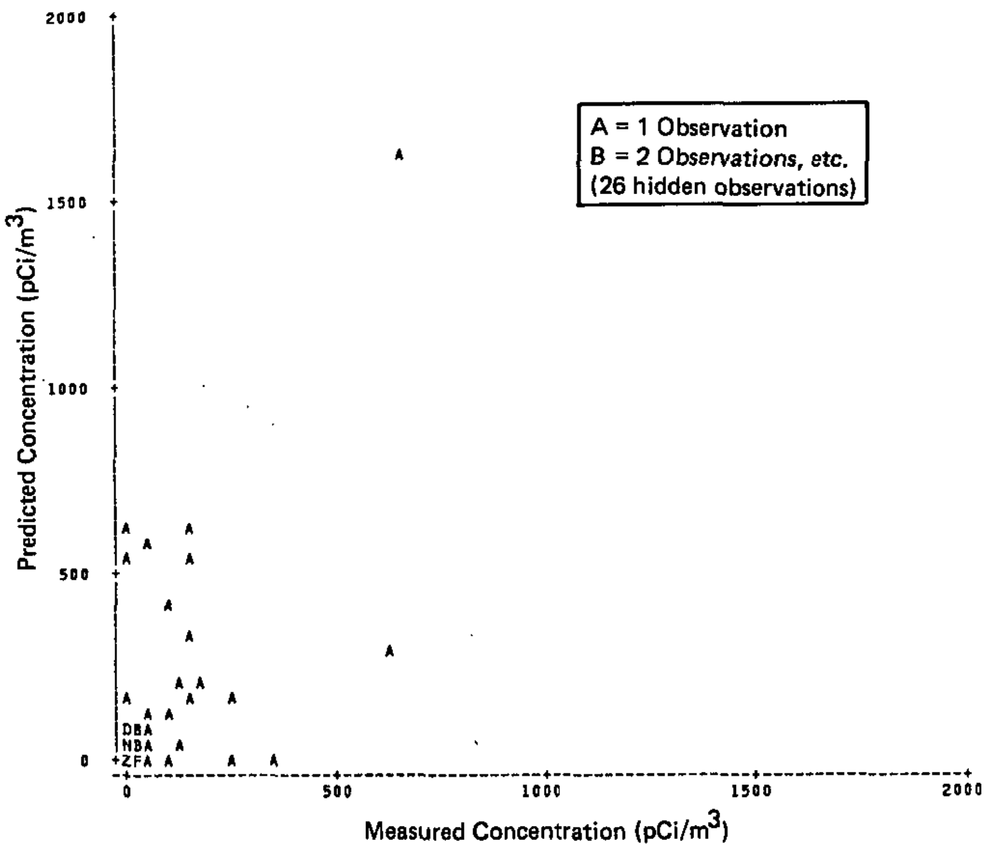

FIGURE C-24. Twice-Daily Predictions for CHAPEAU Model (All Points Included)

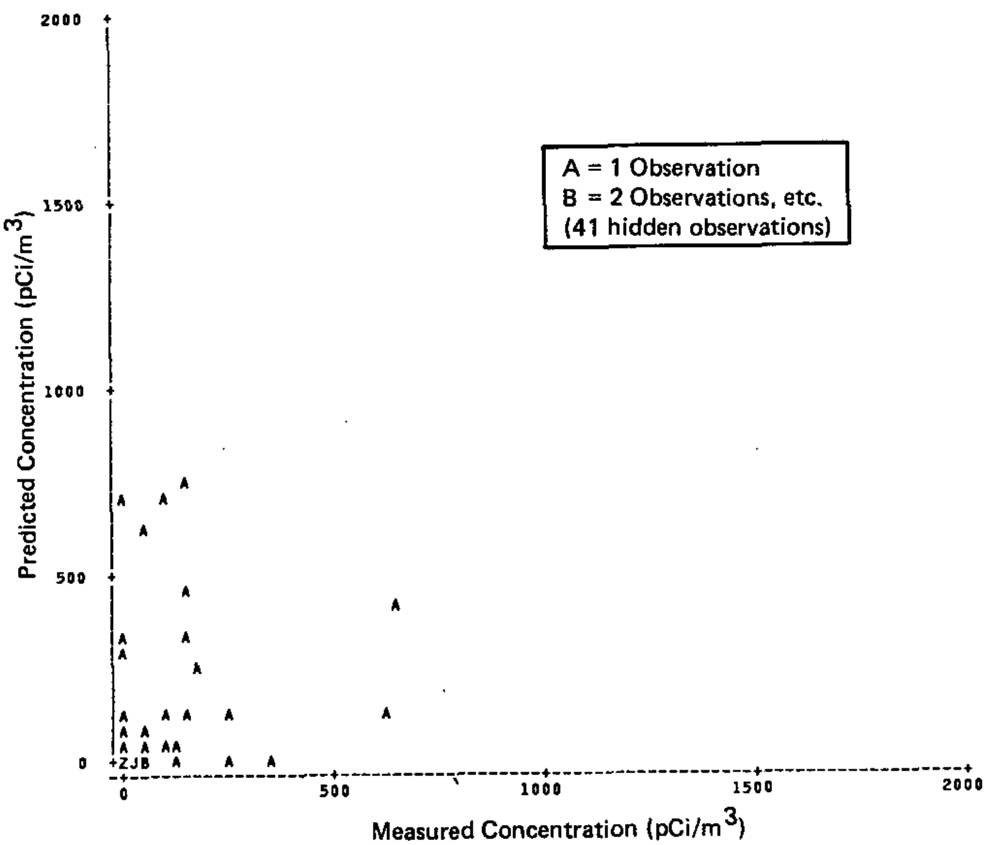

FIGURE C-25. Twice-Daily Predictions for MOMENTS Model (All Points Included)

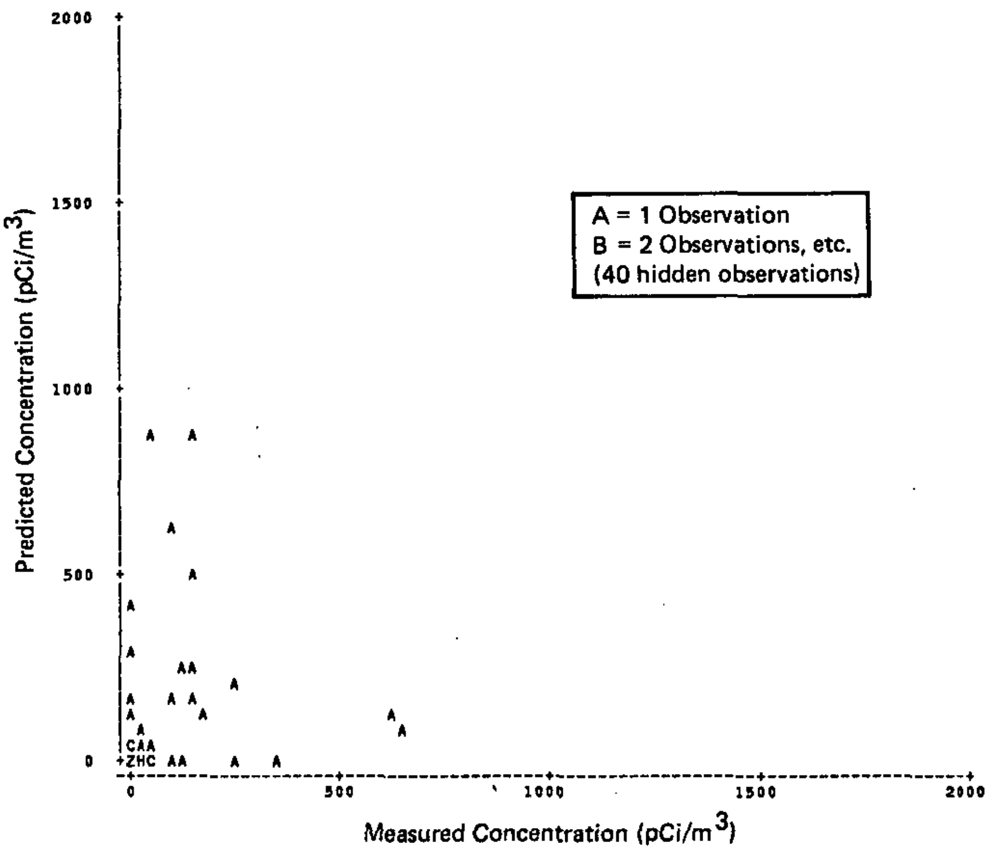

FIGURE C-26. Twice-Daily Predictions for PIC Model (All Points Included)

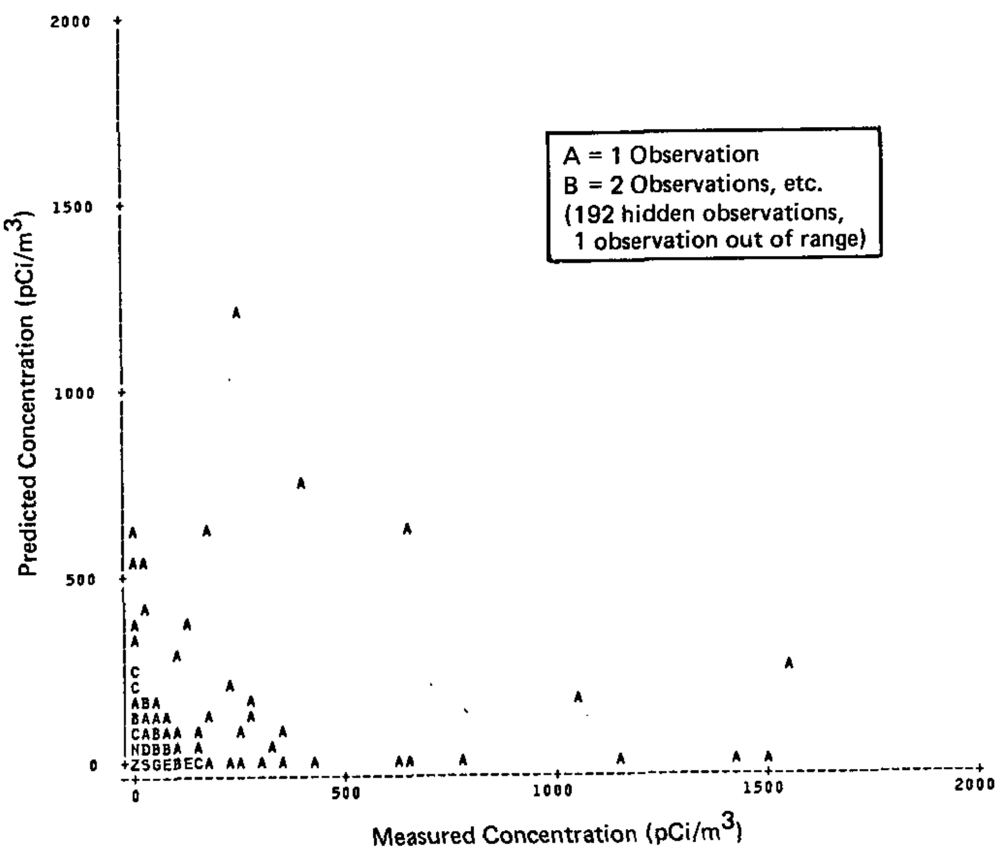

FIGURE C-27. Twice-Daily Predictions for ATAD Model (All Points Included)

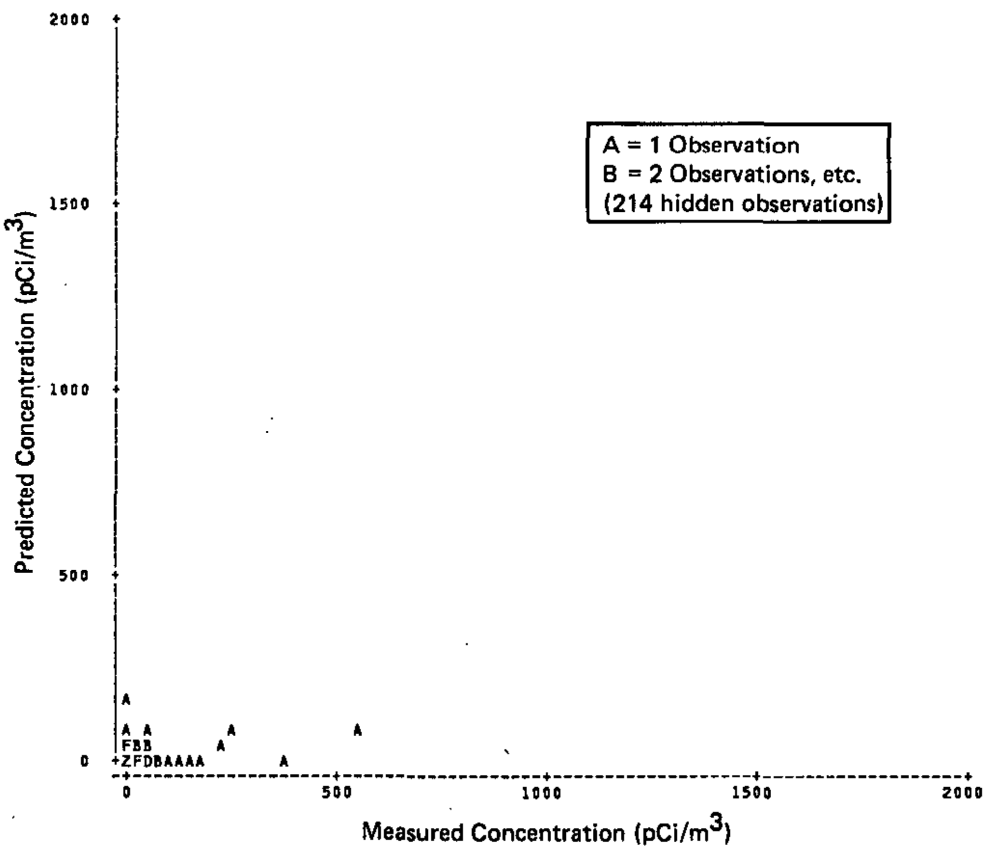

FIGURE C-28. Twice-Daily Predictions for ADPLUM Model (All Points Included)

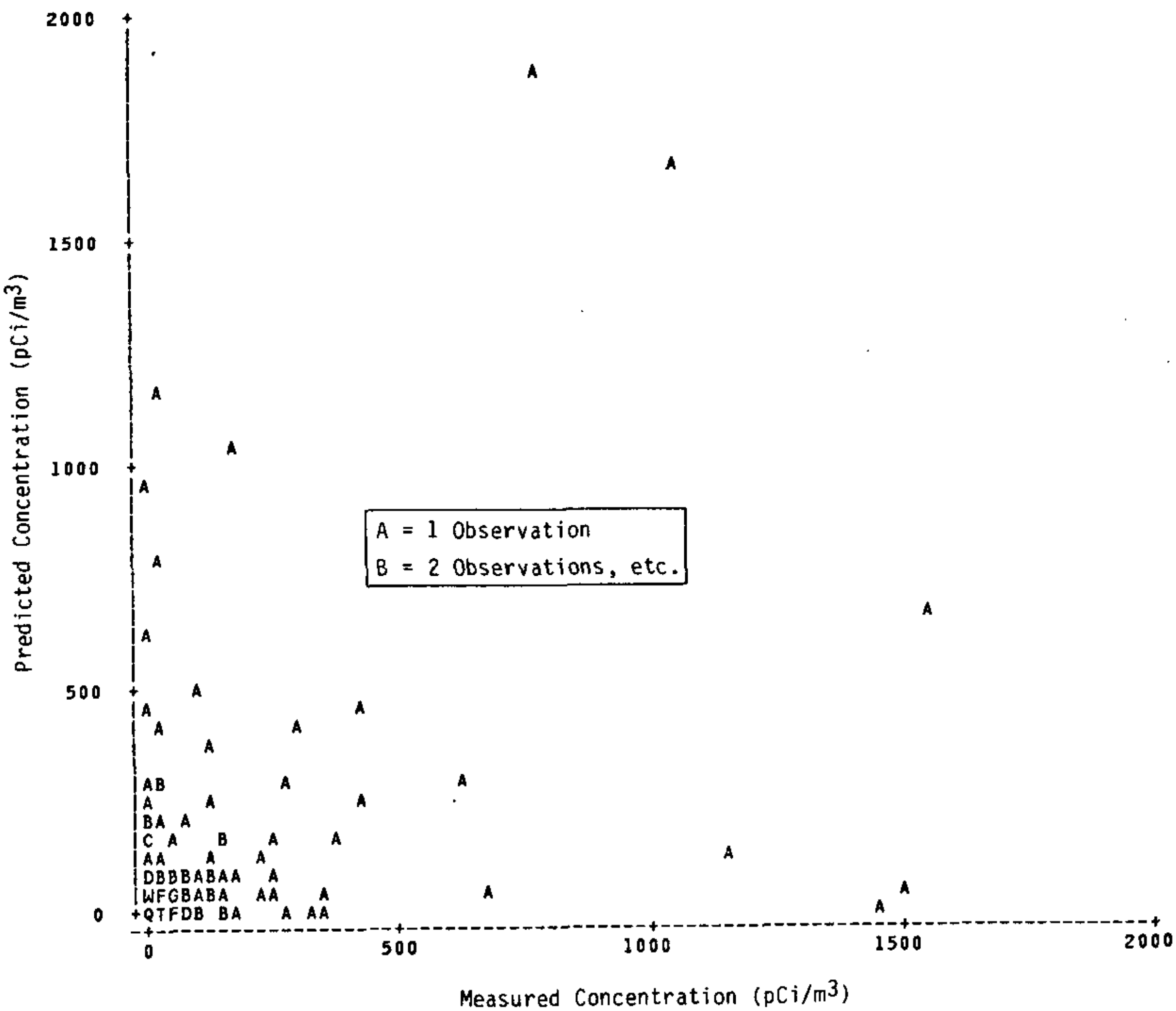

FIGURE C-29. Twice-Daily Predictions for DRAX2 Model (PNOs Excluded)

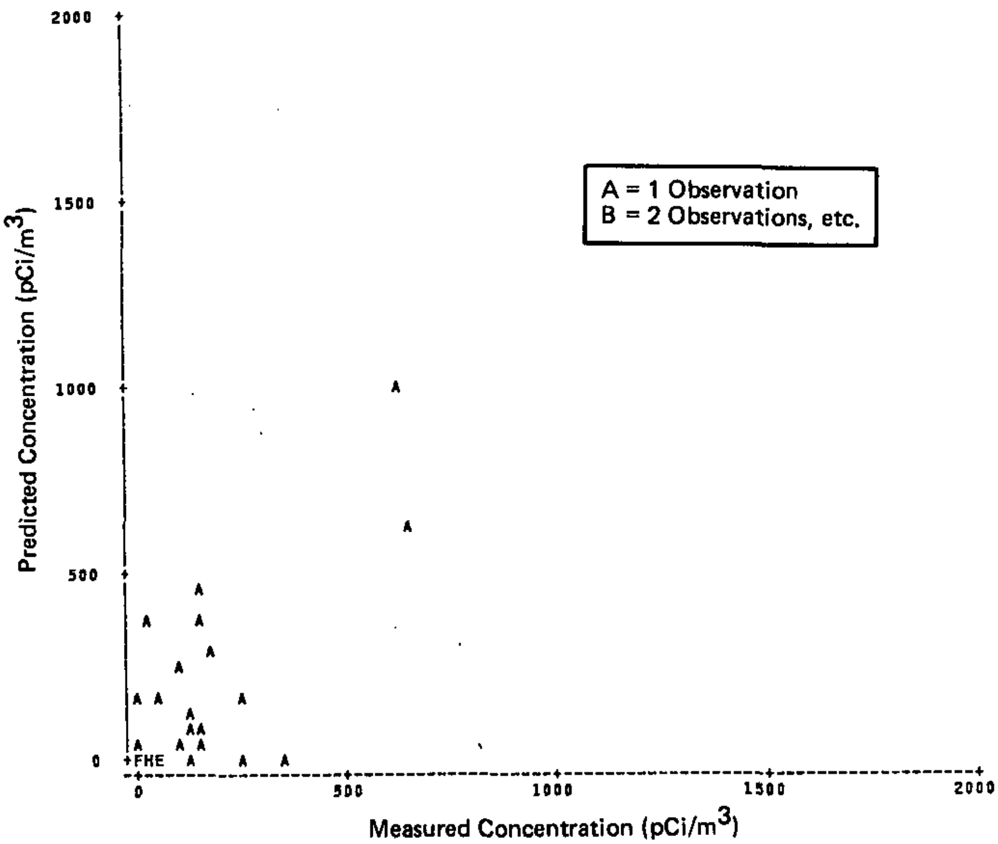

FIGURE C-30. Twice-Daily Predictions for ATMOS Model (PNOs Excluded)

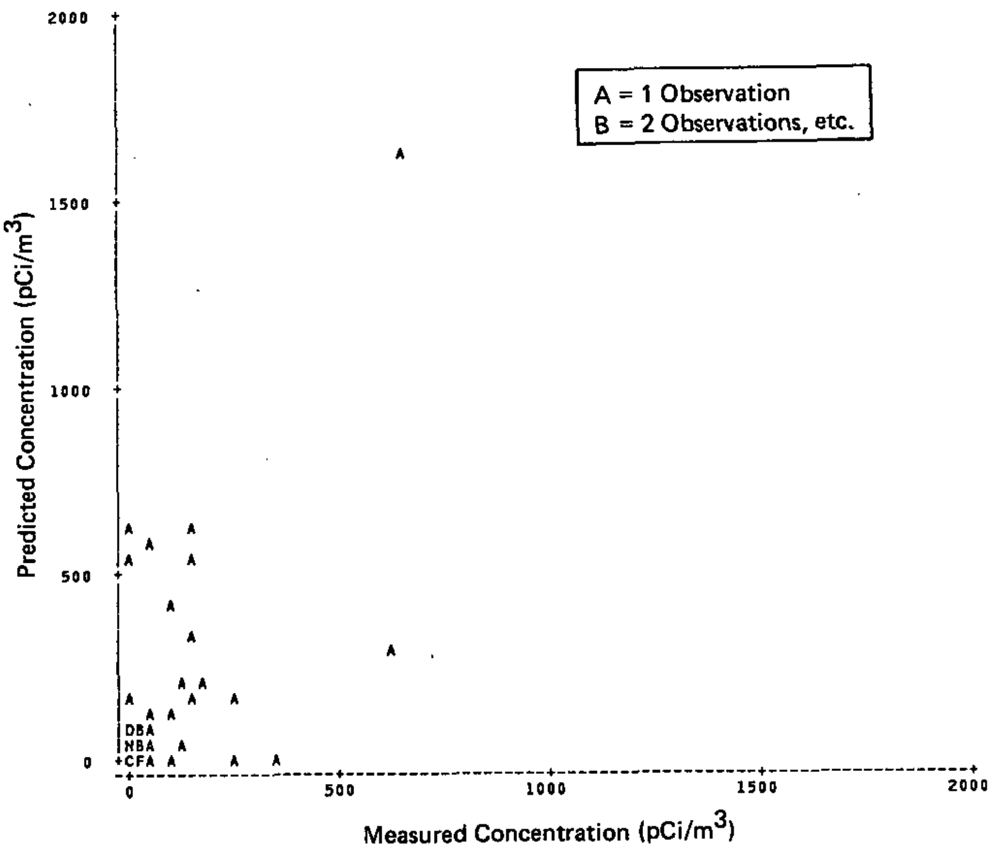

FIGURE C-31. Twice-Daily Predictions for CHAPEAU Model (PNOs Excluded)

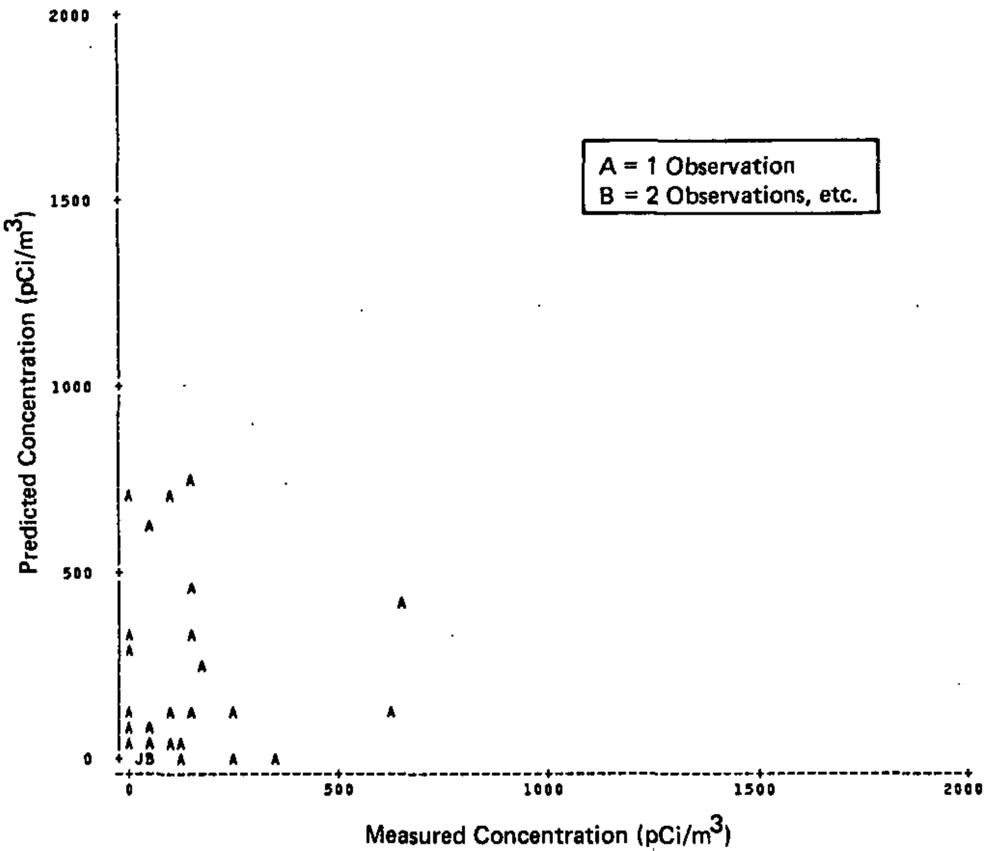

FIGURE C-32. Twice-Daily Predictions for MOMENTS Model (PNOs Excluded)

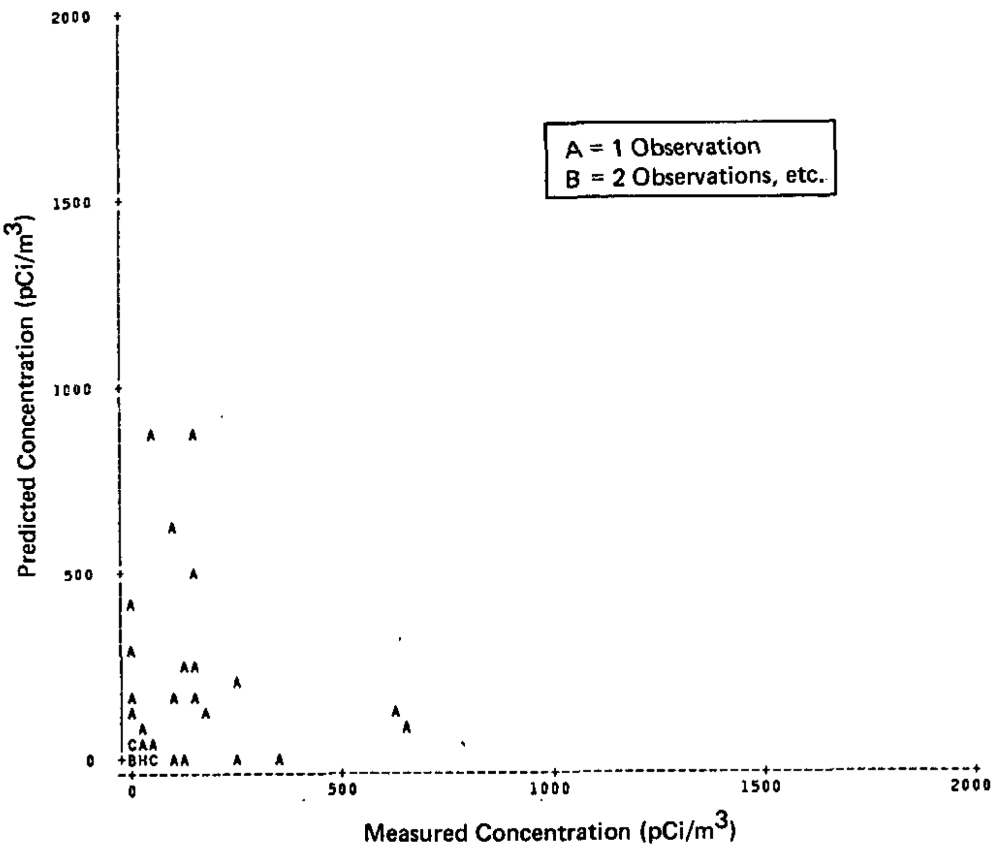

FIGURE C-33. Twice-Daily Predictions for PIC Model (PNOs Excluded)

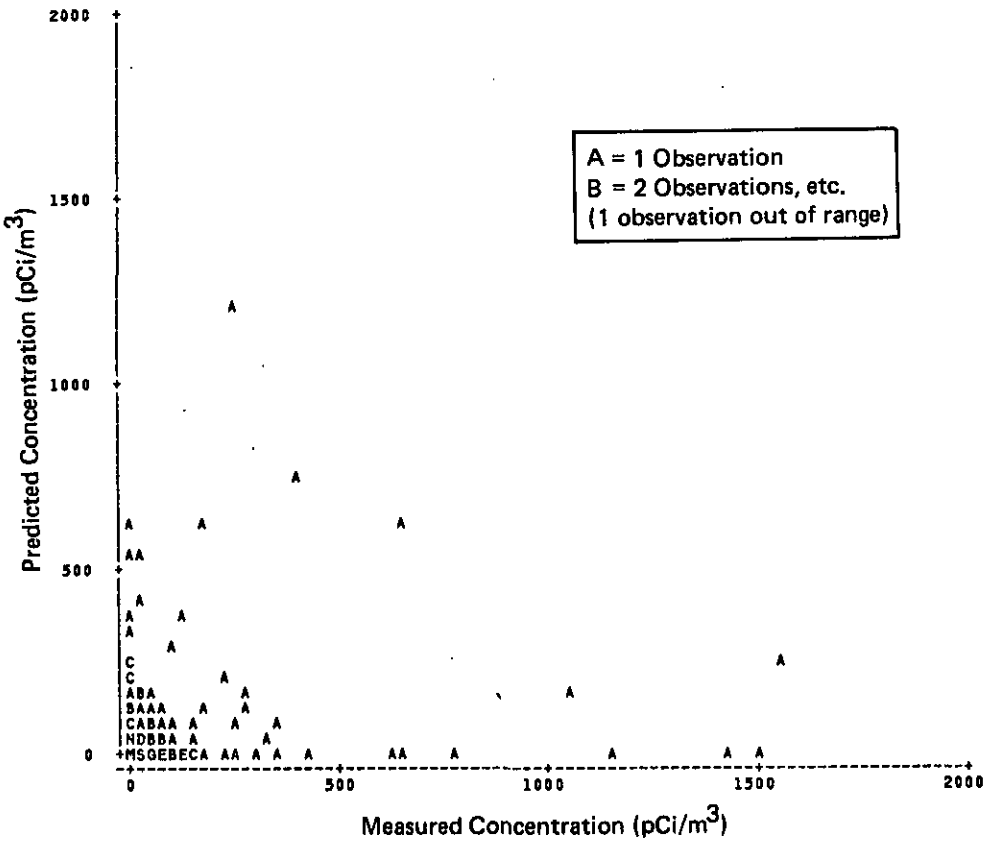

FIGURE C-34. Twice-Daily Predictions for ATAD Model (PNOs Excluded)

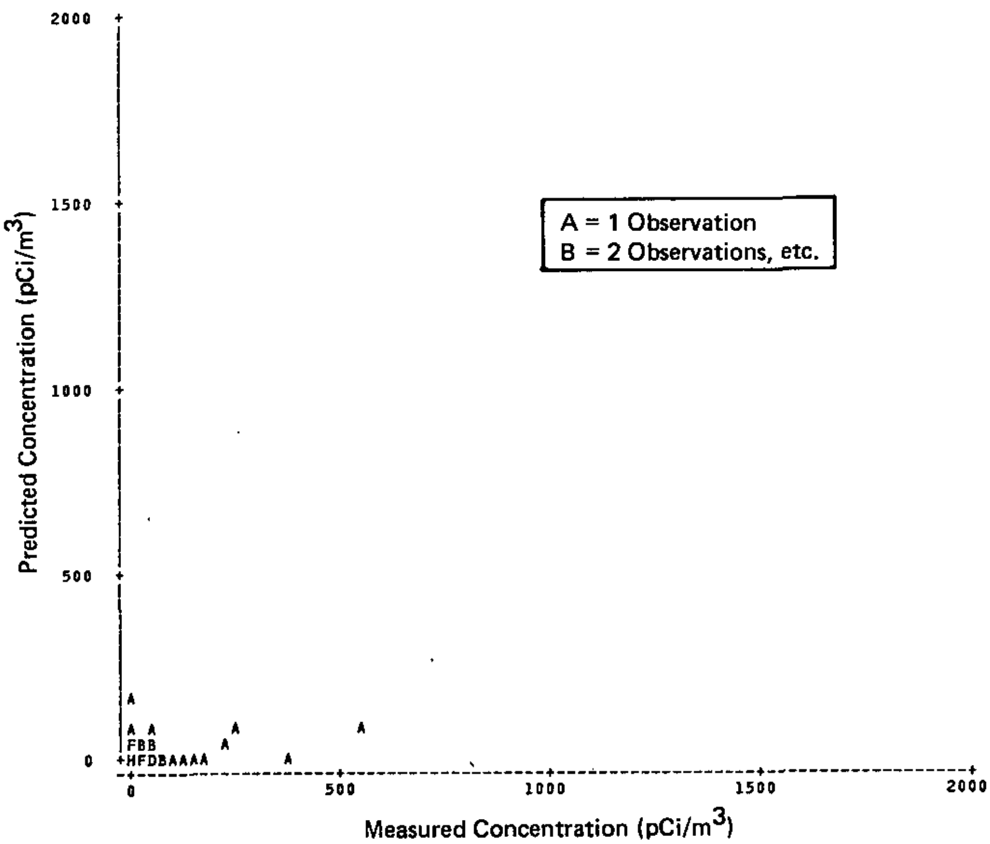

FIGURE C-35. Twice-Daily Predictions for ADPLUM Model (PNOs Excluded)

APPENDIX D. PRIORITY CALCULATIONAL PERIODS

Sampling time periods for both weekly and 10-hour samples were ordered for calculational priority as shown in Tables D-1 and D-2.

TABLE D-1

Calculational Periods and Calculational Order for Weekly Samples

Date of Beginning and/or Ending Sample Collection	Calculational Order	Date of Beginning and/or Ending Sample Collection	Calculational Order	Date of Beginning and/or Ending Sample Collection	Calculational Order
9-29-78 10-6-75 10-13-75 10-20-75 10-27-75	17	4-5-76 4-12-76 4-19-76 4-26-76 5-3-76	15	11-29-76 12-6-76 12-13-76 12-20-76 12-27-76	11
11-3-75 11-10-75 11-17-75 11-24-75 12-1-75	16	5-10-76 5-17-76 5-24-76 5-31-76	12	1-3-77 1-10-77 1-17-77 1-24-77 1-31-77 2-7-77	4
12-8-75 12-15-75 12-22-75 12-29-75	1	6-7-76 6-14-76 6-21-76 6-28-76	2		
1-5-76 1-12-76 1-19-76 1-26-76 2-2-76	10	7-5-76 7-12-76 7-19-76 7-26-76 8-2-76	5	3-7-77 3-14-77 3-21-77 3-28-77 4-4-77	3
2-9-76 2-16-76 2-23-76 3-1-76	7	8-9-76 8-16-76 8-23-76 8-30-76	14	5-9-77 5-16-55 5-23-77 5-30-77	8
3-8-76 3-15-76 3-22-76 3-29-76	9	9-6-76 9-13-76 9-20-76 9-29-76 10-4-76	6	6-6-77 6-13-77 6-20-77 6-27-77 7-1-77	13

TABLE D-2

Calculational Periods and Calculational Order for 10-Hour Samples

Sample Collection Period				Suggested Time Span for Calculations				Calculational Order
Start		End		Start		End		
2200	10-5-76	1200	10-6-76	1800	10-5-76	1800	10-6-76	1
2200	10-14-76	1200	10-16-76	1200	10-14-76	1800	10-16-76	15
0900	10-29-76	0700	10-30-76	0900	10-29-76	1300	10-30-76	5
1000	11-18-76	0800	11-20-76	0100	11-18-76	1400	11-20-76	9
1000	2-2-77	0800	2-4-77	0900	2-2-77	1400	2-4-76	13
2200	2-16-77	0800	2-19-77	0300	2-16-77	1400	2-19-77	2
1000	2-22-77	0800	2-23-77	0100	2-22-77	1400	2-23-77	14
2200	4-5-77	0800	4-9-77	1600	4-5-77	1400	4-9-77	3
1000	4-11-77	0800	4-16-77	2000	4-10-77	1400	4-16-77	10
2200	4-17-77	2000	4-22-77	0600	4-17-77	0200	4-23-77	6
0900	4-27-77	0700	4-29-77	2200	4-25-77	1300	4-29-77	12
0900	7-11-77	0900	7-12-77	2200	7-10-77	0400	7-13-77	4
0900	7-15-77	0700	7-16-77	210	7-14-77	1300	7-16-77	11
2900	7-18-77	1900	7-20-77	1600	7-18-77	0100	7-21-77	8
0900	7-25-77	0700	7-27-77	0400	7-25-77	1300	7027077	7