

United States
Environmental Protection
Agency

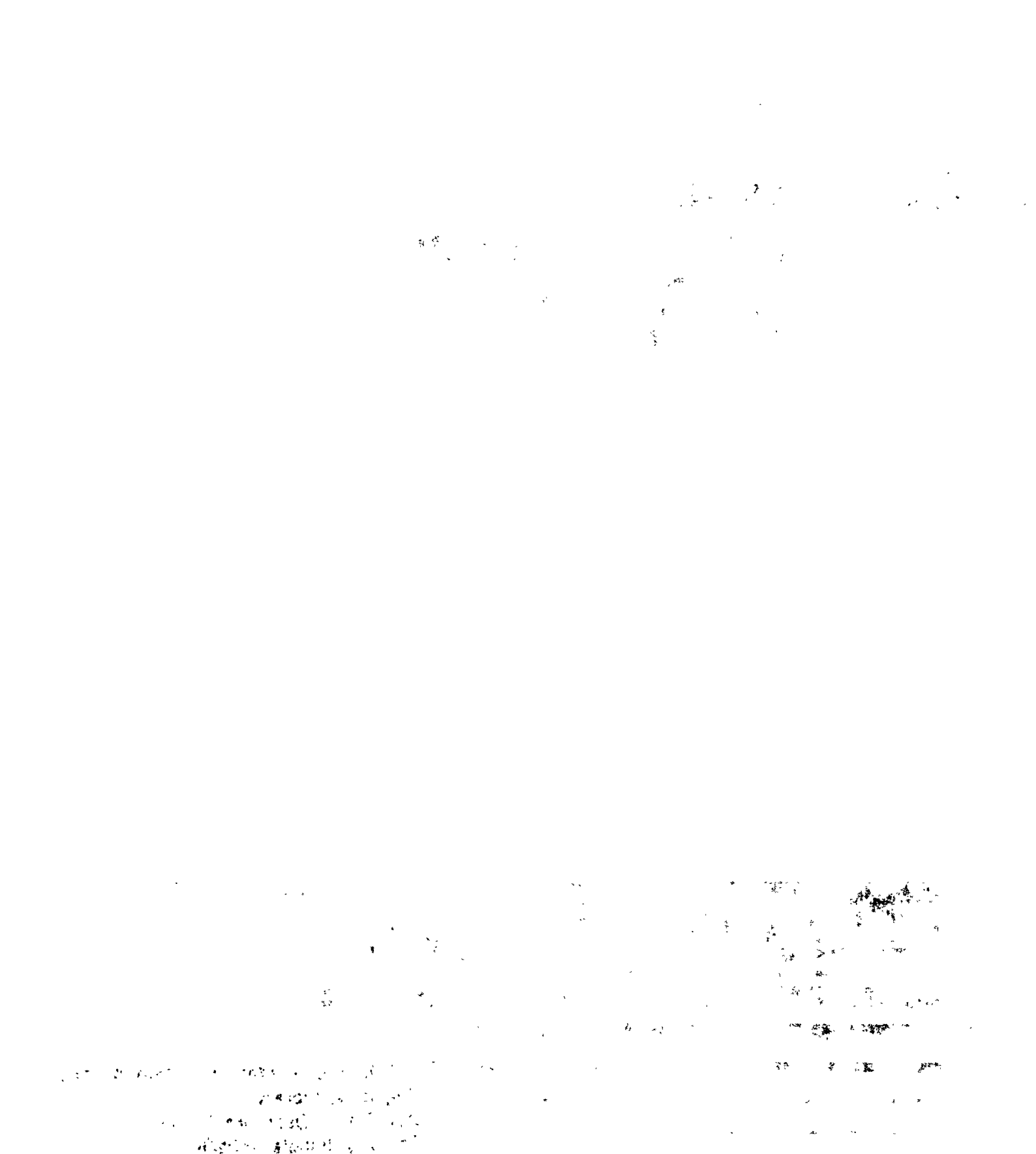
Office of Air Quality
Planning and Standards
Research Triangle Park NC 27711

EPA-450/4-84-017
June 1984

Air



Evaluation of Complex Terrain Air Quality Simulation Models



EPA-450/4-84-017

Evaluation of Complex Terrain Air Quality Simulation Models

by
David Wackter and Richard Londergan

TRC Environmental Consultants, Inc.
800 Connecticut Boulevard
East Hartford, CT 06108

Contract No. 68-02-3514

U.S. Environmental Protection Agency
Region V, Library
230 South Dearborn Street
Chicago, Illinois 60604

Prepared for

U.S. ENVIRONMENTAL PROTECTION AGENCY
Office of Air and Radiation
Office of Air Quality Planning and Standards
Research Triangle Park, NC 27711

June 1984

DISCLAIMER

This report has been reviewed by the Office of Air Quality Planning and Standards, U.S. Environmental Protection Agency, and approved for publication as received from TRC, Environmental Consultants, Inc. Approval does not signify that the contents necessarily reflect the views and policies of the U.S. Environmental Protection Agency, nor does mention of trade names or commercial products constitute endorsement or recommendation for use. Copies of this report are available from the National Technical Information Service, 5285 Port Royal Road, Springfield, Virginia 22161.

U.S. Environmental Protection Agency

TABLE OF CONTENTS

<u>SECTION</u>		<u>PAGE</u>
1.	INTRODUCTION.	1
2.	COMPLEX TERRAIN MODELS	3
	Documentation	3
	Technical Features	4
	Model Input Data Requirements	4
	Source Data	4
	Receptor Date	11
	Meteorological Data	11
3.	DATA BASES FOR COMPLEX TERRAIN EVALUATION	13
	Cinder Cone Butte Data Base	13
	Source Data	16
	Meteorological Data	16
	Tracer Data	21
	Data Selected for Model Input	21
	Tracer Release Information	21
	Ambient Tracer Concentrations	23
	Meteorology	23
	Westvaco-Luke Data Base	27
	Source Data	27
	Meteorology	27
	Data Selected for Model Input	33
	Source Information	33
	Air Quality Data	34
	Meteorology	34
4.	STATISTICS APPROACH	43
	Data Sets for Comparison of Observed and Predicted Concentrations	43
	Peak Concentrations	45
	Comparisons of All Concentrations	46
	Statistical Analysis of Model Performance	46
	Statistical Measures for the Full Westvaco Data Set	50
	IMPACT Model: Analysis of Select Hours for Westvaco	50
	Statistical Measures for the Cinder Cone Butte Data Set	53

TABLE OF CONTENTS (Continued)

<u>SECTION</u>		<u>PAGE</u>
5.	MODEL PERFORMANCE RESULTS	57
	Westvaco Full Year Results	57
	Statistics for 25 Highest Values	57
	Statistics for Highest Concentration at Each Station	63
	Statistics for Highest Concentrations by Event .	66
	Statistics for All Concentrations Paired in Time and Space	66
	Westvaco - Impact Select Hour Results	74
	Statistics for 25 Highest Values	74
	Statistics for Highest Concentrations at Each Station	76
	Statistics for Highest Concentrations by Event .	76
	Statistics for All Concentrations Paired in Time and Space	80
	Cinder Cone Butte Results	83
	Statistics for 25 Highest Values	83
	Statistics for Highest Concentrations by Event .	84
	Statistics for All Comparisons Paired in Time and Space	89
6.	SUMMARY AND CONCLUSIONS	93
	Summary of Results	93
	REFERENCES	95

APPENDICES

A	TEST RUN PACKAGE: DESCRIPTION OF MODELS "AS-RUN" FOR COMPLEX TERRAIN MODEL EVALUATION
B	STATISTICAL TABLES OF MODEL PERFORMANCE FOR WESTVACO
C	STATISTICAL TABLE OF MODEL PERFORMANCE FOR CINCER CONE BUTTE

LIST OF FIGURES

<u>FIGURE</u>		<u>PAGE</u>
3-1	Cinder Cone Butte Field Experiment Layout	15
3-2	Cinder Cone Butte Vertical Cross Section Northwest (315°) to Southeast (135°)	17
3-3	Cinder Cone Tracer Gas Sampler Locations	22
3-4	Map of the Study Area Surrounding the Westvaco Luke Mill .	28
3-5	Westvaco Vertical Cross Sections for radials of 135°, 170°, and 310°. The Westvaco Stack Height Along with Monitor Heights and Distances from the Stack are Superimposed	29

LIST OF TABLES

<u>TABLE</u>		<u>PAGE</u>
2-1	Distinguishing Features of the Complex Terrain Models as Run for the Current Evaluation	5
2-2	Composite of all Meteorological Parameters Expected by the Complex Terrain Models to Exercise Various Models Functions	11
3-1	Periods When Tracer Tests Were Conducted During the Cinder Cone Butte Experiment	14
3-2	Units and Averaging Times Corresponding to Measured Variables Reported in the Cinder Cone Butte Data Base	18
3-3	Cinder Cone Butte Tower Instrumentation and Measures . . .	19
3-4	Summary of Cinder Cone Butte Meteorological Inputs to the Complex Terrain Models	24
3-5	Units and Averaging Times Corresponding to Measured Variables Reported in the Westvaco Data Base	30
3-6	Instrumentation and Parameters Measured on the Westvaco Meteorological Towers	31
3-7	Primary Hourly Meteorological Inputs Included in the Westvaco Modelers' Data Base as Compiled by H.E. Cramer Associates	35
3-8	Data Substitutions Used by H.E. Cramer Associates in Developing Westvaco Hourly Meteorology Inputs	36
3-9	Summary of Westvaco Meteorological Inputs to the Complex Terrain Models	40

LIST OF TABLES

<u>TABLE</u>		<u>PAGE</u>
4-1	Summary of Data Sets for Model Evaluation	44
4-2	Statistical Estimators and Basis for Confidence Limits on Performance Measures	47
4-3	Performance Measures and Statistics Calculated for the Westvaco Unpaired (25 Highest) Data Sets	51
4-4	Performance Measures and Statistics Calculated for Westvaco Data Sets Paired in Time or Location	52
4-5	Performance Measures and Statistics Calculated for the Cinder Cone Butte Unpaired (25 Highest) Data Sets . . .	54
4-6	Performance Measures and Statistics Calculated for the Cinder Cone Butte Data Sets Paired in Time or Location	55
5-1	Comparison of 25 Highest Observed and Predicted SO ₂ Concentration Values (UG/M**3) (Unpaired in Time or Location) for the 1-Hour Averaging Period Westvaco (1980/1981)	58
5-2	Comparison of 25 Highest Observed and Predicted SO ₂ Concentration Values (UG/M**3) (Unpaired in Time or Location) For Various Data Sets Model: Complex I for the 1-Hour Averaging Period Westvaco (1980/1981)	.
60		
5-3	Comparison of 25 Highest Observed and Predicted SO ₂ Concentration Values (UG/M**3) (Unpaired in Time or Location) For the 3-Hour Averaging Period Westvaco (1980/1981)	61
5-4	Comparison of 25 Highest Observed and Predicted SO ₂ Concentration Values (UG/M**3) (Unpaired in Time or Location) For the 24-Hour Averaging Period Westvaco (1980/1981)	62
5-5	Comparison of Highest Observed and Predicted SO ₂ Concentration Values (UG/M**3) Paired by Station for the 1-Hour Averaging Period Westvaco (1980/1981)	64
5-6	Comparison of Second Highest Observed and Predicted SO ₂ Concentration Values (UG/M**3) Paired by Station for the 1-Hour Averaging Period Westvaco (1980/1981)	65
5-7	Comparison of Highest Observed and Predicted SO ₂ Concentration Values (UG/M**3) Event-by-Event (Paired in Time) For the 1-Hour Averaging Period Westvaco (1980/1981)	67

LIST OF TABLES (Continued)

<u>TABLE</u>		<u>PAGE</u>
5-8	Comparison of All Observerd and Predicted SO ₂ Concentration Values (UG/M**3) Paired in Time and Location for the 1-Hour Averaging Period Summary Table (Part 1) Westvaco (1980/1981)	68
5-9	Comparison of all Observed and Predicted SO ₂ Concentration Values (UG/M**3) Paired in Time and Location (For Various Data Sets) Model: COMPLEX I for the 1-Hour Averaging Period Westvaco (1980/1981)	71
5-10	Highest (H) and Highest, Second-High (HSH) 1-Hour Concentrations for Westvaco with Associated Meteorology.	72
5-11	Highest (H) and Highest, Second-High (HSH) 3-Hour and 24-Hour Concentrations for Westvaco Model Runs. . .	73
5-12	Comparison of 25 Highest Observed and Predicted SO ₂ Concentration Values (UG/M**3) (Unpaired in Time or Location) for the 1-Hour Averaging Period Westvaco (1980/1981) Hours Selected for Impact Model Runs. .	75
5-13	Comparison of Highest Observed and Predicted SO ₂ Concentration Values (UG/M**3) (Unpaired in Time or Location) for the 1-Hour Averaging Period Westvaco (1980/1981) Hours Selected for Impact Model Runs. .	77
5-14	Comparison of Second Highest Observed and Predicted SO ₂ Concentration Values (UG/M**3) Paired by Station for the 1-Hour Averaging Period Westvaco (1980/1981) Hours Selected for Impact Model Runs	78
5-15	Comparison of Highest Observed and Predicted SO ₂ Concentration Values (UG/M**3) Event-by-Event (Paired in Time) For the 1-Hour Averaging Period Westvaco (1980/1981) Hours Selected for Impact Model Runs . .	79
5-16	Comparison of All Observed and Predicted SO ₂ Concentration Values (UG/M**3) Paired in Time and Location for the 1-Hour Averaging Period Summary Table (Part 1) Westvaco (1980/1981) Hours Selected for Impact Model Runs . .	81
5-17	Comparison of 25 Highest Observed and Predicted Relative Concentration Values (10**(-6) S/M**3) (Unpaired in Time or Location) For the 1-Hour Averaging Period Cinder Cone Butte (1980)	85

LIST OF TABLES (Continued)

<u>TABLE</u>		<u>PAGE</u>
5-18	Comparison of 25 Highest Observed and Predicted Relative Concentration Values (10**(-6) S/M**3) (Unpaired in Time or Location) for Various Data Sets Model: COMPLEX I For the 1-Hour Averaging Period Cinder Cone Butte (1980)	86
5-19	Comparison of Highest Observed and Predicted Relative Concentration Values (10**(-6) S/M**3) Event-by-Event (Paired in Time) For the 1-Hour Averaging Period Part 1 Cinder Cone Butte (1980)	87
5-20	Comparison of Highest Observed and Predicted Relative Concentration Values (10**(-6) S/M**3) Event-by-Event (For Various Data Sets) Model: COMPLEX I For the 1-Hour Averaging Period Cinder Cone Butte (1980). . .	89
5-21	Comparison of All Observed and Predicted Relative Concentration Values (10**(-6) S/M**3) Paired in Time and Location for the 1-Hour Averaging Period Summary Table (Part 1) Cinder Cone Butte (1980)	91

SECTION 1

INTRODUCTION

The Environmental Protection Agency (EPA) is currently involved in a study to evaluate the performance of air quality dispersion models using statistical measures recommended by the American Meteorological Society. It was EPA's intent, as published in a notice in the March 1980 Federal Register, to provide organizations the opportunity to submit dispersion models for possible inclusion in the next revision of EPA's "Guideline on Air Quality Models".¹ EPA has undertaken a systematic evaluation of these models to decide in an objective manner which models should be included in the guideline and what recommendations should be made concerning the use of these dispersion models for regulatory applications. Several categories of models have been identified including models designed for complex terrain situations. TRC, working under contract to EPA, has assembled the aerometric data sets needed for model input and comparison, set up and run the complex terrain models and produced statistics relating observed and predicted air quality.

In September 1980 the American Meteorological Society (AMS), as a professional organization with expertise in atmospheric dispersion, organized a workshop (sponsored by EPA) to consider the issue of model performance evaluation. The 1980 workshop held at Woods Hole, Massachusetts, produced a report entitled "Judging Air Quality Model Performance."² This report contains recommended statistical procedures for comparing observed air quality with model predictions. The procedures recommended by the Woods Hole workshop provided the basis for the statistical comparisons presented in this report. TRC has performed similar studies for EPA to evaluate eight rural models^{3,4} and six urban models⁵. On the basis of these studies and subsequent comments by the AMS reviewers, a trimmed-down list of statistical comparisons are provided for the complex terrain model evaluation.

In Section 2 the eight complex terrain models are described. The models include COMPLEX I, COMPLEX II, COMPLEX/PFM, 4141, PLUME5, RTDM, SHORTZ and IMPACT. The distinguishing technical features of these models, as run for the current evaluation, are described. Also, the procedures for implementing and testing the models and the unique input data requirements are presented.

The above models have been evaluated with data obtained from two field measurements programs which were carried out in complex terrain environments. The Cinder Cone Butte tracer data base provides air quality measurements with good spatial resolution (94 samplers) for a limited number of study hours (104). The Westvaco data base comes from a rigorous routine-measurements program one year of hourly data at 11 stations, for this study designed for regulatory considerations. These data sets, along with supplemental data, are described in Section 3.

In Section 4 the statistical approach is described. The sets of observed and predicted concentration values have been paired in a variety of ways to provide statistical model performance comparisons that reflect either high concentration values or all concentration values, with and without pairing according to time and space.

The results of this study are presented in Section 5. The tables of statistical comparisons based on the performance measures recommended by the AMS workshop are presented in this section for all eight models run with both data bases.

Three appendices provide additional information. Appendix A is a copy of the TRC document "Test Run Package: Description of the Models 'As Run' for Complex Terrain Model Evaluation" which describes test run procedures, model-by-model code modifications and listings of model input options selected by the model developers for this evaluation. Appendices B and C contain statistical tables for Westvaco and Cinder Cone Butte, respectively. These tables provide statistical results by model for each type of data comparison and for subsets by meteorology and source-receptor geometry.

SECTION 2

COMPLEX TERRAIN MODELS

The following eight complex terrain air quality models have been evaluated by TRC using the performance measures recommended by the American Meteorological Society:

- COMPLEX I
- COMPLEX II
- COMPLEX/PFM
- 4141
- PLUME5
- RTDM
- SHORTZ
- IMPACT

Of these eight models, seven are based on the Gaussian plume assumptions, while IMPACT is a numerical grid model. Specific methods for prescribing plume rise, transport and dispersion differ from model to model, but all of the models require similar basic user-supplied input data describing source characteristics, receptor locations, and representative meteorology. IMPACT generally needs more detailed meteorological input data than the Gaussian models.

DOCUMENTATION

Computer code and documentation for each of the complex terrain models are available to the public. COMPLEX I and COMPLEX II were developed by EPA and are described as screening techniques for applications in complex terrain environments²⁷. Currently no user guides exist for these models. Documentation exists as part of the FORTRAN code and also in the MPTEr user's manual⁶ from which these two models were adapted. COMPLEX/PFM⁷ was developed for EPA by Environmental Research & Technology, Inc. (ERT) as an adaptation of COMPLEX I with provisions for either COMPLEX I, COMPLEX II or potential flow model (PFM) calculations. The model 3141/4141⁸ was developed by Enviroplan, originally as a modified version of CRSTER⁹, and more recently as a modified version of MPTEr. The 4141 option of the MPTEr version was employed in this study. PLUME5¹⁰ was developed by Pacific Gas and Electric, and the Rough Terrain Diffusion Model (RTDM)¹¹ was developed by ERT. SHORTZ¹² was developed by the H.E. Cramer Company. An updated version of SHORTZ which includes an algorithm to account for vertical wind direction shear¹³ was used in this study. Two versions of IMPACT (Integrated Model for Plumes and Atmospheric Chemistry in Complex Terrain)^{14,15} were submitted to EPA. The authors of both versions were contacted and they agreed that very little difference between results from the two versions was likely, at least for the purposes of this evaluation. Therefore, the Fabrick and Haas version was selected for this evaluation.

TECHNICAL FEATURES

Distinguishing features of the complex terrain models as run for the current evaluation are listed in Table 2-1. The information listed in Table 2-1 is presented by model and then by generalized modules including transport, dispersion/stability, plume rise/terrain impaction and limits to vertical mixing. These modules represent physical processes that the models are attempting to simulate. It is not the intent here to fully describe each of the complex terrain models, but rather to list briefly the primary technical features that distinguish one model from another. In-depth technical discussions of each model can be obtained from the appropriate model-user guides. The reader is encouraged to refer to the users manuals for technical details and references.

As part of the model evaluation process, test run packages were prepared and supplied to the model developers for their review and concurrence. A description of this procedure can be found in Appendix A which contains a copy of one of the test run package documents¹⁶. This document also summarizes the model code modifications made by TRC and describes the input options selected by the model developers for each model and data base. Modifications to the models were needed to adapt each model to the EPA UNIVAC computer, to adapt particular models to accept the source-receptor inventories and to format the output of calculated concentrations for input to the statistics system.

It is also noted that ERT (RTDM) and H. E. Cramer Co. (SHORTZ) previously had the opportunity to test their models using at least portions of the data sets selected for this evaluation. Both data sets were previously used by ERT, while only the Westvaco data set was used by the H. E. Cramer Co. According to the developers, the models were not modified based on these evaluations. However, these developers could select model options and model inputs to optimize model performance, based on previous experience.

MODEL INPUT DATA REQUIREMENTS

All of the complex terrain models require basic user-supplied input data describing source characteristics, receptor locations and representative meteorology. Other model inputs control options for data input/output and technical considerations.

Source Data

Each of the models requires that the fixed geographic and geometric characteristics of each source be specified by the model user. The location is generally specified in Cartesian or polar coordinates except for the IMPACT model which requires horizontal source locations to be specified as central cell positions within a Cartesian three-dimensional grid. The stack base elevation, physical stack height, and stack gas exit diameter are fixed variables also required by each of the models.

Pollutant emission rate, stack gas exit velocity and stack gas temperature are generally needed by the complex terrain models in the calculation of plume rise and ambient concentration. The temporal variation of these parameters is available as one-hour averages in the Cinder Cone Butte and Westvaco data bases. Plume rise was not a factor in the Cinder Cone Butte tracer study (passive releases) and therefore stack velocity and temperature are not available. Many of the models had to be modified to accept hourly varying source data.

TABLE 2-1 DISTINGUISHING FEATURES OF THE COMPLEX TERRAIN MODELS AS RUN FOR
THE CURRENT EVALUATION

COMPLEX I

Transport

- Wind speed as input at release height
- Wind direction as input

Dispersion/Stability

- Turner stability categories (class 7 treated as class 6)
- Gaussian vertical distribution using rural, (P-G) σ_z
- 22.5 horizontal sector averaging
- Buoyancy induced vertical dispersion

Plume Rise/Terrain Impaction

- Terrain adjustments = .5, .5, .5, .5, .0, .0 for Stability A-F
- Minimum terrain approach = 10m
- Briggs final plume rise, including momentum rise
- Stack tip downwash for non-passive plumes

Limits to Vertical Mixing

- Full reflection at ground and mixing height
- Uniform vertical mixing beyond where $\sigma_z = 1.6 \times$ mixing height

COMPLEX II

Transport

- Wind speed as input at release height
- Wind direction as input

Dispersion/Stability

- Turner stability categories (class 7 treated as class 6)
- Bivariate Gaussian distribution (PGT σ_y and σ_z)
- Buoyancy induced dispersion

(Continued on next page)

TABLE 2-1 (Continued)

Plume Rise/Terrain Impaction

- Terrain adjustments = .5, .5, .5, .5, .0, .0 for stability A-F
- Minimum terrain approach = 10m
- Briggs final plume rise including momentum rise
- Stack-tip downwash for non-passive plumes
- Linear concentrations drop-off with height above plume centerline

Limits to Vertical Mixing

- Full reflection from ground and mixing height
- Uniform vertical mixing beyond where $\sigma_z = 1.6 \times$ mixing height

COMPLEX/PFM

Transport

- Wind speed as input at release height for COMPLEX I/II calculations
- Wind speed adjusted in potential flow model (PFM) calculations as a function of streamline deformation
- Wind direction as input

Dispersion/Stability

- Turner stability categories (class 7 treated as class 6)
- COMPLEX I (22.5 sector averaging) for D, E or F stability when plume is below dividing streamline height
- COMPLEX II for A, B, or C stability
- PFM (adjusted PGT σ_y and σ_z) for D, E or F stability when plume is above dividing streamline height
- Buoyancy induced vertical dispersion

Plume Rise/Terrain Impaction

- COMPLEX I/II terrain adjustments = .5, .5, .5, .5, .0, .0 for stability A-F
- COMPLEX I/II minimum terrain approach = 10m
- PFM plume height reduced for deformed streamlines
- Modified Briggs layered plume rise
- Stack tip downwash for non-passive plumes

(Continued on next page)

TABLE 2-1 (Continued)

Limits to Vertical Mixing

- Full reflection at ground and mixing height
- Uniform vertical mixing beyond where $\sigma_z = 1.6 \times$ mixing height

4141

Transport

- Wind speed as input at release height
- Wind direction as input

Dispersion/Stability

- Turner stability categories (class G treated as class F)
- Bivariate Gaussian distribution (PGT σ_z and time-enhanced PGT σ_y)
- Buoyancy induced dispersion

Plume Rise/Terrain Impaction

- Terrain adjustments = .5, .5, .5, .5, .25, .25
- Briggs transitional plume rise

Limits to Vertical Mixing

- Full reflection at ground and mixing height
- Uniform vertical mixing beyond where $\sigma_z = 1.6 \times$ mixing height

IMPACT

Transport

- Input wind speed and direction at multiple sites extrapolated and interpolated to 3-dimensional grid cells
- Divergence-free wind field created

(Continued on next page)

TABLE 2-1 (Continued)

Dispersion/Stability

- Finite difference solution to diffusion equation
- Diffusivities from DEPICT model using Smith's (empirical) formulations

Plume Rise/Terrain Impaction

- Plume/terrain approach controlled by wind and diffusivity fields
- Briggs layered plume rise including penetration of stable layers

Limits to Vertical Mixing

- Temperature stratifications incorporated into wind and diffusion fields

PLUME5

Transport

- Wind speed as input at release height
- Wind direction as input

Dispersion/Stability

- Stability categories from horizontal turbulence intensity (σ_θ) and time of day (class A treated as class B; class G treated as class F)
- Bivariate Gaussian distribution (PGT σ_y and σ_z)
- Enhanced horizontal dispersion due to vertical wind directional shear
- Buoyancy induced dispersion

Plume Rise/Terrain Impaction

- Conservative modification to one-half plume height concept
- Briggs final plume rise with determination of stable layer penetration

Limits to Vertical Mixing

- Full reflection at ground and mixing height
- Uniform vertical mixing beyond where $\sigma_z = 1.6 \times$ mixing height

(Continued on next page)

TABLE 2-1 (Continued)

RTDM

Transport

- Wind speed extrapolated from release height to plume height
- Wind direction as input

Dispersion/Stability

- Stability categories from vertical turbulence intensity (σ_z) measured at Westvaco
- Bivariate Gaussian distribution (dispersion coefficients from measured turbulence data)
- Buoyancy induced dispersion
- Enhanced horizontal dispersion for plumes rising through a shearing wind

Plume Rise/Terrain Impaction

- Terrain impingement for stable plumes below critical height
- Half height correction for neutral or unstable conditions and stable conditions when plume exceeds critical height
- Briggs transitional plume rise; hourly potential temperature gradients for stable plume rise
- Stack tip downwash for non-passive plumes

Limits to Vertical Mixing

- Partial terrain reflection; full mixing lid reflection
- Mixing height adjustment for plume path
- Unlimited mixing height for stable conditions

SHORTZ

Transport

- Wind speed extrapolated from release height to plume height
- Wind direction as input

(Continued on next page)

TABLE 2-1 (Continued)

Dispersion/Stability

- Bivariate Gaussian distribution (Cramer dispersion coefficients from measured turbulence data)
- Cramer technique for enhanced horizontal dispersion due to vertical wind direction shear
- Buoyancy induced dispersion

Plume Rise/Terrain Impaction

- Terrain impingement within the mixing layer
- Modified Briggs final plume rise; hourly potential temperature gradient for stable plume rise
- Stack tip downwash for non-passive plumes

Limits to Vertical Mixing

- Full reflection at ground and mixing height
- Uniform mixing beyond where reflection terms ($i=3$) exceed $\exp(-10)$
- Mixing height constant above sea level, for determination of plume penetration
- Minimum actual mixing depth of $H = u \times 200$ meters (u = wind speed) for Westvaco; Height where vertical intensity of turbulence drops below 0.01 radians for Cinder Cone Butte.

Receptor Data

Each of the complex terrain models produces calculated concentrations at multiple receptor locations. In all of the models except IMPACT, discrete receptors at arbitrary locations are defined in Cartesian or polar coordinates. The IMPACT model defines receptor locations internally as the central cell position within each of the 3-dimensional grid "boxes." All of the complex terrain models require receptor elevations above a local reference plane.

Meteorological Data

Meteorological data are used by the models to calculate transport, dispersion, plume rise and limited mixing between sources and receptors. The complex terrain models expect a broad range of meteorological parameters, as summarized in Table 2-2. The IMPACT model allows data from one or multiple meteorological towers to be internally pre-processed into 3-dimensional fields for input to the grid model. The other complex terrain models are exercised with meteorological data from one "representative" station. The representative input data sets used in this evaluation consist of a composite of parameters measured at more than one site. A detailed description appears in Section 3.

TABLE 2-2

COMPOSITE OF ALL METEOROLOGICAL PARAMETERS EXPECTED BY THE
COMPLEX TERRAIN MODELS TO EXERCISE VARIOUS MODEL FUNCTIONS

Transport	Model Function		
	Dispersion (Stability)	Plume Rise	Limited Mixing
Wind Speed	P-G Stability	Temperature	Mixing Height
Wind Direction	σ_θ or I_y	Wind Speed	
Anemometer Height	σ_ϕ or I_z	dT/dZ	
Power Law Exponents	Wind Direction Shear	P-G Stability	
Temperature and Wind Speed for Froude Number and Critical Height			

Some of the complex terrain models contain preprocessor programs that must be exercised in order to obtain a complete set of model-consistent meteorological input data. CRSMET, the CRSTER preprocessor, is used to generate hourly Pasquill-Gifford stability categories from on-site wind speeds and National Weather Service (NWS) cloud observations for input to COMPLEX I, COMPLEX II, COMPLEX/PFM and 4141. RTDM uses this data for the Cinder Cone Butte application. Westvaco mixing heights from CRSMET are used by COMPLEX I, COMPLEX II and 4141. CONVRT, the preprocessor for PLUME5, is used to generate stability class from horizontal turbulence measurements. Westvaco mixing heights are also generated from CONVRT. METZ is the SHORTZ preprocessor which is used to generate mixing heights for Westvaco. The PROFILE preprocessor to COMPLEX/PFM is used with the Westvaco data set to develop vertical profiles of temperature and wind speed which are subsequently needed by the model for calculations of Froude number and critical streamline height. TRC developed preprocessors for providing profiles of meteorological data needed as input to the IMPACT model.

Description of specific model input data for both Westvaco and Cinder Cone Butte are provided in Section 3.

SECTION 3

DATA BASES FOR COMPLEX TERRAIN MODEL EVALUATION

The complex terrain models have been evaluated with data obtained from two field measurements programs which were carried out in complex terrain environments. The Cinder Cone Butte tracer data base provides air quality measurements with good spatial resolution for a limited number of study hours. The Westvaco data base, containing a small number of stations for an extended period of continuous monitoring, results from a rigorous routine-measurements program designed for developing a model to be applied in a regulatory setting. Terrain at the Westvaco-Luke Mill is steep, uneven and rugged; Cinder Cone Butte is a simple, isolated terrain feature.

Both data bases were originally obtained for what might be called research objectives, or diagnostic model evaluation. As a result, there existed an overabundance of meteorological data which was trimmed down to enable operational evaluation of the models. Trimmed down or "modeler's data bases" were recommended for use in this evaluation so that a common set of input data could be used in as many models as possible. The intention was to reduce uncertainties in model predictions resulting from minor differences in input data, and hence allow relative differences between the models to be evaluated strictly on the basis of technical merit. Of course, model input data requirements do differ somewhat from model to model. These model requirements were accounted for in the preparation of test run and final input data sets as described in this section.

CINDER CONE BUTTE DATA BASE

The Cinder Cone Butte experiment represents the first major component of the EPA-sponsored Complex Terrain Model Development Program.^{17,18,19} The broad objective of the experiment was to determine the behavior and impact of an elevated plume in the vicinity of an isolated elevated-terrain feature. During the period between October 16, 1980 and November 12, 1980, 18 multi-hour dual tracer gas experiments were conducted during primarily stable atmospheric conditions. The periods when tracer tests were conducted are listed in Table 3-1.

As can be seen from Figure 3-1, Cinder Cone Butte is a roughly axisymmetric, 100 meter high isolated hill. The hill is located in southeastern Idaho about 50 m south-southeast of Boise. The surrounding Snake River Basin is a broad, nearly level plain.

TABLE 3-1

PERIODS WHEN TRACER TESTS WERE CONDUCTED
DURING THE CINDER CONE BUTTE EXPERIMENT¹⁷

Experiment No.	1980 Date	Experiment Hours (PST)	Hours	Typical Stability
201	10/16	1700-2300	6	E
202	10/17	1700-2300	6	E
203	10/20	0000-0800	8	E-F
204	10/21	0000-0800	8	E-F
205	10/23	0000-0800	8	E
206	10/24	0000-0800	8	E
207	10/25	0000-0800	8	E-F
208	10/27	1700-0100	7	E-F
209	10/28	1700-0100	7	F
210	10/30	0000-0740	7	E-F
211	10/31	0000-0800	8	E-F
213	11/04	0000-0800	8	E-F
214	11/05	0200-1000	8	E-F
215	11/06	0000-0600	6	E-F
216	11/09	0000-0700	7	E-F
217	11/10	0200-1000	8	E-F
218	11/12	0200-1000	8	E

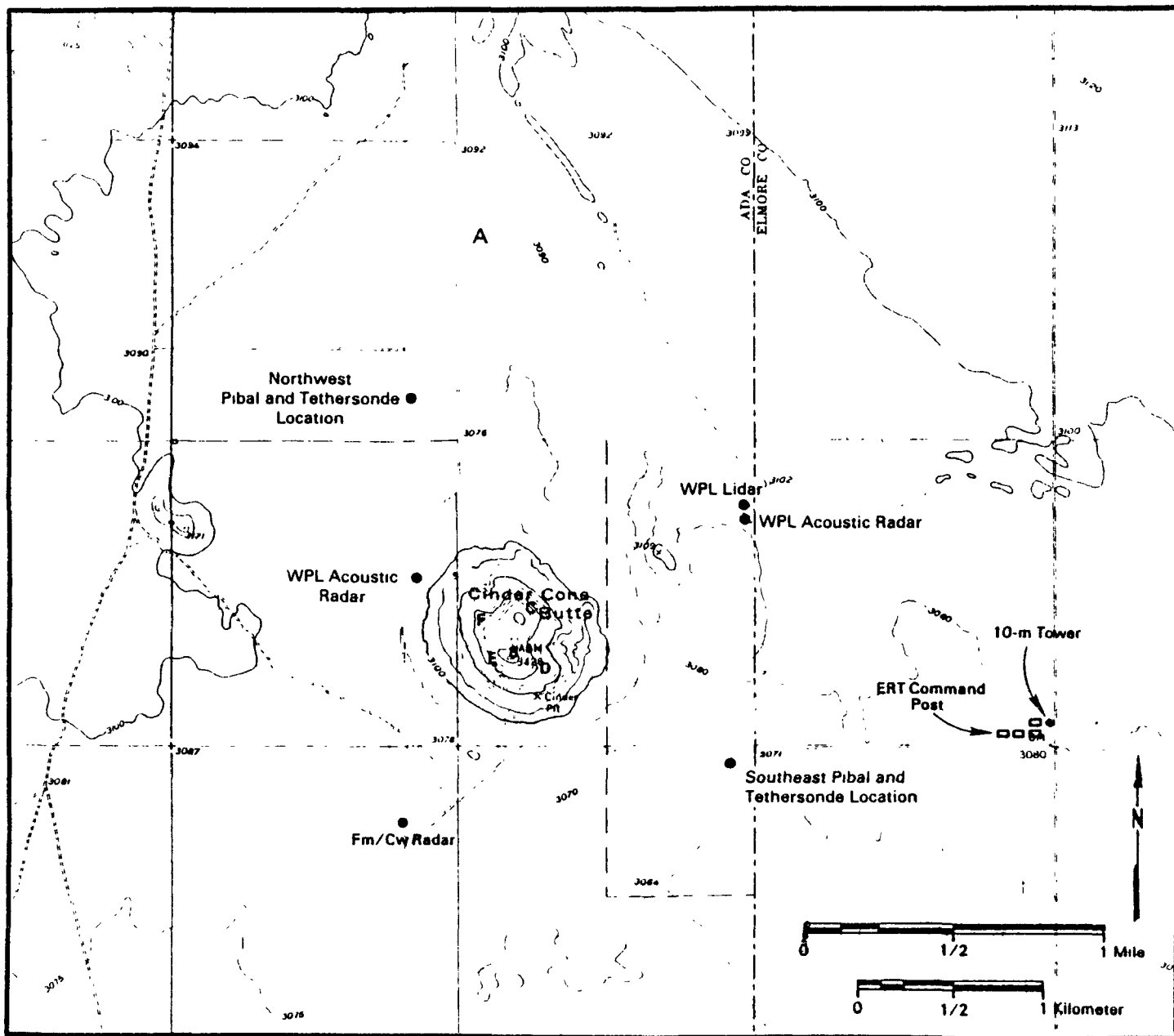


Figure 3-1. Cinder Cone Butte field experiment layout. A is the 150 m tower; B is the 30 m tower; C, D, E, F are 10 m towers(Ref. No. 17).

Ground-level measurements of two tracer gases, sulfur hexafluoride (SF_6) and freon (CF_3Br), were conducted during testing periods. Each test persisted for approximately eight hours with tracer gas releases occurring during five or six of these hours. Of the 111 test hours, 104 were used in this model evaluation. Tracer measurements were accompanied by an extensive collection of meteorological measurements taken on multiple levels of several towers located in the area and on the butte itself. Additionally, plume characteristics were inferred from photography and remote sensing.

The Cinder Cone Butte data base, measured and compiled by Environmental Research and Technology (ERT) under contract to EPA, contains most of the parameters which are needed for the complex terrain model evaluation. The parameters describe source emissions, atmospheric dispersion characteristics and ambient measurements of tracer concentrations.

Source Data

The two tracer gases, SF_6 and CF_3Br , were released passively from different levels utilizing a mobile crane. The range of SF_6 release heights and release distances relative to the butte is displayed in Figure 3-2. The crane release heights ranged from 15 to 57 meters above the local terrain at the base of the butte. Tracer release distances from the butte center ranged from 540 meters to 1420 meters. The mobility afforded by the release system enabled tracer releases directly upwind of the butte, producing a high number of successful hours per test. Although the variability of gas flow for SF_6 and CF_3Br was monitored using separate rotameters, the weight loss of the cylinders was used to determine the emission rate of each tracer. The source data base compiled by ERT consists of the vertical and horizontal crane location (relative to the butte peak) for each release period and average emission rate for each test hour (see Table 3-2).

Meteorological Data

Six instrumented towers were used to measure local meteorology. These included: a 150 meter tower approximately 2 kilometers north of Cinder Cone Butte; a 30 meter tower at the summit of the butte; and four 10 meter towers on the hill. The locations of the towers (A, B, C, D, E, and F) are shown in Figure 3-1. The direct measurements and derived parameters obtained for each of the towers are given in Table 3-3.

Various atmospheric sounding devices were employed during tracer testing periods. A tethersonde was operated usually at a location within 700 m of the primary release point. An ascent-descent sequence conducted at a minimum of once per hour generated profiles of temperature, pressure, wind speed and direction to heights of at least 200 m above the local terrain. When high wind speeds precluded tethersonde operation, profiles were obtained from minisonde flights. Hourly wind profiles were also derived from pilot balloons (pibals). Additionally a frequency-modulated, continuous-wave (FM/CW) radar, and two monostatic acoustic radars were operated near the butte.

The meteorological tower data has been assembled by ERT and currently resides on magnetic tape. Corrections were made by ERT to known errors in the wind speed and wind direction measurements. Temperature corrections were not made, given that the results of two independent audits were

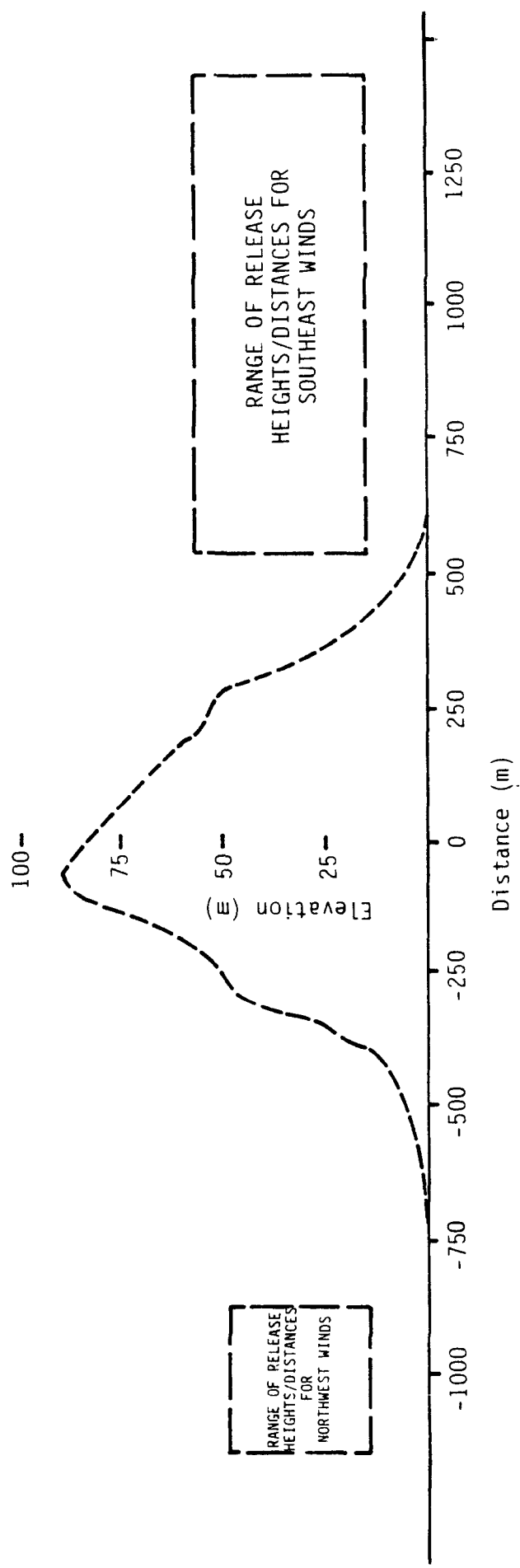


Figure 3-2. Cinder Cone Butte vertical cross section from northwest (315°) to southeast (135°).

TABLE 3-2

UNITS AND AVERAGING TIMES CORRESPONDING TO MEASURED VARIABLES
REPORTED IN THE CINDER CONE BUTTE DATA BASE

Parameter	Source		Meteorological				Tracer	
	Units	Averaging Time	Parameter	Units	Averaging Time	Parameter	Units	Averaging Time
emission rate	gms^{-1}	hourly	wind speed	ms^{-1}	5 minutes	SF_6 concentration	ppt	hourly, 10 minutes depending on mode of sequential sampling used
			wind direction	degrees	5 minutes			
			temperature	$^{\circ}\text{C}$	5 minutes			
			radiation	ly min^{-1}	5 minutes			
			intensity of turbulence	% radians	5 minutes	CF_3Br	ppt	hourly, 10 minutes depending on mode of sequential sampling used

TABLE 3-3

CINDER CONE BUTTE TOWER INSTRUMENTATION AND MEASURES¹⁷

Site	Instruments*	Direct Measures	Derived Measures
Tower A			
Level 0 (1 m)	Pyranometer Net radiometer	Insolation Net radiation	
Level 1 (2 m)	Triaxial props Cup and vane RTD	U, V, W, IX, IY, IZ UX, VX T	WS, WD SP, DR
Level 2 (10 m)	Triaxial props Cup and vane RTD Fast bead thermistor	U, V, W, IX, IY, IZ UX, VX, U, $\sigma\theta$ ΔT (10 m - 2 m) T, σ_T	WS, WD SP, DR T
Level 3 (20 m)	RTD	T	
Level 4 (40 m)	Triaxial props RTD	U, V, W, IX, IY, IZ ΔT (40 m - 2 m)	WS, WD T
Level 5 (60 m)	RTD	T	
Level 6 (80 m)	Triaxial props RTD	U, V, W, IX, IY, IZ ΔT (80 m - 2 m)	WS, WD T
Level 7 (100 m)	RTD	T	
Level 8 (150 m)	Triaxial props Cup and vane RTD Fast bead thermistor	U, V, W, IX, IY, IZ UX, VX ΔT (150 m - 2 m) T, σ_T	WS, WD SP, DR T
Tower B			
2 m	Triaxial props RTD	U, V, W, IX, IY, IZ T	WS, WD

* All temperature sensors were mounted in aspirated radiation shields; an RTD is a Resistance Thermometric Device.

(continued on next page)

TABLE 3-3 (Continued)

CINDER CONE BUTTE TOWER INSTRUMENTATION AND MEASURES¹⁷

Site	Instruments*	Direct Measures	Derived Measures
Tower B (Continued)			
10 m	Triaxial props	U, V, W, IX, IY, IZ	WS, WD
	Cup and vane	UX, VX	SP, DR
	RTD	ΔT	T
30 m	Triaxial props	U, V, W, IX, IY, IZ	WS, WD
	Cup and vane	UX, VX	SP, DR
	RTD	ΔT	T
Towers C, D, E, F			
2 m	Triaxial props	U, V, W, IX, IY, IZ	WS, WD
	RTD	T	
10 m	Triaxial props	U, V, W, IX, IY, IZ	WS, WD
	Cup and vane	UX, VX	SP, DR
	RTD	ΔT	T

* All temperature sensors were mounted in aspirated radiation shields; an RTD is a Resistance Thermometric Device.

Key

U: westerly component of wind measured by east-west oriented propeller
V: southerly component of wind measured by north-south oriented propeller
W: vertical component of wind measured by vertically oriented propeller
SP: horizontal wind speed measured by cup anemometer
DR: horizontal wind direction measured by vane
 $\sigma\theta$: standard deviation of horizontal wind direction calculated from vane output
UX: easterly component of wind calculated from the cup and vane outputs
VX: southerly component of wind calculated from the cup and vane outputs
WS: horizontal wind speed calculated from U and V
WD: horizontal wind direction calculated from U and V
IX: downwind intensity of turbulence
IY: crosswind intensity of turbulence (IY approximates $\sigma\theta$ for small horizontal wind deviations)
IZ: vertical intensity of turbulence (IZ approximates $\sigma\phi$ for small vertical wind deviations)
T: temperature (resistance thermometric device)
 σT : standard deviation of temperature
 ΔT : temperature difference

inconsistent. Turbulence intensity data were also left uncorrected although errors in these data are known to exist due to the response characteristics of the propeller sensors. Other identified errors that remain in the data base are due to the effects of the wake of one instrument on another and the effects of tower wakes on turbulence measurements and wind direction. Users of this data set have been advised by ERT to give precedence where possible to wind measurements from instruments that are more clearly out of wakes. The meteorological tower data has been recorded on tape as five-minute averages for the variables listed in Table 3-2. Data from pibal, mini-sonde, and tether sonde flights are available on a separate magnetic tape.

Tracer Data

Tracer samples were obtained with approximately 90 battery-operated samplers which were sequentially operated for either 10 minute or 1 hour periods. Figure 3-3 shows the locations of the 70 fixed samplers and the 10 movable samplers. The movable samplers were deployed either on the northwest or southeast side of the hill, depending on the prevailing wind direction. For a typical test, 60 of these 80 sites provided 1-hour average samples and 20 were designed to obtain 10-minute average samples. An additional 10 samplers were used: on masts for measuring plume reflection from the ground; for measuring background concentrations; and as collocated samplers for quality assurance purposes.

Bag samples were assayed for SF_6 and CF_3Br concentrations using gas chromatography. After all bags were analyzed, a data base consisting of approximately 14,000 tracer concentration measurements representing the entire experiment was assembled and recorded on magnetic tape. For each 10-minute and 1-hour assayed sample, the experiment number, sample identification, sampling start time, sampling end time, SF_6 concentration and CF_3Br concentration are stored on the data tape (see Table 3-2).

Data Selected for Model Input

A modeler's data base (MDB) was prepared by ERT from the archive of Cinder Cone Butte data. This MDB contains hourly averages of tracer release information, ambient tracer concentrations and meteorological parameters for each of the 111 test hours in which tracer gas was released. Data needed by the models and for the evaluation were selected from the MDB. Supplemental data were also obtained to meet the needs of each of the complex terrain models. These data are described below.

Tracer Release Information

The MDB contains tracer release information for 111 test hours representing 17 different experiments. Freon gas was released along with SF_6 for nine of the experiments. Only the SF_6 releases were modeled in this evaluation, since the SF_6 data had been shown to be of higher quality. The tracer release information included:

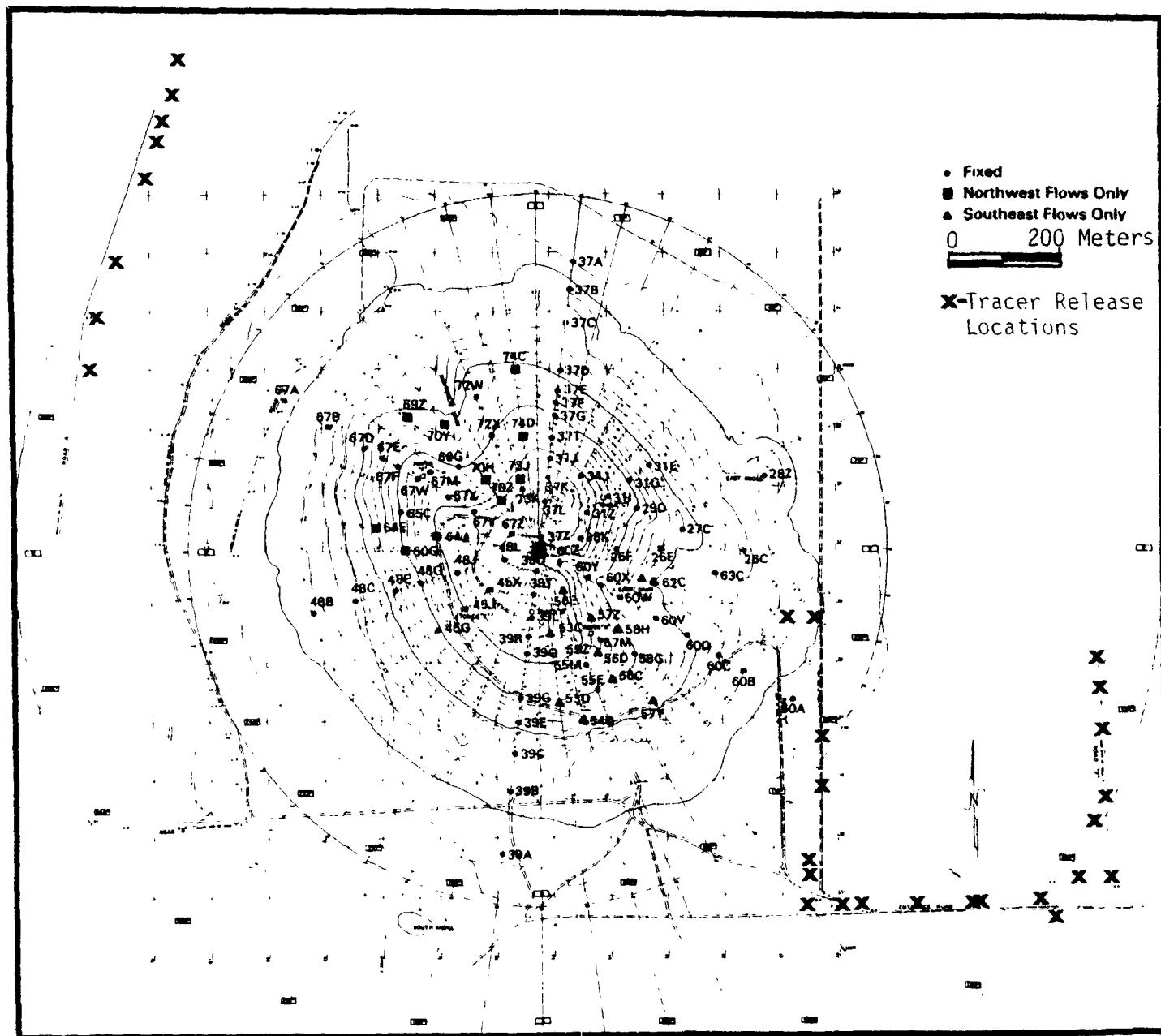


Figure 2-3. Cinder Cone Butte tracer gas sampler locations (Ref. No. 17).
Contour intervals are 5 meters.

- average release rate for the period of each release
- start and end time of each release
- location of the crane (X, Y, Z, L) relative to a local reference frame

Seven of the experiment hours were found to have release periods of less than 40 minutes. These hours were then excluded from the evaluation, since only hourly averages were to be modeled. The net result was that 104 test hours were included in the evaluation.

The model results for Cinder Cone Butte have been evaluated on the basis of relative concentration (X/Q), so emission rates were input to each model as a fixed value of 1.0 g/s. The variable tracer emission rates provided in the data base represent the average tracer release rate for the duration of each release. Some of the experiment hours used in this study had release periods of less than an hour (but greater than 40 minutes). Tracer release rates for these hours were adjusted to hourly average rates. Hourly average tracer release rates were then used to convert the hourly measured concentrations to relative concentrations.

Ambient Tracer Concentrations

Hourly average SF_6 concentrations as measured at each of up to 94 sampler locations are included in the MDB. For the purposes of this evaluation, the measured concentrations (in the units of parts per trillion) were first converted to units of g/m^3 (using hourly on-site temperature; and pressure = 905 mb), and then converted to relative concentration, X/Q (using the release-time-adjusted hourly average tracer release rates).

Meteorology

Table 3-4 summarizes the meteorological inputs to the complex terrain models for Cinder Cone Butte. The input data are primarily from the MDB, but supplemental data were used to provide other required model input data.

The MDB contains hourly averages of measured and derived meteorological parameters representative of tracer release height (which varied from experiment to experiment). ERT used a "spline under tension" method of interpolating tower measurements to release height. Wind speed and direction are provided as both scalar and vector averages. Also provided are hourly values of critical streamline height, Froude number (for the layer between 2m and 150m), and scalar average wind speeds measured at the 10m level of Tower A.

Additional meteorological data were needed for input to some of the models. Vertical profiles using on-site tower measurements of temperature and wind speed were needed by the COMPLEX/PFM model to internally calculate critical streamline height and Froude number. Hourly P-G stability categories based on the Turner method (CRSTER preprocessor) were developed from concurrent Boise National Weather Service cloud cover observations and

TABLE 3-4

SUMMARY OF CINDER CONE BUTTE METEOROLOGICAL INPUTS TO THE COMPLEX TERRAIN MODELS

Model Function	Input Parameter	Model							
		CX1	CX2	PFM	M41	IMP	PL5	RTD	SHZ
Transport	Wind Speed	U-1	U-1	U-1	U-1	U-4	U-1	U-1	U-1
	Wind Direction	0-1	0-1	0-1	0-1	0-2	0-1	0-1	0-1
	Wind Dir. Shear	NR	NR	NR	NR	NR	NR	NR	NR
	Anemometer Ht.	Z-1	Z-1	Z-1	Z-1	Z-1	Z-1	Z-1	Z-1
	Power Law Exponents	NR	NR	NR	NR	P-1	NR	NR	NR
Dispersion	Stability	S-1	S-1	S-1	S-1	S-1	S-2	S-1	NR
	Horiz. Turb.	NR	NR	NR	NR	NR	NR	I _y	I _y
	Vert. Turb.	NR	NR	NR	NR	NR	NR	I _z	I _z
Plume Rise	Temperature	NR			No Plume Rise Calculations for Passive Releases at Cinder Cone Butte				
	Wind Speed	NR							
	dT/dZ	NR							
	Stability	NR							
Limited Mixing	Mixing Height	L-1	L-1	L-1	L-1	NR	L-1	L-1	L-2
Critical Height	Temperature	NR	NR	T-2	NR	NR	NR	DT-1	NR
	Wind Speed	NR	NR	U-3	NR	NR	NR	NR	NR
Key	Description								
Model	CX1	COMPLEX I							
	CX2	COMPLEX II							
	PFM	COMPLEX/PFM							
	M41	4141							
	IMP	IMPACT							
	PL5	PLUMES							
	RTD	RTDM							
	SHZ	SHORTZ							
Wind Speed	U-1	Release height scalar wind speed from Modelers' Data Base (MDB)							
	U-2	Release height vector wind speed from MDB							
	U-3	Profile from 150 m tower							
	U-4	U-1 interpolated to middle of surface grid cell (3.75 m) using P-1							

(continued on next page)

TABLE 3-4 (Continued)

Wind Direction	0-1 0-2	Release height vector wind direction from MDB 0-1 minus 90° for rotated IMPACT grid
Anemometer Height	Z-1	Set to release height for each release
Power Law Exponents	P-1	Internal IMPACT values: $P = .15, .17, .20, .26, .39, .48, .54$ for S-1 (A-G)
Stability	S-1 S-2	P-G category from Turner method (CRSTER preprocessor) using Boise cloud data and Cinder Cone Butte 10 m wind speed P-G category from $\sigma\theta$ (CONVRT preprocessor) using $\sigma_v/U-2$ from MDB where σ_v is horizontal velocity turbulence at release height
Turbulence - Y	I _y	From MDB: ($\sigma_v/U-2$) at release height
Turbulence - Z	I _z	From MDB: ($\sigma_{WH}/U-2$) at release height where σ_{WH} is vertical velocity turbulence scale with Horst correction for non-cosine response
Temperature	T-1 T-2	Release height temperature from MDB Profile from tower
Mixing Height	L-1 L-2	Fixed at 10,000 m Height where tower value of $I_z \leq 0.01$ (radians)
dT/dZ	DT-1	Derived from MDB values of Froude number (2 m - 150 m), critical height, T-1, and U-1
	NR	Not required

10m wind speeds from the MDB. Except for SHORTZ, the effect of mixing height (for these predominantly night time tracer tests) was precluded through the use of a 10,000m mixing depth. SHORTZ requires mixing depth defined as the height above which the vertical turbulence intensity drops below 0.01. These heights were developed from the on-site tower data.

Plume rise calculations for Cinder Cone Butte were not needed due to the passive nature of the tracer releases.

WESTVACO-LUKE DATA BASE

Under an agreement between the Westvaco Corporation, the State of Maryland, and the U.S. EPA²⁰, ambient air quality and meteorological measurements were carried out near the Luke Mill in western Maryland, from December 1, 1979 through November 30, 1981. Data from these measurements are intended to assist in the development of a rough terrain diffusion model applicable in the Luke area.^{21, 22} The complex topography of the area is shown in Figure 3-4. Vertical cross sections of the terrain relative to the Westvaco stack are presented in Figure 3-5 to give the reader a better feel for the source-receptor geometry. As can be seen from this figure, all of the monitors to the southeast of the mill are well above the top of the stack. Most of the monitor distances from the stack range from 0.75 to 1.5 km. The only exception is the Stony Run monitor (No. 10) at 3.4 km northeast.

The effective stack height (physical height plus plume rise) will vary significantly depending on operating load and meteorology. For normal operating loads, the effective stack height can be as low as 250-300 meters for stable conditions, or strong wind, neutral conditions; and can exceed 1000 meters for light wind, unstable conditions, based on Briggs plume rise equations.

Three types of data were measured in order to characterize SO₂ emissions from the stack, atmospheric transport and dispersion, and ambient SO₂ concentrations on the elevated terrain.

Source Data

The Luke Mill utilizes a 190 m stack to vent coal-fired emissions. Flue gas SO₂ concentration and temperature were measured continuously by an emissions monitor.

The source data base for the Westvaco-Luke stack includes sequential hourly-averaged values of SO₂ emission rate, temperature, SO₂ concentration, and steam flow (monitored continuously at the plant). Table 3-5 presents a summary of the measured stack parameters, averaging times and units of measure.

Meteorology

Three instrumented towers were used to measure meteorological parameters (see Figure 3-3). The 100 m Beryl tower had instruments mounted at 10 m and 100 m; the 30 m Luke Hill tower was instrumented at the 10 m and 30 m levels; and the 100 m Met Tower was instrumented at the 10 m, 50 m, and 100 m levels. The parameters measured at each tower are listed in Table 3-6. These include measurements of horizontal wind speed and direction, vertical wind speed, intensity of turbulence in each of the three dimensions with respect to the mean wind, vertical temperature gradient at various levels and ambient temperature. Additionally: measurements of net radiation were obtained with a radiometer at the base of the Met Tower; and an acoustic sounder, operated near the Met Tower, provided mixing depth values.

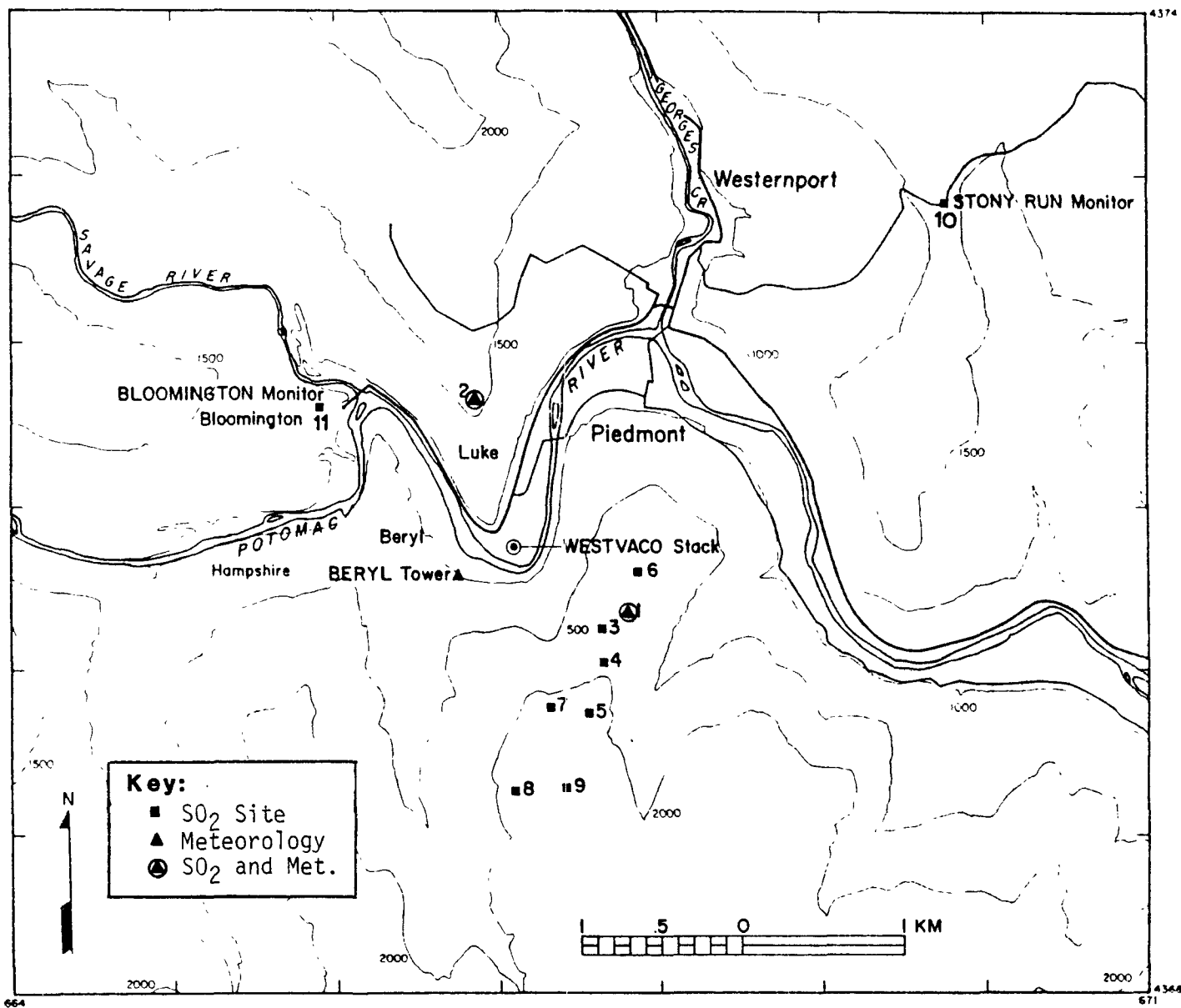


Figure 3-4. Map of the study area surrounding the Westvaco Luke Mill. Elevations are in feet above mean sea level (MSL) and the contour interval is 500 feet (Ref. No. 21).

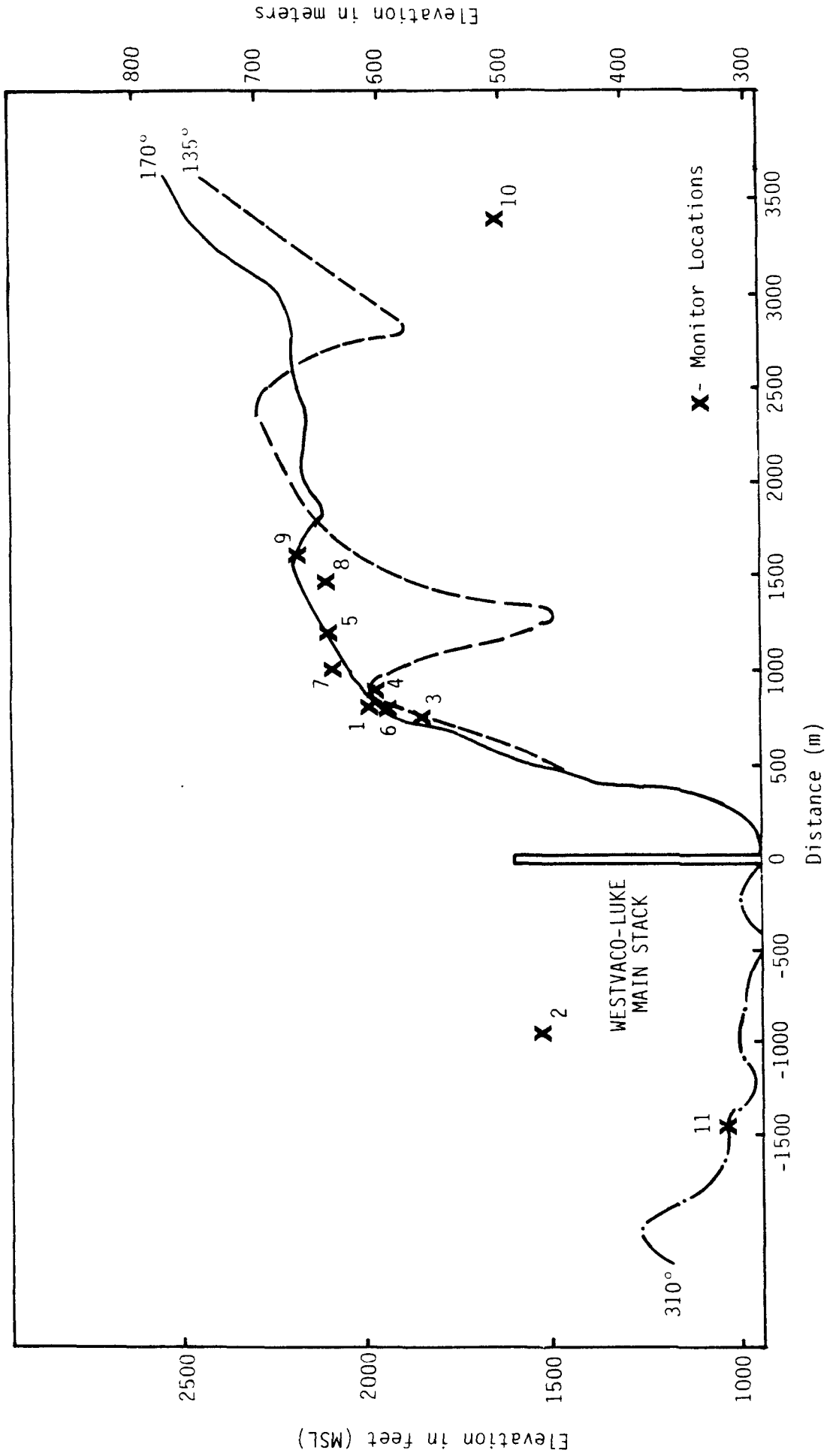


Figure 3-5. Westvaco vertical cross sections for radials of 135°, 170° and 310°. The Westvaco stack height along with monitor heights and distance are superimposed.

TABLE 3-5

UNITS AND AVERAGING TIMES CORRESPONDING TO MEASURED VARIABLES
REPORTED IN THE WESTVACO DATA BASE

Parameter	Source Units	Averaging Time	Meteorological			Ambient Air Quality		
			Parameter	Units	Averaging Time	Parameter	Units	Averaging Time
SO ₂ emission rate	tons hr ⁻¹	1 hour	wind speed	x 10 miles hour ⁻¹	1 hour	SO ₂ concentration	ppm	1 hour
stack temperature	°F	1 hour	wind direction	degrees	1 hour			
stack SO ₂	ppm	1 hour	temperature	°F	1 hour			
steam flow	1000 lbs hour ⁻¹		delta temperature	x 10 °F	1 hour			
			turbulence intensity	x 10 ³ radians	1 hour			
			mixing depth	meters	1 hour			

TABLE 3-6

INSTRUMENTATION AND PARAMETERS MEASURED ON THE WESTVACO METEOROLOGICAL TOWERS

Site	Instruments*	Parameters
Beryl Tower		
Level 0 (10 m)	Cup and vane Propeller anemometer Temperature probe	SP, DR, IX, IY, W, IZ T
Level 1 (100 m)	Cup and vane Propeller anemometer Delta temperature sensor	SP, DR, IX, IY, W, IZ $\Delta T(100 \text{ m} - 10 \text{ m})$
Luke Hill Tower		
Level 0 (10 m)	Cup and vane Propeller anemometer Delta temperature sensor	SP, DR, IX, IY, W, IZ $\Delta T(10 \text{ m} - 2 \text{ m})$
Level 1 (30 m)	Cup and vane Propeller anemometer Delta temperature sensor	SP, DR, IX, IY, W, IZ $\Delta T(30 \text{ m} - 10 \text{ m})$
Met Tower		
Level 0 (10 m)	Cup and vane Propeller anemometer Temperature probe Delta temperature sensor	SP, DR, IX, IY, W, IZ T $\Delta T(10 \text{ m} - 2 \text{ m})$

* All temperature sensors were mounted in aspirated radiation shields.

(continued on next page)

TABLE 3-6 (Continued)

Level 1 (50 m)	Cup and vane Propeller	SP, DR, IX, IY W, IZ
Level 2 (100 m)	Cup and vane Propeller Delta temperature sensor	SP, DR, IX, IY W, IZ ΔT (100 m - 10 m)

Key

W: vertical wind speed
 SP: horizontal wind speed
 DR: horizontal wind direction
 IX: downwind intensity of turbulence
 IY: crosswind intensity of turbulence
 IZ: vertical intensity of turbulence
 T: temperature
 ΔT : temperature difference

The meteorological data base contains sequential hourly-averaged values of the parameters mentioned above. Table 3-5 indicates the units that meteorological data have been reported in.

Ambient Air Quality Data

Monitors for measuring ambient SO₂ concentrations were established at 11 sites (see Figure 3-3). Eight of these sites were located within plant property boundaries (from 800 to 1,500 m from the stack) on the high terrain east and south of the mill. Ground-level elevations at these monitors exceed the physical stack height. Two additional monitors, Luke Hill and Stony Run, were located 900 m north-northwest and 3,300 m northeast of the stack, respectively. Terrain elevations for these two monitors are nearly level with stack top. The remaining monitor, Bloomington, located 1,500 m northwest of the stack, is in a valley where the elevation is comparable to stack base elevation.

The air quality data base reports the sequential hourly-average values of the SO₂ concentrations measured at each of the 11 sites. Units ascribed to each of the variables are given in Table 3-5.

Data Selected for Model Input

The hourly averaged measurements obtained during the Westvaco-Luke field program were first reduced by ERT and then compiled by H.E. Cramer Company into a modelers' data base (MDB) for input to the SHORTZ and LUMM* models.²³ Most of the model inputs were obtained from this MDB, however, some additional data were compiled by TRC in order to meet all technical requirements of the complex terrain models. The data inputs were restricted to the second full year of measurements, December 1980 through November 1981.

Source Information

The source parameters, stack location (x, y, z), stack height and stack diameter, were input as constant values to each of the models. The following source parameters were input to the models on an hourly basis:

Q	Hourly SO ₂ emission rate
T	Hourly stack gas exit temperature
VF	Hourly stack gas volume flow rate, or
V _s	Hourly stack gas exit velocity

In preparing the MDB, any missing values of Q, T, VF, or V_s were substituted with the last reported value.

*The Luke Mill Model (LUMM) was developed specifically for the Westvaco-Luke Mill site.

Air Quality Data

Hourly SO₂ concentrations at each of the eleven monitors were recorded in units of parts per trillion. Prior to the evaluation these concentrations were converted to ug/m³ through the use of hourly on-site temperatures and an average atmospheric pressure (from the U.S. Standard Atmosphere) of 0.96 atmosphere. Receptor locations and elevations were directly input to each of the models, although the horizontal coordinates first had to be converted to source-oriented distance and direction for input to RTDM and COMPLEX/PFM.

Model predictions for the Stony Run monitor (labeled receptor No. 10) could not be made with the IMPACT model due to grid size constraints and computer limitations. The other IMPACT receptors were located in the center of the nearest grid cell.

Meteorology

The Westvaco MDB of meteorological data was developed by H.E. Cramer Company²³ to meet the input needs of the SHORTZ and LUMM models. The specific parameters and their corresponding primary data sources are listed in Table 3-7. In preparing the MDB, alternate sources of meteorological data were preferentially ranked for use when data from the primary source were unavailable or unreliable for certain time periods. These data substitutions are shown in Table 3-8.

The meteorological data provided in the MDB was supplemented with other on-site tower data as well as some off-site data needed as input to the models. Table 3-9 summarizes all of the Westvaco meteorological inputs to the complex terrain models.

Data from off-site locations were used to characterize stability category for four of the models (COMPLEX I, COMPLEX II, COMPLEX/PFM, and 4141), mixing height for most of the models (except IMPACT) and, for COMPLEX/PFM, profiles of wind speed and temperature. The CRSTER preprocessor program was utilized with cloud cover data from the nearest National Weather Service station (Morgantown, WV) in conjunction with Westvaco 10 m wind speeds (averaged from the three towers) to categorize stability. Mixing heights were developed from twice daily Pittsburgh mixing heights as obtained from the National Climatic Center, and interpolated to hourly values using the various model preprocessor programs. (The interpolation scheme used to generate hourly mixing heights for COMPLEX/PFM has been changed since the model was submitted for this study.) The Pittsburgh twice per day radiosonde data (TDF5600 tape) were employed along with Westvaco tower data in the PROFILE program to generate hourly vertical profiles of wind speed and temperature. These profile data are used by COMPLEX/PFM to calculate Froude number and critical streamline height.

TABLE 3-7

PRIMARY HOURLY METEOROLOGICAL INPUTS
INCLUDED IN THE WESTVACO MODELERS' DATA BASE
AS COMPILED BY H.E. CRAMER ASSOCIATES^{2,3}

Input Parameter	Primary Source
Transport Wind Direction	100 m level of Tower 1
Reference Level Wind Speed	30 m level of Tower 2
Wind Profile Exponents	Based on speed difference between upper levels of Tower 1 and 2
Vertical Potential Temperature Gradient	Based on temperature difference between the 10 m level of Tower 2 and 100 m level of Tower 1
Ambient Air Temperature	10 m level of Tower 2
Lateral and Vertical Turbulent Intensities	30 m level of Tower 2
Mixing Depths	A constant value of 1000 m
Stability Class ¹	From vertical turbulent intensity, 10 m level of Tower 2
Vertical Wind Direction Shear ²	Direction difference between upper levels of Tower 1 and 2

¹ Using the stability classification scheme suggested by EPA for a surface roughness length of 15 centimeters: A < 0.2094 (stability class/turbulent intensity in rad); B from 0.1746 to 0.2094; C from 0.1362 to 0.1745; D from 0.0874 to 0.1361; E from 0.0419 to 0.0873; and F < 0.0419.

² Needed only for the modified version of SHORTZ submitted for evaluation.

TABLE 3-8

DATA SUBSTITUTIONS USED BY H.E. CRAMER ASSOCIATES
IN DEVELOPING WESTVACO HOURLY METEOROLOGICAL INPUTS^{2,3}

Input Parameter	Rank of Parameter Source	Parameter Source
Transport Wind Direction ¹	1	100 m Level of Tower No. 1
	2	50 m Level of Tower No. 1
	3	10 m Level of Tower No. 1
	4	30 m Level of Tower No. 2
	5	10 m Level of Tower No. 2
Reference Level Wind Speed ²	1	30 m Level of Tower No. 2
	2	10 m Level of Tower No. 1
	3	50 m Level of Tower No. 1
	4	100 m Level of Tower No. 1
	5	10 m Level of Tower No. 2
Vertical Wind- Direction Shear ³	1	Direction difference between 100 m Level of Tower No. 1 and 30 m Level of Tower No. 2
	2	Direction difference between 50 m Level of Tower No. 1 and 30 m Level of Tower No. 2
	3	Direction difference between 10 m Level of Tower No. 1 and 30 m Level of Tower No. 2
	4	Direction difference between 100 m Level of Tower No. 1 and 10 m Level of Tower No. 2
	5	Direction difference between 50 m Level of Tower No. 1 and 10 m Level of Tower No. 2

(continued on next page)

TABLE 3-8 (continued)

DATA SUBSTITUTIONS USED BY H.E. CRAMER ASSOCIATES
IN DEVELOPING WESTVACO HOURLY METEOROLOGICAL INPUTS^{2 3}

Input Parameter	Rank of Parameter Source	Parameter Source
	6	Direction difference between 10 m Level of Tower No. 1 and 10 m Level of Tower No. 2
	7	Direction difference between 100 m and 10 m levels of Tower No. 1
	8	Direction difference between 50 m and 10 m levels of Tower No. 2
Wind-Profile Exponent ⁴	1	Based on speed difference between 100 m Level of Tower No. 1 and 30 m Level of Tower No. 2
	2	Based on speed difference between 50 m Level of Tower No. 1 and 30 m Level of Tower No. 2
	3	Based on speed difference between 10 m Level of Tower No. 1 and 30 m Level of Tower No. 2
	4	Based on speed difference between 100 m Level of Tower No. 1 and 10 m Level of Tower No. 2
	5	Based on speed difference between 50 m Level of Tower No. 1 and 10 m Level of Tower No. 2

(continued on next page)

TABLE 3-8 (continued)

DATA SUBSTITUTIONS USED BY H.E. CRAMER ASSOCIATES
IN DEVELOPING WESTVACO HOURLY METEOROLOGICAL INPUTS^{2,3}

Input Parameter	Rank of Parameter Source	Parameter Source
	6	Based on speed difference between 10 m Level of Tower No. 1 and 10 m Level of Tower No. 2
	7	Based on speed difference between 100 m Level of Tower No. 1 and 10 m Level of Tower No. 1
	8	Based on speed difference between 50 m Level of Tower No. 1 and 10 m Level of Tower No. 1
Vertical Potential Temperature Gradient ⁵	1	Based on temperature difference between 100 m Level of Tower No. 1 and 10 m Level of Tower No. 2
	2	Based on temperature difference between 10 m Level of Tower No. 1 and 10 m Level of Tower No. 2
	3	Based on temperature difference between 100 m Level of Tower No. 1 and 10 m Level of Tower No. 1
	4	Based on temperature difference between 30 m Level of Tower No. 2 and 10 m Level of Tower No. 2
Ambient Air Temperature	1	10 m Level of Tower No. 2
	2	10 m Level of Tower No. 1
	3	10 m Level of Beryl Tower

(continued on next page)

TABLE 3-8 (continued)

DATA SUBSTITUTIONS USED BY H.E. CRAMER ASSOCIATES
IN DEVELOPING WESTVACO HOURLY METEOROLOGICAL INPUTS^{2 3}

Input Parameter	Rank of Parameter Source	Parameter Source
Lateral and Vertical Turbulent Intensities	1	30 m Level of Tower No. 2
	2	10 m Level of Tower No. 1
	3	50 m Level of Tower No. 1
	4	100 m Level of Tower No. 1
	5	10 m Level of Tower No. 2
Stability Class	1	10 m Level of Tower No. 2
	2	10 m Level of Tower No. 1
	3	30 m Level of Tower No. 2
	4	50 m Level of Tower No. 1
	5	100 m Level of Tower No. 1

¹ When no non-variable wind direction was found, the hour was flagged by setting the wind direction equal to 090 degrees and the mixing depth equal to 1 meter.

² Wind speeds above 0, but less than 1 meter per second, were set equal to 1 meter per second. When all of the wind speeds were calm, the hour was flagged by setting the wind direction equal to 090 degrees and the mixing depth equal to 1 meter.

³ When none of the data substitutions were possible, the wind-direction shear was set equal to zero.

⁴ The wind-profile exponent was set equal to zero when the calculated exponent was negative or if none of the data substitutions were possible. The wind profile exponent was not allowed to exceed unity.

⁵ When none of the data substitutions were possible, the vertical potential temperature gradient was set equal to the moist adiabatic value of 0.003 degrees Kelvin per meter.

⁶ When no turbulence measurements were available, the lateral and/or vertical turbulent intensities substituted were climatological values for the combination of season, wind speed and time-of-day categories.

TABLE 3-9

SUMMARY OF WESTVACO METEOROLOGICAL INPUTS TO THE COMPLEX TERRAIN MODELS

Model Function	Input Parameter	Model							
		CX1	CX2	PFM	M41	IMP	PL5	RTD	SHZ
Transport	Wind Speed	U-1	U-1	U-1	U-1	U-2	U-1	U-3	U-4
	Wind Direction	Θ-1	Θ-1	Θ-1	Θ-1	Θ-2	Θ-1	Θ-1	Θ-1
	Wind Dir. Shear	NR	NR	NR	NR	NR	NR	NR	NR
	Anemometer Ht.	Z-1	Z-1	Z-1	Z-1	Z-1	Z-1	Z-2	Z-1
	Power Law Exponents	NR	NR	NR	NR	NR	NR	P-2	P-1
Dispersion	Stability	S-1	S-1	S-1	S-1	S-4	S-2	S-3	NR
	Horiz. Turb.	NR	NR	NR	NR	NR	NR	Iv2	Iv1
	Vert. Turb.	NR	NR	NR	NR	NR	NR	Iz2	Iz1
Plume Rise	Temperature	T-1	T-1	T-2	T-1	T-1	T-1	T-1	T-1
	Wind Speed	U-1	U-1	U-6	U-1	U-2	U-1	U-5	U-1
	dT/dZ	NR	NR	NR	NR	NR	NR	DT1	DT1
	Stability	S-1	S-1	S-1	S-1	S-4	S-2	S-3	NR
Limited Mixing	Mixing Height	L-1	L-1	L-4	L-1	NR	L-2	L-1	L-3
Critical Height	Temperature	NR	NR	U-6	NR	NR	NR	DT1	NR
	Wind Speed	NR	NR	T-2	NR	NR	NR	U-1	NR
Legend	Description								
Model	CX1	COMPLEX I							
	CX2	COMPLEX II							
	PFM	COMPLEX/PFM							
	M41	4141							
	IMP	IMPACT							
	PL5	PLUME5							
	RTD	RTDM							
	SHZ	SHORTZ							

(continued on next page)

TABLE 3-9 (Continued)

Legend		Description
Wind Speed	U-1	"Stack height" wind speed from Westvaco modelers' data base (MDB)
	U-2	Wind speed from 3 towers, all levels; interpolated to mid-grid cell
	U-3	U-1 extrapolated to plume height from Z-2 using P-2
	U-4	U-1 extrapolated to plume height from Z-2 using P-1
	U-5	U-1 extrapolated to stack height from Z-2 using P-2
	U-6	Profile of speeds from all tower levels merged with Pittsburgh radiosonde data through PROFILE (COMPLEX/PFM preprocessor)
Wind Direction	Θ -1	"Transport height" wind direction from MDB
	Θ -2	Wind direction from 3 towers, all levels; interpolated to mid-grid cell
Wind Direction Shear	$\Delta\Theta$ 1	From MDB
	$\Delta\Theta$ 2	$d\Theta/dz = \Delta\Theta/70$ m
Anemometer Height	Z-1	Set to stack top (189.7 m) since U-1 represents stack top wind
	Z-2	Z = 30 m (Tower 2 height), ZA = 179.6 m (Tower 2 base relative to stack base)
Power Law Exponents	P-1	Hourly from MDB
	P-2	As for P-1 but with observed negative values (from ERT)
Stability	S-1	P-G category from Turner method (CRSTER preprocessor) using Morgantown, WV cloud data and Westvaco 10 m wind speed (Avg. of 3 towers)
	S-2	P-G category from CONVRT (PLUME5 preprocessor) using σ_Θ (I_y from MDB)
	S-3	P-G category using σ_Φ (I_z on 50 m level of Tower 2, from ERT)
	S-4	Vertical profile of P-G category based on $d\Theta/dz$ from temperatures on 3 towers

(Continued on next page)

TABLE 3-9 (Continued)

Key	Description
Turbulence - Y	I _{y1} Horizontal turbulence from MDB I _{y2} Horizontal turbulence measured at 50 m on Tower 1 (from ERT)
Turbulence - Z	I _{z1} Vertical turbulence from MDB I _{z2} Vertical turbulence measured at 50 m on Tower 1 (from ERT)
Temperature	T-1 From MDB T-2 Profile of temperatures from all tower levels merged with Pittsburgh radiosonde data through PROFILE (COMPLEX/PFM preprocessor)
dT/dZ	DT1 Vertical potential temperature gradient from MDB
Mixing Height	L-1 From CRSTER preprocessor with Pittsburgh (Upper) and S-1 L-2 From CONVRT (PLUME5 preprocessor) with Pittsburgh (Upper) and S-2 L-3 From METZ (SHORTZ preprocessor) with Pittsburgh (Upper) and Westvaco 10 m wind speed L-4 From PROFILE (COMPLEX/PFM preprocessor) with Pittsburgh (Upper)
	NR Not required

SECTION 4

STATISTICS APPROACH

The 1980 AMS Woods Hole workshop on model performance evaluation recommended a comprehensive list of performance measures and statistics for evaluating air quality models. The workshop recommended that performance evaluations be based on comparisons of the full set of observed-predicted data pairs, of the highest observed and predicted concentration per event (e.g., 1, 3 or 24 hour time period) and of the highest N values (unpaired in time or space). In addition, comparisons of observed and predicted concentrations are to be carried out on data subsets representing individual monitoring stations or selected meteorological conditions.

TRC and EPA reviewed the workshop report and formulated a statistical approach for the rural model evaluations³ based on workshop recommendations. The approach was modified for the urban model evaluations⁵, primarily to reduce the volume of information by eliminating redundant performance measures and statistics. Additional revisions as appropriate to the complex terrain models were also made, and the statistical approach followed for this evaluation is described below.

DATA SETS FOR COMPARISON OF OBSERVED AND PREDICTED CONCENTRATIONS

The data sets listed in Table 4-1 represent the different types of comparisons recommended by the AMS workshop. In each instance, comparisons were recommended for the basic 1-hour unit for model predictions and also for 3-hour and 24-hour averaging times. The numbering scheme in the table is derived from a summary prepared by William Cox of EPA of the data sets and statistics recommended by the AMS workshop.

To compare observed and predicted air quality values on a common basis, it is necessary to account for background concentration, i.e., contributions to measured air quality from sources whose impact is not modeled. This concern does not arise for the Cinder Cone Butte tracer study, since other sources of SF_6 are non-existent. The effects of background in the Westvaco monitored data were removed from measured SO_2 concentrations before statistical comparisons were made between observed and predicted concentrations. The uncertainty of plume transport in complex terrain poses an uncertainty in attempting to define a method for the determination of background concentrations. High observed concentrations in the Westvaco network tended to occur with light and variable winds which can result in

TABLE 4-1. SUMMARY OF DATA SETS FOR MODEL EVALUATION

Peak Concentration Comparisons		B. All-Concentrations Comparisons	
(A-1)	Compare highest observed value for each event with highest prediction for same event (paired in time, not location)	(B-1)	Compare observed and predicted values at a given station, paired in time (a total of 11 data sets).
(A-2)	Compare highest observed values for the year at each monitoring station with the highest prediction for the year at the same station (paired in location, not time)	(B-2)	Compare observed and predicted values for a given time period, paired in space (not appropriate for data sets with few monitoring sites).
(A-3a)	Compare maximum observed value for the year with highest predicted values representing different time or space pairing (fully unpaired, paired in location; paired in time; paired in space and time)	(B-3)	Compare observed and predicted values at all stations, paired in time and location (one data set) and by time of day.
(A-3b)	Compare maximum predicted value for the year with highest observed values for various pairings, as in (A-3a)	(B-4)	Same as (B-3), but for subsets of events by meteorological conditions (stability and wind speed) and by time of day.
(A-4a)	Compare highest N (=25) observed and highest N predicted values, regardless of time or location		
(A-4b)	Compare highest N (=25) observed and highest N predicted values, regardless of time, for a given monitoring location. (A total of 11 data sets.)		
(A-5)	Same as (A-4a), but for subsets of events by meteorological conditions (stability and wind speed) and by time of day.		

high measured concentrations at monitors located 180° upwind from the stack, using the measured wind direction. It was assumed that the background contribution is evenly distributed over the study area, and can be represented by the lowest measured concentration in the network each hour. Since observed concentrations of less than .005 parts per million (ppm) were set to the minimum instrument detection level of .005 ppm, background concentrations for these hours were set to .0025 ppm. The Luke Mill of Westvaco is relatively isolated from other point sources of SO₂, so this background method should be effective. In Table 4-1, and in the discussions that follow, "observed value" denotes a measured concentration minus background.

For many hours during the year at Westvaco, none of the monitoring stations experienced significant observed or predicted SO₂ impact. These hours of effectively zero observed and zero predicted impact are relatively uninteresting for the evaluation of air quality models for regulatory purposes. Including those hours in statistical analyses adds to the computational burden and tends to dilute the model performance results from hours with significant impact. Consequently, threshold values were imposed to screen the data base for statistical analyses. If, for a given time period, both the observed concentration and the predicted concentration at a station were below the threshold, that data pair was excluded from further analysis. A threshold value of 25 µg/m³ was used for 1-hour and 3-hour averages, and a value of 5 µg/m³ was used for 24-hour averages. Threshold checks were not imposed on the Cinder Cone Butte data.

Peak Concentrations

For peak concentrations, comparisons are made to determine model performance both on an unpaired basis and for various pairings in time and space. The first two items in Table 4-1 represent a comparison of the highest observed and highest predicted concentrations, paired in time (A-1) and paired in location (A-2). For the Westvaco data set, these two comparisons provide quite different measures of performance since the number of events is large (1 year represents 365 days or 8,760 hours) while there are only 11 stations. Meanwhile for the Cinder Cone Butte data set, the number of events is relatively small (104 hours) while the number of stations (94) is relatively large. An additional (A-2) data set was added for the complex terrain evaluation, representing the second-highest values observed and predicted at each station.

Item A-3a represents a comparison of the highest observed concentration values, regardless of time or space, and predicted values representing different time and space pairing. Item A-3b is directly analogous to A-3a, but starts from the highest predicted value. Results for data sets (A-3a) and (A-3b) were relatively uninformative for the rural evaluation. These sets were therefore dropped from subsequent evaluations.

Items A-4 and A-5 involve comparisons of the "N" highest observed and predicted values, unpaired in time or space. The AMS workshop recommended that such comparisons be based on the upper 2 to 5 percent of concentrations, rather than on one or two extreme values. As an alternative

to the percentile approach, TRC recommended using a small number (N=25) which would more appropriately represent the set of highest observed and predicted values, while still providing a statistical basis for establishing confidence limits. On a percentage basis, 25 values represent roughly 7 percent of the 365 24-hour values in a year, about 1 percent of the 3-hour values, and about 0.3 percent of the 1-hour values.

Air quality data often exhibit spatial and temporal correlation, particularly over time periods of a few hours. For 1-hour and 3-hour periods, the highest 25 values were screened to eliminate cases with two or more high values from the same period, or with two consecutive high values (Westvaco only) at the same location. This screening is intended to reduce the effects of auto-correlation and to avoid double-counting a single event. For 24-hour averaging periods, less correlation is expected, and this screening was not included.

Comparisons of the highest 25 observed and predicted values were performed for all stations combined (A-4a), for each station individually (A-4b) and for subsets of events corresponding to selected source-receptor geometry and to selected meteorological conditions (A-5). The subsets selected for the evaluation of each data base are described in more detail later in this section.

Comparisons of All Concentrations

In addition to peak concentration analyses, the AMS workshop recommended that comparisons be made based upon all observed and predicted concentration values. Table 4-1 lists three items of this type. Item B-1 is the comparison of observed and predicted values at a given monitoring station (for all data pairs above the threshold values). Item B-3 represents comparisons based on the set of values from all 11 stations combined. Item B-4 represents subsets of B-3. The same criteria described for item A-5 above (for defining subsets of source-receptor geometry and meteorology) were used to define subsets for comparisons of all concentrations.

STATISTICAL ANALYSIS OF MODEL PERFORMANCE

The AMS workshop report recommended two somewhat different lists of performance measures for comparing model predictions with observed air quality, one appropriate for data sets representing pairs of observed and predicted values, the other appropriate for unpaired data sets. Paired data sets provide a means for assessing how well a model predicts on an event-by-event basis, while unpaired sets do not. Table 4-2 summarizes the basic list of performance measures, and the statistical methods recommended for establishing confidence limits on each measure. At the head of each column (Paired and Unpaired) are listed the data sets from Table 4-1 to which each list of measures and statistical methods has been applied.

TABLE 4-2. STATISTICAL ESTIMATORS AND BASIS FOR CONFIDENCE
LIMITS ON PERFORMANCE MEASURES

Performance Measure	Estimator	Basis for Confidence Interval	
		Paired Comparison (Sets A-1, A-2, B-1, B-3, B-4)*	Unpaired Comparison (Sets A-1, A-4, A-5, B-1, B-3, B-4)
Bias	Average	One sample "t," with adjustment for serial correlation	Two sample "t"
	Median	Wilcoxon match pair	Mann-Whitney
Noise/Scatter	Variance	Chi-squared test on variance of residuals	F test on variance ratio
	Gross variability	None	Not applicable
	Average absolute residual	None	Not applicable
Correlation	Pearson correlation coefficient	Fisher "z"	Not applicable
Frequency distribution comparison	Maximum difference between two cumulative distribution functions	Not Applicable	Kolmogorov-Smirnov (K-S) test on f (obs.) vs. f (pred.)

* These sets refer to Table 4-1.

The data sets from item A-1 (highest observed and predicted values for each event) and from items B-1, B-3, and B-4 all represent observed and predicted values paired in time. For these sets, statistical analyses based on the residual (i.e., the differences between each pair of observed and predicted values) are appropriate for measuring model performance. If the time pairing for these data sets is ignored, however, it is also possible to assess model performance (in aggregate) by comparing the features of the composite set of all observed values to those of the predicted values. Consequently, both paired and unpaired comparisons were recommended by the AMS workshop for these data sets. Data sets representing comparisons of the highest 25 values, regardless of time or space, provide no basis for paired analysis. For these sets (A-4, A-5), only unpaired comparisons were performed. Item A-2 represents comparison of the single highest observed and predicted values from each of the N stations. Only the paired comparison performance measures were computed for this case. No statistics were computed for the single-value comparisons in item A-3.

For paired comparisons, as noted above, the performance measures are based on an analysis of residuals. Model bias is indicated by the average and/or the median residual, with a value of zero representing no bias. The characteristic magnitude of the residuals is an indicator of the scatter between observed and predicted values on an event-by-event basis. Three measures of noise or scatter were computed:

- Variance $\frac{1}{N-1} \sum_{i=1}^N (d_i - \bar{d})^2$
- Gross variability $\frac{1}{N} \sum_{i=1}^N d_i^2$
- Average absolute residual $\frac{1}{N} \sum_{i=1}^N |d_i|$

where d_i is the residual (observed minus predicted) for data pair i , \bar{d} is the average residual, and N is the number of data pairs. The correlation of paired observed and predicted values is measured by the Pearson correlation coefficient.

For unpaired comparisons, the list of performance measures is somewhat shorter. Model bias is indicated by the difference between the average (or median) observed value and the average (median) predicted value. A ratio of the variances of the observed and predicted values is provided to indicate whether the distribution of values in the two data sets is comparable. Similarly, the frequency distribution of observed values is compared with that for predicted values.

Standard statistical methods have been used to estimate confidence limits for each of the performance measures. Discussion of the statistical procedures may be found in most statistics textbooks. For parametric procedures, the reader is referred to Snedecor and Cochran (1967),²⁴ while for nonparametric procedures Hollander and Wolfe (1973)²⁵ provide an appropriate description.

For paired comparisons, the confidence interval on the average residual can be estimated using the one-sample t test. This parametric test incorporates the assumption that the residuals follow a normal distribution, but for large N departures from normality are not critical. Serial correlation can affect results significantly, however, since the number of "independent events" will be overestimated and the calculated variance may understate the magnitude of the actual random error component. The AMS workshop recommended the adjustment of confidence limits for serial correlation. A method described by Hirtzel and Quon (1981)²⁶ has been used to adjust the confidence interval from the one-sample t test. The interval given by the standard one-sample t test is multiplied by the factor $[(1+r)/(1-r)]^{1/2}$, where r is the lag-one autocorrelation coefficient of the residuals.

An analogous nonparametric indicator of model bias is the median residual. The statistical method for estimating a confidence interval on the median residual is provided by the Wilcoxon matched-pairs test. No straightforward method of adjusting the confidence intervals from the Wilcoxon test for serial correlation has been identified.

A confidence interval for the variance of the residuals is calculated using a chi-squared test. No adjustment was made for serial correlation. No standard method is available for estimating confidence intervals for the gross variability or average absolute deviation measures. For the Pearson correlation coefficient, the Fisher z test provides a method of estimating the confidence interval.

Comparison of two cumulative distribution functions is accomplished using the Kolmogorov-Smirnov (K-S) test. For this test, the two distribution functions are compared across the full range of concentration (or residual) values, and the maximum frequency difference between the two functions is identified.

For unpaired comparisons, two bias measures are computed. The average of the observed values is compared with the average of the predicted values. The confidence interval on the difference of the averages is estimated with a two-sample t test. The median difference is also computed, and the confidence interval is estimated using the Mann-Whitney nonparametric test.

The variance of observed values is compared with the variance of predicted values for unpaired data sets. The performance measure is the ratio of the variances; the F test provides confidence limits on the ratio.

The frequency distribution comparison for unpaired data sets provides a measure of the difference between the observed and predicted distribution functions. The K-S test is again used to assess the statistical significance of the maximum frequency difference.

Statistical Measures for the Full Westvaco Data Set

For Westvaco, the full data set represents hourly observed and predicted concentrations at each receptor and hourly associated variables (for subset analysis) for a one-year period of record. The specific performance measures and statistics calculated for each of the unpaired and paired data sets are summarized in Table 4-3 and 4-4. The notation for identifying data sets corresponds to that employed in Table 4-1.

The routine monitoring network at Westvaco, with relatively few stations and a very large number of events lends itself to an evaluation approach focussed on peak values (unpaired in time or location), analysis by station, and analysis for meteorological subsets (by stability and wind speed). The added factor of terrain elevation is reflected in station-by-station results. The performance evaluation considers 1-hour, 3-hour, and 24-hour averaging times. In complex terrain, peak impacts are commonly thought to be associated with stable conditions. Four stability categories, therefore, have been selected: unstable (Class A, B, and C); neutral (Class D); slightly stable (Class E); and stable (Class F).

Table 4-3 indicates that the full set of estimators and confidence interval calculations will be provided for the 25 highest values over all stations and events (A-4a), but only a partial set of measures is provided by station (A-4b) or for subsets by meteorology (A-5).

For the paired data sets (Table 4-4), the highest priority is placed on comparisons of the highest value per station (A-2) and all events paired in time and location (B-3). The remaining data sets received a more limited analysis.

IMPACT Model: Analysis of Select Hours for Westvaco

The IMPACT model runs with Westvaco data were limited to selected periods in order to maintain reasonable computer costs. As previously discussed, the primary basis for evaluating the models (except IMPACT) with the Westvaco data is the set of performance statistics based on the full year of Westvaco data. In order to provide some basis for comparing the performance of the IMPACT model and the other complex terrain models, performance statistics have been prepared for the other models based on the same subset of hours selected for evaluation of the IMPACT model.

Based on benchmark computer costs, it was estimated that approximately 500 hours could be simulated with the IMPACT model. Selection of this many hours allowed the consideration of 24-hour as well as 3-hour and 1-hour averaging periods. However, the number of 24-hour periods, restricted to about twenty is marginal from a statistical standpoint. The selection of twenty 24-hour periods did ensure that a large number of 1-hour and 3-hour

TABLE 4-3. PERFORMANCE MEASURES AND STATISTICS CALCULATED
FOR THE WESTVACO UNPAIRED (25 HIGHEST) DATA SETS

	Average Observed	Average Predicted	Difference of Averages	Median Difference	Variance Ratio
All stations/ all events (A-4a)	✓	✓	✓(C.I.)*	✓(C.I.)	✓(C.I.)
By station/ all events (A-4b)	✓	✓	✓	X	✓
Subsets by met. conditions (A-5)	✓	✓	✓	X	✓

* C.I. = confidence interval

Subsets include: Stability Class (4 groups): Class A, B, C
Class D
Class E
Class F

Wind Speed (3 groups)

Averaging times: 1, 3, 24 hours

TABLE 4-4. PERFORMANCE MEASURES AND STATISTICS CALCULATED FOR
WESTVACO DATA SETS PAIRED IN TIME OR LOCATION

	Highest per event paired in time (A-1)	Highest per station paired by location (A-2)	All data paired in time and location (B-3)	All events at each station paired in time (B-1)	Subsets of events paired in time and location (B-4)
Number of events	✓	✓	✓	✓	✓
Average observed	✓	✓	✓	✓	✓
Average difference	✓(C.I.)*	✓(C.I.)	✓(C.I.)	✓	✓
Fraction Co > Cp	x	✓	✓	x	x
Characteristic Discrepancies					
σ_d	✓(C.I.)	✓(C.I.)	✓(C.I.)	✓	✓
RMSE	x	✓	✓	x	x
AAR	x	✓	✓	x	x
Correlation Coefficients					
Pearson R	x	✓	✓	x	
Spearman ρ	x	✓	✓	x	x
Variance comparison	x	✓(C.I.)	✓(C.I.)	x	x
Maximum frequency difference	✓(C.I.)	x	✓(C.I.)	x	x

* C.I. = confidence interval

periods were modeled. Not all these periods, however, involve significant observed and predicted impact at monitor locations. The following selection criteria were followed:

1. The days with the six highest observed concentrations at each of the 10 monitors to be modeled with the IMPACT model were identified.
2. 20 days (480 hours) were randomly selected from (1).
3. The 3-hour periods with the six highest observed concentrations at each of the 10 monitors were identified as in (1).
4. 20 3-hour periods were randomly selected from (3).

Model results for the hours selected in (2) and (4) above were then analyzed. Implementation of the above criteria resulted in a data set containing 480 hours. Performance statistics for this limited data set include only a portion of the measures listed in Tables 4-3 and 4-4. For unpaired (25 highest) analysis, the all stations/all events case was examined for the 1-hour averaging period. For data sets paired in time or location (Table 4-4), statistics for A-1, A-2, B-1, and B-3 were generated for the 1-hour average, but subsets of events (B-4) were not considered.

Statistical Measures for the Cinder Cone Butte Data Set

The tracer experiments at Cinder Cone Butte represent a different type of data set for evaluating model performance. The number of concentration measurements per hour is much greater, and the number of events much fewer, than those from a long-term, continuous monitoring program. The greater spatial density of measurements make comparisons between observed and predicted values event-by-event (paired in time) more informative for a tracer data set. Analyses for individual hours and/or individual tests are also feasible. By contrast, the number of monitors and the use of movable arrays make it difficult to perform station-by-station analyses.

The evaluation for Cinder Cone Butte shifts the emphasis toward event-by-event analysis. The Cinder Cone Butte data sets representing the 25 highest observed and predicted values (unpaired) received similar treatment to that for Westvaco, as indicated by Table 4-5. No analysis by station has been attempted. Subset analysis included station groups defined by receptor terrain elevation (relative to release height). Receptors were grouped into four categories: below release height; at release height (within 10 meters); between 10 and 30 meters above release height; and more than 30 meters above release height.

The paired data sets analysis for Cinder Cone Butte, summarized in Table 4-6, does not include any analyses by station. The highest-by-event data set (A-1) has been analyzed for the full set of paired performance measures, as was the "all pairs" (B-3) data set.

TABLE 4-5. PERFORMANCE MEASURES AND STATISTICS CALCULATED FOR THE
CINDER CONE BUTTE UNPAIRED (25 HIGHEST) DATA SETS

	Average Observed	Average Predicted	Difference of Averages	Medians Difference	Variance Ratio
All stations/ all events (A-4A)	✓	✓	✓(C.I.)*	✓(C.I.)	✓(C.I.)
Subsets by receptor terrain elevation (A-5)	✓	✓	✓	x	✓

* C.I. = confidence interval

Averaging time: 1 hour only

TABLE 4-6. PERFORMANCE MEASURES AND STATISTICS CALCULATED FOR THE
CINDER CONE BUTTE DATA SETS PAIRED IN TIME OR LOCATION

	Highest per event paired in time (A-1)	Highest per event paired in time- subsets (A-1a)	All data paired in time and location (B-3)	Subsets of events paired in time and location (B-4)
Number of events	✓	✓	✓	✓
Average observed	✓	✓	✓	✓
Average difference	✓(C.I.)*	✓	✓(C.I.)	✓
Fraction Co > Cp	✓	x	✓	x
Characteristic Discrepancies				
σd	✓(C.I.)	✓	✓(C.I.)	✓
RMSE	✓	x	✓	x
AAR	✓	x	✓	x
Correlation Coefficients				
Pearson R	✓	✓	✓	x
Spearman ρ	✓	x	✓	x
Variance comparison	✓(C.I.)	x	✓(C.I.)	x
Maximum frequency difference	✓(C.I.)	x	✓(C.I.)	x

* C.I. = confidence interval

Since the tracer releases for the Cinder Cone Butte experiments were generally shorter than three hours in duration (less than one hour in many instances), it was not feasible to evaluate model performance for averaging times as long as three hours. Analyses were limited to one-hour averaging periods.

For the Cinder Cone Butte data base, analysis of the unpaired 25 highest values for subsets of events was not attempted. Subset analysis was instead performed for the "highest-by-event" paired data set. The recommendation to replace "highest 25" subsets with "highest paired in time" subsets for Cinder Cone Butte reflects two considerations. First, the total number of events is small, and some subsets may contain fewer than 25 hours. Second, the sampler density provides relatively good estimates of peak values for all hours, and the experimental periods were generally selected to provide high impact at receptors.

Paired data subsets for Cinder Cone Butte (for 1-hour periods) were defined by stability group, wind speed, release height and release distance. Stability group wind speed categories for Cinder Cone Butte are the same as those for Westvaco. Three release height categories (relative to the base elevation of 945 meters) were used: below 16 meters; between 16 and 26 meters; and above 26 meters. Two release distance categories were used: less than or greater than 900 meters from the release point to the top of the butte.

SECTION 5

MODEL PERFORMANCE RESULTS

Statistics comparing observed and predicted concentrations have been generated for each of the eight complex terrain models and two data bases. The results are presented by data set for the Westvaco full year model runs, Westvaco-IMPACT select hours, and Cinder Cone Butte tracer tests. Each data set is organized into four types of tables providing statistics for 25 highest values, highest concentrations by station (except for Cinder Cone Butte), highest concentrations by event and comparisons of all observed and predicted concentrations paired in space and time. Tables of statistical subsets by meteorology and source-receptor geometry are provided in Appendices B and C.

WESTVACO FULL YEAR RESULTS

The full year of Westvaco data was run for all of the models except IMPACT. Statistical measures were produced for three averaging times (1-hour, 3-hour, and 24 hours) for each of the seven complex terrain models.

Statistics for 25 Highest Values

Statistics for the set of 25 highest observed and 25 highest predicted 1-hour average SO₂ concentrations are presented for each model in Table 5-1. The first two columns of results are simply the average of the 25 highest observed values and the average of the 25 highest predicted values for each data set. The first performance measure, presented in column three is the difference between the two averages. A positive value implies model underprediction. In parentheses under the calculated differences are 95 percent confidence intervals, determined by using the two-sample Students' t test. These results show that all seven of the complex terrain models overpredicted the 25 highest values at the 95 percent confidence level. The largest overprediction, by a factor of 20, is by COMPLEX II, and the smallest overprediction, by a factor of 1.6, is by RTDM.

The second performance measure is the median difference (313th highest value) between all 625 possible pairings of the 25 highest observed and predicted concentrations. The 95 percent confidence interval is determined with the nonparametric Mann-Whitney test. Results for the median difference are very similar to those for the difference of averages.

TABLE 5-1

COMPARISON OF 25 HIGHEST OBSERVED AND PREDICTED
SO₂ CONCENTRATION VALUES (UG/M³)
(UNPAIRED IN TIME OR LOCATION)
FOR THE 1-HOUR AVERAGING PERIOD
WESTVACO (1969/1931)

MODEL	AVERAGE OBSERVED VALUE	AVERAGE PREDICTED VALUE	DIFFERENCE OF AVERAGES* (OBS-PRED)	MEDIAN DIFFERENCE* (OBS-PRED)	VARIANCE COMPARISON (OBS/PRED)	MAXIMUM FREQUENCY DIFFERENCE
COMPLEX I	1969	14159	-15189 (-17149, -13249)	-15972 (-17149, -14542)	.017 (.009, .039)	1.00 (.365)
COMPLEX II	1969	39638	-35669 (-38555, -34782)	-35616 (-37307, -33968)	.004 (.002, .010)	1.00 (.385)
4141	1969	12205	-10236 (-11549, -8922)	-9559 (-11689, -8080)	.009 (.004, .029)	1.00 (.385)
RTDM	1969	3289	-1219 (-1652, -385)	-655 (-943, -292)	.151 (.057, .344)	.92 (.365)
PLUMES	1969	14525	-12554 (-13923, -11199)	-11472 (-12831, -10749)	.008 (.004, .019)	1.00 (.385)
COMPLEX/PPM	1969	15153	-13193 (-15397, -10989)	-11309 (-12529, -10520)	.003 (.001, .007)	1.00 (.365)
SHORTZ	1969	13563	-11390 (-13075, -10112)	-10153 (-11021, -9576)	.007 (.003, .016)	1.00 (.385)

* 95 PERCENT CONFIDENCE INTERVAL IN PARENTHESES

The third performance measure is the variance comparison. The variance of the 25 highest observed values was divided by the variance of the 25 highest predictions. The F test was used to calculate the 95 percent confidence levels for these comparisons. Results indicate that, for all of the models, the scatter of 25 highest model predicted concentrations is much larger than the scatter of 25 highest observations.

The last performance measure presented in Table 5-1 is the frequency distribution comparison. The cumulative distribution function $f(C)$ represents the fraction of the data set (in this case, the fraction of 25 data points) with concentration values less than or equal to C . The value presented in this column is the largest absolute difference between the observed and predicted distribution functions (for the same concentration value) obtained when the two functions are compared for all concentration values. The value given in parentheses is the maximum difference which is significantly different from zero, at a 95 percent confidence level, as given by the Kolmogorov-Smirnov (K-S) test. This confidence interval is a function of the number of cases. The value is, therefore, the same (0.385) for all models, since the number of cases is always 25. The results for the comparison of maximum frequency differences (1.00 for six of the seven models) indicate there is no overlap between the distributions of 25 highest observations and 25 highest predictions.

Table 5-2 is presented to exemplify how comparisons of the 25 highest observations and 25 highest predictions selected by monitoring station and for various meteorological subsets reveal more detailed aspects of model performance. Results for the COMPLEX I model are depicted in Table 5-2, while results for all of the models are presented in Appendix B. Comparisons of median difference and frequency distributions have been eliminated from the subset tables since they don't provide a great deal of additional information.

While reviewing Table 5-2, the reader should notice from Figure 3-3 that the largest overpredictions by COMPLEX I occur at the close-in monitors (stations 1, 3, 4, and 6) on the ridge southwest of the stack; while underpredictions occur at the two monitors (stations 2 and 11) located northwest of the plant. Overpredictions of the highest 25 concentrations occur on average for all wind speed categories and for stable conditions. Neutral and unstable conditions, however, result in underpredictions of the highest 25 concentrations by COMPLEX I. The average of the 25 highest predictions for stability D is only $8 \mu\text{g}/\text{m}^3$, while the observed average is $1517 \mu\text{g}/\text{m}^3$, resulting in an extremely large variance ratio for this subset. For COMPLEX I (and some other models as well) this result is probably due to the half-height terrain treatment (lifting the plume over terrain) combined with small values of the vertical dispersion coefficients for stability D.

Comparisons of the highest 25 observed and predicted concentrations for data sets of 3-hour and 24-hour averaging periods are presented in Table 5-3 and 5-4. Subset tables for 3-hour and 24-hour averaging periods are

TABLE 5-2

COMPARISON OF 25 HIGHEST OBSERVED AND PREDICTED
SO₂ CONCENTRATION VALUES (US/M**3)
(UNPAIRED IN TIME OR LOCATION)
FOR VARIOUS DATA SETS
MODEL: COMPLEX I
FOR THE 1-HOUR AVERAGING PERIOD
WESTVACO (1987/1981)

DATA SETS	AVERAGE OBSERVED VALUE	AVERAGE PREDICTED VALUE	DIFFERENCE OF AVERAGES* (OBS-PRED)	VARIANCE COMPARISON (OBS/PRED)
ALL	1969	18169	-16199 (-17149,-15249)	.017 (.008, .039)
STATION 1	1316	16574	-15257	.013
STATION 2	318	43	276	11.967
STATION 3	1113	12169	-11257	.264
STATION 4	1072	12189	-11015	.029
STATION 5	1374	8104	-6729	.176
STATION 6	1411	15372	-13960	.029
STATION 7	1547	8398	-7050	.024
STATION 8	1103	2354	-1250	.032
STATION 9	1183	4422	-3239	.056
STATION 10	339	428	-89	30.642
STATION 11	315	191	124	.754

METEOROLOGICAL CONDITION

1. WIND SPEED				
< 2.5 M/S	1576	14169	-16592	.023
2.5 TO 5. M/S	1813	12828	-11013	.001
> 5. M/S	551	5664	-6111	.023
2. STABILITY GROUP				
CLASS A, B & C	1092	419	674	7.232
CLASS D	1517	P	1509	12133.506
CLASS E	1118	11859	-10741	.114
CLASS F	1667	14169	-16501	.027

TABLE 5-3

COMPARISON OF 25 HIGHEST OBSERVED AND PREDICTED
SO₂ CONCENTRATION VALUES (UG/M**3)
(UNPAIRED IN TIME OR LOCATION)
FOR THE 3-HOUR AVERAGING PERIOD
WESTVACO (1987/1991)

MODEL	AVERAGE OBSERVED VALUE	AVERAGE PREDICTED VALUE	DIFFERENCE OF AVERAGES* (OBS-PRED)	MEDIAN DIFFERENCE* (OBS-PRED)	VARIANCE COMPARISON (OBS/PRED)	MAXIMUM FREQUENCY DIFFERENCE
COMPLEX I	1127	12205	-11075 (-11845, -10311)	-10433 (-11000, -10157)	.026 (.011, .058)	1.00 (.383)
COMPLEX II	1127	20557	-19430 (-20871, -17989)	-17793 (-21880, -17031)	.007 (.003, .016)	1.00 (.383)
4101	1127	4769	-3642 (-4283, -3000)	-3552 (-4107, -2712)	.037 (.016, .084)	1.00 (.383)
RTO4	1127	1464	-337 (-545, -127)	-256 (-502, -135)	.473 (.209, 1.075)	.52 (.383)
PLUME5	1127	7817	-5690 (-8031, -5329)	-5554 (-6958, -4625)	.008 (.004, .018)	1.00 (.383)
COMPLEX/PEM	1127	7720	-6601 (-7549, -5652)	-6053 (-6977, -5255)	.617 (.007, .038)	1.00 (.383)
SHORTZ	1127	5330	-5202 (-7780, -4624)	-5043 (-5370, -4323)	.046 (.020, .104)	1.00 (.383)

* 95 PERCENT CONFIDENCE INTERVAL IN PARENTHESES

TABLE 5-4

COMPARISON OF 25 HIGHEST OBSERVED AND PREDICTED
SO₂ CONCENTRATION VALUES (UG/M*H3)
(UNPAIRED IN TIME OR LOCATION)
FOR THE 24-HOUR AVERAGING PERIOD
WESTVALO (1980/1991)

MODEL	AVERAGE OBSERVED VALUE	AVERAGE PREDICTED VALUE	DIFFERENCE OF AVERAGES* (OBS-PRED)	MEDIAN DIFFERENCE* (OBS-PRED)	VARIANCE COMPARISON (OBS/PRED)	MAXIMUM FREQUENCY DIFFERENCE
COMPLEX I	354	3230	(-5101, -2624)	(-2728, -2574)	(.007, .017)	(1.00, .363)
COMPLEX II	354	4482	(-4567, -3587)	(-3504, -3306)	(.002, .004)	(1.00, .383)
4141	354	855	(-544, -357)	(-342, -317)	(.024, .055)	(1.00, .363)
RTM	354	331	(-23, 85)	(32, 92)	(.143, .063)	(.55, .393)
PLUMES	354	1712	(-1357, -574)	(-730, -559)	(.001, .070)	(1.00, .383)
COMPLEX/PPM	354	1594	(-1220, -478)	(-1201, -887)	(.008, .003)	(1.00, .383)
SHORTZ	354	1368	(-1175, -891)	(-944, -824)	(.025, .011)	(1.00, .393)

* 95 PERCENT CONFIDENCE INTERVAL IN PARENTHESES

presented in Appendix B. Results for 3-hour and 24-hour averages are similar to the results for the 1-hour averages. For 24-hour averages, RTDM predicted the average of the 25 highest values with no significant bias, at the 95 percent confidence interval.

Statistics for Highest Concentrations at Each Station

In Table 5-5 performance statistics are presented which compare the maximum concentration values observed and predicted during the year at each monitoring station (a total of 11 observed and 11 predicted values). This table illustrates results for the 1-hour averages, and seven models. Similar comparisons for second highest observed and predicted concentrations are presented in Table 5-6. Caution should be exercised when interpreting the meaning of some of the statistics for these rather small data sets.

The statistics provided in these tables compare observed and predicted values for 11 data pairs as shown in the first column. The next two columns present the average of the 11 observed concentrations and the average difference between observed and predicted values. The 95 percent confidence interval is given in parentheses, as calculated with a one-sample t test. As with the 25 highest concentrations, these results indicate overprediction (negative average differences), especially for COMPLEX II. At the 95 percent confidence level, the RTDM overpredictions are not significant. (The confidence interval is almost as large as the average observed value.)

The fourth column in these tables displays the fraction of positive residuals. This performance measure indicates the fraction of observed-predicted data pairs for which the observed concentration is larger than the predicted concentration. The results indicate overprediction at from 6 of 11 stations (for RTDM) to all 11 stations (COMPLEX/PFM).

The next three performance measures provide estimates of scatter, or characteristic discrepancies. They include the standard deviation of residuals (differences) with 95 percent confidence limits calculated from an F test; root mean square error; and average absolute residual. RTDM has the smallest values for all three measures, and COMPLEX II has the largest.

The Pearson correlation of observed and predicted concentration pairs and the nonparametric Spearman correlation of ranked sets of observed and predicted concentrations provide indications of the spatial correlation of the maximum concentration values at each station. Results from Table 5-5 and 5-6 show Pearson coefficients that range from 0.54 (4141 and SHORTZ) to 0.85 (COMPLEX II).

The last column in Tables 5-5 and 5-6 (variance comparison) presents the ratio of observed variance divided by the predicted variance, with 95 percent confidence bounds in parentheses as calculated by an F test. The 1-hour variance comparisons for highest and second highest by station results are significantly less than unity for all seven models, reflecting the large magnitude and range of predicted values.

TABLE 5-5

COMPARISON OF HIGHEST
OBSERVED AND PREDICTED
SO₂ CONCENTRATION VALUES (UG/M³)
PAIRED BY STATION FOR THE 1 HOUR AVERAGING PERIOD
MEXIVACO (1987/1991)

MODEL	NUMBER OF DATA PAIRS	AVERAGE OBSERVED VALUE	AVERAGE DIFFERENCE*	FRACTION OF POSITIVE RESIDUALS (OBS>PRED)	STANDARD DEVIATION* OF RESIDUALS	ROOT MEAN SQUARE ERROR	AVERAGE ABSOLUTE RESIDUAL	Pearson CORR. COEFF.	Spearman CORR. COEFF.	VARIANCE COMPARISON* (OBS>PRED)
COMPLEX I	11	1P59	-8939 (-14352, -3526)	.27	8058 (5630, 14141)	11789	9149	.79	.74	.007 (.002, .028)
COMPLEX II	11	1P59	-23851 (-35674, -12028)	.18	17600 (12297, 30986)	29154	24393	.85	.74	.002 (.000, .005)
4141	11	1P59	-5513 (-10353, -573)	.36	7204 (5034, 12643)	8809	5165	.54	.49	.010 (.003, .035)
RTDM	11	1P59	-661 (-1552, 230)	.45	1327 (927, 2329)	1428	1106	.76	.69	.171 (.045, .538)
PLUMES	11	1P59	-8879 (-14375, -3394)	.18	8181 (5716, 14357)	11820	9123	.76	.76	.007 (.002, .027)
COMPLEX /PFM	11	1P59	-12032 (-18747, -5317)	.00	9936 (6945, 17547)	15351	12333	.82	.88	.005 (.001, .018)
SHORTZ	11	1P59	-6469 (-11809, -1130)	.18	7949 (5554, 13350)	5965	6525	.59	.72	.009 (.002, .029)

* 95 PERCENT CONFIDENCE INTERVAL IN PARENTHESES

TABLE 5-6

COMPARISON OF SECOND HIGHEST
OBSERVED AND PREDICTED
SO₂ CONCENTRATION VALUES (UG/M*3)
PAIRED BY STATION FOR THE 1 HOUR AVERAGING PERIOD
WESTIVACO (1960/1981)

MODEL	NUMBER OF DATA PAIRS	AVERAGE OBSERVED VALUE	AVERAGE DIFFERENCE*	FRACTION OF POSITIVE RESIDUALS (OBS>PRED)	STANDARD DEVIATION* OF RESIDUALS	ROOT MEAN SQUARE ERROR	AVERAGE ABSOLUTE RESIDUAL	PEARSON CORR. COEFF.	SPEARMAN CORR. COEFF.	VARIANCE COMPARISON* (OBS>PRED)
COMPLEX I	11	1617	-8039 (-12789, -3294)	.27 (4935, 1239F)	7053	10449	8156	.75	.58	.309 (.022, .034)
COMPLEX II	11	1617	-21317 (-31857, -10775)	.18 (10964, 27536)	15691	26044	21440	.83	.58	.302 (.031, .037)
4141	11	1617	-4926 (-9125, -731)	.36 (4365, 10365)	6248	7732	5430	.64	.59	.312 (.033, .045)
RTDN	11	1617	-450 (-1150, 250)	.55 (729, 1830)	1543	1092	918	.75	.55	.245 (.056, .012)
PLUMES	11	1617	-7042 (-11279, -2885)	.18 (4365, 10364)	6248	9255	7191	.79	.70	.312 (.033, .043)
COMPLEX/DFM	11	1617	-8250 (-12262, -4239)	.00 (4172, 10470)	5971	10025	8251	.82	.58	.312 (.033, .045)
SHORTZ	11	1617	-5830 (-10667, -933)	.03 (5031, 12636)	7200	9007	5964	.54	.55	.309 (.033, .035)

* .95 PERCENT CONFIDENCE INTERVAL IN PARENTHESES

Tables of statistics for 3-hour and 24-hour averages of highest and second highest observed and predicted concentrations paired by station are presented in Appendix B. The results for the longer averaging periods are very similar to those for the 1-hour averages.

Statistics for Highest Concentrations by Event

Another data set consists of the highest observed and predicted concentrations over the monitoring network for each sampling period, paired in time (i.e., one pair of values for each 1-hour, 3-hour or 24-hour sampling period). Results for the 1-hour averaging period are presented in Table 5-7. While the data sets discussed up to this point contained relatively few points, event-by-event comparisons for a full year involve much larger volumes of data (i.e., a large "N"), as shown in the first column of this table. The numbers of events is different for each model, because the number of predicted values above the threshold values of $25\mu\text{g}/\text{m}^3$ is different. The performance measures and confidence intervals presented in this table have been discussed previously for Tables 5-1 and 5-5.

The average differences displayed in Table 5-7 indicate that six of the seven models tend to overpredict. The largest overprediction is by COMPLEX II. The average difference predicted by 4141 is not significant at the 95 percent confidence level. RTDM underpredicted by 40 percent.

The standard deviation of residuals is an indicator of the range of residual values encountered for each model. The smallest standard deviation was obtained for RTDM, and the largest for COMPLEX II. Comparisons of observed and predicted frequency distributions of concentration values ignore any time pairing between observed and predicted values. Frequency differences were significantly different from zero for all of the models. The smallest frequency difference was obtained for SHORTZ (0.247), while four of the models gave frequency differences between 0.77 and 0.82.

Tables for 3-hour and 24-hour average highest concentrations by event are provided in Appendix B. The results are generally quite similar to the results for 1-hour values. All of the models except RTDM overpredict, on average, but the differences are not significant for 4141.

Statistics for All Concentrations Paired in Time and Space

The largest data sets considered in this evaluation represent all concentration values paired in time and location. Results for the 1-hour data sets are presented in Table 5-8 (Parts 1 and 2). Due to computer work-space limitations, the size of the data sets for 1-hour values was too large to calculate the maximum difference between observed and predicted frequency distributions.

On average, three of the models overpredicted and four of the models underpredicted. All of the over- and underpredictions are significant at the 95 percent confidence level. The largest average overprediction is by COMPLEX I and COMPLEX II, and the largest average underprediction is by RTDM. The smallest average difference is by PLUME5.

TABLE 5-7

COMPARISON OF HIGHEST OBSERVED AND PREDICTED
SO₂ CONCENTRATION VALUES (UG/M³)
EVENT-BY-EVENT (PAIRED IN TIME)
FOR THE 1-FOUR AVERAGING PERIOD
WESTVACO (1281/1961)

MODEL	NUMBER OF EVENTS	AVERAGE OBSERVED VALUE	AVERAGE DIFFERENCE* (OBS-PRED)	STANDARD DEVIATION* OF RESIDUALS	MAXIMUM FREQUENCY DIFFERENCE
COMPLEXI	7173	154	(-1117, -779)	(3051, 3112)	(.173, .023)
COMPLEXII	7150	155	(-1237, -1033)	(5173, 5158)	(.784, .023)
4141	7132	155	(-73, 1)	(947, 963)	(.303, .023)
RTRM	7411	150	(46, 72)	(326, 337)	(.515, .022)
PLUMES	7305	152	(-213, -94)	(1354, 1376)	(.453, .023)
COMP_EX/PEM	7102	155	(-125, -66)	(1369, 1392)	(.317, .023)
SHORTZ	7785	143	(-415, -315)	(1297, 1317)	(.247, .022)

* 95 PERCENT CONFIDENCE INTERVAL IN PARENTHESES

TABLE 5-8

COMPARISON OF ALL OBSERVED AND PREDICTED
SO₂ CONCENTRATION VALUES (UG/M*3)
PAIRED IN TIME AND LOCATION
FOR THE 1-HOUR AVERAGING PERIOD
SUMMARY TABLE (PART 1)
WESTVACO (1980/1981)

MODE	NUMBER OF EVENTS	AVERAGE OBSERVED VALUE	AVERAGE DIFFERENCE* (OBS-PRED)	STANDARD DEVIATION* OF RESIDUALS	MAXIMUM* FREQUENCY DIFFERENCE
COMPLEXI	30704	95	(-362, -192)	(1436, 1723)	***** (.011)
COMPLEXII	30682	95	(-241, -200)	(2535, 2555)	***** (.011)
4141	30658	95	(33, 50)	(531, 540)	***** (.011)
RTDM	32336	90	(51, 55)	(210, 214)	***** (.011)
PLUMES	31505	93	(1, 26)	(671, 681)	***** (.011)
COMPLEX/PPM	30465	93	(20, 43)	(727, 733)	***** (.011)
SHORTZ	34879	84	(-94, -71)	(686, 696)	***** (.010)

* 95 PERCENT CONFIDENCE INTERVAL IN PARENTHESES

** VALUES COULD NOT BE CALCULATED FOR THESE VERY LARGE DATA SETS DUE TO COMPUTER WORK SPACE LIMITATIONS

TABLE 5-8 (Continued)

COMPARISON OF ALL OBSERVED AND PREDICTED
SO₂ CONCENTRATION VALUES (US/M**3)
PAIRED IN TIME AND LOCATION
FOR THE 1-HOUR AVERAGING PERIOD
SUMMARY TABLE (PART 2)
WESTVACO (1985/1991)

MODEL	FRACTION OF POSITIVE RESIDUALS (OBS>PRED)	ROOT MEAN SQUARE ERROR	AVERAGE ABSOLUTE RESIDUAL	PEARSON CORRELATION COEFFICIENT	SPEARMAN CORRELATION COEFFICIENT	VARIANCE COMPARISON* (OBS/PRED)
COMPLEXI	.95	1724	406	.008	.115	(.007, .008)
COMPLEXII	.95	2547	421	.015	.115	(.003, .004)
4141	.95	537	138	.059	.095	(.005, .003)
RIDM	.87	219	102	.079	-.004	(.044, .028)
PLUME*	.87	576	145	.051	.069	(.047, .056)
COMPLEX/PPM	.96	713	151	.009	.151	(.041, .050)
SHORTZ	.70	596	216	.046	-.138	(.045, .050)

* .95 PERCENT CONFIDENCE INTERVAL IN PARENTHESES

Values for standard deviation of residuals, root mean square error and average absolute residual are larger than average observed concentrations for all seven models. The largest values for all three measures occur with COMPLEX II. The smallest values of the standard deviation and root mean square error were obtained for RTDM. The smallest average absolute residual was obtained for 4141.

More than 50 percent of all residuals are positive, indicating that while all of the models tend to overpredict in terms of the average differences, there are more hours with underprediction than overprediction. COMPLEX/PFM underpredicted 96 percent of the values, while SHORTZ underpredicted 70 percent of the values.

As shown in previous studies, predicted concentrations correlate poorly with concentrations observed at the same time and place. Pearson correlations range from 0.008 (COMPLEX I and COMPLEX/PFM) to 0.079 (RTDM). Spearman correlations range from -0.138 (SHORTZ) to 0.151 (COMPLEX/PFM). Variance ratios are consistently less than 0.1 (except for 0.844 for RTDM) and significantly different from unity.

Similar results are found for the 3-hour and 24-hour average statistics for all concentrations paired in time and space (Appendix B). The same models over- and underpredict as for the 1-hour averages. Correlation coefficients improve for the 24-hour averages, but remain quite low ranging from 0.1 (COMPLEX/PFM) to 0.38 (RTDM).

Table 5-9 is presented here to exemplify the results for data subsets of observed and predicted concentrations paired in time and space. Subsets are presented by station and for various meteorological conditions. Subset tables for each of the models are presented in Appendix B. Table 5-9 shows how COMPLEX I produces a mixture of over- and underpredictions, with all overpredictions at the close-in receptors southeast of the stack. Underpredictions are noted at more distant receptors and receptors located in different directions from the plant. Overpredictions occur for all wind speed categories and for stable (E and F) conditions. Neutral and unstable hours produced underpredictions, on average.

Highest and Highest, Second-High Values

In many regulatory applications, model predictions of the highest or highest, second-high concentrations are of interest. Observed and predicted highest and highest, second-high 1-hour concentrations are presented in Table 5-10. These values clearly show an overprediction by all of the models with the largest 1-hour overprediction by COMPLEX II (nearly a factor of 20 for the highest prediction) and the smallest 1-hour overprediction by RTDM (a factor of just under two for both values). Table 5-11 shows similar results for 3-hour and 24-hour averages with the largest overpredictions again by COMPLEX II and smallest overpredictions by RTDM.

TABLE 5-9

COMPARISON OF ALL OBSERVED AND PREDICTED
SO₂ CONCENTRATION VALUES (UG/M*H*3)
PAIRED IN TIME AND LOCATION
(FOR VARIOUS DATA SETS)
MODEL: COMPLEYI
FOR THE 1-HOUR AVERAGING PERIOD
WESTVACO (1980/1981)

DATA SET	NUMBER OF EVENTS	AVERAGE OBSERVED VALUE	AVERAGE DIFFERENCE (OBS-PRED)	STANDARD DEVIATION OF RESIDUALS
ALL	3704	95	-227	1709
STATION 1	3722	112	-589	2610
STATION 2	2247	52	51	44
STATION 3	3155	94	-302	1983
STATION 4	2423	104	-209	1742
STATION 5	2568	97	-45	998
STATION 6	3864	161	-958	3012
STATION 7	2344	106	-6	989
STATION 8	2840	78	53	383
STATION 9	2411	85	32	495
STATION 10	2364	57	16	128
STATION 11	2766	56	53	46

METEOROLOGICAL CONDITION

1. WIND SPEED				
< 2.5 M/S	926	130	-168	44
2.5 TO 5.0 M/S	15227	80	-359	44
> 5.0 M/S	7451	70	-20	26
2. STABILITY GROUP				
CLASS A, B & C	5867	94	86	11
CLASS D	14821	84	84	11
CLASS E	3431	86	-830	49
CLASS F	6385	125	-890	56

TABLE 5-10 - HIGHEST (H) AND HIGHEST, SECOND-HIGH (HSH)
1-HOUR CONCENTRATIONS FOR WESTVACO WITH
ASSOCIATED METEOROLOGY

1-HOUR AVERAGES					
Model		Concentration (ug/m ³)	Receptor Number	Stability Category*	Wind Speed(m/s)*
OBSERVED	H	2570	4	4	2.9
	HSH	2344	7	6	3.1
COMPLEX I	H	23678	1	6	1.2
	HSH	21063	1	6	1.3
COMPLEX II	H	50705	6	6	1.6
	HSH	46260	1	6	2.0
4141	H	18714	9	6	2.1
	HSH	18020	9	6	1.8
RTDM	H	5073	6	5	1.0
	HSH	4312	1	5	1.5
PLUME5	H	26630	7	6	1.0
	HSH	16946	1	4	4.3
COMPLEX/PFM	H	34281	4	4	1.0
	HSH	20960	1	6	1.5
SHORTZ	H	24200	6	6*	3.8
	HSH	21810	6	6*	3.3

* The SHORTZ model uses intensity of turbulence (Iy and Iz) to define dispersion. The stability categories presented here were the ones used to define meteorological subsets.

TABLE 5-11 - HIGHEST (H) AND HIGHEST, SECOND-HIGH (HSH)
3-HOUR AND 24-HOUR CONCENTRATIONS FOR WESTVACO
FULL YEAR MODEL RUNS

Model	3-HOUR			24-HOUR	
		Concentration (ug/m ³)	Receptor Number	Concentration (ug/m ³)	Receptor Number
OBSERVED	H	2066	7	487	1
	HSH	1509	6	401	6
COMPLEX I	H	17973	1	4647	1
	HSH	16827	1	4102	1
COMPLEX II	H	26960	6	8854	1
	HSH	25537	6	6338	1
4141	H	10088	9	2026	9
	HSH	6238	9	1260	5
RTDM	H	2564	6	766	6
	HSH	1954	6	596	6
PLUME 5	H	15268	1	8450	6
	HSH	11901	6	3843	6
COMPLEX/PFM	H	14007	1	3024	6
	HSH	11485	4	2949	6
SHORTZ	H	10751	3	2227	3
	HSH	7605	6	1811	6

WESTVACO - IMPACT SELECT HOUR RESULTS

Performance statistics have been prepared for all models for the subset of hours selected from the Westvaco data set for IMPACT model runs. Using the criteria discussed in Section 4, a total of 20 days representing 480 hours were selected. The days selected for this analysis all contained high observed concentrations at one or more monitors, while at the same time other monitors recorded zero concentrations.

The 3-dimensional grid which was constructed for the IMPACT runs was constrained, due to computer limitations and model resolution requirements, to exclude the most distant monitor at Stony Run (receptor No. 10 in the full Westvaco model runs). Therefore the statistical comparisons for each model are based on data sets representing predictions made at 10 receptors for 480 hours (4800 receptor-hours/model).

Statistical comparisons were produced for the 1-hour, 3-hour and 24-hour averaging periods, except for the 25 highest data sets which do not contain 24-hour averages. Since only twenty 24-hour periods were analyzed, the highest by event data sets provide similar information for this averaging period.

Subsets of events by station or for various meteorological conditions are not presented for the Westvaco-IMPACT selected hour analysis.

Although the early test run package for IMPACT was approved by the model developer, the results suggest that the model did not operate properly for all prediction runs. In his review of the draft report, the model developer (Alan Fabrick) commented "the predicted concentrations are so large that they could not have occurred if the model was running correctly. For some reason the model's numerical algorithm for simulating advection and diffusion went unstable for a few hours of Westvaco simulations." The model input data for these periods of high concentrations have been reviewed along with the model code, however, to date, the specific technical problem has not been identified.

Statistics for 25 Highest Values

Table 5-12 presents statistics for the comparison of 25 highest observed and predicted SO₂ concentrations for 1-hour averages. The performance measures and confidence intervals are the same as those described for Table 5-1.

The largest overpredictions, as depicted by the difference of averages, are by COMPLEX II and IMPACT. The smallest overpredictions were obtained for 4141 and RTDM. The overpredictions are significant at a 95 percent confidence level for all models except RTDM.

Overpredictions are similarly indicated by the comparison of median differences, with two exceptions. The median differences predicted by 4141 and RTDM are not significant at the 95 percent confidence level. The IMPACT model has a much improved (but still poor) performance for this measure indicating that the average is affected by extreme overpredictions for a few hours.

TABLE 5-12

COMPARISON OF 25 HIGHEST OBSERVED AND PREDICTED
SO₂ CONCENTRATION VALUES (UG/M*3)
(UNPAIRED IN TIME OR LOCATION)
FOR THE 1-HOUR AVERAGING PERIOD
WESTVACO (1980/1981)
HOURS SELECTED FOR IMPACT MODEL RUNS

MODEL	AVERAGE OBSERVED VALUE	AVERAGE PREDICTED VALUE	DIFFERENCE OF AVERAGES* (OBS-PRED)	MEDIAN DIFFERENCE* (OBS-PRED)	VARIANCE COMPARISON (OBS/PRED)	MAXIMUM FREQUENCY DIFFERENCE
COMPLEXI	1792	11420	-9627 (-11043, -8212)	-8504 (-10169, -7752)	.015 (.006, .033)	1.00 (.383)
COMPLEXII	1792	20558	-18765 (-22874, -14557)	-18139 (-20821, -15630)	.002 (.001, .004)	1.00 (.383)
4141	1792	3430	-1637 (-3257, -17)	-475 (-1570, 237)	.011 (.005, .025)	.42 (.383)
RTDM	1792	2031	-238 (-810, 332)	200 (-255, 559)	.096 (.042, .217)	.35 (.383)
PLUME5	1792	5413	-3520 (-5034, -2206)	-2470 (-3835, -1617)	.015 (.006, .033)	.89 (.383)
COMPLEX/PFM	1792	9011	-7216 (-9537, -4899)	-6433 (-9785, -4617)	.005 (.002, .012)	.04 (.383)
SHORTZ	1792	7448	-3555 (-7213, -3498)	-4404 (-6854, -2151)	.005 (.003, .014)	.83 (.383)
IMPACT	1786	17829	-16042 (-26484, -5500)	-4441 (-8189, -3115)	.000 (.000, .001)	1.00 (.383)

* 95 PERCENT CONFIDENCE INTERVAL IN PARENTHESES

Again, predicted variances are large relative to observed variances. The variance ratio for RTDM (0.096) is highest, while the lowest value occurs with IMPACT (0.000).

For the comparison of observed and predicted frequency distributions reveal that there is very little overlap between them for most of the models. Differences between the observed and predicted distributions are shown to be significantly different from zero at the 95 percent confidence level for all models except RTDM.

Results for the 25 highest 3-hour averages (Appendix B) are quite similar to those for the 1-hour values. The main exception is that 4141 underpredicts the median difference for 3-hour values.

Statistics for Highest Concentrations at Each Station

Comparison of the sets of highest concentrations by station for the 1-hour values can be seen in Table 5-13. Results for second highest values are presented in Table 5-14. For these comparisons, each data set consists of only 10 data pairs.

Results indicate overprediction by all eight models for the highest values, and by all models except RTDM for the second highest values. However, for four models, the overpredictions are not significant at the 95 percent confidence level. The largest overpredictions occurred with the IMPACT model.

Results for the fraction of positive residuals indicate that IMPACT overpredicted the highest and second highest values at all 10 stations. PLUME5 underpredicted second highest values at 7 stations. Measures of scatter were largest for IMPACT and smallest for RTDM.

The variance comparison indicates that the variance of predicted values is significantly larger than the variance of observed values for all eight models.

Statistics for the 3-hour average and 24-hour average highest concentrations at each station are given in Appendix B. The results are similar to those for 1-hour values.

Statistics for Highest Concentrations by Event

Statistics for the comparison of highest observed and predicted concentration values event-by-event (paired in time) are provided in Table 5-15 for the 1-hour values.

The number of events (418-463), representing the number of hours analyzed for the 1-hour data sets, is less than the number of hours modeled (480) primarily as the result of screening for threshold values. Results for the average difference indicate that all of the models except 4141 and RTDM tend to overpredict the highest values each hour. However, three of the models neither over- nor underpredict significantly at the 95 percent confidence level. Large overpredictions (factor of three times observed values) occur for COMPLEX II, while the average underprediction for RTDM is about 50 percent of the average observed value.

TABLE 5-13

COMPARISON OF HIGHEST
OBSERVED AND PREDICTED
SO₂ CONCENTRATION VALUES (UG/M³)
PAIRED BY STATION FOR THE 1 HOUR AVERAGING PERIOD
WESTIVACO (1980/1991)
HOURS SELECTED FOR IMPACT MODEL RUNS

MODEL	NUMBER OF DATA PAIRS	AVERAGE OBSERVED VALUE	AVERAGE DIFFERENCE*	FRACTION OF POSITIVE RESIDUALS (OBS>PRED)	STANDARD DEVIATION OF RESIDUALS	ROOT MEAN SQUARE ERROR	AVERAGE ABSOLUTE RESIDUAL	PEARSON CORR. COEFF.	SPEARMAN CORR. COEFF.	VARIANCE COMPARISON (OBS>PRED)
COMPLEX I	10	1876	-7556 (-12685, -2425)	.50	7171 (4932, 13092)	10153	7757	.65	.66	.012 (.003, .049)
COMPLEX II	10	1876	-17123 (-28531, -5715)	.20	15948 (10069, 29117)	21394	17253	.53	.65	.003 (.001, .011)
4141	10	1876	-3865 (-8676, 944)	.40	6725 (4525, 12278)	7726	4354	.34	.32	.013 (.004, .059)
FTDM	10	1876	-164 (-1116, 787)	.70	1331 (915, 2430)	3250	893	.60	.73	.259 (.054, 1.043)
FLUMES	10	1876	-3138 (-6573, 295)	.40	4802 (3303, 8767)	6076	3980	.55	.66	.025 (.005, .105)
COMPLEX/DFM	10	1876	-7320 (-13104, -1937)	.30	7806 (5363, 14251)	10505	7918	.50	.54	.010 (.003, .042)
SHORTZ	10	1876	-6025 (-11029, -1023)	.10	6994 (4811, 12753)	9063	6075	.59	.70	.013 (.003, .051)
IMPACT	10	1876	-43709 (-54209, -22589)	.00	29392 (20311, 53115)	40171	43400	.57	.58	.001 (.000, .003)

* 95 PERCENT CONFIDENCE INTERVAL IN PARENTHESES

TABLE 5-14

COMPARISON OF SECOND HIGHEST
OBSERVED AND PREDICTED
SO₂ CONCENTRATION VALUES (US/M**3)
PAIRED BY STATION FOR THE 1 HOUR AVERAGING PERIOD
WESTVACO (1981/1981)
HOURS SELECTED FOR IMPACT MODEL RUNS

MODEL	NUMBER OF DATA PAIRS	AVERAGE OBSERVED VALUE	AVERAGE DIFFERENCE*	FRACTION OF POSITIVE RESIDUALS (OBS>PRED)	STANDARD DEVIATION* OF RESIDUALS	ROOT MEAN SQUARE ERROR	AVERAGE ABSOLUTE RESIDUAL	PEARSON CORR. COEFF.	SPEARMAN CORR. COEFF.	VARIANCE COMPARISON* (OBS>PRED)
COMPLEX I	10	1654	-5652 (-10085, -1220)	.20 (4262, 11314)	6197	8340	5871	.53	.45	.015 (.003, .053)
COMPLEX II	10	1654	-10808 (-19398, -2217)	.40 (8260, 21928)	12009	15274	11526	.45	.41	.004 (.001, .015)
4141	10	1654	-1725 (-4008, 558)	.50 (2195, 5823)	3193	4437	2350	.55	.54	.045 (.011, .181)
RTM	10	1654	112 (-726, 951)	.60 (807, 2142)	1173	3198	932	.48	.45	.317 (.079, 1.279)
FLUME 5	10	1654	-588 (-3275, 2097)	.70 (2584, 6858)	3755	4577	2288	.33	.37	.035 (.009, .147)
COMPLEX/DFM	10	1654	-4490 (-9392, 411)	.40 (4714, 12513)	5853	8115	5040	.52	.50	.011 (.003, .044)
SHORTZ	10	1654	-2390 (-5507, 725)	.40 (2907, 7258)	4357	5461	2779	.41	.45	.227 (.007, .107)
IMPACT	10	1654	-30108 (-45216, -15180)	.80 (14441, 30331)	20995	34524	34194	.52	.54	.001 (.000, .005)

* 95 PERCENT CONFIDENCE INTERVAL IN PARENTHESES

TABLE 5-15

COMPARISON OF HIGHEST OBSERVED AND PREDICTED
SO₂ CONCENTRATION VALUES (US/M³)
EVENT-BY-EVENT (PAIRED IN TIME)
FOR THE 1-HOUR AVERAGING PERIOD
WESTVACO (1980/1981)
HOURS SELECTED FOR IMPACT MODEL RUNS

MODEL	NUMBER OF EVENTS	AVERAGE OBSERVED VALUE	AVERAGE DIFFERENCE* (OBS-PRED)	STANDARD DEVIATION* OF RESIDUALS	MAXIMUM FREQUENCY DIFFERENCE
COMP_EXI	460	373	(-1331, -259)	(3258, 3485)	(.352, .090)
COMP_EXII	461	372	(-1136, -482)	(5435, 5814)	(.357, .090)
4141	461	372	(-27, 283)	(1269, 1350)	(.352, .090)
RTDM	461	372	(75, 301)	(682, 730)	(.531, .090)
PLUMES	461	372	(-135, 198)	(1557, 1772)	(.557, .090)
COMPLEX/PFM	461	372	(-236, 174)	(2572, 2751)	(.433, .090)
SHORTZ	463	370	(-323, -47)	(2048, 2233)	(.432, .090)
IMPACT	418	363	(-1050, 177)	(7452, 7993)	(.345, .094)

* .95 PERCENT CONFIDENCE INTERVAL IN PARENTHESES

Standard deviations of residuals indicate the largest scatter for IMPACT (20 times average observed value), with the smallest scatter by RTDM. Maximum frequency differences indicate a distinct difference among the models. For four models (COMPLEX I, COMPLEX II, 4141, and COMPLEX/PFM) there is little overlap between observed and predicted distributions, and the maximum difference is close to 1. The lowest value, for IMPACT, is 0.385.

Tables of 3-hour and 24-hour comparisons of the highest concentrations by event are displayed in Appendix B. The results are quite similar to the 1-hour comparisons. The average observed value drops rather slowly with increasing averaging time (338-349 $\mu\text{g}/\text{m}^3$ for 3-hour periods; 261-269 $\mu\text{g}/\text{m}^3$ for 24-hour periods).

Statistics for All Concentrations Paired in Time and Space

Table 5-16 (Parts 1 and 2) presents the comparison of all observed and predicted 1-hour concentration values paired in time and location for the Westvaco IMPACT select hours. The total number of events (2476-2595) implies that roughly half of the hourly observed-predicted pairs (4800 total) passed the tests for threshold and/or missing data. Average observed values are quite high (about 200 $\mu\text{g}/\text{m}^3$) due to the nature of the data selection criteria.

Results for the average differences show considerable variability among the models. From the 95 percent confidence intervals, one model overpredicts significantly (IMPACT), four models underpredict significantly (4141, RTDM, PLUME5 and COMPLEX/PFM), and three models show no significant tendency to over- or underpredict (SHORTZ, COMPLEX I and COMPLEX II). The magnitude of the average differences represents from 12-71 percent of the average observed values, except for IMPACT (343 percent). The prediction biases indicated by these results should be interpreted with caution, since the selection criteria favored hours with high observed concentrations. Results for the full data set (for all models except IMPACT) are more reliable for judging bias, because they are not subject to this limitation.

Values for the standard deviation of residuals, root mean square error and average absolute residual all exceed the average observed values. The largest measures of scatter occur for IMPACT, followed by COMPLEX II; while the smallest values occur for RTDM, and also 4141 and PLUME5.

Maximum frequency differences and fractions of positive residuals are all quite large.

Correlations of observed and predicted concentrations are extremely low, and negative in many cases. Variance ratios indicate variances for predicted values are much greater than variances for observed values.

Results for the 3-hour and 24-hour concentrations paired in time and space can be found in Appendix B. The results are generally similar to the results for 1-hour values.

TABLE 5-16

COMPARISON OF ALL OBSERVED AND PREDICTED
SO₂ CONCENTRATION VALUES (UG/M**3)
PAIRED IN TIME AND LOCATION
FOR THE 1-HOUR AVERAGING PERIOD
SUMMARY TABLE (PART 1)
WESTVACO (1980/1981)
HOURS SELECTED FOR IMPACT MODEL RUNS

MODE-	NUMBER OF EVENTS	AVERAGE OBSERVED VALUE	AVERAGE DIFFERENCE* (OBS-PRED)	STANDARD DEVIATION* OF RESIDUALS	MAXIMUM FREQUENCY DIFFERENCE
COMPLEXI	2477	203	(-126, -58 11)	(1524, 1638)	(.953 .033)
COMPLEXII	2476	204	(-191, -92 6)	(2404, 2542)	(.954 .033)
4141	2478	203	(115, 145 174)	(724, 745)	(.954 .033)
RTDM	2531	199	(120, 137 154)	(398, 421)	(.904 .030)
PLUMES	2508	201	(69, 100 131)	(762, 805)	(.370 .038)
COMPLEX/PEM	2474	204	(18, 67 117)	(1252, 1303)	(.945 .033)
SHORTZ	2595	195	(-16, 23 63)	(921, 1014)	(.740 .078)
IMPACT	2526	190	(-517, -797, -437)	(4527, 4750)	(.505 .034)

* 95 PERCENT CONFIDENCE INTERVAL IN PARENTHESES

TABLE 5-16 (Continued)

COMPARISON OF ALL OBSERVED AND PREDICTED
SO₂ CONCENTRATION VALUES (UG/M**3)
PAIRED IN TIME AND LOCATION
FOR THE 1-HOUR AVERAGING PERIOD
SUMMARY TABLE (PART 2)
WESTVACO (1980/1981)
HOURS SELECTED FOR IMPACT MODEL RUNS

MODEL	FRACTION OF POSITIVE RESIDUALS (OBS>PRED)	ROOT MEAN SQUARE ERROR	AVERAGE ABSOLUTE RESIDUAL	PEARSON CORRELATION COEFFICIENT	SPEARMAN CORRELATION COEFFICIENT	VARIANCE COMPARISON* (OBS/PRED)
COMPLEX I	.97	1639	453	-.002	-.009	(.037, .045)
COMPLEX II	.97	2472	498	.018	-.060	(.017, .019)
4141	.97	739	250	.052	-.074	(.234, .253)
RTM	.90	431	217	.125	.059	(1.180, 1.393)
PLUMES	.92	789	269	.109	-.039	(.185, .204)
COMPLEX/PFM	.96	1258	327	.017	.013	(.063, .077)
SHORT7	.82	991	306	.051	-.091	(.111, .123)
IMPACT	.70	4557	872	-.020	.029	(.005, .005)

* .95 PERCENT CONFIDENCE INTERVAL IN PARENTHESES

CINDER CONE BUTTE RESULTS

All eight complex terrain models were run with the full Cinder Cone Butte data set, consisting of 104 hours of SF₆ tracer and meteorological data. Ambient tracer samples were observed at up to 94 receptor locations. Statistical performance measures were generated for the 1-hour average values, only. Results are not presented for highest concentrations by station. Otherwise, the performance measures and confidence intervals presented for Cinder Cone Butte are the same as the ones described previously for Westvaco. Slightly different subsets by meteorology and source-receptor geometry were selected for the Cinder Cone Butte analysis. All observed and predicted values and the corresponding performance measures are for relative concentrations (i.e., mass concentration per unit of emission rate, χ/Q). No screening was performed for threshold values of observed and/or predicted concentrations.

Cinder Cone Butte results for the IMPACT model did not show any evidence of the instability suspected for Westvaco. However, the model developer's comments to the draft report indicated that the eddy diffusivity algorithm in the IMPACT model is not appropriate for the grid resolution (50m horizontal; 10m vertical) used for the Cinder Cone Butte model runs. (This issue was not raised when the test package was reviewed).

Statistics for 25 Highest Values

Statistics for the comparison of 25 highest observed and predicted data sets are given in Table 5-17. From the difference of averages this table shows that six of the eight models overpredict on average, and that these differences between observed and predicted averages are non-zero at a 95 percent confidence level. The IMPACT model average underprediction is also significant at the 95 percent confidence level. Only the RTDM model shows no significant bias. Results for median difference are similar to the results for difference of averages.

Variance ratios are below 0.5 except for COMPLEX I and IMPACT. The confidence interval for COMPLEX I indicates that no significant difference exists between the variance of COMPLEX I predictions and the variance of observations at a 95 percent level of confidence.

Observed and predicted frequency distributions differ significantly for all of the models except RTDM and SHORTZ.

It should be noted that interpretation of the 25 highest observed and predicted concentrations for Cinder Cone Butte is not quite as simple as for Westvaco. This is because, in addition to the unpairing in space and time, the experiments included changes in source-receptor geometries since a mobile crane was used for the releases. One group of subsets based on source-receptor geometries was selected for investigation with the 25 highest Cinder Cone Butte data sets. Table 5-18 is presented here to exemplify the subset results for COMPLEX I. Additional subset tables are provided for all models in Appendix C. As shown in Table 5-18, the four subsets selected for the 25 highest comparisons are based on receptor height. The intention was to investigate whether model performance varied with receptor height. No pronounced differences in performance were identified.

Statistics for Highest Concentrations by Event

Comparisons of highest observed and predicted concentrations event-by-event for Cinder Cone Butte are found in Table 5-19 (Parts 1 and 2). This table is identical in form to the Westvaco tables for the full data sets paired in space and time. For this tracer data set, no threshold screening was performed. The number of events and average observed values are identified for all models.

Results for the average difference indicate overprediction by all of the models except IMPACT, which underpredicted by an average of 50 percent, and RTDM which exhibited no significant bias. The largest overprediction (by a factor of 3.6) occurred with COMPLEX II.

Measures of variability between observed and predicted concentrations (standard deviation of residuals, root mean square error and average absolute residual) are largest for COMPLEX II and smallest for IMPACT and RTDM.

The predicted frequency distributions are all significantly different from the observed distributions for all models except RTDM and SHORTZ. The largest frequency difference occurs for COMPLEX II.

From the fraction of positive residuals, COMPLEX II overpredicted for 74 percent of the highest concentrations by event, while IMPACT overpredicted for only 28 percent. The best performance for this measure was by SHORTZ which overpredicted 52 percent of the events.

Correlation coefficients for Cinder Cone Butte show some improvement over Westvaco, but remain fairly low. Pearson coefficients range from 0.26 (SHORTZ) to 0.60 (RTDM), while Spearman coefficients range from 0.32 (COMPLEX II) to 0.51 (RTDM).

The variance ratios are significantly different from unity for all the models, with the variance of predictions larger than the variance of observations for all models except IMPACT.

Table 5-20 is presented here to exemplify, for COMPLEX I, the evaluation of model performance for various subsets of source-hill characteristics and meteorological conditions. Similar tables for each model are presented in Appendix C. Six of the subsets are based on two release distance categories (less or greater than 900 m from source to butte top) and three release height categories. Wind speed and stability categories are also evaluated. The number of events in some categories is quite small.

For COMPLEX I overpredictions occurred for five of the six distance/height categories, and for low wind speeds and stable conditions. Underpredictions, on average, occurred for the higher wind speeds and non-stable conditions.

TABLE 5-17

COMPARISON OF 25 HIGHEST OBSERVED AND PREDICTED
RELATIVE CONCENTRATION VALUES (19**(-6) S/M**3)
(UNPAIRED IN TIME OR LOCATION)
FOR THE 1-HOUR AVERAGING PERIOD
CINDER CONE BUTTE (1980)

MODEL	AVERAGE OBSERVED VALUE	AVERAGE PREDICTED VALUE	DIFFERENCE OF AVERAGES* (OBS-PRED)	MEDIAN DIFFERENCE* (OBS-PRED)	VARIANCE COMPARISON (OBS/PRED)	MAXIMUM FREQUENCY DIFFERENCE
COMPLFYI	66	105	(-50, -38) (-15)	(-56, -31) (-18)	(.234, .532) (.1, 2.07)	(.52) (.385)
COMPLEXII	66	250	(-231, -163) (-135)	(-207, -148) (-115)	(.084) (.037, .191)	(.95) (.385)
4141	66	196	(-129, -158, -100) (-100)	(-120, -154, -92) (-92)	(.255) (.112, .578)	(.92) (.385)
RTDM	66	67	(-23, -110) (-55)	(-12, -57) (-45)	(.475) (.210, 1.080)	(.23) (.385)
PLUMES	66	177	(-165, -90) (-63)	(-103, -87) (-57)	(.062) (.027, .140)	(.63) (.385)
COMPLEX/PPM	66	166	(-135, -72) (-1)	(-121, -19) (-3)	(.151) (.067, .343)	(.63) (.385)
SHORTZ	66	139	(-143, -31) (47)	(-50, 27) (42)	(.237) (.016, .084)	(.35) (.385)
IMPACT	66	34	(15, 31) (47)	(13, 27) (42)	(2.645) (1.165, 5.003)	(.75) (.385)

* 95 PERCENT CONFIDENCE INTERVAL IN PARENTHESES

TABLE 5-12

COMPARISON OF 25 HIGHEST OBSERVED AND PREDICTED
RELATIVE CONCENTRATION VALUES (10⁻⁶ (-5) S/M³)
(UNPAIRED IN TIME OR LOCATION)
FOR VARIOUS DATA SETS
MODEL: COMPLEYI
FOR THE 1-HOUR AVERAGING PERIOD
CINDER CONE BUTTE (1980)

DATA SETS	AVERAGE OBSERVED VALUE	AVERAGE PREDICTED VALUE	DIFFERENCE OF AVERAGES* (OBS-PRED)	VARIANCE COMPARISON (OBS/PRED)
ALL	66	105	(-60, -38	.532 (.234, 1.207)
RECEPTOR ELEVATION RELATIVE TO SOURCE RELEASE HEIGHT				
<10. M	39	64	-24	.351
10. M TO 10. M	51	93	-41	.579
10. M TO 30. M	41	74	-32	.471
>30. M	43	59	-14	1.270

TABLE 5-19

COMPARISON OF HIGHEST OBSERVED AND PREDICTED
RELATIVE CONCENTRATION VALUES (10**(-5) S/M**3)
EVENT-BY-EVENT (PAIRED IN TIME)
FOR THE 1-HOUR AVERAGING PERIOD

PART 1

CINDER CONE BUTTE (1930)

MODEL	NUMBER OF EVENTS	AVERAGE OBSERVED VALUE	AVERAGE DIFFERENCE* (OBS-PRED)	STANDARD DEVIATION* OF RESIDUALS	MAXIMUM FREQUENCY DIFFERENCE
COMPLEX I	104	26	(-25, -16)	(36, 41)	(.212, .183)
COMPLEX II	104	25	(-95, -68)	(91, 103)	(.442, .183)
4141	104	25	(-67, -47)	(56, 75)	(.345, .183)
RTDM	104	25	(-8, 0)	(26, 30)	(.387, .183)
PLUMES	104	25	(-62, -40)	(78, 88)	(.413, .183)
COMPLEX/PPM	104	25	(-51, -34)	(58, 66)	(.298, .183)
SHORTZ	104	25	(-40, -20)	(83, 94)	(.135, .183)
IMPACT	104	25	(3, 13)	(23, 26)	(.298, .183)

* 95 PERCENT CONFIDENCE INTERVAL IN PARENTHESES

TABLE 5-19 (Continued)

COMPARISON OF HIGHEST OBSERVED AND PREDICTED
RELATIVE CONCENTRATION VALUES (10**(-5) S/M**3)
EVENT-DY-EVENT (PAIRED IN TIME)
FOR THE 1-HOUR AVERAGING PERIOD
PART 2
CINDER CONE BUTTE (1980)

MODEL	FRACTION OF POSITIVE RESIDUALS (OBS>PRED)	ROOT MEAN SQUARE ERROR	AVERAGE ABSOLUTE RESIDUAL	PEARSON CORRELATION COEFFICIENT	SPEARMAN CORRELATION COEFFICIENT	VARIANCE COMPARISON* (OBS/PRED)
COMPLEX I	.43	44	29	.454	.331	(.287, .337)
COMPLEX II	.25	123	74	.345	.317	(.043, .058)
4141	.36	88	55	.383	.355	(.090, .125)
RTDM	.53	30	19	.593	.510	(.450, .523)
P-UMEF	.31	26	47	.278	.438	(.037, .070)
COMPLEX/PPM	.38	74	42	.305	.408	(.144, .144)
SHORTZ	.48	96	35	.255	.474	(.005, .052)
IMPACT	.72	29	19	.914	.537	(.223, .223)
						(2.315, 4.444)

* 95 PERCENT CONFIDENCE INTERVAL IN PARENTHESES

TABLE 5-20

COMPARISON OF HIGHEST OBSERVED AND PREDICTED
RELATIVE CONCENTRATION VALUES (10*(-6) S/M*3)
EVENT-BY-EVENT (FOR VARIOUS DATA SETS)
MODEL: COMPLEX1
FOR THE 1-HOUR AVERAGING PERIOD
CINDER CONE BUTTE (1980)

DATA SET	NUMBER OF EVENTS	AVERAGE OBSERVED VALUE	AVERAGE DIFFERENCE (OBS-PRED)	STANDARD DEVIATION OF RESIDUALS	PEARSON CORRELATION COEFFICIENT
HIGHEST CONCENTRATION EVENT BY EVENT	104	26	-16	41	.454
BY RELEASE DISTANCE/ RELEASE HEIGHT					
DISTANCE < 900. M					
H< 15. M	4	59	-32	62	.188
H=15. M TO 26. M	12	27	-40	37	.730
H> 26. M	8	69	-13	55	.567
DISTANCE > 900. M					
H< 15. M	6	37	14	23	.649
H=15. M TO 26. M	46	13	-19	44	-.070
H> 26. M	24	13	-4	24	-.127
METEOROLOGICAL CONDITION:					
1. WIND SPEED					
< 2.5 M/S	52	29	-27	47	.488
2.5 TO 5. M/S	27	22	-1	25	-.010
> 5. M/S	15	22	6	13	.464
2. STABILITY GROUP					
CLASS C+D	30	31	4	36	.529
CLASS F	38	26	-25	45	.556
CLASS F	36	22	-21	36	.351

Statistics for All Comparisons Paired in Time and Space

Statistics for the full set of paired observed and predicted concentrations are presented in Table 5-21. These data sets have the largest populations (3836 data pairs) of any group for the Cinder Cone Butte data base.

As with the high-by-event data group, average differences for all concentrations indicate overprediction by all of the models except IMPACT, which underpredicts by about 50 percent, and RTDM, which exhibits no significant bias. The largest average overpredictions are by 4141 (by a factor of over two).

Measures of variability between observed and predicted concentrations are largest for COMPLEX II, and smallest for IMPACT and RTDM. Frequency distributions of observed and predicted values are significantly different (at a 95 percent confidence level) for all eight models.

Correlation coefficients for Cinder Cone Butte model results are substantially better than for Westvaco results for all concentrations. Pearson coefficients range from 0.22 (PLUME5) to 0.43 (RTDM), while Spearman coefficients range from 0.33 (COMPLEX I) to 0.45 (SHORTZ).

The variance ratio for RTDM was not significantly different from unity (at a 95 percent level of confidence). For the other models, the variance of predictions was significantly larger than the variance of observations, although IMPACT, the opposite relationship was true.

TABLE 5-21

COMPARISON OF ALL OBSERVED AND PREDICTED
RELATIVE CONCENTRATION VALUES (10*(-5) S/M**3)
PAIRED IN TIME AND LOCATION
FOR THE 1-HOUR AVERAGING PERIOD
SUMMARY TABLE (PART 1)
CINDER CONE ROUTE (1980)

MODE	NUMBER OF EVENTS	AVERAGE OBSERVED VALUE	AVERAGE DIFFERENCE* (OBS-PRED)	STANDARD DEVIATION* OF RESIDUALS	MAXIMUM FREQUENCY DIFFERENCE
COMPLEX I	3836	5	(-5, -5)	(20, 21)	(.348, .331)
COMPLEX II	3836	5	(-7, -5)	(34, 35)	(.293, .331)
4141	3836	6	(-10, -7)	(30, 31)	(.121, .331)
RTOM	3836	5	(0, 1)	(12, 13)	(.355, .331)
PLUMES	3836	5	(-5, -3)	(28, 29)	(.301, .331)
COMPLEX/PFM	3836	5	(-5, -4)	(26, 27)	(.363, .331)
SHORTZ	3836	6	(-2, 0)	(23, 24)	(.107, .331)
IMPACT	3836	5	(2, 3)	(11, 12)	(.132, .331)

* 95 PERCENT CONFIDENCE INTERVAL IN PARENTHESES

TABLE 5-21 (Continued)

COMPARISON OF ALL OBSERVED AND PREDICTED
RELATIVE CONCENTRATION VALUES (10**(-6) S/M**3)
PAIRED IN TIME AND LOCATION
FOR THE 1-HOUR AVERAGING PERIOD
SUMMARY TABLE (PART 2)
CINDER CONE ROUTE (1990)

MODEL	FRACTION OF POSITIVE RESIDUALS (OPS>PRED)	ROOT MEAN SQUARE ERROR	AVERAGE ABSOLUTE RESIDUAL	PEARSON CORRELATION COEFFICIENT	SPEARMAN CORRELATION COEFFICIENT	VARIANCE COMPARISON* (OPS/PRED)
COMPLEX I	.49	21	11	.309	.333	(.238, .327) (.350)
COMPLEX II	.56	35	13	.236	.301	(.114 (.139, .125)
4141	.42	32	14	.277	.377	(.143 (.130, .137)
RICH	.47	13	5	.425	.409	(1.035 (.640, 1.130)
PLUMF5	.56	28	10	.223	.409	(.176 (.150, .134)
COMPLEX/PEM	.55	27	11	.313	.353	(.130 (.173, .213)
SHORTZ	.40	23	7	.236	.447	(.251 (.238, .247)
IMPACT	.54	12	6	.294	.422	(4.531 (4.174, 5.030)

* 95 PERCENT CONFIDENCE INTERVAL IN PARENTHESES

SECTION 6

SUMMARY AND CONCLUSIONS

The performance evaluation of the complex terrain models has produced an imposing array of statistical measures to compare observed and predicted concentration values. The principal objective of this project is to produce performance statistics so that EPA and a group of reviewers may judge the relative merits of different models. In this report, the results have been discussed and explained, but no attempt has been made to compare the performance of one model versus another. Many of the model developers, upon reviewing this report, indicated the desire to see more detailed depictions of the results such as scatter plots of observed and predicted concentrations, histograms, cumulative frequency plots, isopleth analyses and time series displays. Graphical displays can be useful in exploring possible causes of poor model performance and are particularly desirable in diagnostic model evaluations. One of the difficulties encountered in the presentation of operational evaluation statistics is selecting meaningful graphical or tabular displays with limited report space. An abundance of useful information remains to be extracted from the results of this study and it is hoped that further analyses are pursued in the future. The conclusions and recommendations presented below are concerned with model evaluation methods and with the performance of the models as a group.

The complex terrain models were evaluated using two data bases representing different terrain settings and experimental approaches. The Westvaco data set consisted of one year of measurements at eleven SO₂ monitoring stations in the rugged terrain of western Maryland and northeastern West Virginia, for a buoyant tall-stack release. The Cinder Cone Butte experiments were conducted for 104 hours using a non-buoyant tracer release, with impacts measured from a 94-station sampling grid on an isolated small hill.

SUMMARY OF RESULTS

The results discussed in Section 5, plus those in Appendices B and C, contain a wealth of information concerning the performance of each of the eight complex terrain models. Distinct differences in performance are evident among the models. The patterns of results changed between the two data sets and, to a lesser extent, with averaging time (for Westvaco). A few key results are highlight below.

Westvaco. For Westvaco, seven of the models overpredicted the 25 highest concentration values for 1, 3, and 24-hour averaging times, by factors ranging from 2 to 20. RTDM predicted with less bias than the other models for all three averaging times. (The IMPACT model was evaluated only for selected hours from Westvaco.) The COMPLEX II model and the IMPACT model gave the largest overpredictions. COMPLEX I also overpredicted the average of the 25 highest 1-hour values by almost a factor of 10.

Cinder Cone Butte. Six of the eight models overpredicted the 25 highest 1-hour values. IMPACT underpredicted, and RTDM predicted with no significant bias. COMPLEX II again gave the largest overprediction, roughly a factor of 4 times observed.

Thus, COMPLEX II showed the most consistent and pronounced tendency to overpredict peak concentrations; RTDM showed the least bias for estimating peak 1-hour values; and IMPACT showed the greatest inconsistency between the two data sets.

Model performance results for the two data sets showed several striking differences:

- The models showed a much greater tendency to overpredict peak 1-hour concentrations for the Westvaco data set than for Cinder Cone Butte.
- Comparisons between predicted and observed concentrations, paired in time and location, showed smaller discrepancies and higher correlation for Cinder Cone Butte than for Westvaco.
- For Westvaco, model performance was very different for stable and neutral conditions (for most of the models). For Cinder Cone Butte, model performance was generally similar for both stability categories.

These differences point to the importance of the source characteristics and the local terrain setting (as well as other design factors) for model performance in complex terrain.

The Westvaco data set permitted model performance to be evaluated by monitoring station and for several averaging times. From these analyses, the following conclusions could be drawn:

- Distinct differences in model performance were found between those monitors within 2 km of the plant and those at greater distances. Overprediction was more pronounced at monitors close to the plant.
- Results for 1-hour and 3-hour averages were quite similar. For 24-hour averages, however, distinct differences in model performance were found for estimating peak concentrations.

REFERENCES

1. United States Environment Protection Agency, 1978. Guideline On Air Quality Models. EPA-450/2-78-027. OAQPS, Research Triangle Park, NC.
2. Fox, D.G., 1981. Judging Air Quality Model Performance (A Summary of the AMS Workshop on Dispersion Model Performance, Woods Hole, MA, 8-11 September 1980). Bull. Am. Meteorol. Soc., 62, 599-609.
3. Londergan, R.J., D.H., Minott, D.J. Wackter, T.M. Kincaid and D.M. Bonitata, 1982. Evaluation of Rural Air Quality Simulation Models. Prepared for EPA by TRC Environmental Consultants, EPA-450/4-83-003, OAQPS, Research Triange Park, NC.
4. Minott, D.H., R.J. Londergan, W.M. Cox, and J.A. Tikvart, 1982. Comparative Performance Evaluations of MPTEr and Alternative Rural Models. Presented at the 75th Annual Meeting of the Air Pollution Control Association, New Orleans, LA.
5. Londergan, R.J., D.H. Minott, D.J. Wackter and R.R. Fizz, 1983. Evaluation of Urban Air Quality Simulation Models. Prepared for EPA by TRC Environmental Consultants, EPA-450/4-83-020, OAQPS, Research Triangle Park, NC.
6. Pierce, T.D. and D. B. Turner, 1980. User's Guide for MPTEr. EPA-600/8-80-016, U.S. Environmental Protection Agency, Research Triangle Park, NC.
7. Strimaitis, D.G., J.S. Scire and A. Bass, 1982. User's Guide for COMPLEX/PFM Air Quality Model. EPA-600/8-83-015, Environmental Protection Agency, Research Triangle Park, NC.
8. Enviroplan, Inc., 1981. User's Manual for Enviroplan's Model 3141 and Model 4141. Enviroplan, Inc., West Orange, NJ.
9. United States Environmental Protection Agency, 1977. User's Manual for Single Source (CRSTER) Model. EPA-450/2-77-013, OAQPS, Research Triangle Park, NC.
10. Pacific Gas and Electric, 1981. User's Manual for Pacific Gas and Electric PLUME5 Model. Pacific Gas and Electric, San Francisco, CA.
11. Environmental Research & Technology, Inc., 1982. User's Guide for the Rough Terrain Diffusion Model (RTDM, Rev. 3.00). ERT Report No. M 2209-585. Environmental Research & Technology, Inc., Concord, MA.

12. Bjorklund, J.R., and J.F. Bowers, 1982. User's Instructions for the SHORTZ and LONGZ Computer Programs, Volumes 1 and 2. EPA 903/9-82-004, U.S. Environmental Protection Agency, Research Triangle Park, NC.
13. Cramer, H.E., et al., 1972. Development of Dosage Models and Concepts. Final Report under Contract DAAD 09-67-C-00 20 (R) with the U.S. Army, Dessert Test Center Report DTC-TR-72-609, Fort Douglas, UT.
14. Fabrick, A.J. and P.J. Haas, 1980. User Guide to IMPACT: An Integrated Model for Plumes and Atmospheric Chemistry in Complex Terrain. Radian Corporation, Austin, TX.
15. Tran, K.T., R.C. Sklarew, 1979. User Guide To IMPACT: An Integrated Model For Plumes And Atmospheric Chemistry In Complex Terrain. Form & Substance, Inc., Westlake Village, CA.
16. Wackter, D.J., 1983. Test Run Package: Description of Models "As-Run" for Complex Terrain Model Evaluation. Prepared for EPA by TRC Environmental Consultants under Contract 68-02-3514, W.A. 27, OAQPS, Research Triangle Park, NC.
17. Lavery, T.F., A. Bass, D.G. Strimaitis, A. Venkatrom, B.R. Greene, P.J. Drivas and B.A. Egan, 1982. EPA Complex Terrain Model Development: First Milestone Report - 1981. EPA-600/3-82-036, Environmental Protection Agency, Research Triangle Park, NC.
18. Strimaitis, D.G., A. Venkatrom, B.R. Greene, S. Hanna, S. Hesler, T.F. Lavery, A. Bass and B.A. Egan, 1983. EPA Complex Terrain Model Development: Second Milestone Report - 1982. EPA-600/3-83-015 Environmental Protection Agency, Research Triangle Park, NC.
19. Truppi, L.E., and G.C. Holzworth, 1983. EPA Complex Terrain Model Development: Description of a Computer Data Base from Small Hill Impaction Study No. 1, Cinder Cone Butte, Idaho. Environmental Sciences Research Laboratory, Research Triangle Park, NC.
20. Maryland State Department of Health and Mental Hygiene, 1979. Westvaco Corporation Amended Consent Order.
21. Cramer, H.E., 1981. Westvaco-Luke, Maryland Monitoring Program: Data Analysis and Dispersion Model Evaluation (First Two Quarters). H.E. Cramer Company, Inc., Salt Lake City, UT.
22. Hanna, S., C. Vaudo, A. Curreri, J. Beebe, B. Egan, and J. Mahoney, 1982. Diffusion Model Development and Evaluation, and Emission Limitations at the Westvaco Luke Mill. Document PA439 prepared for the Westvaco Corporation by Environmental Research & Technology, Inc., Concord, MA.

23. Cramer, H.E., 1982. Portocol for the Evaluation of the SHORTZ and LUMM Dispersion Models Using the Westvaco Data Set. H.E. Cramer Company, Inc., Salt Lake City, UT.
24. Snedecor, G.W. and W.G. Cochran, 1967. Statistical Methods, 6the Edition. Iowa State University Press, Ames, Iowa.
25. Hollander, M. and R.A. Wolfe, 1973. Nonparametric Statistical Methods. John Wiley and Sons, New York, NY.
26. Hirtzel, C.S. and J.E. Quon, 1981. Estimating Precision of Autocorrelated Air Quality Measurements. Summary of Proceedings Environmetrics 81, 200-201.
27. United States Environmental Protection Agency, 1981. Regional Workshops on Air Quality Modeling: A Summary Report. EPA-450/4-82-015, EPA/OAQPS, Research Triangle Park, NC.

APPENDIX A

TEST RUN PACKAGE: DESCRIPTION OF MODELS "AS-RUN"
FOR COMPLEX TERRAIN MODEL EVALUATION

TEST RUN PACKAGE:
DESCRIPTION OF MODELS "AS-RUN"
FOR COMPLEX TERRAIN MODEL EVALUATION



TRC Project No. 2164--R81

David Wackter
Project Manager

September, 1983

800 Connecticut Blvd.
East Hartford, CT 06108
(203) 289-8631

TABLE OF CONTENTS

<u>SECTION</u>		<u>PAGE</u>
1.0	INTRODUCTION	1
2.0	COMPLEX-I AND COMPLEX-II	3
2.1	Technical Modifications to COMPLEX-I and COMPLEX-II	3
2.2	COMPLEX-I and COMPLEX-II: Input Options and Variables for Cinder Cone Butte	4
2.3	COMPLEX-I and COMPLEX-II: Input Options and Variables for Westvaco	4
2.4	TRC Changes to COMPLEX-I for Cinder Cone Butte . .	5
2.5	TRC Changes to COMPLEX-I for Westvaco	5
2.6	TRC Changes to COMPLEX-II for Cinder Cone Butte . .	6
2.7	TRC Changes to COMPLEX-II for Westvaco	6
3.0	PLUME5	7
3.1	Technical Modifications to PLUME5	7
3.2	PLUME5: Input Options and Variables	8
3.3	TRC Changes to PLUME5 Code for Cinder Cone Butte .	9
3.4	TRC Changes to PLUME5 Code for Westvaco	10
4.0	RTDM	11
4.1	Technical Modifications to RTDM	11
4.2	RTDM: Input Options and Variables for Cinder Cone Butte	12
4.3	RTDM: Input Options and Variables for Westvaco . .	13
4.4	TRC Changes to RTDM for Cinder Cone Butte	14
4.5	TRC Changes to RTDM for Westvaco	15
5.0	SHORTZ	16
5.1	Technical Modifications to SHORTZ	16
5.2	SHORTZ: Input Options and Variables for Cinder Cone Butte	16
5.3	SHORTZ: Input Options and Variables for Westvaco .	17
5.4	TRC Changes to SHORTZ for Cinder Cone Butte	18
5.5	TRC Changes to SHORTZ for Westvaco	18
6.0	4141	19
6.1	Technical Modifications to 4141	19
6.2	4141: Input Options and Variables for Cinder Cone Butte	19
6.3	4141: Input Options and Variables for Westvaco . .	20
6.4	TRC Changes to 4141 for Cinder Cone Butte	21
6.5	TRC Changes to 4141 for Westvaco	22
7.0	COMPLEX/PFM	23
7.1	Technical Modifications to COMPLEX/PFM	23
7.2	COMPLEX/PFM: Input Options and Variables for Cinder Cone Butte	24
7.3	COMPLEX/PFM: Input Options and Variables for Westvaco	24
7.4	TRC Changes to COMPLEX/PFM for Cinder Cone Butte .	25
7.5	TRC Changes to COMPLEX/PFM for Westvaco	26

TABLE OF CONTENTS
(continued)

<u>SECTION</u>		<u>PAGE</u>
8.0	IMPACT	27
8.1	Technical Modifications to IMPACT	27
8.2	IMPACT: Input Options and Variables for Cinder Cone Butte	28
8.3	IMPACT: Input Options and Variables for Westvaco .	29
8.4	TRC Changes to IMPACT (Version 1 from Radian) for Cinder Cone Butte	30
8.5	TRC Changes to IMPACT (Version 1 from Radian) for Westvaco	30

1.0 INTRODUCTION

EPA has contracted with TRC to evaluate the performance of complex terrain air quality simulation models using performance measures recommended by the American Meteorological Society. Eight models are to be evaluated: COMPLEX-I, COMPLEX-II, PLUME5, RTDM, SHORTZ, 4141, COMPLEX/PPM, and IMPACT. Prior to running the complex terrain models for evaluation, it is desirable to confirm that the models have been implemented in accordance with the expectations of the model developers. To accomplish this, test-run packages were prepared and are being supplied to the model developers for their formal review and concurrence. The package supplied to each model developer contains the following information:

- Descriptions of the complex terrain model evaluation data bases (Cinder Cone Butte and Westvaco);
- Summary of model-code modifications;
- Summary of input options;
- Test-run data (listings of all input and output data) for the model developer's particular model;
- Complete listing of the model code "as run," (for the model developer's particular model) to enable the model developer to confirm the code line-by-line.

Also provided as part of the test case package are three other relevant documents:

- "Data Archiving Recommendations for Complex Terrain Model Evaluations" (TRC, November 1982).
- "Addendum to: Data Archiving Recommendations for Complex Terrain Model Evaluations (Response to Comments from Model Developers)" (TRC, July 1983).
- "Statistical Evaluation for Complex Terrain Models" (TRC, June 1983).

This document summarizes the model code modifications made by TRC and input options selected by the model developers for each model and data base. Modifications to the models were needed for three basic reasons:

- To adapt the model to the EPA UNIVAC computer.
- To adopt particular models to accept the source-receptor inventories.
- To format calculated concentrations for input to the statistics system.

Detailed summaries of line-by-line changes made by TRC to each model's computer code are also described in this document.

Computer code listings for the models "as run," plus the test run input and output data listings are supplied separately.

2.0 COMPLEX-I AND COMPLEX-II

2.1 Technical Modifications to COMPLEX-I and COMPLEX-II

TRC altered COMPLEX-I and COMPLEX-II to accept input data from the model input file on Unit 18 rather than Unit 5. Statements were added to facilitate writing calculated concentrations to a work file for future statistical analysis. These changes were made for both the Westvaco and Cinder Cone Butte data bases.

To accommodate the Westvaco data base, TRC modified COMPLEX-I and COMPLEX-II in three areas. The models were altered to accept hourly input of source exit velocity and exit temperature. TRC made changes to circumvent problems that could be caused by the Westvaco data starting in one calendar year and ending in the next calendar year. Code was added to check for hours with missing stability during which no concentrations were calculated.

When COMPLEX-I and COMPLEX-II were tested with the Cinder Cone Butte data base, one technical modification was needed. The models were altered so that only the source with a source number (1-111) equal to the hour (1-111) being modeled has an impact on the calculated concentrations. This modification, consistent with the input emissions inventory, was needed because a single emission point was moved each hour in the Cinder Cone Butte study.

2.2 COMPLEX-I and COMPLEX-II: Input Options and Variables for Cinder Cone Butte

<u>Variable Name</u>	<u>Input Value</u>	<u>Description</u>
IOPT(1)	1	Use terrain adjustments.
IOPT(2)	1	No stack downwash.
IOPT(3)	1	No gradual plume rise.
IOPT(4)	1	Calculate initial plume size.
IOPT(25)	1	Use complex terrain option.
HANE	0.90	Anemometer height in meters.
PL	0.,0.,0.,0.,0.,0.	Wind profile power law exponents.
CONTER	0.5,0.5,0.5,0.5,0.,0.	Terrain adjustment factors.
ZMIN	10.	Distance limit for plume centerline from ground.
HAFL	0.	No pollutant loss.

2.3 COMPLEX-I and COMPLEX-II: Input Options and Variables for Westvaco

<u>Variable Name</u>	<u>Input Value</u>	<u>Description</u>
IOPT(1)	1	Use terrain adjustments.
IOPT(2)	0	Use stack downwash.
IOPT(3)	1	No gradual plume rise.
IOPT(4)	1	Calculate initial plume size.
IOPT(25)	1	Use complex terrain option.
HANE	189.7	Anemometer height in meters.
PL	0.,0.,0.,0.,0.,0.	Wind profile power law exponents.
CONTER	0.5,0.5,0.5,0.5,0.,0.	Terrain adjustment factors.
ZMIN	10.	Distance limit for plume centerline from ground.
HAFL	0.	No pollutant loss.

2.4 TRC Changes to COMPLEX-I for Cinder Cone Butte

<u>Line Number</u>	<u>Description of Modification</u>
1-2, 134-137	Comments.
358-360	Dimension TRC variables.
377-381	Define work file.
451-455, 466-475	Initialize I/O units and hour counter. Check data base ID.
736-740	Do not read met station identifiers.
945-948	Increment the TRC hour counter.
1061-1064, 1568-1570	Transfer TRC hour counter to subroutine PTR.
1065-1074	Write to hourly work file.
1617-1619	Ignore sources other than the one which corresponds to the hour of simulation.
1702-1703	Set distance to final plume rise equal to zero.
1734	Allow for stack temperature equal to ambient.

2.5 TRC Changes to COMPLEX-I for Westvaco

<u>Line Number</u>	<u>Description of Modification</u>
1-3, 135-138, 472	Comments.
359-362	Dimension TRC variables.
379-384	Define work file.
454-462, 474-485	Initialize I/O units. Check data base ID.
900-905, 910-912, 917-919, 924-931, 934-936, 1084-1087, 1482-1483	Changes to accommodate data from two calendar years.
978-987	Flag missing stability data.
1088-1101, 1722-1726	Read in hourly source data.
1108-1118	Write to work file.

2.6 TRC Changes to COMPLEX-II for Cinder Cone Butte

<u>Line Number</u>	<u>Description of Modification</u>
1-2, 132-135	Comments.
356-358	Dimension TRC variables.
375-379	Define work file.
449-454, 465-474	Initialize I/O units and hour counter. Check data base ID.
735-749	Do not read met station identifiers.
943-946	Increment the TRC hour counter.
1059-1062, 1565-1567	Transfer TRC hour counter to subroutine PTR.
1063-1071	Write to hourly work file.
1614-1616	Ignore sources other than the one which corresponds to the hour of simulation.
1699-1700	Set distance to final plume rise equal to zero.
1731	Allow for stack temperature equal to ambient.

2.7 TRC Changes to COMPLEX-II for Westvaco

<u>Line Number</u>	<u>Description of Modification</u>
1-3, 133-136, 465	Comments.
357-359	Dimension TRC variables.
376-381	Define work file.
451-455, 467-478	Initialize I/O units. Check data base ID.
893-897, 902-904, 909-911, 921-923, 926-928, 1077-1079, 1472-1473	Changes to accommodate data from two calendar years.
970-980	Flag missing stability data.
1080-1091, 1712-1716	Read in hourly source data.
1098-1108	Write to work file.

3.0 PLUME5

3.1 Technical Modifications to PLUME5

TRC added code to PLUME5 to write calculated concentrations to a work file for future statistical analysis. The model was altered to allow input from a disk file rather than cards. The meteorological data input unit has been set to 11. To reduce computer core requirements, receptor arrays dimensioned by 500 were reduced to the number of receptors in each respective data base.

For the Westvaco data base only, TRC modified PLUME5 to accept hourly values of emission rate, stack exit velocity, and stack exit temperature.

Several changes were made to adapt PLUME5 to the Cinder Cone Butte data base. Code was added to skip the reading of station identifiers on the disk file containing meteorological data and to read the meteorological data one hour at a time. The DO loops on days and hours were merged into a single loop to handle the non-sequential nature of the Cinder Cone Butte experiment hours. Daily and annual average output were skipped. Plume rise was set equal to zero. TRC also modified the model so that only the source with a source number equal to the consecutive hour number has an impact on calculated concentrations (See Section 2.1).

3.2 PLUME5: Input Options and Variables

<u>Variable Name</u>	<u>Input Value</u>		<u>Description</u>
	<u>Westvaco</u>	<u>CCB</u>	
<u>CONVRT (PLUME5 preprocessor):</u>			
ISTAT	2	2	Stability classified by σ_A .
MST	1	1	Modify unstable stability at night as a function of wind speed.
DTHDZ	0.01	0.01	Default value for change of potential temperature with height through stable layer.
THICK	800.	NA	Default value for the thickness of stable layer.
SIGMAF	1	1	Default multiplier for sigma value.
LAT	39.5	43.0	Latitude of surface station.
LONG	79.3	115.5	Longitude of surface station.
ZONE	5	7	Standard time zone.
NCCOFF	0	NA	NCC mixing height data used.
<u>PLUME5:</u>			
IUR	1	1	RURAL1 mixing heights used.
BKGRD	1.E-30	1.E-30	Background concentration in $\mu\text{g}/\text{m}^3$.
IGRID	0	0	Do not use receptor grid.
ICIRC	0	0	Do not generate receptors using radial rings.
IATOB	1	1	Changes Class A stability to Class B.
IPLUME	0	0	No hourly plume rise input.
ISGFLG	1	1	Initial plume expansion allowed.
MODFLG	1	1	Pasquill modification to the crosswind spread of plumes due to vertical wind directional shear allowed.
WINDHT	189.7	10.	Wind speed measurement height (meters).
MSLFLG	1	NA	Mixing heights are above ground level.

3.3 TRC Changes to PLUME5 Code for Cinder Cone Butte

General: Receptor array arguments reduced from 500 to 94 to reduce core requirements. The number of point source locations was raised from 10 to 111, while the number of release heights per location was reduced from 15 to 1. One source per hour of simulation. Mixing height set to 9999 meters.

<u>Line Number</u>	<u>Description of Modification</u>
1-13	Comments.
26-28, 523-524	Define TRC COMMON block.
47-60	Initialize I/O units. Define work file. Check data base ID.
84	Change loop on sources from 10 to 111.
117-119, 138-139	Skip section which reads station identifiers from meteorological data file.
145-146, 1402-1403	Change maximum number of sources allowed.
150-151	Change maximum number of heights per source.
178-180, 480-481, 485-486	Change write statement.
521-522	Dimension TRC variables.
552-554	Reduce maximum number of receptors allowed from 500 to 94.
628-636, 723, 728-730	Change the day and hour loops since CCB data is not in 24 hour groups.
651-652	Change unit number for input of meteorological data.
656-672	Read in the meteorological data, one hour at a time.
694-714	Change write statement and format for output of meteorological data.
766-769, 857	Separate the loops on source location and release height.

3.3 TRC Changes to PLUME5 Code for Cinder Cone Butte (Continued)

<u>Line Number</u>	<u>Description of Modification</u>
110-113, 889-893	Ignore sources other than the one which corresponds to the hour of simulation.
1211-1220	Write to the work file.
1222-1226	Skip output of daily and annual averages.
1855-1857	Set plume rise to zero.

3.4 TRC Changes to PLUME5 Code for Westvaco

General: Receptor array arguments reduced from 500 to 11 to reduce core requirements.

<u>Line Number</u>	<u>Description of Modification</u>
1-5	Comments.
18-20, 515-517	Define TRC common block.
39-60	Initialize I/O units. Define work file. Check data base ID.
119-123, 638-642	Change unit number for input of meteorological data.
511-514	Dimension TRC variables.
545-549	Change maximum number of receptors allowed from 500 to 11.
691-700	Read and print the hourly point source data.
1167-1173	Write to the work file.

4.0 RTDM

4.1 Technical Modifications to RTDM

TRC made general and data base specific modifications to RTDM. For both the Westvaco and Cinder Cone Butte data bases, code was added to write calculated concentrations to a work file, and to read model input data on Unit 18 rather than Unit 5. Meteorological data is read from Unit 10 for Cinder Cone Butte, and Units 10 and 11 for Westvaco, instead of Unit 7. For both data bases, assignment of the PR005 parameter has been fixed to properly correspond to wind profile exponents, not terrain factors.

Modifications specific to the Westvaco data base include reading hourly source data from Unit 15, reading meteorological station identifiers from Unit 10, and checking for hours with missing stability. Concentrations are not calculated for the hours with missing stability.

For the Cinder Cone Butte data base, RTDM was modified to set plume rise and wind profile exponents equal to zero, to set anemometer height equal to release height, and to allow hours which are out of sequence. TRC modified RTDM so that only one source contributes to the calculated concentration in any given hour (See Section 2.1).

4.2 RTDM: Input Options and Variables for Cinder Cone Butte

<u>Variable Name</u>	<u>Input Value</u>	<u>Description</u>
ZWIND1	Release height	Anemometer height (m).
ZWIND2	Not used	
IDILUT	0	Wind speed at level 1 is used for plume rise and transport calculations.
EXPON	0.,0.,0.,0.,0.,0.	Wind speed profile power law exponents.
ICOEF	3	ASME (1979) stability-dependent dispersion parameters.
IPPP	0	No partial plume penetration.
IBUOY	1	Use buoyancy-enhanced dispersion.
IALPHA	3.162	
IDMX	1	Unlimited mixing height in stable conditions.
ITRANS	1	Use transitional plume rise.
TERCOR	0.5,0.5,0.5, 0.5,0.5,0.5	Plume path correction factors.
RVPTG	0.02, 0.035	Default VPTG for stabilities 5 and 6.
ITIPD	0	No stack-tip downwash.
IY	1	User-supplied I_y .
IZ	1	User-supplied I_z .
IRVPTG	0	Default VPTG for plume rise calculations.
IHVPTG	1	User-supplied VPTG for H_{crit} calculations.
ISHEAR	0	Wind direction shear is not used in σ_y computation.
IEPS	0	No hourly wind profile exponents.
IREFL	1	Use partial reflection algorithm.
IHORIZ	1	Off-centerline horizontal distribution function.
IEMIS	0	Use constant emission rate.

4.3 RTDM: Input Options and Variables for Westvaco

<u>Variable Name</u>	<u>Input Value</u>	<u>Description</u>
ZWIND1	30.	Anemometer height (m) above ZA, for plume rise.
ZWIND2	Not used	Anemometer height for transport.
IDILUT	0	Wind speed at level 1 extrapolated to stack top for plume rise calculations and to plume height for transport calculations.
ZA	179.6	Height above stack base where the wind profile originates.
EXPON	0.,0.,0.,0.,0.,0.	Wind speed profile power law exponents.
ICOEF	3	ASME (1979) stability-dependent dispersion parameters.
IPPP	0	No partial plume penetration.
IBUOY	1	Use buoyancy-enhanced dispersion.
IALPHA	3.162	
IDMX	1	Unlimited mixing height in stable conditions.
ITRANS	1	Use transitional plume rise.
TERCOR	0.5,0.5,0.5, 0.5,0.5,0.5	Plume path correction factors.
RVPTG	0.02, 0.035	Default VPTG for stabilities 5 and 6.
ITIPD	1	Use stack-tip downwash.
IY	1	User-supplied I_y .
IZ	1	User-supplied I_z .
IRVPTG	1	User-supplied VPTG for plume rise calculations.
IHVPTG	1	User-supplied VPTG for H_{crit} calculations.
ISHEAR	1	Wind direction shear is used in σ_y computation.

4.3 RTDM: Input Options and Variables for Westvaco (Continued)

<u>Variable Name</u>	<u>Input Value</u>	<u>Description</u>
IEPS	1	User-supplied hourly wind profile exponents.
IREFL	1	Use partial reflection algorithm.
IHORIZ	1	Off-centerline horizontal distribution function.
IEMIS	1	User-supplied hourly emission rate.

4.4 TRC Changes to RTDM for Cinder Cone Butte

<u>Line Number</u>	<u>Description of Modification</u>
1-4	Comments.
21	Define work file.
22-32	Check data base ID.
33-41	Read and print the experiment hours being modeled.
474-475	PR005 should read wind profile exponents, not terrain factors.
1177-1178	Change requested by ERT.
1365-1367, 1695-1696	Define TRC common block.
1436-1448, 1452-1453	Read meteorological data.
1463-1464	Allow hours which are out of sequence.
1510-1514, 1546-1547, 1549-1550, 1583-1586	Change output formats.
1697-1698	Dimension TRC variables.
1712-1717	Allow source contribution from only one source per hour.
1738-1734	Set wind profile exponents equal to zero and wind measurement height equal to release height.
1759, 1763	Set plume rise equal to zero.
1836, 1850-1856	Write to the work file.

4.5 TRC Changes to RTDM for Westvaco

<u>Line Number</u>	<u>Description of Modification</u>
1-4	Comments.
21	Define work file.
22-34	Check data base ID.
35-36	Read station identifiers from meteorological data file.
471-472	PR005 should be reading wind profile exponents, not terrain factors.
1175-1176	Change requested by ERT.
1365-1374, 1736-1739	Define TRC common block.
2891	Dimension TRC variables.
1443-1475, 1479, 1485-1486	Read meteorological data from two files.
1480-1484, 1742-1748, 2897-2902	Flag hours with missing stability.
1491-1507	Read point source data file.
1610-1618, 1624-1627	Change error message formats.
1871-1874, 1887-1893	Write to work file.

5.0 SHORTZ

5.1 Technical Modifications to SHORTZ

The SHORTZ model was modified to accept input data from a disk file, and to write calculated concentrations to a work file for subsequent statistical analysis. For the Westvaco data base run, an hour counter and an alternate output format for the time period in question were added. Modifications specific to the Cinder Cone Butte data base include setting plume rise equal to zero, adding an array to hold calculated concentrations, and allowing the maximum number of hours in a case to equal 111.

5.2 SHORTZ: Input Options and Variables for Cinder Cone Butte

<u>Variable Name</u>	<u>Input Value</u>	<u>Description</u>
ISW(7)	1	Terrain elevation data are input.
ISW(9)	0	Wind speed is not terrain following.
ISW(17)	0	Rural option.
G	9.80	Acceleration of gravity (m/s^2).
ZR	9.99	Wind speed measurement height (m).
GAMMA1	0.60	Entrainment coefficient for unstable atmosphere.
GAMMA2	0.66	Entrainment coefficient for stable atmosphere.
XRY	50.	Distance (m) over which rectilinear expansion occurs downwind of source.
DECAY	0.	No pollutant loss.
HA	99.9	Elevation (m) of base of weather station.

5.3 SHORTZ: Input Options and Variables for Westvaco

<u>Variable Name</u>	<u>Input Value</u>	<u>Description</u>
ISW(7)	1	Terrain elevation data are input.
ISW(9)	0	Wind speed is not terrain following.
ISW(17)	0	Rural option.
G	9.80	Acceleration of gravity (m/s ²).
ZR	30.0	Wind speed measurement height (m).
GAMMA1	0.60	Entrainment coefficient for unstable atmosphere.
GAMMA2	0.66	Entrainment coefficient for stable atmosphere.
XRY	50.	Distance (m) over which rectilinear expansion occurs downwind of source.
DECAY	0.	No pollutant loss.
HA	467.6	Elevation (m) of base of weather station.

5.4 TRC Changes to SHORTZ for Cinder Cone Butte

<u>Line Number</u>	<u>Description of Modification</u>
2-14, 118-135	Comments.
26-55, 656-684	Define TRC COMMON block EVAL.
86-94	Initialize I/O units.
98-114	Define work file.
136-171	Check data base ID.
202-210	Set TRC variable NMON=NXXYY.
232	Set MKQ=111, maximum number of hours.
1194-1199	Zero the TRCONC array each hour.
1211	Let maximum number of hours = 111.
1483-1488	Set plume rise equal to zero.
1797-1802	Put calculated concentrations into array TRCONC.
1812-1834	Write to the work file.

5.5 TRC Changes to SHORTZ for Westvaco

<u>Line Number</u>	<u>Description of Modification</u>
2-14, 118-135	Comments.
26-55, 656-684, 2043-2048	Define TRC COMMON block EVAL.
86-94, 154	Initialize I/O units.
98-114	Define work file.
136-171	Check data base ID.
202-210	Set TRC variable NMON=NXXYY.
1795-1817	Write to work file.
1875-1876	Set hour counter IHRTRC.
2120-2125	Change the output hour format.

6.0 4141

6.1 Technical Modifications to 4141

Modifications to 4141 are the same as for COMPLEX-I and COMPLEX-II.

6.2 4141: Input Options and Variables for Cinder Cone Butte

<u>Variable Name</u>	<u>Input Value</u>	<u>Description</u>
MODEL	4141	Select 4141 Model Option. Sets CONTER = 0.5,0.5,0.5,0.5, 0.25,0.25. Sets IOPT(4) = 1. Sets IOPT(1) = 1.
IOPT(1)	1	Use terrain adjustments.
IOPT(2)	1	No stack downwash.
IOPT(3)	0	Gradual plume rise.
IOPT(4)	1	Calculate initial plume size.
HANE	0.9	Anemometer height in meters.
PL	0.,0.,0.,0.,0.,0.	Wind speed profile power law exponents.
HAFL	0.	No pollutant loss.

6.3 4141: Input Options and Variables for Westvaco

<u>Variable Name</u>	<u>Input Value</u>	<u>Description</u>
MODEL	4141	Select 4141 Model Option. Sets CONTER - 0.5,0.5,0.5,0.5, 0.25,0.25. Sets IOPT(4) = 1. Sets IOPT(1) = 1.
IOPT(1)	1	Use terrain adjustments.
IOPT(2)	1	No stack downwash.
IOPT(3)	0	Gradual plume rise.
IOPT(4)	1	Calculate initial plume size.
HANE	189.7	Anemometer height in meters.
PL	0.,0.,0.,0.,0.,0.	Wind speed profile power law exponents.
HAFL	0.	No pollutant loss.

6.4 TRC Changes to 4141 for Cinder Cone Butte

<u>Line Number</u>	<u>Description of Modification</u>
1-2, 82-85, 185-188	Comments.
304-306	Dimension TRC variables.
325-329	Define work file.
404-409, 421-430	Initialize I/O units and hour counter. Check data base ID.
689-692	Do not read met station identifiers.
899-902	Increment the TRC hour counter.
1015-1018, 1597-1599	Transfer TRC hour counter to subroutine PTR.
1019-1028	Write to hourly work file.
1645-1647	Ignore sources other than the one which corresponds to the hour of simulation.
1729-1731	Set distance to final plume rise equal to zero.
1761-1762	Allow for stack temperature equal to ambient.

6.5 TRC Changes to 4141 for Westvaco

<u>Line Number</u>	<u>Description of Modification</u>
1-3, 83-86, 186-189	Comments.
305-307	Dimension TRC variables.
326-331	Define work file.
406-410, 423-434	Initialize I/O units. Check data base ID.
848-853, 858-860, 865-867, 872-879, 882-884, 1033-1035	Changes to accommodate data from two calendar years.
926-936	Flag missing stability data.
1036-1047	Read in hourly source data.
1054-1064	Write to work file.

7.0 COMPLEX/PFM

7.1 Technical Modifications to COMPLEX/PFM

The technical modifications to COMPLEX/PFM consist of the same changes made to COMPLEX-I and COMPLEX-II, plus several alterations specific to COMPLEX/PFM. For both the Westvaco and Cinder Cone Butte data bases, COMPLEX/PFM was modified to read receptor data from a unique disk file. Also, array sizes were reduced in accordance with data base requirements in order to reduce the need for computer core storage.

Some modifications were needed only for the Cinder Cone Butte data base. These include reading the potentially non-sequential list of experiment hours to be modeled; reading hourly values of critical streamline height (H_{crit}) and Froude number from a disk file; and accounting for the absence of vertical wind and temperature profiles in the Cinder Cone Butte input data set.

7.2 COMPLEX/PFM: Input Options and Variables for Cinder Cone Butte

<u>Variable Name</u>	<u>Input Value</u>	<u>Description</u>
IOPT(1)	1	Use terrain adjustments.
IOPT(2)	1	No stack downwash.
IOPT(3)	1	No gradual plume rise.
IOPT(4)	1	Calculate initial plume size.
IOPT(25)	1	Use complex terrain option.
IOPT(26)	1	Long-term PFM option.
HANE	0.90	Anemometer height in meters.
PL	0.,0.,0.,0.,0.,0.	Wind profile power law exponents.
CONTER	0.5,0.5,0.5,0.5,0.,0.	Terrain adjustment factors.
ZMIN	10.	Distance limit for plume centerline from ground.
HAFL	0.	No pollutant loss.

7.3 COMPLEX/PFM: Input Options and Variables for Westvaco

<u>Variable Name</u>	<u>Input Value</u>	<u>Description</u>
IOPT(1)	1	Use terrain adjustments.
IOPT(2)	0	Use stack downwash.
IOPT(3)	1	No gradual plume rise.
IOPT(4)	1	Calculate initial plume size.
IOPT(25)	1	Use complex terrain option.
IOPT(26)	1	Long-term PFM option.
HANE	189.7	Anemometer height in meters.
PL	.10,.15,.20,.25,.25,.25	Wind profile power law exponents.
CONTER	0.5,0.5,0.5,0.5,0.,0.	Terrain adjustment factors.
ZMIN	10.	Distance limit for plume centerline from ground.
HAFL	0.	No pollutant loss.

7.4 TRC Changes to COMPLEX/PFM for Cinder Cone Butte

<u>Line Number</u>	<u>Description of Modification</u>
1-18, 183-186, 314-316, 373-374, 429-430, 602, 2322, 4141-4142, 5960-5961.	Comments.
453-455, 2323-2327, 5495-5497	TRC common block definition .
458-460	Dimension TRC variables.
484-489	Define work file.
569-573, 4172-4175	Change the maximum number of receptors from 180 to 99 to reduce core requirements.
582-587	I/O device initialization.
604-625	Read and verify data base and work file identifiers. Read in the experiment hours to be modeled.
920-923, 1258-1264, 1298-1299	Modifications to account for the absence of wind and temperature profiles.
1141-1147	Read Hcrit and Froude number from TRC disk file.
1318-1328	Write calculated concentrations to work file.
1887	Write format change.
2423-2426	Print Hcrit and Froude number.
5549-5552, 5581-5584, 5856-5858	Do not call subroutines which calculate Hcrit and Froude number.
5607-5612	Allow source contributions from only one source per hour.
5714-5716, 5747-5748	Allow for ambient temperature identical to stack temperature.
6005-6010	Change format and input unit of statements which read receptor data.

7.5 TRC Changes to COMPLEX/PFM for Westvaco

<u>Line Number</u>	<u>Description of Modification</u>
1-11, 176-179, 307-309, 366-367 422-423, 592, 5933-5934	Comments.
448-450	Dimension TRC variables.
474-479	Define files.
559-563, 4166-4169	Change maximum number of receptors allowed from 180 to 15 to reduce computer core requirements.
572-577	Device initializations.
594-605	Read and verify data base and work file identifiers.
1064-1068, 1073-1075, 1080-1082, 1087-1094, 1098-1100, 1297-1298	Changes to accommodate data from two calendar years.
1142-1152	Check for missing stability. Set calculated concentration to missing.
1299-1311, 5659-5663	Read hourly point source data.
1318-1329	Write calculated concentrations to the work file.
5978-5983	Change format of statements which read receptor data.

8.0 IMPACT

8.1 Technical Modifications to IMPACT

TRC inserted additional codes within specific sections of the IMPACT model to produce the following two results:

- i) Identify and write to the output work file those 1-hour average surface level concentrations for calls corresponding to monitor sites. These changes were included for both the Westvaco and Cinder Cone Butte versions of the model.
- ii) Redimension arrays in the COMMON block TREFOR to accommodate the number of cells utilized in the X-, Y-, and Z- directions for each data base. In the case of Westvaco, the number of cells are 13, 15, and 20, respectively, with corresponding cell dimensions of 200, 200, and 60.96m. In the case of Cinder Cone Butte, the number of cells are 36, 45 and ~~14~~²⁰, respectively, with corresponding cell dimensions of 50m, 50m and 10m.

The IMPACT model allows for a maximum of 40 cells in the "X-" direction. The actual grid developed by TRC for Cinder Cone Butte contains 45 cells in the East-West direction. In order to avoid additional code revisions, the grid was rotated 90° counter-clockwise. There are now 36 cells in the X- direction (north-south) and 45 cells in the Y- direction (east-west).

Another modification to the IMPACT model was required for the Cinder Cone Butte application. The minimum time step, DTMIN (specified in a Data statement located in subroutine DIFFUS), was reduced from 3.6 seconds to ~~1.0~~^{0.5} seconds. This change allows the model to calculate a time step appropriate for the small grid spacing defined for Cinder Cone Butte.

8.2 IMPACT: Input Options and Variables for Cinder Cone Butte

<u>Variable Name</u>	<u>Input Value</u>	<u>Description</u>
DX	50.	E-W cell size in m.
DY	50.	N-S cell size in m.
DZ	10. 7.5	Vertical cell size in m. 1/81
NX	36	Number of grid cells in x-direction
NY	45	Number of grid cells in y-direction
NZ	14 20.	Number of grid cells in z-direction 1/84
IDOWND	1	WEST wind Model
IDOCEN	1	1 tracer effluent
IDOPLM	1	User specified ΔH for plume rise ($\Delta H=0.$)
IDODIF	3	DEPICT algorithm diffusivities
IDOBK	1	User specified background (background =0.)
NUMHRS	1	Number of hours to be modeled
IDOPLT	0	No contour plots
IDOPRN	1	Printer edit every hour for test run
IDOCAL	0	No CALCOMP plots
HRSAUG	1	Hourly printout for test run
IDOSUR	0	Hourly printout for vertical levels

8.3 IMPACT: Input Options and Variables for Westvaco

<u>Variable Name</u>	<u>Input Value</u>	<u>Description</u>
DX	200.	E-W cell size in m.
DY	200.	N-S cell size in m.
DZ	60.96	Vertical cell size in m.
NX	13	Number of grid cells in x-direction
NY	15	Number of grid cells in y-direction
NZ	20	Number of grid cells in z-direction
IDOWND	1	WEST wind model
IDOLEM	1	1 tracer effluent
IDOPLM	0	Briggs' '74 Plume Rise
IDODIF	3	DEPICT algorithm diffusivities
IDOBAL	1	User specified background set to 0.0
NUMHRS	25	Number of hours to be modeled
IDOPLT	0	No contour plots
IDOPRN	1	Printer edit every hour for test run
IDOCAL	0	No CALCOMP plots
HRSAUG	1	Hourly printout for test run
IDOSUR	1	Print surface values only

8.4 TRC Changes to IMPACT (Version 1 from Radian) for Cinder Cone Butte

<u>Line Number</u>	<u>Description of Modification</u>
1-18	Comments
113-130, 386-402, 898-915, 998-1014, 1325-1341, 1735-1751, 1975-1991, 2180-2196, 2569-2585, 2813-2829, 2962-2978, 3069-3085, 3145-3161	Common TREFR1, TREFR2
131-265	Comments, TRC COMMON verify input files, load I, J of receptors
2197-2224	TRC COMMON
2230-2239	DTMIN, minimum time step, set to 1.0 sec.
2481-2514	Write to work file

8.5 TRC Changes to IMPACT (Version 1 from Radian) for Westvaco

<u>Line Number</u>	<u>Description of Modification</u>
1-18	Comments
113-124, 381-392, 888-900, 983-994, 1305-1316, 1710-1721, 1945-1956, 2145-2152, 2531-2542, 2770-2781, 2914-2925, 3016-3027, 3087-3098	Common TREFOR
125-260	Comments, TRC COMMON, verify input files, load I, J of receptors
1969-1984	Set unset variable
2153-2186	TRC COMMON
2443-2476	Write to work file

APPENDIX B

STATISTICAL TABLES OF MODEL PERFORMANCE FOR WESTVACO

<u>Table</u>	<u>Page</u>
Westvaco Comparison of 25 Highest, 1 Hour	B-1
Westvaco Comparison of 25 Highest, 3 Hour	B-9
Westvaco Comparison of 25 Highest, 24 Hour	B-17
Westvaco Comparison of Highest by Station	B-25
Westvaco Comparison of Second Highest by Station	B-28
Westvaco Comparison of Highest by Event	B-31
Westvaco Comparison of All Events Paired in Space and Time	B-34
Westvaco-IMPACT Hours Comparison of 25 Highest	B-61
Westvaco IMPACT Hours Comparison of Highest by Station	B-63
Westvaco IMPACT Hours Comparison of Second Highest	B-66
Westvaco IMPACT Hours Comparison of Highest by Event	B-69
Westvaco IMPACT Hours Comparison of All Events Paired in Space and Time	B-72

COMPARISON OF 25 HIGHEST OBSERVED AND PREDICTED
SO₂ CONCENTRATION VALUES (UG/M**3)
(UNPAIRED IN TIME OR LOCATION)
FOR THE 1-HOUR AVERAGING PERIOD
WESTVACO (1980/1981)

MODEL	AVERAGE OBSERVED VALUE	AVERAGE PREDICTED VALUE	DIFFERENCE OF AVERAGES* (OBS-PRED)	MEDIAN DIFFERENCE* (OBS-PRED)	VARIANCE COMPARISON (OBS/PRED)	MAXIMUM FREQUENCY DIFFERENCE
COMPLEX I	1969	10159	-15104 (-17149,-15249)	-15972 (-17144,-14542)	.017 (.008,.039)	1.00 (.383)
COMPLEX II	1969	30634	-35566 (-38555,-34782)	-35616 (-37807,-33968)	.004 (.002,.010)	1.00 (.383)
4141	1969	12205	-10226 (-11549,-8922)	-9558 (-11689,-8000)	.009 (.004,.029)	1.00 (.383)
RTDM	1969	3289	-1319 (-1652,-985)	-655 (-945,-282)	.151 (.057,.344)	.92 (.383)
PLUMES	1969	14525	-12556 (-13923,-11188)	-11472 (-12831,-10748)	.008 (.004,.019)	1.00 (.383)
COMPLEX/PPM	1969	15153	-13193 (-15397,-10989)	-11389 (-12329,-10520)	.003 (.001,.007)	1.00 (.383)
SHORTZ	1969	13563	-11394 (-13075,-10112)	-10153 (-11021,-9576)	.007 (.003,.015)	1.00 (.383)

* 95 PERCENT CONFIDENCE INTERVAL IN PARENTHESES

COMPARISON OF 25 HIGHEST OBSERVED AND PREDICTED
SO₂ CONCENTRATION VALUES (US/M**3)
(UNPAIRED IN TIME OR LOCATION)
FOR VARIOUS DATA SETS
MODEL: COMPLEYI
FOR THE 1-HOUR AVERAGING PERIOD
WESTVACO (1981/1981)

DATA SETS	AVERAGE OBSERVED VALUE	AVERAGE PREDICTED VALUE	DIFFERENCE OF AVERAGES* (OBS-PRED)	VARIANCE COMPARISON (OBS/PRED)
ALL	1969	18169	-16199 (-17149,-15249)	.017 (.008,.039)
STATION 1	1316	16574	-15257	.013
STATION 2	318	43	276	11.967
STATION 3	1110	12768	-11257	.264
STATION 4	1072	12089	-11015	.029
STATION 5	1374	8134	-6729	.176
STATION 6	1411	15372	-13969	.028
STATION 7	1347	8198	-7050	.024
STATION 8	1103	2354	-1250	.032
STATION 9	1183	4422	-3238	.056
STATION 10	539	428	-89	30.642
STATION 11	315	191	124	.754

METEOROLOGICAL CONDITION

1. WIND SPEED				
< 2.5 M/S	1576	14169	-16592	.023
2.5 TO 5. M/S	1813	12828	-11013	.801
> 5. M/S	551	4664	-6111	.023

2. STABILITY GROUP				
CLASS A, B & C	1092	418	674	7.232
CLASS D	1517	F	1509	12133.506
CLASS E	1118	11858	-10741	.114
CLASS F	1667	14169	-16501	.027

COMPARISON OF 25 HIGHEST OBSERVED AND PREDICTED
SO2 CONCENTRATION VALUES (UG/M*3)
(UNPAIRED IN TIME OR LOCATION)
FOR VARIOUS DATA SETS
MODEL: COMPLEXII
FOR THE 1-HOUR AVERAGING PERIOD
WESTVACO (1980/1981)

DATA SETS	AVERAGE OBSERVED VALUE	AVERAGE PREDICTED VALUE	DIFFERENCE OF AVERAGES* (OBS-PRED)	VARIANCE COMPARISON (OBS/PRED)
ALL	1959	38538	-36558 (-38555,-34782)	.004 (.002,.010)
STATION 1	1316	35157	-33840	.005
STATION 2	318	39	279	34.062
STATION 3	1110	24883	-23872	.002
STATION 4	1372	23135	-22051	.004
STATION 5	1374	9890	-8515	.003
STATION 6	1411	32664	-31252	.009
STATION 7	1347	11575	-10228	.001
STATION 8	1103	25118	-1414	.007
STATION 9	1183	5253	-4068	.004
STATION 10	339	1722	-1382	.369
STATION 11	315	140	174	1.965

METEOROLOGICAL CONDITION

1. WIND SPEED				
< 2.5 M/S	1576	37325	-35749	.004
2.5 TO 5. M/S	1813	32874	-31060	.028
> 5. M/S	551	15344	-14792	.001
2. STABILITY GROUP				
CLASS A, H & C	1092	276	816	28.050
CLASS D	4517	10	1508	3750.474
CLASS E	1118	2177	-21588	.120
CLASS F	1667	39639	-37972	.007

COMPARISON OF 25 HIGHEST OBSERVED AND PREDICTED
SO₂ CONCENTRATION VALUES (U3/M**3)
(UNPAIRED IN TIME OR LOCATION)
FOR VARIOUS DATA SETS
MODEL: COMPLEX/PPM
FOR THE 1-HOUR AVERAGING PERIOD
WFSIVACO (1987/1981)

DATA SETS	AVERAGE OBSERVED VALUE	AVERAGE PREDICTED VALUE	DIFFERENCE OF AVERAGES* (OBS-PRED)	VARIANCE COMPARISON (OBS/PRED)
ALL	1969	15163	-13193 (-15397,-10389)	.093 (.001,.607)
STATION 1	1314	10509	-9192	.005
STATION 2	318	318	0	.169
STATION 3	1110	4937	-3826	.004
STATION 4	1072	5136	-4062	.003
STATION 5	1374	4229	-2854	.007
STATION 6	1411	9667	-8455	.030
STATION 7	1347	3885	-2538	.007
STATION 8	1103	1510	-407	.048
STATION 9	1183	2285	-1100	.028
STATION 10	339	769	-429	.107
STATION 11	315	421	-105	.191

METEOROLOGICAL CONDITION

1. WIND SPEED				
< 2.5 M/S	1570	1420	-12713	.003
2.5 TO 5. M/S	1813	17258	-8444	.60
> 5. M/S	591	2643	-2091	.002

2. STABILITY GROUP

CLASS A, B & C	1092	2547	-1454	.194
CLASS D	1517	7205	-5688	.003
CLASS E	1118	9218	-8100	.027
CLASS F	1667	12700	-11032	.014

COMPARISON OF 25 HIGHEST OBSERVED AND PREDICTED
SO2 CONCENTRATION VALUES (UG/M**3)
(UNPAIRED IN TIME OR LOCATION)
FOR VARIOUS DATA SETS
MODEL: 4141
FOR THE 1-HOUR AVERAGING PERIOD
WESTVACO (1980/1981)

DATA SETS	AVERAGE OBSERVED VALUE	AVERAGE PREDICTED VALUE	DIFFERENCE OF AVERAGES* (OBS-PRED)	VARIANCE COMPARISON (OBS/PRED)
ALL	1959	12205	-10236 (-11549, -8922)	.009 (.004, .020)
STATION 1	1316	5173	-3757	.111
STATION 2	318	33	285	44.168
STATION 3	1110	183	921	45.264
STATION 4	1072	3205	-2132	.199
STATION 5	1374	6968	-5593	.012
STATION 6	1411	2241	-829	1.529
STATION 7	1347	6821	-5473	.006
STATION 8	1103	2173	-970	.018
STATION 9	1183	7498	-6314	.094
STATION 10	339	75	269	42.523
STATION 11	315	104	211	5.478

METEOROLOGICAL CONDITION

1. WIND SPEED				
< 2.5 M/S	1576	8220	-6643	.005
2.5 TO 5. M/S	1813	2331	-7517	.012
> 5. M/S	551	1925	-1373	.026

2. STABILITY GROUP				
CLASS A, B & C	1092	214	888	56.172
CLASS D	1517	2	1516	85105.351
CLASS E	1118	3203	-2081	.058
CLASS F	1667	1205	-11537	.14

COMPARISON OF 25 HIGHEST OBSERVED AND PREDICTED
SO2 CONCENTRATION VALUES (UG/M**3)
(UNPAIRED IN TIME OR LOCATION)
FOR VARIOUS DATA SETS
MODEL: PLUMF5
FOR THE 1-HOUR AVERAGING PERIOD
WFSIVACO (1980/1981)

DATA SETS	AVERAGE OBSERVED VALUE	AVERAGE PREDICTED VALUE	DIFFERENCE OF AVERAGES* (OBS-PRED)	VARIANCE COMPARISON (OBS/PRED)
ALL	1969	14525	-12556 (-13923,-11198)	.008 (.004,.019)
STATION 1	1316	9096	-8379	.008
STATION 2	318	80	238	5.903
STATION 3	1110	1887	-776	.008
STATION 4	1072	2154	-1082	.019
STATION 5	1374	2787	-1412	.016
STATION 6	1411	12332	-10920	.025
STATION 7	1347	2831	-1482	.004
STATION 8	1103	680	223	.122
STATION 9	1183	1232	-48	.025
STATION 10	339	327	12	.516
STATION 11	315	59	256	21.932

METEOROLOGICAL CONDITION

1. WIND SPEED				
< 2.5 M/S	1576	9831	-8254	.005
2.5 TO 5. M/S	1813	11487	-9593	.012
> 5. M/S	551	15317	-9765	.001
2. STABILITY GROUP				
CLASS A, B & C	1092	4346	-3252	.002
CLASS D	1517	13745	-12227	.042
CLASS E	1118	4555	-3436	.013
CLASS F	1667	2520	-852	.018

COMPARISON OF 25 HIGHEST OBSERVED AND PREDICTED
SO2 CONCENTRATION VALUES (UG/M**3)
(UNPAIRED IN TIME OR LOCATION)
FOR VARIOUS DATA SETS
MODEL: RTDM
FOR THE 1-HOUR AVERAGING PERIOD
WESTVACO (1987/1991)

DATA SETS	AVERAGE OBSERVED VALUE	AVERAGE PREDICTED VALUE	DIFFERENCE OF AVERAGES* (OBS-PRED)	VARIANCE COMPARISON (OBS/PRED)
ALL	1935	3054	(-2212, -1823)	(.722, .314, 1.438)
STATION 1	1269	2780	-1511	.172
STATION 2	269	284	-15	84.369
STATION 3	1930	1985	-985	.515
STATION 4	976	2245	-1268	.871
STATION 5	1284	3135	-1751	.262
STATION 6	1333	2554	-1219	.309
STATION 7	1316	3741	-2424	.000
STATION 8	1700	1790	-80	4.503
STATION 9	1113	1619	-805	.099
STATION 10	275	315	-40	9.551
STATION 11	306	219	84	30.855

METEOROLOGICAL CONDITION

1. WIND SPEED			
< 2.5 M/S	1450	3944	-2492
2.5 TO 5. M/S	1787	2774	-1985
> 5. M/S	534	1460	-326
			1.030
			13.163
			.021

2. STABILITY GROUP			
CLASS A, E & C	809	3741	-2941
CLASS D	1456	2742	-2384
CLASS F	1025	2618	-1593
CLASS F	1506	2742	-2145
			.170
			.649
			.200
			8.697

COMPARISON OF 25 HIGHEST OBSERVED AND PREDICTED
SO₂ CONCENTRATION VALUES (UG/M**3)
(UNPAIRED IN TIME OR LOCATION)
FOR VARIOUS DATA SETS
MODEL: SHORIZ
FOR THE 1-HOUR AVEAGING PERIOD
WESTVACO (1980/1981)

DATA SETS	AVERAGE OBSERVED VALUE	AVERAGE PREDICTED VALUE	DIFFERENCE OF AVERAGES* (OBS-PRED)	VARIANCE COMPARISON (OBS/PRED)
ALL	1959	13553	-11594 (-13075,-10112)	.007 (.003,.016)
STATION 1	1316	10132	-8715	.012
STATION 2	318	280	-61	4.755
STATION 3	1110	6491	-5380	.005
STATION 4	1072	5641	-4569	.031
STATION 5	1374	2700	-1325	.303
STATION 6	1411	10251	-9439	.012
STATION 7	1337	2542	-1594	.137
STATION 8	1103	1254	-150	.379
STATION 9	1183	1490	-306	.263
STATION 10	339	410	-70	1.077
STATION 11	315	215	100	2.227

METEOROLOGICAL CONDITION

1. WIND SPEED				
< 2.5 M/S	1576	8401	-6823	.013
2.5 TO 5. M/S	1813	13060	-11246	.010
> 5. M/S	551	2458	-1906	.001
2. STABILITY GROUP				
CLASS A, B & C	1092	2678	-2585	.017
CLASS D	1517	7912	-6394	.022
CLASS E	1118	6513	-5395	.026
CLASS F	1667	10367	-10695	.019

COMPARISON OF 25 HIGHEST OBSERVED AND PREDICTED
SO₂ CONCENTRATION VALUES (UG/M**3)
(UNPAIRED IN TIME OR LOCATION)
FOR THE 3-HOUR AVERAGING PERIOD
WESTVACO (1986/1991)

MODEL	AVERAGE OBSERVED VALUE	AVERAGE PREDICTED VALUE	DIFFERENCE OF AVERAGES* (OBS-PRED)	MEDIAN DIFFERENCE* (OBS-PRED)	VARIANCE COMPARISON (OBS/PRED)	MAXIMUM FREQUENCY DIFFERENCE
COMPLEX I	1127	12205	-11076 (-11845, -10311)	-10433 (-11000, -10157)	.026 (.011, .058)	1.03 (.383)
COMPLEX II	1127	27557	-17430 (-20871, -17988)	-17793 (-21880, -17031)	.007 (.003, .015)	1.03 (.383)
4141	1127	4769	-3642 (-4283, -3000)	-3552 (-4107, -2712)	.037 (.015, .084)	1.03 (.383)
RTM	1127	1464	-337 (-545, -127)	-256 (-502, -135)	.473 (.209, 1.075)	.52 (.383)
PLUMES	1127	7817	-6690 (-8051, -5329)	-5534 (-6958, -4625)	.008 (.004, .018)	1.03 (.383)
COMPLEX/PEM	1127	7720	-6601 (-7545, -5652)	-6053 (-6977, -5255)	.017 (.007, .038)	1.03 (.383)
SHORTZ	1127	5330	-5202 (-5740, -4624)	-5043 (-5370, -4323)	.046 (.020, .104)	1.03 (.383)

* 95 PERCENT CONFIDENCE INTERVAL IN PARENTHESES

COMPARISON OF 25 HIGHEST OBSERVED AND PREDICTED
 SO2 CONCENTRATION VALUES (UG/M**3)
 (UNPAIRED IN TIME OR LOCATION)
 FOR VARIOUS DATA SETS
 MODEL: COMPLEX I
 FOR THE 3-HOUR AVERAGING PERIOD
 WESTVACO (1980/1981)

DATA SETS	AVERAGE OBSERVED VALUE	AVERAGE PREDICTED VALUE	DIFFERENCE OF AVERAGES* (OBS-PRED)	VARIANCE COMPARISON (OBS/PRED)
ALL	1127	12205	-11078 (-11845,-10311)	.026 (.011,.059)
STATION 1	759	10432	-9672	.010
STATION 2	165	9	155	7.322
STATION 3	614	7685	-7065	.008
STATION 4	615	6134	-5518	.008
STATION 5	717	3480	-2762	.039
STATION 6	788	9951	-9161	.044
STATION 7	718	2862	-2142	.018
STATION 8	526	854	-327	.632
STATION 9	578	1354	-775	.047
STATION 10	204	245	-141	2.308
STATION 11	200	73	127	1.713

COMPARISON OF 25 HIGHEST OBSERVED AND PREDICTED
 SO2 CONCENTRATION VALUES (UG/M*3)
 (UNPAIRED IN TIME OR LOCATION)
 FOR VARIOUS DATA SETS
 MODEL: COMPLEX II
 FOR THE 3-HOUR AVERAGING PERIOD
 WESTVACO (1981/1981)

DATA SETS	AVERAGE OBSERVED VALUE	AVERAGE PREDICTED VALUE	DIFFERENCE OF AVERAGES* (OBS-PRED)	VARIANCE COMPARISON (OBS/PRED)
ALL	1127	20557	-19430 (-20871,-17988)	.007 (.003,.016)
STATION 1	759	16609	-15939	.004
STATION 2	165	11	155	20.051
STATION 3	618	9689	-9270	.002
STATION 4	615	7453	-6837	.002
STATION 5	717	3541	-2823	.007
STATION 6	788	17242	-16453	.005
STATION 7	718	3164	-2444	.007
STATION 8	526	787	-259	.012
STATION 9	578	1571	-992	.017
STATION 10	204	677	-472	.119
STATION 11	205	63	137	5.019

COMPARISON OF 25 HIGHEST OBSERVED AND PREDICTED
SO2 CONCENTRATION VALUES (UG/M**3)
(UNPAIRED IN TIME OR LOCATION)
FOR VARIOUS DATA SETS
MODEL: COMPLEX/PEM
FOR THE 3-HOUR AVERAGING PERIOD
WESTVACO (1980/1991)

DATA SETS	AVERAGE OBSERVED VALUE	AVERAGE PREDICTED VALUE	DIFFERENCE OF AVERAGES* (OBS-PRED)	VARIANCE COMPARISON (OBS/PRED)
ALL	1127	7728	-6601 (-7549, -5652)	.017 (.007, .038)
STATION 1	759	4137	-3376	.008
STATION 2	155	105	58	.128
STATION 3	613	1775	-1157	.007
STATION 4	615	1608	-1192	.005
STATION 5	717	1557	-840	.023
STATION 6	788	5516	-4727	.026
STATION 7	718	1285	-567	.042
STATION 8	526	497	30	.083
STATION 9	578	778	-200	.117
STATION 10	204	340	-135	.377
STATION 11	200	193	7	.540

COMPARISON OF 25 HIGHEST OBSERVED AND PREDICTED
 SO2 CONCENTRATION VALUES (UG/M**3)
 (UNPAIRED IN TIME OR LOCATION)
 FOR VARIOUS DATA SETS
 MODEL: 4141
 FOR THE 3-HOUR AVERAGING PERIOD
 WESTVACO (1981/1981)

DATA SETS	AVERAGE OBSERVED VALUE	AVERAGE PREDICTED VALUE	DIFFERENCE OF AVERAGES* (OBS-PRED)	VARIANCE COMPARISON (OBS/PRED)
ALL	1127	4769	(-4283, -3000)	(.037, .084)
STATION 1	759	2240	-1480	.088
STATION 2	165	10	155	22.623
STATION 3	618	84	534	82.409
STATION 4	615	1160	-544	.134
STATION 5	717	2465	-1748	.029
STATION 6	788	1246	-457	.515
STATION 7	718	2701	-1981	.023
STATION 8	526	582	-54	.027
STATION 9	578	2200	-1622	.011
STATION 10	204	31	173	23.916
STATION 11	209	50	159	12.871

COMPARISON OF 25 HIGHEST OBSERVED AND PREDICTED
 SO2 CONCENTRATION VALUES (UG/M**3)
 (UNPAIRED IN TIME OR LOCATION)
 FOR VARIOUS DATA SETS
 MODEL: PLUMFS
 FOR THE 3-HOUR AVERAGING PERIOD
 WESTVACO (1980/1981)

DATA SETS	AVERAGE OBSERVED VALUE	AVERAGE PREDICTED VALUE	DIFFERENCE OF AVERAGES* (OBS-PRED)	VARIANCE COMPARISON (OBS/PRED)
ALL	1127	7817	(-8051, -5329)	(.004, .019)
STATION 1	761	3852	-3090	.007
STATION 2	165	25	139	2.134
STATION 3	618	885	-265	.021
STATION 4	615	645	-23	.064
STATION 5	717	1283	-567	.012
STATION 6	788	574	-4951	.010
STATION 7	718	830	-210	.027
STATION 8	526	289	237	.252
STATION 9	578	427	151	.115
STATION 10	204	125	78	1.899
STATION 11	200	28	172	25.630

COMPARISON OF 25 HIGHEST OBSERVED AND PREDICTED
 SO2 CONCENTRATION VALUES (UG/M**3)
 (UNPAIRED IN TIME OR LOCATION)
 FOR VARIOUS DATA SETS
 MODEL: RTDM
 FOR THE 3-HOUR AVERAGING PERIOD
 WESTVACO (1980/1981)

DATA SETS	AVERAGE OBSERVED VALUE	AVERAGE PREDICTED VALUE	DIFFERENCE OF AVERAGES (OBS-PRED)	VARIANCE COMPARISON (OBS/PRED)
ALL	1388	3587	(-2700, -2283)	.531 (.234*1.206)
STATION 1	708	1466	-957	.151
STATION 2	131	225	-93	2.760
STATION 3	538	1287	-748	.312
STATION 4	525	1513	-1006	.203
STATION 5	575	1638	-961	.085
STATION 6	721	1314	-593	.395
STATION 7	681	2064	-2283	.083
STATION 8	475	651	-473	5.187
STATION 9	536	1538	-1001	.267
STATION 10	160	228	-66	1.315
STATION 11	184	189	-4	3.597

COMPARISON OF 25 HIGHEST OBSERVED AND PREDICTED
 SO2 CONCENTRATION VALUES (UG/M**3)
 (UNPAIRED IN TIME OR LOCATION)
 FOR VARIOUS DATA SETS
 MODEL: SHORIZ
 FOR THE 3-HOUR AVERAGING PERIOD
 WESTVACO (1980/1981)

DATA SETS	AVERAGE OBSERVED VALUE	AVERAGE PREDICTED VALUE	DIFFERENCE OF AVERAGES* (OBS-PRED)	VARIANCE COMPARISON (OBS/PRED)
ALL	1127	6330	-5202 (-5780, -4624)	.045 (.020, .104)
STATION 1	761	4510	-3748	.041
STATION 2	165	171	-6	1.730
STATION 3	610	3079	-2469	.010
STATION 4	615	2685	-1969	.024
STATION 5	717	1129	-411	.924
STATION 6	780	5010	-4230	.043
STATION 7	718	1290	-570	.310
STATION 8	526	510	-12	.395
STATION 9	578	647	-69	.540
STATION 10	204	252	-47	.570
STATION 11	200	112	88	4.740

COMPARISON OF 25 HIGHEST OBSERVED AND PREDICTED
SO₂ CONCENTRATION VALUES (UG/M*3)
(UNPAIRED IN TIME OR LOCATION)
FOR THE 24-HOUR AVERAGING PERIOD
WESTVACO (1989/1991)

MODEL	AVERAGE OBSERVED VALUE	AVERAGE PREDICTED VALUE	DIFFERENCE OF AVERAGES* (OBS-PRED)	MEDIAN DIFFERENCE* (OBS-PRED)	VARIANCE COMPARISON (OBS/PRED)	MAXIMUM FREQUENCY DIFFERENCE
COMPLEXI	354	3230	(-3141, -2624)	(-2886, -2574)	(.003, .017)	(1.00 (.385)
COMPLEXII	354	4482	(-4127, -3597)	(-3504, -3306)	(.002, .004)	(1.00 (.385)
4141	354	855	(-560, -357)	(-392, -317)	(.024, .055)	(1.00 (.385)
RTD4	354	331	(-37, 85)	(32, 92)	(.143, .324)	(.55 (.395)
PLUME5	354	1712	(-1357, -574)	(-730, -559)	(.001, .002)	(1.00 (.385)
COMPLEX/PEM	354	1584	(-1220, -978)	(-1201, -887)	(.308, .019)	(1.00 (.385)
SHORTZ	354	1388	(-1033, -891)	(-344, -824)	(.025, .057)	(1.00 (.385)

* 95 PERCENT CONFIDENCE INTERVAL IN PARENTHESES

COMPARISON OF 25 HIGHEST OBSERVED AND PREDICTED
 SO₂ CONCENTRATION VALUES (UG/M**3)
 (UNPAIRED IN TIME OR LOCATION)
 FOR VARIOUS DATA SETS
 MODEL: COMPLEX I
 FOR THE 24-HOUR AVERAGING PERIOD
 WESTVACO (1981/1981)

DATA SETS	AVERAGE OBSERVED VALUE	AVERAGE PREDICTED VALUE	DIFFERENCE OF AVERAGES* (OBS-PRED)	VARIANCE COMPARISON (OBS/PRED)
ALL	354	3238	(-3141, -2624)	(.003, .017)
STATION 1	201	2358	-2155	.010
STATION 2	61	2	61	22.734
STATION 3	172	1489	-1314	.028
STATION 4	156	1533	-876	.021
STATION 5	169	591	-422	.024
STATION 6	282	2824	-2541	.012
STATION 7	152	435	-282	.099
STATION 8	137	122	15	.087
STATION 9	138	264	-65	.059
STATION 10	66	75	-9	.649
STATION 11	67	13	55	5.566

COMPARISON OF 25 HIGHEST OBSERVED AND PREDICTED
 SO2 CONCENTRATION VALUES (UG/M**3)
 (UNPAIRED IN TIME OR LOCATION)
 FOR VARIOUS DATA SETS
 MODEL: COMPLEX II
 FOR THE 24-HOUR AVERAGING PERIOD
 WESTVACO (1980/1981)

DATA SETS	AVERAGE OBSERVED VALUE	AVERAGE PREDICTED VALUE	DIFFERENCE OF AVERAGES* (OBS-PRED)	VARIANCE COMPARISON (OBS/PRED)
ALL	354	4482	(-4667, -3587)	(.001, .004)
STATION 1	201	3058	-2856	.003
STATION 2	63	2	61	51.305
STATION 3	172	1655	-1481	.011
STATION 4	156	1114	-956	.008
STATION 5	169	502	-332	.013
STATION 6	282	3010	-3527	.004
STATION 7	152	489	-336	.004
STATION 8	137	111	26	.036
STATION 9	139	234	-95	.024
STATION 10	65	109	-42	.121
STATION 11	67	12	56	14.680

COMPARISON OF 25 HIGHEST OBSERVED AND PREDICTED
 SO₂ CONCENTRATION VALUES (UG/M**3)
 (UNPAIRED IN TIME OR LOCATION)
 FOR VARIOUS DATA SETS
 MODEL: COMPLEX/PFM
 FOR THE 24-HOUR AVERAGING PERIOD
 WESTVACO (1980/1981)

DATA SETS	AVERAGE OBSERVED VALUE	AVERAGE PREDICTED VALUE	DIFFERENCE OF AVERAGES* (OBS-PRED)	VARIANCE COMPARISON (OBS/PRED)
ALL	354	1584	(-1400, -978)	(.003, .018)
STATION 1	201	710	-507	.024
STATION 2	63	14	49	.333
STATION 3	172	267	-94	.044
STATION 4	156	237	-80	.023
STATION 5	169	209	-39	.078
STATION 6	282	1495	-763	.006
STATION 7	152	152	0	.050
STATION 8	137	70	56	.321
STATION 9	138	108	30	.279
STATION 10	55	55	11	.934
STATION 11	67	37	31	1.289

COMPARISON OF 25 HIGHEST OBSERVED AND PREDICTED
 SO2 CONCENTRATION VALUES (UG/M*3)
 (UNPAIRED IN TIME OR LOCATION)
 FOR VARIOUS DATA SETS
 MODEL: 4141
 FOR THE 24-HOUR AVERAGING PERIOD
 WESTVACO (1480/1981)

DATA SETS	AVERAGE OBSERVED VALUE	AVERAGE PREDICTED VALUE	DIFFERENCE OF AVERAGES+ (OBS-PRED)	VARIANCE COMPARISON (OBS/PRED)
ALL	354	855	(-644, -357)	(.024, .035)
STATION 1	201	410	-208	.214
STATION 2	63	2	62	43.534
STATION 3	172	16	156	188.667
STATION 4	156	174	-16	.314
STATION 5	169	374	-204	.940
STATION 6	282	286	-3	.215
STATION 7	152	295	-143	.114
STATION 8	137	94	43	.055
STATION 9	138	243	-205	.015
STATION 10	66	7	59	38.465
STATION 11	57	0	58	59.597

COMPARISON OF 25 HIGHEST OBSERVED AND PREDICTED
 SO₂ CONCENTRATION VALUES (UG/M**3)
 (UNPAIRED IN TIME OR LOCATION)
 FOR VARIOUS DATA SETS
 MODEL: PLUMES
 FOR THE 24-HOUR AVERAGING PERIOD
 WESTVACO (1987/1981)

DATA SETS	AVERAGE OBSERVED VALUE	AVERAGE PREDICTED VALUE	DIFFERENCE OF AVERAGES* (OBS-PRED)	VARIANCE COMPARISON (OBS/PRED)
ALL	354	1712	(-2040, -674)	(.000, .002)
STATION 1	201	719	-516	.J17
STATION 2	63	5	59	4.006
STATION 3	172	193	-20	.095
STATION 4	156	129	29	.159
STATION 5	169	184	-15	.037
STATION 6	282	1290	-1008	.001
STATION 7	152	127	25	.628
STATION 8	137	49	97	.911
STATION 9	138	61	77	.311
STATION 10	65	25	41	1.605
STATION 11	67	5	62	102.463

COMPARISON OF 25 HIGHEST OBSERVED AND PREDICTED
 SO2 CONCENTRATION VALUES (UG/M**3)
 (UNPAIRED IN TIME OR LOCATION)
 FOR VARIOUS DATA SETS
 MODEL: RTDM
 FOR THE 24-HOUR AVERAGING PERIOD
 WESTVACO (1980/1981)

DATA SETS	AVERAGE OBSERVED VALUE	AVERAGE PREDICTED VALUE	DIFFERENCE OF AVERAGES* (OBS-PRED)	VARIANCE COMPARISON (OBS/PRED)
ALL	346	260	(-211, -1355)	(.004, .010)
STATION 1	192	695	-501	.048
STATION 2	57	116	-58	.555
STATION 3	161	639	-477	.049
STATION 4	141	683	-742	.039
STATION 5	163	633	-469	.016
STATION 6	272	405	-133	.082
STATION 7	147	1296	-1149	.001
STATION 8	124	665	-540	.142
STATION 9	129	114	-584	.011
STATION 10	57	107	-49	.165
STATION 11	63	99	-35	.155

COMPARISON OF 25 HIGHEST OBSERVED AND PREDICTED
 SO2 CONCENTRATION VALUES (UG/M**3)
 (UNPAIRED IN TIME OR LOCATION)
 FOR VARIOUS DATA SETS
 MODEL: SHORTZ
 FOR THE 24-HOUR AVERAGING PERIOD
 WESTVACO (1980/1981)

DATA SETS	AVERAGE OBSERVED VALUE	AVERAGE PREDICTED VALUE	DIFFERENCE OF AVERAGES (OBS-PRED)	VARIANCE COMPARISON (OBS/PRED)
ALL	354	1368	(-1175, -691)	(.025, .057)
STATION 1	291	934	-731	.065
STATION 2	63	37	27	.511
STATION 3	172	560	-387	.054
STATION 4	156	443	-286	.105
STATION 5	169	225	-55	.621
STATION 6	282	1190	-907	.040
STATION 7	152	211	-59	.151
STATION 8	137	83	54	1.259
STATION 9	138	99	39	1.197
STATION 10	65	68	-1	.572
STATION 11	67	30	37	4.086

COMPARISON OF HIGHEST
OBSERVED AND PREDICTED
SO₂ CONCENTRATION VALUES (U3/M**3)
PAIRED BY STATION FOR THE 1 HOUR AVERAGING PERIOD
WESTVACO (1980/1981)

MODEL	NUMBER OF DATA PAIRS	AVERAGE OBSERVED VALUE	AVERAGE DIFFERENCE*	FRACTION OF POSITIVE RESIDUALS (OBS>PRED)	STANDARD DEVIATION* OF RESIDUALS	ROOT MEAN SQUARE ERROR	AVERAGE ABSOLUTE RESIDUAL	PEARSON CORR. COEFF.	SPEARMAN CORR. COEFF.	VARIANCE COMPARISON* (OBS>PRED)
COMPLEX I	11	1859	-8939 (-14352, -3525)	.27 (5630, 14141)	8058	11788	9143	.79	.74	.057 (.002, .028)
COMPLEX II	11	1859	-23851 (-35674, -12028)	.18 (12297, 30986)	17680	29154	24393	.85	.74	.002 (.000, .005)
4141	11	1859	-5513 (-10353, -673)	.36 (5034, 12543)	7204	8879	6155	.54	.49	.010 (.003, .035)
RTDM	11	1859	-561 (-1552, 230)	.45 (927, 2320)	1327	1428	1105	.75	.68	.171 (.045, .538)
PLUMES	11	1859	-8779 (-14375, -3384)	.18 (5715, 14357)	8141	11820	9123	.76	.76	.007 (.002, .027)
COMPLEX/PPM	11	1859	-12032 (-18747, -5317)	.20 (6945, 17547)	9996	15351	12033	.82	.84	.005 (.001, .018)
SHORTZ	11	1859	-6469 (-11809, -1130)	.18 (5554, 13750)	7943	5965	6525	.59	.72	.003 (.002, .023)

* 95 PERCENT CONFIDENCE INTERVAL IN PARENTHESES

COMPARISON OF HIGHEST
OBSERVED AND PREDICTED
SO₂ CONCENTRATION VALUES (UG/M*3)
PAIRED BY STATION FOR THE 3 HOUR AVERAGING PERIOD
WESTVACO (1+8/1941)

MODEL	NUMBER OF DATA PAIRS	AVERAGE OBSERVED VALUE	AVERAGE DIFFERENCE*	FRACTION OF POSITIVE RESIDUALS (OBS>PRED)	STANDARD DEVIATION* OF RESIDUALS	ROOT MEAN SQUARE ERROR	AVERAGE ABSOLUTE RESIDUAL	PEARSON CORR. COEFF.	SPEARMAN CORR. COEFF.	VARIANCE COMPARISON* (OBS>PRED)
COMPLEX I	11	1229	-6391 (-10126, -2553)	.27	5553 (3887, 9762)	8306	6482	.72	.56	.009 (.022, .034)
COMPLEX II	11	1229	-11006 (-17281, -4732)	.18	9340 (6526, 15391)	14159	11120	.70	.53	.503 (.011, .013)
4141	11	1229	-2495 (-4621, -364)	.36	3153 (2211, 5554)	3915	2894	.73	.74	.025 (.037, .035)
RTDM	11	1229	-54 (-409, 280)	.54	513 (359, 911)	494	401	.81	.73	.443 (.113, 1.544)
FLUMES	11	1229	-4864 (-8582, -1147)	.27	5534 (3867, 9712)	7177	5000	.73	.77	.003 (.032, .034)
COMPLEX/DFM	11	1229	-4863 (-7953, -1773)	.00	4600 (3214, 8073)	6549	4864	.60	.53	.013 (.024, .049)
SHORTZ	11	1229	-2725 (-5129, -343)	.18	3562 (2469, 5251)	4362	2801	.45	.45	.022 (.006, .033)

* 95 PERCENT CONFIDENCE INTERVAL IN PARENTHESES

COMPARISON OF HIGHEST
OBSERVED AND PREDICTED
SO₂ CONCENTRATION VALUES (UG/M*3)
PAIRED BY STATION FOR THE 24 HOUR AVERAGING PERIOD
WESTVACO (1987/1991)

MODEL	NUMBER OF DATA PAIRS	AVERAGE OBSERVED VALUE	AVERAGE DIFFERENCE*	FRACTION OF POSITIVE RESIDUALS (OBS>PRED)	STANDARD DEVIATION* OF RESIDUALS	ROOT MEAN SQUARE ERROR	AVERAGE ABSOLUTE RESIDUAL	PEARSON CORR. COEFF.	SPEARMAN CORR. COEFF.	VARIANCE COMPARISON* (OBS>PRED)
COMPLEX I	11	317	(-1416 (-2425, -407)	.18	(1502 (1050, 2636)	2015	1453	.92	.89	(.022, .029)
COMPLEX II	11	317	(-2401 (-4152, -650)	.18	(2505 (1821, 4574)	3956	2942	.77	.84	(.003 (.001, .010)
4141	11	317	(-455 (-677, 5)	.35	(658 (460, 1154)	754	572	.93	.92	(.040 (.011, .147)
PTON	11	317	(-105, 7 (-105, 113)	.73	(158 (117, 200)	160	139	.74	.72	(.030 (.033, .127)
FLUMES	11	317	(-1272 (-2486, 341)	.36	(2402 (1679, 4218)	2521	1336	.52	.84	(.093 (.001, .012)
COMPLEX/DEM	11	317	(-823 (-1481, -165)	.69	(979 (564, 1717)	1245	937	.81	.84	(.015 (.004, .061)
SHORTZ	11	317	(-584 (-695, -13)	.36	(731 (511, 1247)	851	555	.75	.83	(.123 (.035, .174)

* 95 PERCENT CONFIDENCE INTERVAL IN PARENTHESES

COMPARISON OF SECOND HIGHEST
OBSERVED AND PREDICTED
SO₂ CONCENTRATION VALUES (UG/M*3)
PAIRED BY STATION FOR THE 1 HOUR AVERAGING PERIOD
WESTVACO (1980/1981)

MODEL	NJMRCR OF DATA PAIRS	AVERAGE OBSERVED VALUE	AVERAGE DIFFERENCE*	FRACTION OF POSITIVE RESIDUALS (OBS>PRED)	STANDARD DEVIATION* OF RESIDUALS	ROOT MEAN SQUARE ERROR	AVERAGE ABSOLUTE RESIDUAL	PEARSON CORR. COEFF.	SPEARMAN CORR. COEFF.	VARIANCE COMPARISON* (OBS>PRED)
COMPLEX I	11	1617	-8039 (-12784, -3294)	.27 (4335, 12395)	7053 (4335, 12395)	10449	8156	.75	.58 (.022, .034)	.009 (.022, .034)
COMPLEX II	11	1617	-21317 (-31857, -10776)	.18 (10964, 27536)	15691 (10964, 27536)	26044	21440	.83	.58 (.011, .007)	.002 (.011, .007)
4141	11	1617	-4928 (-3125, -731)	.36 (4366, 10365)	6248 (4366, 10365)	7732	5430	.64	.59 (.013, .045)	.012 (.013, .045)
28 RTDM	11	1617	-450 (-1150, 250)	.55 (729, 1430)	1043 (729, 1430)	1092	918	.75	.55 (.055, .012)	.245 (.055, .012)
PLUMES	11	1617	-7082 (-11279, -2885)	.18 (4365, 10364)	6248 (4365, 10364)	9255	7191	.79	.70 (.003, .043)	.012 (.003, .043)
COMPLEX/PPM	11	1617	-8250 (-12262, -4239)	.00 (4172, 10470)	5971 (4172, 10470)	10025	8251	.82	.58 (.033, .016)	.012 (.033, .016)
SHORTZ	11	1617	-5830 (-10667, -933)	.03 (5031, 12636)	7200 (5031, 12636)	9007	5964	.54	.55 (.033, .013)	.009 (.033, .013)

* 95 PERCENT CONFIDENCE INTERVAL IN PARENTHESES

COMPARISON OF SECOND HIGHEST
OBSERVED AND PREDICTED
SO₂ CONCENTRATION VALUES (UG/M**3)
PAIRED BY STATION FOR THE 3 HOUR AVERAGING PERIOD
WESTIVACO (1980/1981)

MODEL	NUMBER OF DATA PAIRS	AVERAGE OBSERVED VALUE	AVERAGE DIFFERENCE*	FRACTION OF POSITIVE RESIDUALS (OBS>PRED)	STANDARD DEVIATION* OF RESIDUALS	ROOT MEAN SQUARE ERROR	AVERAGE ABSOLUTE RESIDUAL	PEARSON CORR. COEFF.	SPEARMAN CORR. COEFF.	VARIANCE COMPARISON* (OBS>PRED)
COMPLEX I	11	990	(-5756 -9441, -2071)	.18	(5485 3433, 9526)	7778	5833	.73	.72	(.002, .028)
COMPLEX II	11	990	(-9387 -16045, -3928)	.18	(9019 6301, 15027)	13179	10073	.76	.76	(.003 .071, .011)
4141	11	790	(-1851 -3367, -335)	.36	(2255 1577, 3960)	2839	2150	.68	.71	(.039 .011, .146)
RTDM	11	990	(-238, 332) 47	.54	(423 297, 746)	409	346	.92	.97	(.435 .133, .044)
PLUMES	11	990	(-2930 -5538, -322)	.27	(3883 2713, 6914)	4722	3032	.71	.83	(.014 .004, .034)
COMPLEX/DFM	11	990	(-2242 -6236, -1493)	.09	(3533 2469, 5201)	5125	3954	.67	.67	(.017 .005, .055)
HORIZ	11	990	(-2139 -3899, -379)	.09	(2613 1830, 4597)	3289	2177	.61	.74	(.031 .038, .114)

* .95 PERCENT CONFIDENCE INTERVAL IN PARENTHESES

COMPARISON OF SECOND HIGHEST
OBSERVED AND PREDICTED
SO₂ CONCENTRATION VALUES (JG/M**3)
PAIRED BY STATION FOR THE 24 HOUR AVEPAGING PERIOD
WESTVACO (1980/1991)

MODEL	NJMPER OF DATA PAIRS	AVERAGE OBSERVED VALUE	AVERAGE DIFFERENCE*	FRACTION OF POSITIVE RESIDUALS (OBS>PRED)	STANDARD DEVIATION* OF RESIDUALS	ROOT MEAN SQUARE ERROR	AVERAGE ABSOLUTE RESIDUAL	PEARSON CORR. COEFF.	SPEARMAN CORR. COEFF.	VARIANCE COMPARISON* (OBS>PRED)
COMPLEX I	11	256	(-1275 -2147, -323)	.18	(1357 948, 2392)	1790	1252	.87	.90	(.005 .002, .024)
COMPLEX II	11	256	(-1891 -3337, -445)	.18	(2152 1504, 3777)	2791	1921	.84	.92	(.003 .001, .010)
4141	11	255	(-238 -496, 19)	.36	(384 268, 674)	437	350	.47	.35	(.075 .020, .279)
RTDM	11	255	(-38 -19, 95)	.82	(87 61, 152)	91	74	.85	.86	(.529 .142, 1.958)
FLUMES	11	256	(-635 -1383, 112)	.36	(1114 778, 1955)	1239	580	.73	.95	(.009 .003, .035)
COMPLEX/SPM	11	256	(-578 -1120, -37)	.27	(806 563, 1415)	963	591	.78	.88	(.017 .005, .053)
SHORTZ	11	256	(-366 -743, 10)	.36	(562 392, 985)	549	400	.92	.91	(.032 .009, .118)

* 95 PERCENT CONFIDENCE INTERVAL IN PARENTHESES

COMPARISON OF HIGHEST OBSERVED AND PREDICTED
SO₂ CONCENTRATION VALUES (UG/M**3)
EVENT-BY-EVENT (PAIRED IN TIME)
FOR THE 1-HOUR AVERAGING PERIOD
WESTVACO (1981/1982)

MODEL	NUMBER OF EVENTS	AVERAGE OBSERVED VALUE	AVERAGE DIFFERENCE* (OBS-PRED)	STANDARD DEVIATION* OF RESIDUALS	MAXIMUM FREQUENCY DIFFERENCE
COMP_EXI	7175	154	(-1117, -779)	(3051, 3112)	(.773, .023)
COMP_EXII	7160	155	(-1237, -1033)	(573, 5158)	(.784, .023)
4141	7132	155	(-73, 1)	(947, 963)	(.305, .023)
RTCM	7411	150	(46, 72)	(326, 337)	(.516, .022)
PLUMES	7305	152	(-213, -94)	(1354, 1376)	(.453, .023)
COMP_EX/PEM	7102	155	(-125, -5)	(1359, 1392)	(.417, .023)
SHORT2	7785	143	(-415, -315)	(1297, 1317)	(.247, .022)

* .95 PERCENT CONFIDENCE INTERVAL IN PARENTHESES

COMPARISON OF HIGHEST OBSERVED AND PREDICTED
SO₂ CONCENTRATION VALUES (UG/M*3)
EVENT-BY-EVENT (PAIRED IN TIME)
FOR THE 3-HOUR AVERAGING PERIOD
WESTVACO (1-8-1981)

MODEL	NUMBR OF EVENTS	AVERAGE OBSERVED VALUE	AVERAGE DIFFERENCE* (OBS-PRED)	STANDARD DEVIATION* OF RESIDUALS	MAXIMUM FREQUENCY DIFFERENCE
COMPLEX I	2445	139	(-1095, -570)	(2208, 2437)	(.573, .543)
COMPLEX II	2429	140	(-1077, -860)	(3475, 3575)	(.715, .039)
4141	2415	140	(-62, 17)	(609, 644)	(.743, .033)
RTDM	2514	136	(32, 53)	(229, 242)	(.424, .039)
PLUMES	2477	138	(-215, -58)	(1029, 1052)	(.381, .039)
COMPLEX/PPM	2415	140	(-113, 2)	(850, 1015)	(.752, .033)
SHORTZ	2612	131	(-388, -281)	(878, 927)	(.235, .039)

* .95 PERCENT CONFIDENCE INTERVAL IN PARENTHESES

COMPARISON OF HIGHEST OBSERVED AND PREDICTED
SO₂ CONCENTRATION VALUES (UG/M³)
EVENT-BY-EVENT (PAIRED IN TIME)
FOR THE 24-HOUR AVERAGING PERIOD
WESTVAC (1-6/1981)

MODE-	NUMBER OF EVENTS	AVERAGE OBSERVED VALUE	AVERAGE DIFFERENCE* (OBS-PRED)	STANDARD DEVIATION* OF RESIDUALS	MAXIMUM FREQUENCY DIFFERENCE
COMPLEXI	363	98	(-729, -471)	(445, 1023)	(.465, .101)
COMPLEXII	364	98	(-705, -581)	(1320, 1425)	(.411, .101)
4141	363	98	(-52, 19)	(235, 242)	(.455, .101)
RTDM	365	98	(24, 50)	(30, 104)	(.327, .101)
PLUNED	365	98	(-162, -35)	(574, 621)	(.255, .101)
COMPLEX/PPM	362	98	(-81, 17)	(357, 425)	(.519, .101)
SHORTZ	365	98	(-300, -210)	(335, 387)	(.479, .101)

* 95 PERCENT CONFIDENCE INTERVAL IN PARENTHESES

COMPARISON OF ALL OBSERVED AND PREDICTED
SO₂ CONCENTRATION VALUES (UG/M*3)
PAIRED IN TIME AND LOCATION
FOR THE 1-HOUR AVERAGING PERIOD
SUMMARY TABLE (PART 1)
WESTIVACO (1980/1981)

MODEL	NUMBER OF EVENTS	AVERAGE OBSERVED VALUE	AVERAGE DIFFERENCE* (OBS-PRED)	STANDARD DEVIATION* OF RESIDUALS	MAXIMUM FREQUENCY DIFFERENCE
COMP_EX1	30764	75	(-227 -252, -192)	(1709 1626, 1723)	***** (.011)
COMP_EX11	30682	85	(-241 -282, -200)	(2535 2515, 2555)	***** (.011)
4141	30656	95	(42 35, 50)	(535 511, 549)	***** (.011)
RTOM	32236	90	(55 51, 59)	(212 210, 214)	***** (.011)
PLUMES	31505	93	(14 1, 26)	(675 671, 681)	***** (.011)
COMP_EX/PPM	30463	85	(31 29, 43)	(723 727, 733)	***** (.011)
SHORT2	34879	84	(-22 -24, -71)	(621 605, 595)	***** (.010)

* 95 PERCENT CONFIDENCE INTERVAL IN PARENTHESES

COMPARISON OF ALL OBSERVED AND PREDICTED
SO2 CONCENTRATION VALUES (UG/M**3)
PAIRED IN TIME AND LOCATION
FOR THE 1-HOUR AVERAGING PERIOD
SUMMARY TABLE (PART 2)
WESTIVACO (1985/1991)

MODEL	FRACTION OF POSITIVE RESIDUALS (OBS>PRED)	ROOT MEAN SQUARE ERROR	AVERAGE ABSOLUTE RESIDUAL	PEARSON CORRELATION COEFFICIENT	SPEARMAN CORRELATION COEFFICIENT	VARIANCE COMPARISON* (OBS/PRED)
COMPLEX I	.95	1724	406	.008	.115	(.007, .002)
COMPLEX II	.95	2547	421	.015	.115	(.004, .004)
4141	.95	537	138	.059	.295	(.005, .033)
RT9M	.87	219	152	.079	-.004	(.044, .028)
PLUMES	.87	576	145	.051	.069	(.051, .056)
COMPLEX/PPM	.96	723	151	.009	.151	(.045, .030)
SHORTZ	.70	596	206	.046	-.128	(.045, .033)

* .95 PERCENT CONFIDENCE INTERVAL IN PARENTHESES

COMPARISON OF ALL OBSERVED AND PREDICTED
SO₂ CONCENTRATION VALUES (UG/M**3)
PAIRED IN TIME AND LOCATION
(FOR VARIOUS DATA SETS)
MODEL: COMPLY1
FOR THE 1-HOUR AVERAGE PERIOD
WESTVACO (12/80/1981)

DATA SET	NUMBER OF EVENTS	AVERAGE OBSERVED VALUE	AVERAGE DIFFERENCE (OBS-PRED)	STANDARD DEVIATION OF RESIDUALS
ALL	37704	95	-227	1703
STATION 1	3722	112	-589	2510
STATION 2	2247	52	51	44
STATION 3	3155	94	-302	1983
STATION 4	2423	104	-203	1742
STATION 5	2568	97	-45	898
STATION 6	3864	161	-953	3512
STATION 7	2344	106	-6	989
STATION 8	2840	71	53	383
STATION 9	2411	88	32	495
STATION 10	2364	57	16	128
STATION 11	2766	56	53	45

METEOROLOGICAL CONDITION

1. WIND SPEED			
< 2.5 M/S	926	130	44
2.5 TO 5.0 M/S	15227	80	44
> 5.0 M/S	7451	7	25

2. STABILITY GROUP			
CLASS A, B & C	5867	94	11
CLASS D	17021	64	11
CLASS E	3431	48	49
CLASS F	1585	12	56

COMPARISON OF ALL OBSERVED AND PREDICTED
SO2 CONCENTRATION VALUES (UG/M*3)
PAIRED IN TIME AND LOCATION
(FOR VARIOUS DATA SETS)
MODEL: COMPLEX11
FOR THE 1-HOUR AVERAGING PERIOD
WESTVACO (1980/1981)

DATA SET	NUMBER OF EVENTS	AVERAGE OBSERVED VALUE	AVERAGE DIFFERENCE (OBS-PRED)	STANDARD DEVIATION OF RESIDUALS
ALL	30682	9E	-241	2535
STATION 1	7731	112	-552	4072
STATION 2	2240	52	51	44
STATION 3	2166	94	-273	2680
STATION 4	2424	104	-213	2609
STATION 5	2567	97	-18	1369
STATION 6	2688	16E	-1029	4977
STATION 7	2346	106	-23	1642
STATION 8	2838	78	56	619
STATION 9	2414	8E	27	804
STATION 10	2289	54	13	239
STATION 11	2770	56	53	45

METEOROLOGICAL CONDITION

1. WIND SPEED				
< 2.5 M/S	8326	130	-187	53
2.5 TO 5.0 M/S	15198	80	-371	54
> 5.0 M/S	7458	7E	-34	33
2. STABILITY GROUP				
CLASS A, P & C	5901	9E	84	11
CLASS D	14623	84	84	11
CLASS E	2453	8E	-059	54
CLASS F	6315	124	-359	59

COMPARISON OF ALL OBSERVED AND PREDICTED
SO₂ CONCENTRATION VALUES (UG/M**3)
PAIRED IN TIME AND LOCATION
(FOR VARIOUS DATA SETS)
MODEL: COMPLEX/FFM
FOR THE 1-HOUR AVERAGING PERIOD
WESTVACO (1980/1981)

DATA SET	NUMBER OF EVENTS	AVERAGE OBSERVED VALUE	AVERAGE DIFFERENCE (OBS-PRED)	STANDARD DEVIATION OF RESIDUALS
ALL	37465	95	31	733
STATION 1	3690	117	-13	154
STATION 2	2242	50	48	76
STATION 3	3109	95	42	678
STATION 4	2413	104	31	107
STATION 5	2578	97	48	703
STATION 6	3752	165	-25	1210
STATION 7	2346	105	61	654
STATION 8	2836	70	63	239
STATION 9	2418	85	58	347
STATION 10	2264	55	33	116
STATION 11	2817	55	44	67

METEOROLOGICAL CONDITION

1. WIND SPEED				
< 2.5 M/S	1108	120	27	31
2.5 TO 5.0 M/S	14900	90	21	27
> 5.0 M/S	7449	70	57	16
2. STABILITY GROUP				
CLASS A, P & C	6070	91	33	16
CLASS D	14895	87	65	22
CLASS E	3273	80	-53	32
CLASS F	4227	131	-8	35

COMPARISON OF ALL OBSERVED AND PREDICTED
SO₂ CONCENTRATION VALUES (UG/M**3)
PAIRED IN TIME AND LOCATION
(FOR VARIOUS DATA SETS)
MODEL: 4141
FOR THE 1-HOUR AVERAGING PERIOD
WESTVACO (1980/1981)

DATA SET	NUMBER OF EVENTS	AVERAGE OBSERVED VALUE	AVERAGE DIFFERENCE (OBS-PRED)	STANDARD DEVIATION OF RESIDUALS
ALL	30658	95	42	535
STATION 1	3758	111	-4	594
STATION 2	238	50	51	44
STATION 3	3143	95	91	149
STATION 4	2435	103	52	401
STATION 5	2573	97	10	838
STATION 6	3902	160	68	370
STATION 7	2343	100	27	886
STATION 8	2640	78	60	415
STATION 9	2414	85	0	974
STATION 10	2228	56	54	51
STATION 11	2784	56	53	45

METEOROLOGICAL CONDITION

1. WIND SPEED				
< 2.5 M/S	7997	130	78	26
2.5 TO 5.0 M/S	15183	80	18	24
> 5.0 M/S	7478	70	54	13
2. STABILITY GROUP				
CLASS A, B & C	5933	97	87	11
CLASS D	14621	84	84	11
CLASS E	1448	85	-14	20
CLASS F	2456	127	-63	73

COMPARISON OF ALL OBSERVED AND PREDICTED
SO₂ CONCENTRATION VALUES (UG/M**3)
PAIRED IN TIME AND LOCATION
(FOR VARIOUS DATA SETS)
MODEL: PLUMES
FOR THE 1-HOUR AVERAGING PERIOD
WESTVACO (1980/1981)

DATA SET	NUMBER OF EVENTS	AVERAGE OBSERVED VALUE	AVERAGE DIFFERENCE (OBS-PRED)	STANDARD DEVIATION OF RESIDUALS
ALL	31005	93	14	675
STATION 1	3970	106	-56	1004
STATION 2	2245	50	50	43
STATION 3	3241	90	49	417
STATION 4	2491	101	55	308
STATION 5	2593	97	53	622
STATION 6	4231	140	-151	1252
STATION 7	2367	105	72	698
STATION 8	2853	70	70	207
STATION 9	2429	85	69	295
STATION 10	2320	50	43	59
STATION 11	2765	56	55	44

METEOROLOGICAL CONDITION

1. WIND SPEED				
< 2.5 M/S	8247	127	61	27
2.5 TO 5. M/S	15023	87	18	25
> 5. M/S	7635	60	-46	27
2. STABILITY GROUP				
CLASS A, P & C	6091	91	30	22
CLASS D	15470	81	-37	29
CLASS E	3421	86	31	23
CLASS F	6488	127	103	18

COMPARISON OF ALL OBSERVED AND PREDICTED
SO2 CONCENTRATION VALUES (UG/M**3)
PAIRED IN TIME AND LOCATION
(FOR VARIOUS DATA SETS)
MODEL: RTDM
FOR THE 1-HOUR AVERAGING PERIOD
WESTVACO (1980/1981)

DATA SET	NUMBER OF EVENTS	AVERAGE OBSERVED VALUE	AVERAGE DIFFERENCE (OBS-PRED)	STANDARD DEVIATION OF RESIDUALS
ALL	3028	66	-82	394
STATION 1	4303	83	-80	408
STATION 2	2452	40	2	85
STATION 3	2535	70	-86	350
STATION 4	2271	64	-165	452
STATION 5	2179	67	-108	489
STATION 6	4372	122	-16	333
STATION 7	2599	61	-211	706
STATION 8	2831	52	-100	282
STATION 9	2514	52	-116	388
STATION 10	2753	37	-4	82
STATION 11	2219	42	11	68

METEOROLOGICAL CONDITION

1. WIND SPEED	8732	84	-104	22
< 2.5 M/S	20290	60	-88	20
2.5 TO 5.0 M/S	8006	58	-48	16
> 5.0 M/S				

2. STABILITY GROUP

CLASS A, F & C	7743	50	-125	21
CLASS D	1685	60	-52	18
CLASS E	4229	60	-65	13
CLASS F	8044	87	-106	22

COMPARISON OF ALL OBSERVED AND PREDICTED
SO₂ CONCENTRATION VALUES (UG/M³)
PAIRED IN TIME AND LOCATION
(FOR VARIOUS DATA SETS)
MODEL: SHORTZ
FOR THE 1-HOUR AVERAGING PERIOD
WE STIVACO (1980/1981)

DATA SET	NUMBER OF EVENTS	AVERAGE OBSERVED VALUE	AVERAGE DIFFERENCE (OBS-PRED)	STANDARD DEVIATION OF RESIDUALS
ALL	34679	84	-82	691
STATION 1	4580	93	-235	898
STATION 2	2433	45	24	71
STATION 3	3698	82	-94	795
STATION 4	2944	87	-78	691
STATION 5	2766	91	22	352
STATION 6	4918	128	-385	1157
STATION 7	2455	102	34	305
STATION 8	2900	77	57	191
STATION 9	2490	83	52	223
STATION 10	2700	47	12	91
STATION 11	2425	52	39	58

METEOROLOGICAL CONDITION

1. WIND SPEED				
< 2.5 M/S	9326	117	-63	26
2.5 TO 5. M/S	17139	80	-115	23
> 5. M/S	8414	67	-37	17
2. STABILITY GROUP				
CLASS A, B & C	4562	85	8	18
CLASS D	17215	77	-65	22
CLASS E	7841	78	-126	27
CLASS F	7197	116	-175	34

COMPARISON OF ALL OBSERVED AND PREDICTED
SO2 CONCENTRATION VALUES (UG/M**3)
PAIRED IN TIME AND LOCATION
FOR THE 3-HOUR AVERAGING PERIOD
SUMMARY TABLE (PART 1)
WESTVACO (1980/1991)

MODEL	NUMBER OF EVENTS	AVERAGE OBSERVED VALUE	AVERAGE DIFFERENCE* (OBS-PRED)	STANDARD DEVIATION* OF RESIDUALS	MAXIMUM FREQUENCY DIFFERENCE
COMPLEX I	10600	89	(-262, -181)	(1322, 1340)	(.391, .319)
COMPLEX II	10556	89	(-237, -188)	(1806, 1831)	(.385, .319)
4141	10510	89	(29, 47)	(359, 364)	(.393, .319)
RIDM	11134	85	(47, 55)	(157, 162)	(.395, .319)
PLUMES	10825	87	(-5, 27)	(517, 521)	(.745, .319)
COMPLEX/PPM	10487	89	(14, 41)	(529, 543)	(.399, .319)
SHORTZ	12096	79	(-34, -67)	(501, 514)	(.555, .317)

* 95 PERCENT CONFIDENCE INTERVAL IN PARENTHESES

COMPARISON OF ALL OBSERVED AND PREDICTED
SO₂ CONCENTRATION VALUES (UG/M**3)
PAIRED IN TIME AND LOCATION
FOR THE 3-HOUR AVERAGING PERIOD
SUMMARY TABLE (PART 2)
WESTVACO (1980/1991)

MODEL	FRACTION OF POSITIVE RESIDUALS (OBS>PRED)	ROOT MEAN SQUARE ERROR	AVERAGE ABSOLUTE RESIDUAL	PEARSON CORRELATION COEFFICIENT	SPEARMAN CORRELATION COEFFICIENT	VARIANCE COMPARISON* (OBS>PRED)
COMPLX I	.91	1340	302	.010	.162	(.008, .039)
COMPLX II	.92	1921	309	.019	.106	(.005, .035)
4141	.94	361	125	.064	.097	(.023, .123)
RTD4	.86	157	90	.108	.130	(.067, .137)
P-JME5	.85	524	132	.074	.081	(.049, .054)
COMPLX/PPM	.94	537	140	.003	.134	(.043, .054)
SHORTZ	.65	514	156	.172	-.001	(.043, .059)

* 95 PERCENT CONFIDENCE INTERVAL IN PARENTHESES

COMPARISON OF ALL OBSERVED AND PREDICTED
 SO2 CONCENTRATION VALUES (UG/M*3)
 PAIRED IN TIME AND LOCATION
 (FOR VARIOUS DATA SETS)
 MODEL: COMPLEX I
 FOR THE 3-HOUR AVERAGING PERIOD
 WESTVACO (1980/1981)

DATA SET	NUMBER OF EVENTS	AVERAGE OBSERVED VALUE	AVERAGE DIFFERENCE (OBS-PRED)	STANDARD DEVIATION OF RESIDUALS
ALL	1600	88	-222	1322
STATION 1	1339	102	-547	1978
STATION 2	737	56	49	36
STATION 3	1112	87	-288	1459
STATION 4	850	94	-202	1283
STATION 5	869	91	-50	747
STATION 6	1420	144	-870	2281
STATION 7	794	99	-11	699
STATION 8	937	75	50	277
STATION 9	821	70	28	341
STATION 10	818	47	12	101
STATION 11	903	54	51	37

COMPARISON OF ALL OBSERVED AND PREDICTED
 SO₂ CONCENTRATION VALUES (UG/M**3)
 PAIPEL IN TIME AND LOCATION
 (FOR VARIOUS DATA SETS)
 MODEL: COMPLEX II
 FOR THE 3-HOUR AVERAGING PERIOD
 WESTVACO (1980/1991)

DATA SET	NUMBER OF EVENTS	AVERAGE OBSERVED VALUE	AVERAGE DIFFERENCE (OBS-PRED)	STANDARD DEVIATION OF RESIDUALS
ALL	17556	89	-237	1806
STATION 1	1335	102	-609	2825
STATION 2	739	57	49	37
STATION 3	1113	87	-261	1794
STATION 4	850	94	-207	1674
STATION 5	869	91	-22	895
STATION 6	1420	144	-941	3221
STATION 7	795	90	-28	987
STATION 8	938	77	53	392
STATION 9	623	70	22	477
STATION 10	760	57	9	159
STATION 11	905	54	51	37

COMPARISON OF ALL OBSERVED AND PREDICTED
SO₂ CONCENTRATION VALUES (UG/M**3)
PAIRED IN TIME AND LOCATION
(FOR VARIOUS DATA SETS)
MODEL: COMPLEX/PPM
FOR THE 3-HOUR AVERAGING PERIOD
WESTVACO (1980/1981)

DATA SET	NUMBER OF EVENTS	AVERAGE OBSERVED VALUE	AVERAGE DIFFERENCE (OBS-PRED)	STANDARD DEVIATION OF RESIDUALS
ALL	17487	89	27	536
STATION 1	1319	103	-14	764
STATION 2	743	49	46	47
STATION 3	1085	89	38	517
STATION 4	847	98	26	705
STATION 5	872	93	44	451
STATION 6	1378	148	-25	914
STATION 7	797	98	55	391
STATION 8	941	75	61	183
STATION 9	831	78	52	216
STATION 10	749	51	30	87
STATION 11	925	53	42	52

COMPARISON OF ALL OBSERVED AND PREDICTED
 SO₂ CONCENTRATION VALUES (UG/M**3)
 PAIRED IN TIME AND LOCATION
 (FOR VARIOUS DATA SETS)
 MODEL: 4141
 FOR THE 3-HOUR AVERAGING PERIOD
 WESTVACO (1980/1981)

DATA SET	NUMBER OF EVENTS	AVERAGE OBSERVED VALUE	AVERAGE DIFFERENCE (OBS-PRED)	STANDARD DEVIATION OF RESIDUALS
ALL	10510	80	38	359
STATION 1	1346	102	-6	423
STATION 2	739	50	49	30
STATION 3	1094	80	85	117
STATION 4	855	94	45	279
STATION 5	870	91	5	555
STATION 6	1425	144	60	285
STATION 7	794	90	21	560
STATION 8	939	70	56	282
STATION 9	822	79	-4	615
STATION 10	719	50	51	40
STATION 11	907	54	51	37

COMPARISON OF ALL OBSERVED AND PREDICTED
SO2 CONCENTRATION VALUES (UG/M**3)
PAIRED IN TIME AND LOCATION
(FOR VARIOUS DATA SETS)
MODEL: PLUMES
FOR THE 3-HOUR AVERAGING PERIOD
WESTVACO (1980/1981)

DATA SET	NUMBER OF EVENTS	AVERAGE OBSERVED VALUE	AVERAGE DIFFERENCE (OBS-PRED)	STANDARD DEVIATION OF RESIDUALS
ALL	17825	87	11	524
STATION 1	1415	90	-62	746
STATION 2	739	57	48	30
STATION 3	1132	86	45	370
STATION 4	869	97	60	252
STATION 5	881	91	48	549
STATION 6	1526	135	-146	995
STATION 7	805	90	66	415
STATION 8	948	70	55	139
STATION 9	835	70	63	186
STATION 10	770	40	30	51
STATION 11	697	54	53	35

COMPARISON OF ALL OBSERVED AND PREDICTED
SO2 CONCENTRATION VALUES (UG/M**3)
PAIRED IN TIME AND LOCATION
(FOR VARIOUS DATA SETS)
MODEL: PTDM
FOR THE 3-HOUR AVERAGING PERIOD
WESTVACO (1980/1981)

DATA SET	NUMBER OF EVENTS	AVERAGE OBSERVED VALUE	AVERAGE DIFFERENCE (OBS-PRED)	STANDARD DEVIATION OF RESIDUALS
ALL	11360	62	-85	375
STATION 1	1342	76	-78	359
STATION 2	716	38	0	77
STATION 3	1068	65	-86	328
STATION 4	980	58	-166	420
STATION 5	923	65	-118	493
STATION 6	1403	112	-17	268
STATION 7	1049	58	-223	787
STATION 8	1140	40	-102	267
STATION 9	1026	55	-120	379
STATION 10	772	35	-5	75
STATION 11	941	45	0	64

COMPARISON OF ALL OBSERVED AND PREDICTED
 SO2 CONCENTRATION VALUES (UG/M**3)
 PAIRED IN TIME AND LOCATION
 (FOR VARIOUS DATA SETS)
 MODEL: SHORTZ
 FOR THE 3-HOUR AVERAGING PERIOD
 WESTVACO (1980/1981)

DATA SET	NUMBER OF EVENTS	AVERAGE OBSERVED VALUE	AVERAGE DIFFERENCE (OBS-PRED)	STANDARD DEVIATION OF RESIDUALS
ALL	12096	79	-81	507
STATION 1	1658	85	-216	694
STATION 2	820	45	32	51
STATION 3	1305	76	-90	576
STATION 4	1058	78	-73	505
STATION 5	945	86	19	245
STATION 6	1748	110	-360	824
STATION 7	642	94	29	287
STATION 8	958	74	54	140
STATION 9	657	76	47	163
STATION 10	917	42	10	75
STATION 11	988	50	36	47

COMPARISON OF ALL OBSERVED AND PREDICTED
SO₂ CONCENTRATION VALUES (UG/M³)
PAIRED IN TIME AND LOCATION
FOR THE 24-HOUR AVERAGING PERIOD
SUMMARY TABLE (PART 1)
WESTVACO (1346/1981)

MODEL	NUMBER OF EVENTS	AVERAGE OBSERVED VALUE	AVERAGE DIFFERENCE* (OBS-PRED)	STANDARD DEVIATION* OF RESIDUALS	MAXIMUM FREQUENCY DIFFERENCE
COMPLEX I	3463	39	(-95, -75)	(401, 421)	(.341, .333)
COMPLEX II	3463	39	(-103, -81)	(525, 537)	(.351, .333)
4141	3463	39	(15, 20)	(95, 100)	(.353, .333)
RTM	3482	39	(23, 25)	(48, 51)	(.301, .333)
PLUMES	3482	39	(2, 10)	(134, 203)	(.783, .333)
COMPLEX/PPM	3456	39	(13, 16)	(154, 161)	(.351, .333)
SHORTZ	3486	39	(-37, -29)	(171, 176)	(.341, .333)

* 95 PERCENT CONFIDENCE INTERVAL IN PARENTHESES

COMPARISON OF ALL OBSERVED AND PREDICTED
SO₂ CONCENTRATION VALUES (UG/M**3)
PAIRED IN TIME AND LOCATION
FOR THE 24-HOUR AVERAGING PERIOD
SUMMARY TABLE (PART 2)
WESTVACO (1980/1981)

MODEL	FRACTION OF POSITIVE RESIDUALS (OBS>PRED)	ROOT MEAN SQUARE ERROR	AVERAGE ABSOLUTE RESIDUAL	PEARSON CORRELATION COEFFICIENT	SPEARMAN CORRELATION COEFFICIENT	VARIANCE COMPARISON* (OBS/PRED)
COMPLEX I	.86	417	133	.223	.320	(.012, .013)
COMPLEX II	.89	531	142	.205	.320	(.007, .009)
4141	.94	100	46	.194	.327	(.237, .244)
RTM	.90	55	23	.384	.406	(1.425, 1.554)
PLUMED	.90	203	49	.222	.335	(.054, .059)
COMPLEX/PPM	.93	155	52	.105	.316	(.034, .037)
SHORTZ	.73	174	70	.329	.407	(.071, .074)

* .95 PERCENT CONFIDENCE INTERVAL IN PARENTHESES

COMPARISON OF ALL OBSERVED AND PREDICTED
SO₂ CONCENTRATION VALUES (UG/M**3)
PAIRED IN TIME AND LOCATION
(FOR VARIOUS DATA SETS)
MODEL: COMPLEX1
FOR THE 24-HOUR AVERAGING PERIOD
WFSIVACO (1980/1991)

DATA SET	NUMBER OF EVENTS	AVERAGE OBSERVED VALUE	AVERAGE DIFFERENCE (OBS-PRED)	STANDARD DEVIATION OF RESIDUALS
ALL	3463	39	-75	411
STATION 1	317	57	-277	712
STATION 2	287	22	21	10
STATION 3	264	51	-147	479
STATION 4	317	37	-56	317
STATION 5	319	37	-11	290
STATION 6	285	91	-499	689
STATION 7	321	35	1	160
STATION 8	336	32	23	66
STATION 9	341	31	15	79
STATION 10	349	21	9	27
STATION 11	327	24	23	19

COMPARISON OF ALL OBSERVED AND PREDICTED
 SO2 CONCENTRATION VALUES (UG/M**3)
 PAIRED IN TIME AND LOCATION
 (FOR VARIOUS DATA SETS)
 MODEL: COMPLEXII
 FOR THE 24-HOUR AVERAGING PERIOD
 WESTVAC (1981/1981)

DATA SET	NUMBER OF EVENTS	AVERAGE OBSERVED VALUE	AVERAGE DIFFERENCE (OBS-PRED)	STANDARD DEVIATION OF RESIDUALS
ALL	3463	39	-91	525
STATION 1	317	57	-309	971
STATION 2	287	22	21	19
STATION 3	264	57	-135	557
STATION 4	317	37	-52	789
STATION 5	319	37	-2	217
STATION 6	285	91	-551	1167
STATION 7	321	35	-3	227
STATION 8	336	32	24	91
STATION 9	341	37	13	117
STATION 10	349	27	8	38
STATION 11	327	24	23	19

COMPARISON OF ALL OBSERVED AND PREDICTED
SO₂ CONCENTRATION VALUES (UG/M**3)
PAIRED IN TIME AND LOCATION
(FOR VARIOUS DATA SETS)
MODEL: COMPLEX/PEM
FOR THE 24-HOUR AVERAGING PERIOD
WESTVACO (1980/1981)

DATA SET	NUMBER OF EVENTS	AVERAGE OBSERVED VALUE	AVERAGE DIFFERENCE (OBS-PRED)	STANDARD DEVIATION OF RESIDUALS
ALL	1456	39	16	157
STATION 1	316	57	-5	257
STATION 2	287	22	27	20
STATION 3	263	57	23	162
STATION 4	316	37	18	163
STATION 5	319	37	21	100
STATION 6	285	91	-12	398
STATION 7	320	35	23	72
STATION 8	335	32	27	47
STATION 9	340	37	22	57
STATION 10	349	27	14	22
STATION 11	326	24	27	21

COMPARISON OF ALL OBSERVED AND PREDICTED
SO₂ CONCENTRATION VALUES (UG/M³)
PAIRED IN TIME AND LOCATION
(FOR VARIOUS DATA SETS)
MODEL: 4141
FOR THE 24-HOUR AVERAGING PERIOD
WESTVACO (1980/1981)

DATA SET	NUMBER OF EVENTS	AVERAGE OBSERVED VALUE	AVERAGE DIFFERENCE (OBS-PRED)	STANDARD DEVIATION OF RESIDUALS
ALL	1463	39	20	98
STATION 1	317	57	2	135
STATION 2	287	22	21	19
STATION 3	264	57	48	54
STATION 4	317	37	22	73
STATION 5	319	37	8	140
STATION 6	285	91	41	118
STATION 7	321	35	12	122
STATION 8	336	30	25	75
STATION 9	341	37	5	143
STATION 10	349	27	19	17
STATION 11	327	24	23	19

COMPARISON OF ALL OBSERVED AND PREDICTED
SO₂ CONCENTRATION VALUES (UG/M**3)
PAIRED IN TIME AND LOCATION
(FOR VARIOUS DATA SETS)
MODEL: PLUMF5
FOR THE 24-HOUR AVERAGING PERIOD
WESTVACO (1987/1981)

DATA SET	NUMBER OF EVENTS	AVERAGE OBSERVED VALUE	AVERAGE DIFFERENCE (OBS-PRED)	STANDARD DEVIATION OF RESIDUALS
ALL	1482	39	10	203
STATION 1	319	57	-29	272
STATION 2	289	22	21	18
STATION 3	265	50	27	120
STATION 4	318	37	25	79
STATION 5	321	37	22	124
STATION 6	287	00	-90	596
STATION 7	323	35	25	82
STATION 8	338	32	29	41
STATION 9	343	30	25	45
STATION 10	351	20	17	18
STATION 11	328	24	23	19

COMPARISON OF ALL OBSERVED AND PREDICTED
 SO2 CONCENTRATION VALUES (UG/M**3)
 PAIRED IN TIME AND LOCATION
 (FOR VARIOUS DATA SETS)
 MODEL: RTDM
 FOR THE 24-HOUR AVERAGING PERIOD
 WESTVACO (1980/1981)

DATA SET	NUMBER OF EVENTS	AVERAGE OBSERVED VALUE	AVERAGE DIFFERENCE (OBS-PRED)	STANDARD DEVIATION OF RESIDUALS
ALL	2676	37	-43	251
STATION 1	258	56	-55	241
STATION 2	241	20	3	43
STATION 3	223	47	-59	240
STATION 4	269	35	-83	289
STATION 5	268	36	-40	271
STATION 6	234	90	-11	164
STATION 7	268	34	-119	513
STATION 8	284	31	-57	197
STATION 9	282	30	-57	265
STATION 10	291	18	0	37
STATION 11	267	24	0	36

COMPARISON OF ALL OBSERVED AND PREDICTED
SO₂ CONCENTRATION VALUES (UG/M*3)
PAIRED IN TIME AND LOCATION
(FOR VARIOUS DATA SETS)
MODEL: SHORTZ
FOR THE 24-HOUR AVERAGING PERIOD
WESTVACO (1986/1991)

DATA SET	NUMBER OF EVENTS	AVERAGE OBSERVED VALUE	AVERAGE DIFFERENCE (OBS-PRED)	STANDARD DEVIATION OF RESIDUALS
ALL	1486	39	-29	171
STATION 1	319	57	-137	267
STATION 2	289	22	16	20
STATION 3	265	50	-50	206
STATION 4	321	37	-21	135
STATION 5	321	37	12	71
STATION 6	287	90	-255	349
STATION 7	323	35	14	64
STATION 8	338	30	25	40
STATION 9	343	30	21	41
STATION 10	352	20	8	23
STATION 11	328	24	18	20

COMPARISON OF 25 HIGHEST OBSERVED AND PREDICTED
SO₂ CONCENTRATION VALUES (UG/M**3)
(UNPAIRED IN TIME OR LOCATION)
FOR THE 1-HOUR AVERAGING PERIOD
WESTVACO (1980/1991)
HOURS SELECTED FOR IMPACT MODEL RUNS

MODEL	AVERAGE OBSERVED VALUE	AVERAGE PREDICTED VALUE	DIFFERENCE OF AVERAGES* (OBS-PRED)	MEDIAN DIFFERENCE* (OBS-PRED)	VARIANCE COMPARISON (OBS/PRED)	MAXIMUM FREQUENCY DIFFERENCE
COMPLEXI	1792	11420	-9527 (-11043, -8212)	-8594 (-10169, -7752)	.015 (.006, .033)	1.00 (.385)
COMPLEXII	1792	20558	-18765 (-22874, -14557)	-18139 (-20821, -15630)	.002 (.001, .004)	1.00 (.385)
4141	1792	3430	-1637 (-3257, -17)	-475 (-1570, 237)	.011 (.005, .125)	.42 (.385)
RTCM	1792	2031	-234 (-810, 332)	200 (-255, 559)	.096 (.042, .217)	.35 (.385)
PLUM15	1792	5413	-3520 (-5034, -2205)	-2470 (-3835, -1617)	.015 (.006, .033)	.88 (.385)
COMPLEX/PEM	1792	9011	-7218 (-9537, -4899)	-6433 (-9785, -4617)	.005 (.002, .012)	.94 (.385)
SHORTZ	1792	7448	-5552 (-7813, -3493)	-4404 (-6854, -2151)	.005 (.003, .014)	.87 (.385)
IMPACT	1796	17820	-16042 (-26484, -5500)	-4441 (-8189, -3115)	.000 (.000, .001)	1.00 (.385)

* 95 PERCENT CONFIDENCE INTERVAL IN PARENTHESES

COMPARISON OF 25 HIGHEST OBSERVED AND PREDICTED
SO₂ CONCENTRATION VALUES (UG/M³)
(UNPAIRED IN TIME OR LOCATION)
FOR THE 3-HOUR AVERAGING PERIOD
WESTVACO (1984/1991)
HOURS SELECTED FOR IMPACT MODEL RUNS

MODEL	AVERAGE OBSERVED VALUE	AVERAGE PREDICTED VALUE	DIFFERENCE* (OBS-PRED)	MEDIAN DIFFERENCE* (OBS-PRED)	VARIANCE COMPARISON (OBS/PRED)	MAXIMUM FREQUENCY DIFFERENCE
COMPLEXI	941	5310	(-4375 -5610, -3141)	(-3371 -5253, -2634)	(.015 .007, .035)	(.92 (.385)
COMPLEXII	941	7898	(-5955 -9077, -4834)	(-6377 -9133, -4796)	(.005 .002, .012)	(.83 (.385)
4101	941	1277	(-234 -1010, 341)	(179 -150, 306)	(.053 .023, .121)	(.40 (.385)
RTD4	941	934	(107 -230, 445)	(305 -20, 509)	(.243 .107, .553)	(.52 (.385)
PLUMES	941	1868	(-925 -1918, 55)	(-54 -961, 352)	(.024 .011, .055)	(.40 (.385)
COMPLEX/PEM	941	2871	(-1920 -3378, -479)	(-132 -2854, 431)	(.011 .005, .025)	(.44 (.385)
SHORTZ	941	2669	(-1727 -2675, -779)	(-549 -1337, -328)	(.026 .012, .050)	(.52 (.385)
IMPACT	022	5693	(-5770 -10860, -580)	(-1355 -2202, -658)	(.001 .000, .002)	(.53 (.385)

* 95 PERCENT CONFIDENCE INTERVAL IN PARENTHESES

COMPARISON OF HIGHEST
OBSERVED AND PREDICTED
SO₂ CONCENTRATION VALUES (UG/M³)
PAIRED BY STATION FOR THE 1 HOUR AVERAGING PERIOD
WESTVACO (1980/1991)
HOURS SELECTED FOR IMPACT MODEL RUNS

MODEL	NUMBER OF DATA PAIRS	AVERAGE OBSERVED VALUE	AVERAGE DIFFERENCE*	FRACTION OF POSITIVE RESIDUALS (OBS>PRED)	STANDARD DEVIATION* OF RESIDUALS	ROOT MEAN SQUARE ERROR	AVERAGE ABSOLUTE RESIDUAL	PEARSON CORR. COEFF.	SPEARMAN CORR. COEFF.	VARIANCE COMPARISON* (OBS>PRED)
COMPLEX I	10	1876	-7556 (-12685, -2425)	.30	7171 (4932, 13092)	10153	7767	.66	.66	.012 (.003, .043)
COMPLEX II	10	1876	-17123 (-28531, -5715)	.20	15248 (10969, 29117)	21394	17253	.53	.53	.003 (.001, .011)
4141	10	1876	-3865 (-8676, 944)	.40	6725 (4525, 12279)	7726	4354	.34	.32	.015 (.004, .052)
RTDM	10	1876	-164 (-1116, 787)	.70	1331 (915, 2430)	3250	893	.60	.73	.239 (.054, 1.043)
FLUMEL5	10	1876	-3138 (-5573, 295)	.40	4872 (3373, 9767)	6076	3390	.55	.56	.025 (.005, .175)
COMPLEX/2FM	10	1876	-7520 (-13104, -1937)	.30	7886 (5369, 14251)	10506	7318	.60	.64	.012 (.003, .042)
SHORTZ	10	1876	-6026 (-11729, -1023)	.10	6994 (4811, 12769)	9163	6075	.59	.70	.013 (.003, .051)
IMPACT	10	1876	-43749 (-54209, -22589)	.50	24032 (20011, 53115)	49131	43400	.57	.58	.001 (.000, .003)

* 95 PERCENT CONFIDENCE INTERVAL IN PARENTHESES

COMPARISON OF HIGHEST
OBSERVED AND PREDICTED
SO₂ CONCENTRATION VALUES (UG/M*3)
PAIRED BY STATION FOR THE 3 HOUR AVERAGING PERIOD
WESTVACO (1980/1981)
HOURS SELECTED FOR IMPACT MODEL RUNS

MODEL	NUMBER OF DATA PAIRS	AVERAGE OBSERVED VALUE	AVERAGE DIFFERENCE*	FRACTION OF POSITIVE RESIDUALS (OBS>PRED)	STANDARD DEVIATION* OF RESIDUALS	ROOT MEAN SQUARE ERROR	AVERAGE ABSOLUTE RESIDUAL	PEARSON CORR. COEFF.	SPEARMAN CORR. COEFF.	VARIANCE COMPARISON* (OBS>PRED)
COMPLEX I	10	1273	(-3421 (-6652, -183)	.30	(4518 (3108, 9240)	6036	3567	.37	.35	(.034, .061)
COMPLEX II	10	1273	(-6178 (-10765, -1590)	.30	(6413 (4411, 11708)	8900	5388	.48	.39	(.032, .030)
4141	10	1273	(-1074 (-2754, 604)	.60	(2342 (1615, 4288)	3828	1652	.51	.54	(.012, .061)
FTJ4	10	1273	(242 (-282, 867)	.80	(804 (553, 1467)	3114	704	.45	.43	(.110, 1.779)
FLUMES	10	1273	(-1031 (-3201, 1138)	.60	(3033 (2085, 5538)	4194	1702	.48	.73	(.032, .127)
COMPLEX/OPM	10	1273	(-2684 (-5761, 331)	.40	(4217 (2900, 7594)	5495	3176	.41	.54	(.017, .059)
SHORTZ	10	1273	(-1562 (-3434, 269)	.60	(2529 (1761, 4726)	4135	1947	.41	.47	(.011, .175)
IMPACT	10	1273	(-23096 (-35063, -11110)	.00	(16743 (11516, 35560)	26969	23097	.73	.73	(.000, .005)

* 95 PERCENT CONFIDENCE INTERVAL IN PARENTHESES

COMPARISON OF HIGHEST
OBSERVED AND PREDICTED
SO₂ CONCENTRATION VALUES (UG/M**3)
PAIRED BY STATION FOR THE 24 HOUR AVERAGING PERIOD
WESTVACO (1280/1981)
HOURS SELECTED FOR IMPACT MODEL RUNS

MODEL	NUMBER OF DATA PAIRS	AVERAGE OBSERVED VALUE	AVERAGE DIFFERENCE*	FRACTION OF POSITIVE RESIDUALS (OBS>PRED)	STANDARD DEVIATION* OF RESIDUALS	ROOT MEAN SQUARE ERROR	AVERAGE ABSOLUTE RESIDUAL	PEARSON CORR. COEFF.	SPEARMAN CORR. COEFF.	VARIANCE COMPARISON* (OBS>PRED)
COMPLEXI	10	326	(-626 (-1447, 199)	.40	(1149 (799, 2097)	3245	721	.55	.79	(.033, .043)
COMPLEXII	10	326	(-1069 (-2350, 172)	.40	(1764 (1213, 3220)	3566	1214	.50	.71	(.005 (.031, .013)
4141	10	326	(44 (-164, 252)	.80	(292 (201, 532)	3027	235	.16	.33	(.195 (.044, .757)
RTDM	10	326	(45 (-79, 170)	.80	(175 (126, 320)	3020	154	.78	.91	(.244 (.031, .935)
FLUMES	10	326	(-257 (-1069, 554)	.60	(1135 (781, 2072)	3195	532	.34	.54	(.011 (.033, .045)
COMPLEX/PFM	10	325	(-357 (-1003, 258)	.40	(889 (611, 1527)	3140	531	.52	.64	(.013 (.034, .071)
SHORTZ	10	326	(-255 (-737, 225)	.60	(673 (463, 1220)	3086	404	.64	.84	(.028 (.037, .114)
IMPACT	10	325	(-3432 (-5061, -1803)	.00	(2279 (1567, 4150)	4904	3433	.32	.27	(.903 (.031, .012)

* 95 PERCENT CONFIDENCE INTERVAL IN PARENTHESES

COMPARISON OF SECOND HIGHEST
OBSERVED AND PREDICTED
SO₂ CONCENTRATION VALUES (UG/M**3)
PAIRED BY STATION FOR THE 1 HOUR AVERAGING PERIOD
WESTVACO (11/87/1981)
HOURS SELECTED FOR IMPACT MODEL RUNS

MODEL	NUMBER OF DATA PAIRS	AVERAGE OBSERVED VALUE	AVERAGE DIFFERENCE*	FRACTION OF POSITIVE RESIDUALS (OBS>PRED)	STANDARD DEVIATION* OF RESIDUALS	ROOT MEAN SQUARE ERROR	AVERAGE ABSOLUTE RESIDUAL	PEARSON CORR. COEFF.	SPEARMAN CORR. COEFF.	VARIANCE COMPARISON* (OBS>PRED)
COMPLEX I	10	1654	-5652 (-10083, -1220)	.30 (4262, 11314)	6197	8340	5871	.53	.45	.013 (.003, .053)
COMPLEX II	10	1654	-10368 (-19398, -2217)	.40 (8260, 21426)	12009	15274	11526	.45	.41	.064 (.001, .015)
COMPLEX III	10	1654	-1725 (-4008, 558)	.50 (2196, 5829)	3193	4437	2350	.55	.54	.045 (.011, .101)
RTCM	10	1654	112 (-726, 951)	.60 (807, 2142)	1173	2198	332	.48	.45	.317 (.079, 1.279)
FLUMES	10	1654	-548 (-3275, 2097)	.70 (2524, 6858)	3755	4577	2288	.33	.37	.035 (.008, .107)
COMPLEX/PPM	10	1654	-4490 (-9392, 411)	.40 (4714, 12513)	5853	8115	5040	.52	.50	.011 (.003, .044)
SHORTZ	10	1654	-2300 (-5507, 725)	.40 (2907, 7955)	4357	5461	2779	.41	.45	.027 (.007, .107)
IMPACT	10	1654	-3164 (-45216, -15180)	.50 (14441, 30231)	20995	34524	30199	.52	.54	.001 (.000, .005)

* 95 PERCENT CONFIDENCE INTERVAL IN PARENTHESES

COMPARISON OF SECOND HIGHEST
OBSERVED AND PREDICTED
SO₂ CONCENTRATION VALUES (UG/M**3)
PAIRED BY STATION FOR THE 3 HOUR AVERAGING PERIOD
WESTVACO (1980/1981)
HOURS SELECTED FOR IMPACT MODEL RUNS

MODEL	NUMBER OF DATA PAIRS	AVERAGE OBSERVED VALUE	AVERAGE DIFFERENCE*	FRACTION OF POSITIVE RESIDUALS (CRSDPRED)	STANDARD DEVIATION* OF RESIDUALS	ROOT MEAN SQUARE ERROR	AVERAGE ABSOLUTE RESIDUAL	PEARSON CORR. COEFF.	SPEARMAN CORR. COEFF.	VARIANCE COMPARISON* (03SDPRED)
COMPLEX I	10	1021	(-2036 (-3848, -224)	.30	2533 (1742, 4624)	4256	2185	.65	.71	.033 (.038, .132)
COMPLEX II	10	1021	(-4219 (-8293, -145)	.40	5695 (3917, 10390)	7198	4559	.50	.74	.007 (.002, .030)
4141	10	1021	(-62 (-676, 511)	.60	930 (571, 1316)	3108	581	.76	.89	.199 (.049, .802)
RTM	10	1021	(-206 (-224, 637)	.70	502 (414, 1099)	3070	480	.60	.64	.459 (.115, .894)
FLUMES	10	1021	(-129 (-1720, 1452)	.60	2225 (1530, 4762)	3627	1251	.42	.59	.045 (.011, .137)
COMPLEX/PEM	10	1021	(-1374 (-3235, 985)	.50	2601 (1789, 4742)	4043	1928	.70	.83	.331 (.038, .124)
SHORTZ	10	1021	(-937 (-2688, 713)	.60	2378 (1635, 4341)	3522	1442	.53	.67	.339 (.010, .155)
IMPACT	10	1021	(-11931 (-17150, -6712)	.00	7297 (5719, 13322)	13494	11932	.53	.50	.003 (.001, .019)

* 95 PERCENT CONFIDENCE INTERVAL IN PARENTHESES

COMPARISON OF SECOND HIGHEST
OBSERVED AND PREDICTED
SO₂ CONCENTRATION VALUES (UG/M**3)
PAIRED BY STATION FOR THE 24 HOUR AVERAGING PERIOD
WESTVACO (1986/1991)
HOURS SELECTED FOR IMPACT MODEL RUNS

MODEL	NUMBER OF DATA PAIRS	AVERAGE OBSERVED VALUE	AVERAGE DIFFERENCE*	FRACTION OF POSITIVE RESIDUALS (OBS>PRED)	STANDARD DEVIATION* OF RESIDUALS	ROOT MEAN SQUARE ERROR	AVERAGE ABSOLUTE RESIDUAL	PEARSON CORR. COEFF.	SPEARMAN CORR. COEFF.	VARIANCE COMPARISON* (OBS>PRED)
COMPLEX I	10	251	(-366, 224) (-956, 224)	.40	(825, 150F) (566, 150F)	3126	425	.72	.92	.015 (.004, .034)
COMPLEX II	10	251	(-337, 50) (-726, 50)	.40	(543, 391) (373, 391)	3072	462	.78	.98	.030 (.006, .122)
414J	10	251	(140, 253) (26, 253)	.90	(159, 290) (109, 290)	3021	103	.34	.58	.455 (.115, 1.675)
RTDM	10	251	(106, 191) (22, 191)	.90	(114, 215) (81, 215)	3019	145	.74	.90	.390 (.037, 1.574)
FLJME5	10	251	(105, 254) (-53, 254)	.90	(222, 406) (153, 406)	3023	204	.65	.94	.153 (.038, .515)
COMPLEX/DFM	10	251	(-138, 272) (-548, 272)	.80	(573, 1047) (394, 1047)	3052	239	.73	.91	.224 (.007, .113)
SHORTZ	10	251	(-69, 157) (-305, 157)	.70	(331, 604) (227, 604)	3031	130	.79	.99	.072 (.017, .242)
IMPACT	10	251	(-2148, -1250) (-3047, -1250)	.50	(1256, 2294) (854, 2294)	3310	2149	.21	.25	.907 (.032, .033)

* 95 PERCENT CONFIDENCE INTERVAL IN PARENTHESES

COMPARISON OF HIGHEST OBSERVED AND PREDICTED
SO₂ CONCENTRATION VALUES (UG/M**3)
EVENT-BY-EVENT (PAIRED IN TIME)
FOR THE 1-HOUR AVERAGING PERIOD
WESTVACO (1980/1981)
HOURS SELECTED FOR IMPACT MODEL RUNS

MODE-	NUMBER OF EVENTS	AVERAGE OBSERVED VALUE	AVERAGE DIFFERENCE* (OBS-PRED)	STANDARD DEVIATION* OF RESIDUALS	MAXIMUM FREQUENCY DIFFERENCE
COMPLEX I	460	373	(-1331, -795)	(3062, 3445)	(.352 (.090)
COMPLEX II	461	372	(-1790, -1136)	(5108, 5814)	(.357 (.090)
4141	461	372	(-27, 128)	(1193, 1350)	(.352 (.090)
RTDM	461	372	(75, 301)	(641, 730)	(.531 (.090)
PLUMES	461	372	(-457, 198)	(1557, 1772)	(.557 (.090)
COMPLEX/PPM	461	372	(-546, 174)	(2417, 2751)	(.323 (.090)
SHORTZ	463	370	(-323, -47)	(2098, 2233)	(.332 (.090)
IMPACT	418	363	(-2278, 177)	(5982, 7903)	(.345 (.094)

* 95 PERCENT CONFIDENCE INTERVAL IN PARENTHESES

COMPARISON OF HIGHEST OBSERVED AND PREDICTED
 SO₂ CONCENTRATION VALUES (UG/M**3)
 EVENT-BY-EVENT (PAIRED IN TIME)
 FOR THE 3-HOUR AVERAGING PERIOD
 WESTVACO (1980/1981)
 HOURS SELECTED FOR IMPACT MODEL RUNS

MODEL	NUMBER OF EVENTS	AVERAGE OBSERVED VALUE	AVERAGE DIFFERENCE* (OBS-PRED)	STANDARD DEVIATION* OF RESIDUALS	MAXIMUM FREQUENCY DIFFERENCE
COMPLEX I	150	349	(-1280, -244)	(2496, 2821)	(.767, .157)
COMPLEX II	150	349	(-1755, -443)	(3664, 4142)	(.773, .157)
4141	150	349	(-41, 288)	(856, 968)	(.783, .157)
RTDM	151	347	(55, 293)	(471, 592)	(.503, .157)
PLUMES	152	344	(-111, 353)	(1339, 1512)	(.467, .155)
COMPLEX/PPH	152	344	(-205, 170)	(1858, 2092)	(.730, .155)
SHORTZ	152	344	(-301, -28)	(1350, 1525)	(.335, .155)
IMPACT	137	338	(-1048, 18)	(5785, 6580)	(.328, .164)

* 95 PERCENT CONFIDENCE INTERVAL IN PARENTHESES

COMPARISON OF HIGHEST OBSERVED AND PREDICTED
SO2 CONCENTRATION VALUES (UG/M**3)
EVENT-BY-EVENT (PAIRED IN TIME)
FOR THE 24-HOUR AVERAGING PERIOD
WESTVACO (1986/1991)
HOURS SELECTED FOR IMPACT MODEL RUNS

MODEL	NUMBER OF EVENTS	AVERAGE OBSERVED VALUE	AVERAGE DIFFERENCE* (OBS-PRED)	STANDARD DEVIATION* OF RESIDUALS	MAXIMUM FREQUENCY DIFFERENCE
COMP-EXI	20	269	(-1049, -564)	(888, 1159)	(.500)
COMP-EXII	20	269	(-1222, -693)	(1129, 1473)	(.500)
4141	20	269	(42, 123)	(190, 248)	(.550)
RTDM	20	269	(40, 138)	(162, 211)	(.700)
PLUMES	20	269	(-501, -115)	(641, 836)	(.500)
COMP-EX/PPM	20	269	(-397, -90)	(510, 796)	(.550)
SHORTZ	20	269	(-499, -242)	(402, 524)	(.400)
IMPACT	10	261	(-2406, -958)	(1554, 2354)	(.500)

* 95 PERCENT CONFIDENCE INTERVAL IN PARENTHESES

COMPARISON OF ALL OBSERVED AND PREDICTED
SO₂ CONCENTRATION VALUES (UG/M³)
PAIRED IN TIME AND LOCATION
FOR THE 1-HOUR AVERAGING PERIOD
SUMMARY TABLE (PART 1)
WESTVACO (1980/1981)
HOURS SELECTED FOR IMPACT MODEL RUNS

MODEL	NUMBER OF EVENTS	AVERAGE OBSERVED VALUE	AVERAGE DIFFERENCE* (OBS-PRED)	STANDARD DEVIATION* OF RESIDUALS	MAXIMUM FREQUENCY DIFFERENCE
COMPLEX I	2477	203	(-126, -59 11)	(1538, 1685)	(.958, .039)
COMPLEX II	2476	204	(-191, -92 6)	(2471, 2542)	(.953, .032)
4141	2478	203	(115, 145 174)	(724, 745)	(.954, .033)
RTDM	2531	199	(137, 154)	(409, 421)	(.804, .039)
PLUMES	2508	201	(69, 100 131)	(762, 783)	(.370, .038)
COMPLEX/PPM	2474	204	(67, 117)	(1267, 1373)	(.948, .032)
SHORTZ	2595	195	(-16, 23 63)	(991, 1019)	(.740, .033)
IMPACT	2526	190	(-517, -797, -437)	(4527, 4753)	(.925, .038)

* 95 PERCENT CONFIDENCE INTERVAL IN PARENTHESES

COMPARISON OF ALL OBSERVED AND PREDICTED
SO₂ CONCENTRATION VALUES (UG/M**3)
PAIRED IN TIME AND LOCATION
FOR THE 1-HOUR AVERAGING PERIOD
SUMMARY TABLE (PART 2)
WESTIVACO (1980/1981)
HOURS SELECTED FOR IMPACT MODEL RUNS

MODEL	FRACTION OF POSITIVE RESIDUALS (OR>PRED)	ROOT MEAN SQUARE ERROR	AVERAGE ABSOLUTE RESIDUAL	PEARSON CORRELATION COEFFICIENT	SPEARMAN CORRELATION COEFFICIENT	VARIANCE COMPARISON* (OBS/PRED)
COMPLEXI	.97	1639	453	-.002	-.009	(.037, .041)
COMPLEXII	.97	2472	498	.018	-.063	(.015, .017)
4141	.97	739	250	.062	-.074	(.023, .034)
RTOW	.90	431	217	.125	.058	(1.180, 1.303)
P_JMES	.92	789	269	.109	-.132	(.185, .204)
COMPLX/PTM	.95	1268	327	.017	.013	(.063, .077)
SHORT7	.82	301	306	.051	-.091	(.111, .123)
IMPACT	.70	4557	872	-.020	.022	(.005, .005)

* 95 PERCENT CONFIDENCE INTERVAL IN PARENTHESES

COMPARISON OF ALL OBSERVED AND PREDICTED
SO2 CONCENTRATION VALUES (UG/M**3)
PAIRED IN TIME AND LOCATION
FOR THE 3-HOUR AVERAGING PERIOD
SUMMARY TABLE (PART 1)
WESTVACO (1980/1991)
HOURS SELECTED FOR IMPACT MODEL RUNS

MODEL	NUMBER OF EVENTS	AVERAGE OBSERVED VALUE	AVERAGE DIFFERENCE* (OBS-PRED)	STANDARD DEVIATION* OF RESIDUALS	MAXIMUM FREQUENCY DIFFERENCE
COMP_EXI	861	193	(-160, 44) -58	(1166, 1282) 1221	(.912 , .065)
COMPLEXII	858	193	(-220, 37) -92	(1621, 1782) 1597	(.937 , .065)
4141	860	193	(102, 171) 137	(454, 400) 475	(.933 , .055)
RTDM	883	189	(109, 157) 129	(307, 337) 321	(.745 , .065)
PLUMES	877	189	(15, 172) 94	(588, 546) 516	(.928 , .055)
COMPLEX/PEM	867	191	(-9, 132) 62	(850, 934) 890	(.911 , .065)
SHORTZ	913	182	(-36, 77) 21	(530, 723) 589	(.563 , .054)
IMPACT	865	173	(-85, -332) -501	(3505, 3852) 3669	(.477 , .045)

* 95 PERCENT CONFIDENCE INTERVAL IN PARENTHESES

COMPARISON OF ALL OBSERVED AND PREDICTED
SO₂ CONCENTRATION VALUES (US/M**3)
PAIRED IN TIME AND LOCATION
FOR THE 3-HOUR AVERAGING PERIOD
SUMMARY TABLE (PART 2)
WESTVACO (1980/1991)
HOURS SELECTED FOR IMPACT MODEL RUNS

MODEL	FRACTION OF POSITIVE RESIDUALS (OBS>PRED)	ROOT MEAN SQUARE ERROR	AVERAGE ABSOLUTE RESIDUAL	PEARSON CORRELATION COEFFICIENT	SPEARMAN CORRELATION COEFFICIENT	VARIANCE COMPARISON* (OBS/PRED)
COMPLEXI	.94	1222	421	-.019	-.021	(.042, .048)
COMPLEXII	.95	1598	457	.005	-.051	(.024, .027)
4141	.95	494	230	.062	-.048	(.392, .445)
RTD*	.88	345	194	.134	.195	(1.253, 1.430)
PLUMES	.90	623	242	.132	-.032	(.143, .214)
COMPLEX/PPM	.94	832	300	.009	.022	(.032, .104)
S40R17	.77	559	270	.074	-.071	(.150, .149)
IMPACT	.69	1716	872	.000	.102	(.005, .005)

* .95 PERCENT CONFIDENCE INTERVAL IN PARENTHESES

COMPARISON OF ALL OBSERVED AND PREDICTED
SO₂ CONCENTRATION VALUES (UG/M**3)
PAIRED IN TIME AND LOCATION
FOR THE 24-HOUR AVERAGING PERIOD
SUMMARY TABLE (PART 1)
WESTVACO (12HC/1981)
HOURS SELECTED FOR IMPACT MODEL RUNS

MODEL	NUMBR OF EVENTS	AVERAGE OBSERVED VALUE	AVERAGE DIFFERENCE* (OBS-PRED)	STANDARD DEVIATION* OF RESIDUALS	MAXIMUM FREQUENCY DIFFERENCE
COMP-EXI	165	124	(-117, 50) -33	(454, 564) 502	(.303 .150)
COMP-EXII	165	124	(-133, 47) -44	(556, 691) 615	(.303 .150)
4141	165	124	(72, 117) 95	(129, 160) 143	(.314 .150)
RTOM	165	124	(57, 105) 86	(110, 136) 121	(.553 .150)
PLUMES	165	124	(8, 114) 61	(281, 350) 311	(.721 .150)
COMPLEX/PFM	165	124	(-5, 91) 43	(311, 345) 344	(.773 .150)
SHORTZ	165	124	(-34, 65) 15	(246, 306) 273	(.391 .150)
IMPACT	150	122	(-543, -226) -435	(1102, 1365) 1225	(.340 .157)

* 95 PERCENT CONFIDENCE INTERVAL IN PARENTHESES

COMPARISON OF ALL OBSERVED AND PREDICTED
SO₂ CONCENTRATION VALUES (UG/M**3)
PAIRED IN TIME AND LOCATION
FOR THE 24-HOUR AVERAGING PERIOD
SUMMARY TABLE (PART 2)
WESTVACO (1980/1981)
HOURS SELECTED FOR IMPACT MODEL RUNS

MODEL	FRACTION OF POSITIVE RESIDUALS (OBS>PRED)	ROOT MEAN SQUARE ERROR	AVERAGE ABSOLUTE RESIDUAL	PEARSON CORRELATION COEFFICIENT	SPEARMAN CORRELATION COEFFICIENT	VARIANCE COMPARISON* (OBS/PRED)
COMPLFXI	.82	502	222	.007	.170	(.050, .050) (.039, .065)
COMPLFXII	.85	615	245	.012	.222	(.033, .033) (.025, .042)
4141	.95	171	123	.126	.299	(.075, .075) (.029, 1.332)
RTDM	.92	148	105	.354	.400	(.127, .127) (.058, 1.064)
PLUMES	.90	316	135	.284	.235	(.115, .115) (.054, .143)
COMPLEX/PTM	.80	345	165	.075	.333	(.104, .104) (.033, .140)
SHORTZ	.80	272	143	.315	.407	(.147, .147) (.113, .131)
IMPACT	.59	1236	530	.361	.551	(.009, .009) (.005, .011)

* 95 PERCENT CONFIDENCE INTERVAL IN PARENTHESES

APPENDIX C

STATISTICAL TABLE OF MODEL PERFORMANCE FOR CINDER CONE BUTTE

<u>Table</u>	<u>Page</u>
Cinder Cone Butte Comparison of 25 Highest	C-1
Cinder Cone Butte Comparison of Highest by Event	C-10
Cinder Cone Butte Comparison of All Events Paired in Space and Time	C-20

COMPARISON OF 25 HIGHEST OBSERVED AND PREDICTED
RELATIVE CONCENTRATION VALUES (13**(-6) S/M**3)
(UNPAIRED IN TIME OR LOCATION)
FOR THE 1-HOUR AVERAGING PERIOD
CINDER CONE BUTTE (1980)

MODEL	AVERAGE OBSERVED VALUE	AVERAGE PREDICTED VALUE	DIFFERENCE OF AVERAGES* (OBS-PRED)	MEDIAN DIFFERENCE* (OBS-PRED)	VARIANCE COMPARISON (OBS/PRED)	MAXIMUM FREQUENCY DIFFERENCE
COMPLEX I	66	105	(-38, -15)	(-31, -18)	(.532, .234, 1.207)	(.52, .385)
COMPLEX II	66	250	(-183, -133)	(-148, -115)	(.084, .037, .191)	(.95, .385)
4141	66	196	(-129, -100)	(-120, -92)	(.255, .112, .578)	(.92, .385)
RTSM	66	67	(-23, 22)	(-12, 5)	(.475, .210, 1.080)	(.23, .385)
PLUME 5	66	177	(-110, -53)	(-57, -45)	(.062, .027, .140)	(.63, .385)
COMPLEX/PFM	66	166	(-90, -53)	(-87, -57)	(.151, .067, .343)	(.63, .385)
SHORT Z	66	139	(-72, -1)	(-19, -3)	(.737, .016, .684)	(.35, .385)
IMPACT	66	34	(31, 47)	(13, 42)	(2.645, 1.165, 5.083)	(.75, .385)

* 95 PERCENT CONFIDENCE INTERVAL IN PARENTHESES

COMPARISON OF 25 HIGHEST OBSERVED AND PREDICTED
RELATIVE CONCENTRATION VALUES (10**(-6) S/M**2)
(UNPAIRED IN TIME OR LOCATION)
FOR VARIOUS DATA SETS
MODEL: COMPLEX I
FOR THE 1-HOUR AVERAGING PERIOD
CINDER CONE ROUTE (1980)

DATA SETS	AVERAGE OBSERVED VALUE	AVERAGE PREDICTED VALUE	DIFFERENCE OF AVERAGES* (OBS-PRED)	VARIANCE COMPARISON (OBS/PRED)
ALL	66	105	(-60, -38	(.532 .234*1.207)
RECEPTOR ELEVATION RELATIVE TO SOURCE RELEASE HEIGHT				
<-10. M	39	64	-24	.351
-10. M TO 10. M	51	63	-41	.579
10. M TO 30. M	41	74	-32	.471
>30. M	43	59	-14	1.270

COMPARISON OF 25 HIGHEST OBSERVED AND PREDICTED
RELATIVE CONCENTRATION VALUES (10**(-4) S/M**3)
(UNPAIRED IN TIME OR LOCATION)
FOR VARIOUS DATA SETS
MODEL: COMPLEX II
FOR THE 1-HOUR AVERAGING PERIOD
CINDER CONE BUTTE (1980)

DATA SETS	AVERAGE OBSERVED VALUE	AVERAGE PREDICTED VALUE	DIFFERENCE OF AVERAGES (OBS-PRED)	VARIANCE COMPARISON (OBS/PRED)
ALL	64	25	(-231, -133)	(.037, .131)
RECEPTOR ELEVATION RELATIVE TO SOURCE RELEASE HEIGHT				
<10. M	39	114	-74	.033
10. M TO 10. M	51	151	-138	.003
10. M TO 30. M	41	147	-105	.189
>30. M	43	146	-102	.158

COMPARISON OF 25 HIGHEST OBSERVED AND PREDICTED
RELATIVE CONCENTRATION VALUES (10*(-6) S/M**2)
(OBTAINED IN TIME & LOCATION)
FOR VARIOUS DATA SETS
MODEL: COMPLEX/7FM
FOR THE 1-HOUR AVERAGING PERIOD
CINDER CONE BUTTE (1983)

DATA SETS	AVERAGE OBSERVED VALUE	AVERAGE PREDICTED VALUE	DIFFERENCE OF AVERAGES* (OBS-PRED)	VARIANCE COMPARISON (OBS/PRED)
ALL	46	155	(-135, -89	.151 (.767, .243)

RECEPTOR ELEVATION RELATIVE
TO SOURCE RELEASE HEIGHT

<-10. M	39	67	-27	.349
10. M TO 10. M	51	129	-77	.137
10. M TO 30. M	41	115	-73	.092
>30. M	43	114	-69	.134

COMPARISON OF 25 HIGHEST OBSERVED AND PREDICTED
 RELATIVE CONCENTRATION VALUES (13**(-6) S/M**3)
 (UNPAIRED IN TIME OR LOCATION)
 FOR VARIOUS DATA SETS
 MODEL: 4141
 FOR THE 1-HOUR AVERAGING PERIOD
 CINDER CONE BUTTE (1960)

DATA SETS	AVERAGE OBSERVED VALUE	AVERAGE PREDICTED VALUE	DIFFERENCE OF AVERAGES* (OBS-PRED)	VARIANCE COMPARISON (OBS/PRED)
ALL	65	195	(-15P* -129	.255 (.112* .579)

RECEPTOR ELEVATION RELATIVE
 TO SOURCE RELEASE HEIGHT

<-10. M	39	64	-24	.194
-10. M TO 10. M	51	142	-90	.278
10. M TO 30. M	41	155	-113	.161
>30. M	43	174	-89	.251

COMPARISON OF 25 HIGHEST OBSERVED AND PREDICTED
 RELATIVE CONCENTRATION VALUES (10**(-6) S/M**3)
 (UNFAIRFD IN TIME OR LOCATION)
 FOR VARIOUS DATA SETS
 MODEL: PLUMEE
 FOR THE 1-HOUR AVEAGING PERIOD
 CINDER CONE BUTTE (1980)

DATA SETS	AVERAGE OBSERVED VALUE	AVERAGE PREDICTED VALUE	DIFFERENCE OF AVERAGES* (OBS-PRED)	VARIANCE COMPARISON (OBS/PRED)
ALL	66	177	(-165, -55)	(.027, .140)
RECEPTOR ELEVATION RELATIVE TO SOURCE RELEASE HEIGHT				
<10. M	39	176	-67	.027
10. M TO 10. M	51	173	-51	.243
10. M TO 30. M	41	59	-57	.180
>30. M	43	112	-67	.078

COMPARISON OF 25 HIGHEST OBSERVED AND PREDICTED
RELATIVE CONCENTRATION VALUES (10**(-6) S/M**3)
(UNPAIRED IN TIME OR LOCATION)
FOR VARIOUS DATA SETS

MODEL: RTDM
FOR THE 1-HOUR AVERAGING PERIOD
CINDER CONE BUTTE (1980)

DATA SETS	AVERAGE OBSERVED VALUE	AVERAGE PREDICTED VALUE	DIFFERENCE OF AVERAGES* (OBS-PRED)	VARIANCE COMPARISON (OBS/PRED)
ALL	55	57	(-27, 25)	(.332 .145, .754)

RECEPTOR ELEVATION RELATIVE
TO SOURCE RELEASE HEIGHT

<-10. M	39	35	4	.166
-10. M TO 10. M	51	50	1	1.053
10. M TO 30. M	41	43	-1	.633
>30. M	43	43	0	1.398

COMPARISON OF 25 HIGHEST OBSERVED AND PREDICTED
RELATIVE CONCENTRATION VALUES (12+*(-5) 5/4+*3)
(UNPAIRED IN TIME OR LOCATION)
FOR VARIOUS DATA SETS
MODEL: SHORTZ
FOR THE 1-HOUR AVERAGING PERIOD
CINDER CONE BUTTE (1988)

DATA SETS	AVERAGE OBSERVED VALUE	AVERAGE PREDICTED VALUE	DIFFERENCE OF AVERAGES* (OBS-PRED)	VARIANCE COMPARISON (OBS/PRED)
ALL	65	139	(-143, -72 -1)	(.037 .016, .004)
RECEPTOR ELEVATION RELATIVE TO SOURCE RELEASE HEIGHT				
<-10. M	39	77	?	.419
-10. M TO 10. M	51	84	-42	.141
10. M TO 30. M	41	93	-51	.021
>30. M	43	79	-34	.071

COMPARISON OF 25 HIGHEST OBSERVED AND PREDICTED
RELATIVE CONCENTRATION VALUES (10**(-6) S/M**3)
(UNPAIRED IN TIME OR LOCATION)
FOR VARIOUS DATA SETS
MODEL: IMPACT
FOR THE 1-HOUR AVERAGING PERIOD
CINDER CONE BUTTE (1980)

DATA SETS	AVERAGE OBSERVED VALUE	AVERAGE PREDICTED VALUE	DIFFERENCE OF AVERAGES* (OBS-PRED)	VARIANCE COMPARISON (OBS/PRED)
ALL	65	34	(16, 31 47)	2.645 (1.165,5.003)
RECEPTOR ELEVATION RELATIVE TO SOURCE RELEASE HEIGHT				
<-10. " 39		23	6	1.250
-10. " TO 10. M 51		20	31	16.390
10. M TO 30. M 41		12	29	21.332
>30. " 43		10	34	23.097

COMPARISON OF HIGHEST OBSERVED AND PREDICTED
RELATIVE CONCENTRATION VALUES (10**(-5) S/1**+3)
EVENT-PY-EVENT (PAIRED IN TIME)
FOR THE 1-HOUR AVEAGING PERIOD

PART 1
CINDER CONE BUTTE (1980)

MODE	NUMBER OF EVENTS	AVERAGE OBSERVED VALUE	AVERAGE DIFFERENCE* (OBS-PRED)	STANDARD DEVIATION* OF RESIDUALS	MAXIMUM FREQUENCY DIFFERENCE
COMPLEXI	104	25	(-25, -16 -6)	(36, 41 43)	(.212 (.183)
COMPLEXII	104	25	(-93, -68 -33)	(91, 103 120)	(.442 (.149)
4141	104	25	(-67, -47 -26)	(56, 75 87)	(.345 (.189)
RTCM	104	25	(-2, 0 9)	(26, 30 35)	(.347 (.149)
PLUMES	104	25	(-62, -40 -10)	(78, 98 102)	(.417 (.189)
COMPLEX/PPM	104	25	(-31, -34 -16)	(58, 66 74)	(.294 (.149)
SHORTZ	104	25	(-40, -20 0)	(83, 94 110)	(.135 (.189)
IMPACT	104	25	(3, 13 20)	(23, 26 31)	(.294 (.189)

* 95 PERCENT CONFIDENCE INTERVAL IN PARENTHESES

COMPARISON OF HIGHEST OBSERVED AND PREDICTED
RELATIVE CONCENTRATION VALUES (10**(-6) S/M**3)
EVENT-BY-EVENT (PAIRED IN TIME)
FOR THE 1-HOUR AVERAGING PERIOD

PART 2

CINDER CONE BUTTE (1980)

MODEL	FRACTION OF POSITIVE RESIDUALS (OBS>PRED)	ROOT MEAN SQUARE ERROR	AVERAGE ABSOLUTE RESIDUAL	PEARSON CORRELATION COEFFICIENT	SPEARMAN CORRELATION COEFFICIENT	VARIANCE COMPARISON* (OBS/PRED)
COMPLEX I	.43	44	29	.454	.331	(.287, .357)
COMPLEX II	.26	123	74	.345	.317	(.049, .394)
4141	.36	88	55	.385	.365	(.125, .173)
RTD"1	.53	30	19	.599	.510	(.450, .964)
P-UMEF	.31	46	47	.278	.438	(.070, .133)
COMPLEX/PFM	.30	74	42	.305	.406	(.104, .149)
SHORTZ	.48	96	35	.255	.474	(.065, .111)
IMPACT	.72	29	19	.414	.397	(.202, .444)

* 95 PERCENT CONFIDENCE INTERVAL IN PARENTHESES

COMPARISON OF HIGHEST OBSERVED AND PREDICTED
RELATIVE CONCENTRATION VALUES (C/O) (-6) S/M*3)
EVENT-BY-EVENT (FOR VARIOUS DATA SETS)
MODEL: COMPLEX1
FOR THE 1-HOUR AVERAGING PERIOD
LINCOLN COLE BUTTE (1960)

DATA SET	NUMBER OF EVENTS	AVERAGE OBSERVED VALUE	AVERAGE DIFFERENCE (OBS-PRED)	STANDARD DEVIATION OF RESIDUALS	PEARSON CORRELATION COEFFICIENT
HIGHEST CONCENTRATION EVENT BY EVENT	174	26	-16	41	.454
BY RELEASE DISTANCE/ RELEASE HEIGHT					
DISTANCE < 900 M					
HK 15. M	4	59	-32	62	.168
H=15. M TO 26. M	12	27	-42	37	.70
H> 25. M	8	69	-13	55	.567
DISTANCE > 900 M					
HK 15. M	8	27	14	23	.649
H=15. M TO 26. M	46	19	-13	44	-.370
H> 25. M	24	13	-8	24	-.127

METEOROLOGICAL CORRELATION

1. WIND SPEED					
< 2.5 M/S	52	29	-27	47	.488
2.5 TO 5. M/S	27	22	-1	25	-.012
> 5. M/S	15	22	5	13	.454
2. STABILITY GROUP					
CLASS C+D	30	31	4	26	.529
CLASS F	38	26	-25	42	.556
CLASS F	36	22	-21	34	.361

COMPARISON OF HIGHEST OBSERVED AND PREDICTED
RELATIVE CONCENTRATION VALUES (10**(-6) S/M**3)
EVENT-BY-EVENT (FOR VARIOUS DATA SETS)
MODEL: COMPLEX II
FOR THE 1-HOUR AVERAGING PERIOD
CINDER CONE BUTTE (1980)

DATA SET	NUMBER OF EVENTS	AVERAGE OBSERVED VALUES	AVERAGE DIFFERENCE (OBS-PRED)	STANDARD DEVIATION OF RESIDUALS	PEARSON CORRELATION COEFFICIENT
HIGHEST CONCENTRATION EVENT BY EVENT	104	25	-58	172	.545
BY RELEASE DISTANCE/ RELEASE HEIGHT					
DISTANCE < 900. M					
HC 15. M	4	59	-178	154	.128
H=16. M TO 26. M	12	27	-55	42	.439
H> 25. M	9	59	-145	145	.417
DISTANCE > 900. M					
HC 15. M	6	37	-4	24	.691
H=16. M TO 26. M	46	19	-72	114	-.066
H> 25. M	24	13	-41	61	-.124

METEOROLOGICAL CONDITIONS

1. WIND SPEED					
< 2.5 M/S	62	29	-97	121	.752
2.5 TO 5. M/S	27	22	-31	49	.545
> 5. M/S	15	22	-15	12	.463
2. STABILITY GROUP					
CLASS C+D	30	51	-9	76	.658
CLASS E	34	26	-27	107	.524
CLASS F	36	22	-86	20	.172

COMPARISON OF HIGHEST OBSERVED AND PREDICTED
RELATIVE CONCENTRATION VALUES (10**(-6) S/M**3)
EVENT-BY-EVENT (FOR VARIOUS DATA SETS)
MODEL: COMPLEX/PEM
FOR THE 1-HOUR AVERAGING PERIOD
CINDER CONE ROUTE (1900)

DATA SET	HIGHER OF EVENTS	AVERAGE OBSERVED VALUE	AVERAGE DIFFERENCE (OBS-PRED)	STANDARD DEVIATION OF RESIDUALS	PEARSON CORRELATION COEFFICIENT
HIGHEST CONCENTRATION EVENT BY EVENT	104	26	-34	65	.605
BY RELEASE DISTANCE/ RELEASE HEIGHT					
DISTANCE < 900. M					
H< 15. M	4	59	-68	63	.247
H=16. M TO 26. M	12	27	-47	45	.177
H> 26. M	9	59	-93	121	.577
DISTANCE > 900. M					
H< 15. M	9	37	5	23	.657
H=16. M TO 26. M	46	19	-32	52	-.049
H> 26. M	24	13	-14	45	-.032

METEOROLOGICAL COLLECTION

1. WIND SPEED					
< 4.5 M/S	52	29	-25	75	.534
4.5 TO 5. M/S	27	22	-4	20	.334
> 5. M/S	15	22		1	.425
2. STABILITY GROUP					
CLASS C+D	30	31	-6	29	.431
CLASS E	38	26	-37	73	.073
CLASS F	36	22	-53	73	.093

COMPARISON OF HIGHEST OBSERVED AND PREDICTED
RELATIVE CONCENTRATION VALUES (10**(-6) S/M**3)
EVENT-BY-EVENT (FOR VARIOUS DATA SETS)
MODEL: 4141
FOR THE 1-HOUR AVERAGING PERIOD
CINDER CONE BUTTE (1990)

DATA SET	NUMBER OF EVENTS	AVERAGE OBSERVED VALUE	AVERAGE DIFFERENCE (OBS-PRED)	STANDARD DEVIATION OF RESIDUALS	PEARSON CORRELATION COEFFICIENT
HIGHEST CONCENTRATION EVENT BY EVENT	104	26	-47	75	.349
RELEASE DISTANCE/ RELEASE HEIGHT					
DISTANCE < 900. M					
< 15. M	4	59	-22	71	.216
15. M TO 26. M	12	27	-57	72	.625
> 26. M	9	69	-92	72	.316
DISTANCE > 900. M					
< 15. M	6	37	5	13	.867
15. M TO 26. M	46	19	-51	84	-.002
> 26. M	24	13	-24	47	-.191

LOGICAL CONDITION

WIND SPEED					
< 1.5 M/S	52	29	-73	85	.402
1.5 TO 5. M/S	27	22	-13	33	.054
> 5. M/S	15	22	-2	27	.430
STABILITY GROUP					
CLASS C+D	37	31	1	20	.699
CLASS E	34	26	-49	29	.575
CLASS F	33	22	-94	45	.614

COMPARISON OF HIGHEST OBSERVED AND PREDICTED
RELATIVE CONCENTRATION VALUES (11**(-6) G/M**3)
EVENT-BY-EVENT (FOR VARIOUS DATA SITES)
MODEL: PLUMFE
FOR THE 1-HOUR AVERAGING PERIOD
CINDER CONE BUTTE (1950)

DATA SET	NUMBER OF EVENTS	AVERAGE OBSERVED VALUE	AVERAGE DIFFERENCE (OBS-PRED)	STANDARD DEVIATION OF RESIDUALS	PEARSON CORRELATION COEFFICIENT
HIGHEST CONCENTRATION EVENT BY EVENT	104	26	-40	80	.278
BY RELEASE DISTANCE/ RELEASE HEIGHT					
DISTANCE < 900. M					
H< 15. M	4	29	-204	255	-.033
H=15. M TO 25. M	12	27	-49	43	.420
H> 25. M	9	69	-13	20	.918
DISTANCE > 900. M					
H< 15. M	9	37	2	25	.731
H=15. M TO 25. M	46	19	-43	35	-.038
H> 25. M	24	13	-18	20	.151

METEOROLOGICAL CONDITION

1. WIND SPEED					
< 2.5 M/S	62	29	-55	100	.267
2.5 TO 5. M/S	27	22	-20	40	.108
> 5. M/S	15	22	-12	10	.431
2. STABILITY GROUP					
CLASS C+D	30	31	-25	78	.651
CLASS E	38	25	-71	151	.221
CLASS F	36	22	-28	40	.298

COMPARISON OF HIGHEST OBSERVED AND PREDICTED
RELATIVE CONCENTRATION VALUES (10+(-6) S/M+2)
EVENT-BY-EVENT (FOR VARIOUS DATA SETS)

MODEL: R10W

FOR THE 1-HOUR AVERAGING PERIOD
CINFER CONE BUTTE (1980)

DATA SET	NUMBER OF EVENTS	AVERAGE OBSERVED VALUE	AVERAGE DIFFERENCE (OBS-PRED)	STANDARD DEVIATION OF RESIDUALS	PEARSON CORRELATION COEFFICIENT
HIGHEST CONCENTRATION EVENT BY EVENT	104	26	1	52	.551
BY RELEASE DISTANCE/ RELEASE HEIGHT					
DISTANCE < 910. M					
HC 15. M	4	59	46	34	-.000
H=16. M TO 26. M	12	27	-2	42	.367
H> 26. M	0	69	-31	65	.558
DISTANCE > 910. M					
HC 15. M	0	37	24	24	.508
H=16. M TO 26. M	46	19	2	17	.411
H> 26. M	24	13	-4	15	.242

METEOROLOGICAL CONDITIONS

1. WIND SPEED					
< 5.5 M/S	62	29	-3	73	.549
2. TO 10. M/S	27	22	4	12	.623
> 10. M/S	16	22	3	12	.540
2. STABILITY GROUP					
CLASS C+D	39	21	4	20	.605
CLASS E	24	26	1	20	.610
CLASS F	26	22	-4	20	.413

COMPARISON OF HIGHEST OBSERVED AND PREDICTED
RELATIVE CONCENTRATION VALUES (10**(-6) G/M**3)
EVENT-BY-EVENT (FOR VARIOUS DATA SETS)
MODEL: SHORT7
FOR THE 1-HOUR AVERAGING PERIOD
(INHER CONE BUTTE (1980))

DATA SET	NUMBER OF EVENTS	AVERAGE OBSERVED VALUE	AVERAGE DIFFERENCE (OBS-PRED)	STANDARD DEVIATION OF RESIDUALS	PEARSON CORRELATION COEFFICIENT
HIGHEST CONCENTRATION EVENT BY EVENT	124	26	-20	94	.256
BY RELEASE DISTANCE/ RELEASE HEIGHT					
DISTANCE < 900. M					
H< 15. M	4	59	37	30	-.253
H=15. M TO 24. M	12	27	-10	40	.404
H> 25. M	9	69	-115	112	.155
DISTANCE > 900. M					
H< 15. M	9	37	24	22	.724
H=15. M TO 26. M	46	19	-3	19	.517
H> 25. M	24	13	-40	165	.249

METEOROLOGICAL CONDITION

1. WIND SPEED < 2.5 M/S 2.5 TO 5. M/S > 5. M/S	60 27 15	29 22 22	-14 -17 -40	57 43 213	.520 .314 -.128
2. STABILITY GROUP CLASS C+D CLASS F CLASS F	3 38 36	31 26 22	-7 -13 -40	27 50 148	.775 .484 .120

COMPARISON OF HIGHEST OBSERVED AND PREDICTED
RELATIVE CONCENTRATION VALUES (10*(-6) S/M*3)
EVENT-BY-EVENT (FOR VARIOUS DATA SETS)
MODEL: IMPACT
FOR THE 1-HOUR AVERAGING PERIOD
CINDER CONE BUTTE (1980)

DATA SET	NUMBER OF EVENTS	AVERAGE OBSERVED VALUE	AVERAGE DIFFERENCE (OBS-PRED)	STANDARD DEVIATION OF RESIDUALS	PEARSON CORRELATION COEFFICIENT
----------	------------------------	------------------------------	-------------------------------------	---------------------------------------	---------------------------------------

HIGHEST CONCENTRATION EVENT BY EVENT	104	26	13	26	.414
---	-----	----	----	----	------

BY RELEASE DISTANCE /
RELEASE HEIGHT

DISTANCE < 9.0 M					
H<15. M	4	59	42	20	.471
H=15. M TO 26. M	12	27	9	32	.369
H>26. M	9	59	37	44	.456

DISTANCE > 9.0 M					
H<15. M	9	37	33	24	.403
H=15. M TO 26. M	46	19	7	21	-.103
H>26. M	24	13	4	12	.015

METEOROLOGICAL CONDITION

1. WIND SPEED					
< 3.5 M/S	52	20	11	31	.433
2.5 TO 5. M/S	27	22	15	21	-.275
> 5. M/S	15	22	15	14	.711

2. STABILITY GROUP					
CLASS C+D	30	31	21	33	.452
CLASS E	30	26	11	25	.459
CLASS F	16	22	7	21	.420

COMPARISON OF ALL OBSERVED AND PREDICTED
RELATIVE CONCENTRATION VALUES (10**(-5) S/M**3)
PAIRED IN TIME AND LOCATION
FOR THE 1-HOUR AVERAGING PERIOD
SUMMARY TABLE (PART 1)
CINDER CONE RJTTE (1990)

MODE -	NUMBER OF EVENTS	AVERAGE OBSERVED VALUE	AVERAGE DIFFERENCE* (OBS-PRED)	STANDARD DEVIATION* OF RESIDUALS	MAXIMUM FREQUENCY DIFFERENCE
COMP_LXI	3836	5	(-5, -5)	(20, 21)	(.349, .031)
COMP_EXII	5839	5	(-7, -5)	(34, 35)	(.293, .031)
4141	3836	5	(-10, -7)	(30, 31)	(.121, .031)
RIDM	3836	5	(0, 1)	(12, 13)	(.055, .031)
PLUMES	3836	5	(-5, -3)	(28, 29)	(.301, .031)
COMPLEX/PFM	3836	5	(-5, -4)	(26, 27)	(.305, .031)
SHORTZ	3836	5	(-2, 0)	(23, 24)	(.107, .031)
IMPACT	3836	5	(2, 3)	(11, 12)	(.132, .031)

* .05 PERCENT CONFIDENCE INTERVAL IN PARENTHESES

COMPARISON OF ALL OBSERVED AND PREDICTED
RELATIVE CONCENTRATION VALUES (10**(-5) S/M**3)
PAIRED IN TIME AND LOCATION
FOR THE 1-HOUR AVERAGING PERIOD
SUMMARY TABLE (PART 2)
CINDER CONE ROUTE (1980)

MODEL	FRACTION OF POSITIVE RESIDUALS (OPS>PRED)	ROOT MEAN SQUARE ERROR	AVERAGE ABSOLUTE RESIDUAL	PEARSON CORRELATION COEFFICIENT	SPEARMAN CORRELATION COEFFICIENT	VARIANCE COMPARISON* (OBS/PRED)
COMPLEX I	.49	21	11	.509	.333	(.238, .327)
COMPLEX II	.56	35	13	.236	.391	(.114, .125)
4141	.42	32	14	.277	.377	(.143, .157)
RTW	.47	13	5	.425	.409	(1.035, 1.138)
PLUMF	.56	28	10	.223	.403	(.175, .194)
COMPLEX/PEM	.55	27	11	.313	.353	(.173, .213)
SHORTZ	.49	23	7	.236	.447	(.251, .287)
IMPACT	.54	12	6	.294	.422	(4.531, 5.053)

* 95 PERCENT CONFIDENCE INTERVAL FOR SPEARMAN'S

COMPARISON OF ALL OBSERVED AND PREDICTED
RELATIVE CONCENTRATION VALUES (IC**(-6) S/M**3)
PAIRED IN TIME AND LOCATION
(FOR VARIOUS DATA SETS)
MODEL: COMPLEX
FOR THE 1-HOUR AVERAGING PERIOD
CINDER COVE PUTTE (1980)

DATA SET	NUMBER OF EVENTS	AVERAGE OBSERVED VALUE	AVERAGE DIFFERENCE (OPS-PRED)	STANDARD DEVIATION OF RESIDUALS
ALL	1836	8	-6	20
BY RELEASE DISTANCE/ RELEASE HEIGHT				
DISTANCE < 900. M				
HC 15. M	155	8	-1	22
H=16. M TO 26. M	414	7	-7	24
H> 26. M	269	16	-12	30
DISTANCE > 900. M				
HC 16. M	308	8	2	13
H=16. M TO 26. M	1771	8	-5	22
H> 26. M	914	7	-6	13

METEOROLOGICAL CONDITION

1. WIND SPEED				
< 2.5 M/S	2272	8	-8	24
2.5 TO 5. M/S	1333	5	-2	13
> 5. M/S	531	7	-1	7
2. STABILITY GROUP				
CLASS C+D	1247	8	1	15
CLASS E	1478	5	-3	23
CLASS F	1111	4	-9	21

COMPARISON OF ALL OBSERVED AND PREDICTED
RELATIVE CONCENTRATION VALUES (10**(-6) S/M**3)
PAIRED IN TIME AND LOCATION
(FOR VARIOUS DATA SETS)
MODEL: COMPLEXII
FOR THE 1-HOUR AVERAGING PERIOD
CINDER CONE BUTTE (1990)

STANDARD
DEVIATION
OF RESIDUALS

AVERAGE
DIFFERENCE
(OBS-PRED)

AVERAGE
OBSERVED
VALUE

NUMBER
OF
EVENTS

DATA SET

34

-5

0

2636

ALL

BY RELEASE DISTANCE/
RELEASE HEIGHT

DISTANCE < 900. M
HC 15. W
H=16. W TO 26. M
H> 26. W

44

25

54

-1

-5

-15

0

0

14

155

413

269

DISTANCE > 900. M
HC 16. W
H=16. W TO 26. M
H> 26. W

19

38

21

2

-7

-6

0

0

3

508

1771

914

METEOROLOGICAL CONDITION

1. WIND SPEED
< 1.5 M/S
2.5 TO 5. M/S
> 5. M/S

42

20

11

-9

-3

-1

0

0

0

1272

1033

531

2. STABILITY GROUP
CLASS C+D
CLASS F
CLASS F

18

40

29

1

-10

-9

0

0

4

1247

1476

1111

COMPARISON OF ALL OBSERVED AND PREDICTED
RELATIVE CONCENTRATION VALUES (10**(-6)) S/M**3)
PAIRED IN TIME AND LOCATION)
(FOR VARIOUS DATA SETS)
MODEL: COMPLEX/DEM
FOR THE 1-HOUR AVERAGING PERIOD
CINDER CONE BUTTE (1900)

DATA SET	NUMBER OF EVENTS	AVERAGE OBSERVED VALUE	AVERAGE DIFFERENCE (OBS-PRED)	STANDARD DEVIATION OF RESIDUALS
----------	------------------------	------------------------------	-------------------------------------	---------------------------------------

ALL	7836	4	-5	26
-----	------	---	----	----

BY RELEASE DISTANCE/
RELEASE HEIGHT

DISTANCE < 900. M				
H < 16. M	155	5	-2	33
H=16. M TO 26. M	418	5	-5	29
H > 26. M	259	15	-14	53
DISTANCE > 900. M				
H < 16. M	509	6	2	15
H=16. M TO 26. M	1771	5	-5	26
H > 26. M	914	7	-3	12

METEOROLOGICAL CONDITION

1. WIND SPEED				
< 2.5 M/S	7272	5	-8	32
2.5 TO 5. M/S	1534	5	-	12
> 5. M/S	531	5	1	3
2. STABILITY GROUP				
CLASS C/D	1247	5	1	16
CLASS E	1478	5	-8	29
CLASS F	1111	4	-7	50

COMPARISON OF ALL OBSERVED AND PREDICTED
RELATIVE CONCENTRATION VALUES (10**(-5) S/M**3)
PAIRED IN TIME AND LOCATION
(FOR VARIOUS DATA SETS)
MODEL: 4141
FOR THE 1-HOUR AVERAGING PERIOD
CINDER CONE SUITE (1980)

DATA SET	NUMBER OF EVENTS	AVERAGE OBSERVED VALUE	AVERAGE DIFFERENCE (OBS-PRED)	STANDARD DEVIATION OF RESIDUALS
ALL	1836		-R	39
BY RELEASE DISTANCE/ RELEASE HEIGHT				
DISTANCE < 900. M				
H< 15. M	155		-2	29
H=15. M TO 26. M	419		-9	29
H> 26. M	269	15	-25	52
DISTANCE > 900. M				
H< 16. M	308		0	17
H=16. M TO 26. M	1771		-9	33
H> 26. M	914		-7	17

METEOROLOGICAL CONDITION

1. WIND SPEED				
< 2.5 M/S	2272		-12	37
2.5 TO 6. M/S	1335		-3	17
> 6. M/S	521		-5	11
2. STABILITY GROUP				
CLASS C+D	1247			15
CLASS F	1470		-11	30
CLASS E	1111		-14	40

COMPARISON OF ALL OBSERVED AND PREDICTED
RELATIVE CONCENTRATION VALUES (10**(-5) G/M**3)
PAIRED IN TIME AND LOCATION
(FOR VARIOUS DATA SETS)
MODEL: PLUMER
FOR THE 1-HOUR AVERAGING PERIOD
CINDER CONE BUTTE (1990)

DATA SET	NUMBER OF EVENTS	AVERAGE OBSERVED VALUE	AVERAGE DIFFERENCE (OBS-PRED)	STANDARD DEVIATION OF RESIDUALS
ALL	7836	4	-4	28
BY RELEASE DISTANCE/ RELEASE HEIGHT				
DISTANCE < 900. M				
HC 15. "	155	8	-1	53
H=10. M TO 26. M	419	8	-5	26
H> 26. "	269	14	-1	32
DISTANCE > 900. M				
HC 15. "	308	8	2	17
H=10. M TO 26. M	1771	8	-3	32
H> 26. "	914	7	-4	13

METEOROLOGICAL CONDITION

1. WIND SPEED				
< 2.5 M/S	2472	8	-5	33
2.5 TO 5. M/S	1430	8	-2	20
> 5. M/S	531	8	-1	11
2. STABILITY GROUP				
CLASS C+D	1447	8	-1	21
CLASS E	1478	8	-7	28
CLASS F	1111	4	-3	18

COMPARISON OF ALL OBSERVED AND PREDICTED
RELATIVE CONCENTRATION VALUES (10**(-9) S/M**43)
PAIRED IN TIME AND LOCATION
(FOR VARIOUS DATA SETS)
MODEL: RTDM
FOR THE 1-HOUR AVERAGING PERIOD
CINDER CONE BUTTE (1930)

DATA SET	NUMBER OF EVENTS	AVERAGE OBSERVED VALUE	AVERAGE DIFFERENCE (OBS-PRED)	STANDARD DEVIATION OF RESIDUALS
----------	------------------------	------------------------------	-------------------------------------	---------------------------------------

ALL	3036	5	0	13
-----	------	---	---	----

BY RELEASE DISTANCE /
RELEASE HEIGHT

DISTANCE < 900. M				
HC 16. M	155	5	5	15
H=16. M TO 26. M	416	5	-1	15
H> 26. M	469	15	-4	20
DISTANCE > 900. M				
HC 16. M	308	5	5	13
H=16. M TO 26. M	1771	5	1	3
H> 26. M	314	7	-2	3

METEOROLOGICAL CONDITION

1. WIND SPEED				
< 2.5 M/S	2272	5	-1	15
2.5 TO 5. M/S	1032	5	1	5
> 5. M/S	331	5	1	7
2. CLOUDILITY GROUP				
CLASS C+D	1247	5	2	13
CLASS E	1470	5	0	12
CLASS F	1111	4	-2	13

COMPARISON OF ALL OBSERVED AND PREDICTED
RELATIVE CONCENTRATION VALUES (1300(-6) 5/11/83)
PAIRED IN TIME AND LOCATION
(FOR VARIOUS DATA SETS)
MODEL: SHORTZ
FOR THE 1-HOUR AVERAGING PERIOD
CHURR CONE SITE (1300)

DATA SET	NUMBER OF EVENTS	AVERAGE OBSERVED VALUE	AVERAGE DIFFERENCE (OBS-PRED)	STANDARD DEVIATION OF RESIDUALS
ALL	3656	1	-1	23
BY RELEASE DISTANCE/ RELEASE HEIGHT				
DISTANCE < 900. M				
HC 16. M	155	8	4	15
H=16. M TO 26. M	410	15	-1	16
H> 26. M	269	15	-13	50
DISTANCE > 900. M				
HC 16. M	306	5	5	13
H=16. M TO 26. M	1771	5	1	7
H> 26. M	514	7	-5	23

METEOLOGICAL CONDITION

1. WIND SPEED				
< 2.5 M/S	2272	5	-1	19
2.5 TO 5. M/S	1357	5	-1	19
> 5. M/S	331	5	-1	43
2. STABILITY GROUP				
CLASS C+D	1247	5	2	14
CLASS E	1478	5	-1	19
CLASS F	1111	4	-4	35

COMPARISON OF ALL OBSERVED AND PREDICTED
RELATIVE CONCENTRATION VALUES (12**(-5) S/M**3)
PAIRED IN TIME AND LOCATION
(FOR VARIOUS DATA SETS)
MODEL: IMPACT
FOR THE 1-HOUR AVERAGING PERIOD
CINFER CONE BUTTE (1960)

DATA SET

NUMBER
OF
EVENTS

AVERAGE
OBSERVED
VALUE

AVERAGE
DIFFERENCE
(OBS-PRED)

STANDARD
DEVIATION
OF RESIDUALS

ALL

1636

6

3

12

BY RELEASE DISTANCE/
RELEASE HEIGHT

DISTANCE < 900. M
H< 16. " 155
H=16. " 10 26. " 410
H> 26. " 260

6
5
10

7
2
13

15
12
23

DISTANCE > 900. M
H< 16. " 308
H=16. " 10 26. " 1771
H> 26. " 214

6
6
3

7
3
3

12
10
5

METEOROLOGICAL CONDITION

1. WIND SPEED
< 0.5 M/S 2472
0.5 TO 1. M/S 1037
> 1. M/S 331

6
6
6

3
3
3

13
10
5

2. STABILITY GROUP
CLASS C+D 1247
CLASS E 1478
CLASS F 1111

6
6
4

6
3
2

13
11
10

TECHNICAL REPORT DATA <i>(Please read Instructions on the reverse before completing)</i>		
1. REPORT NO. EPA-450/4-84-017	2.	3. RECIPIENT'S ACCESSION NO.
4. TITLE AND SUBTITLE Evaluation of Complex Terrain Air Quality Simulation Models	5. REPORT DATE June 1984	6. PERFORMING ORGANIZATION CODE
	8. PERFORMING ORGANIZATION REPORT NO.	
7. AUTHOR(S) David J. Wackter & Richard J. Londergan	10. PROGRAM ELEMENT NO.	
9. PERFORMING ORGANIZATION NAME AND ADDRESS TRC Environmental Consultants 800 Connecticut Boulevard East Hartford, CT 06108	11. CONTRACT/GRANT NO. 68-02-3514	
	13. TYPE OF REPORT AND PERIOD COVERED	
12. SPONSORING AGENCY NAME AND ADDRESS U.S. Environmental Protection Agency OAQPS, MDAD, SRAB (MD-14) Research Triangle Park, N.C. 27711	14. SPONSORING AGENCY CODE EPA-450/4-84-017	
	15. SUPPLEMENTARY NOTES	
16. ABSTRACT <p>This report summarizes the results of a comprehensive evaluation of eight air quality models applicable to complex terrain. Seven of the models are "Gaussian" and one is "numerical." The models are evaluated with data obtained from two field measurements programs. The Cinder Cone Butte data base is for tracers released upwind of a dense sampler network for a limited number of hours. The Westvaco data base contains a year of routine hourly SO₂ measurements for an 11 station network. The report includes numerous tabulations of each model's performance in terms of statistical measures of performance recommended by the American Meteorological Society.</p> <p>The purpose of the report is two-fold. First, it serves to document for the models considered, and similar models, their relative performance. Second, it provides the basis for a peer scientific review of the models. To stay within the spirit of this latter purpose, the report is limited to a factual presentation of information and performance statistics. No attempt is made to interpret the statistics or to provide direction to the reader, lest reviewers might be biased.</p>		
17. KEY WORDS AND DOCUMENT ANALYSIS		
a. DESCRIPTORS	b. IDENTIFIERS/OPEN ENDED TERMS	c. COSATI Field/Group
Air Pollution Mathematical modeling Meteorology Power Plants Sulfur Dioxide Statistical Measures Performance Evaluation	Air Quality Impact Assessment New Source Review	
18. DISTRIBUTION STATEMENT Release to public	19. SECURITY CLASS (This Report) Unclassified	21. NO. OF PAGES 244
	20. SECURITY CLASS (This page) Unclassified	22. PRICE

U.S. Environmental Protection Agency
Region V, Library
230 South Dearborn Street
Chicago, Illinois 60604