United States
Environmental Protection
Agency

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

EPA-454/R-95-006
December 1995

AIR

INTERAGENCY WORKGROUP ON AIR QUALITY MODELING (IWAQM): ASSESSMENT OF PHASE 1 RECOMMENDATIONS REGARDING THE USE OF MESOPUFF II

INTERAGENCY WORKGROUIP ON AIR QUALITY MODELING (IWAQM): ASSESSMENT OF PHASE 1 RECOMMENDATIONS REGARDING THE USE OF MESOPUFF II

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April 1995

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PREFACE

A memorandum of understanding (MOU) was developed by interested Federal agencies, viz. the Environmental Protection Agency, the U.S. Forest Service, the National Park Service, and the U.S. Fish and Wildlife Service, to provide a focus for development of technically sound, regional air quality models for regulatory assessments of pollutant source impacts on Federal Class I areas. Based on this MOU the Interagency Workgroup on Air Quality Modeling (IWAQM) was formed. Although no States are signatories, their participation in IWAQM functions is explicitly noted in the MOU.

The Guideline on Air Quality Models (Code of Federal Regulations, Appendix W to Part 51) suggests MESOPUFF II may be considered on a case-by-case basis for use for assessing long range transport impacts. In the interim recommendations (EPA, 1993), IWAQM outlined a manner in which MESOPUFF II might be applied in such instances. This report documents results from a case study to apply the MESOPUFF II air quality modeling system following the IWAQM interim recommendations.

As will be seen in the discussion, limitations in resources necessitated only partial implementation of the interim recommendations. This was deemed acceptable because the purpose of the exercise was not to develop a meaningful assessment of actual air pollution impacts, but was to identify and summarize the decisions made; record and summarize the resolution process for these decision; and provide a written record of the resources used to complete the effort. The contractor was given a free hand in suggesting and implementing strategies to automate processes and to accelerate the computations. Acceptance of these or similar strategies in an actual assessment can only be addressed on a case-by-case basis involving the relevant review authorities in the context of an actual situation.

IWAQM concludes that the findings confirm the need for active interaction between applicant and all the reviewing authorities (EPA, State, Federal Land Managers), and that this interaction should occur as soon as is feasible. Such interaction is needed to confirm the assessment endpoints of interest from the Federal Land Managers. Assessments involving Air Quality Related Values are evolving as experience is gained. It would be erroneous to believe that the previous report, EPA (1993), and this report provides all the information needed to define the modeling requirements. For instance, when IWAQM first issued its suggestions regarding regional haze assessment, (EPA, 1993), one hour visibility impacts were considered appropriate by the Federal Land Managers participating in IWAQM. When IWAQM asked the contractor to perform the analyses summarized in this report, 3-hour visibility impacts were deemed appropriate. As of the release of this report, consideration is being given to 24-hour impacts as providing a better representation of regional haze impacts than 3-hour impacts.

The IWAQM members anticipate issuing additional publications related to progress toward meeting the IWAQM goals and objectives, the results of model evaluation studies, proposed and recommendations on modeling systems for regulatory applications, and other topics related to specific objectives in the MOU.

ACKNOWLEDGEMENTS

The members of IWAQM acknowledge the special efforts of H. Andrew Gray, Mary P. Ligocki and Christopher A. Emery of Systems Applications International in conducting the analyses and summarizing the results presented in this report under EPA Contract No. 68-D-30019, Work Assignment 2-94 with John S. Irwin as the Work Assignment Manager.

The members of IWAQM acknowledge the peer review comments provided by several separate groups. We found the comments to be insightful and helpful towards providing a complete and understandable description of work. Recognizing the constraints of resources and time, every effort was made to address the comments received. Despite everyone's assistance, however, some errors and inadequacies no doubt exist, which of course are IWAQM's sole responsibility. Review comments were received from:

Utility Air Regulatory Group (UARG) comments received from Robert J. Paine and David W. Heinold of ENSR Consulting & Engineering, commissioned by Lucinda Minton Langworthy of Hunton & Williams.

Stephen F. Mueller of the Tennessee Valley Authority.

Northeastern States for Coordinated Air Use Management (NESCAUM) comments coordinated by Paul Wishinski of the Vermont Air Pollution Control Division.

Southern Appalachian Mountains Initiative (SAMI) comments received from Kenneth L. McBee of the Virginia Department of Environmental Quality.

Western States Air Resources (WESTAR) comments from Clint Bowman of Washington Department of Ecology, Patrick Hanrahan of the Oregon Department of Environmental Quality, and Steven F. Weber of the North Dakota Division of Environmental Engineering.

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Acronyms and Abbreviations

AIRS	Aerometric Information Retrieval System
AQRV	Air Quality Related Value
BBS	Bulletin Board Service
CD144	standard 144 column format for surface weather observation data
DRI	Desert Research Institute (University of Nevada, Reno)
EPA	Environmental Protection Agency (U.S.)
FLM	Federal Land Manager
IMPROVE	Interagency Monitoring of Protected Visual Environments
IWAQM	Interagency Workgroup on Air Quality Modeling
JRFW	James River Face Wilderness
km	kilometer
MB	mega-byte (computer disk storage)
mb	millibar (atmospheric pressure)
MESOFILE	postprocessing program for MESOPUFF II
MESOPAC	meteorological preprocessing program for MESOPUFF II (the version used is MESOPAC II)
MESOPUFF II	mesoscale puff model; version II (all other program names in this report are **boldface**)
MHz	megahertz
MM4	mesoscale meteorological model (four-dimensional data assimilation)
NCDC	National Climatic Data Center
NFS	National Forest Service (U.S.)
NPS	National Park Service (U.S.)
OAQPS	Office of Air Quality Planning and Standards (U.S. EPA)
PC	personal computer
PM_{10}	particulate matter with aerodynamic diameters less than or equal to 10 microns
QA	quality assurance
SAI	Systems Applications International (San Rafael, California)
SCRAM	Support Center for Regulatory Air Models
SNP	Shenandoah National Park
TD-3240	standard format for precipitation measurement data
TD-6200	standard format for upper air sounding data
UTM	Universal Transverse Mercator (coordinate projection)
VDEQ	Virginia Department of Environmental Quality
WBAN	National Weather Service station identifier
WRCC	Western Regional Climate Center (@DRI)

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1 INTRODUCTION

Recognizing the immediate need within the permitting community for evaluating the impacts of sources of air pollution located more than 50 kilometers from Class I wilderness areas and national parks, the Interagency Workgroup on Air Quality Modeling (IWAQM) drafted an interim Phase 1 recommendation from existing "off-the-shelf-techniques" (EPA, 1993). The interim approach recommended the use of the Lagrangian puff model, MESOPUFF-II (Scire et al., 1984), to evaluate the impacts of pollutants from sources located more than 50 kilometers from Class I areas, and up to several hundred kilometers from Class I areas. The impacts of concern are the allowable Prevention of Significant Deterioration (PSD) Class I increases in pollutants (increments), the National Ambient Air Quality Standards (NAAQS), and the Air Quality Related Values (AQRVs). AQRV impacts include such effects as visibility degradation and acidic deposition. The interim recommendation was envisioned as suitable for single source impact analyses, as well as for multiple source (cumulative) impact analyses.

It is important to note that by restricting the modeling techniques to "off-the-shelf," certain limitations were incurred. These include limits in considering the effects of terrain on long range transport and dispersion, an underestimation of the conversion of sulfur dioxide to sulfate when polluted air interacts with clouds, and an overestimation of particulate nitrate when a limited number of sources are considered. Furthermore, the estimations of the impacts of sources on regional visibility are simplistic and do not account for all of the processes important to regional visibility. Nonetheless, the IWAQM considers the techniques to provide a useful assessment of air quality impacts in Class I areas.

In the course of developing the Phase 1 interim recommendations, it was recognized that even if the modeling techniques could be agreed upon between the various federal agencies, there would still remain both technical and policy issues in implementing an assessment of pollutant impacts on a Class I area. In general, the fact that Class I area analyses focus on a fixed piece of real estate sets them apart from Class II analyses. In Class II analyses, the area of concern is a circular area (typically of radius 50 kilometers or less) centered on the source in question; whereas in Class I analyses the source and the Class I area are usually separated by a significant distance. This occasions a unique set of issues which need consideration from and cooperation among a variety of organizations, given the need to assess the incremental increase in concentration values, the need to evaluate AQRVs, and the added role of the Federal Land Mangers (FLMs).

STUDY OBJECTIVES

In an attempt to address some of the concerns unique to Class I area analyses, it was decided that a case study would be conducted to apply the MESOPUFF II air quality modeling system following the IWAQM interim recommendations (EPA, 1993). This study would identify and summarize the decisions made, would record and summarize the resolution process for these decisions, and would provide a written record of the resources used to complete the effort. The objective was to learn by experience where the difficulties are in the process of conducting such an analysis, and when possible, to provide a means for resolving these difficulties. It was not an objective to provide a meaningful assessment of PSD, NAAQS or AQRV impacts for the Class I areas considered in the study. As will be seen in the following discussion, on several occasions significant departures were made in conducting this study from that which would be expected if a realistic assessment were to be developed. For instance, the source inventory considered only some of the states surrounding the Shenandoah National Park and the James River Face Wilderness, and thus is incomplete. And in order to conserve resources, the sources were consolidated into ten surrogate sources for the purposes of this study. These departures allowed the emphasis of the project to be focused on a critique of the process and resource needs, which were the primary study objectives.

A realistic assessment, following the interim IWAQM recommendations, would require that all important sources be modeled (without consolidation). If the modeling objective is to determine PSD impacts, then all relevant sources that consume PSD increment must be considered. If one desires to determine the impact of a single new (or modified) source, then the PSD increment from the new source must be added to all pre-existing PSD sources. It would be possible to model the impacts from a single source and then add those impacts to prior MESOPUFF II results, assuming the prior results were available. If not, it would be necessary to model all relevant PSD sources to assess the total PSD increment consumed.

The demonstration modeling assessment described in this report did not completely follow IWAQM's interim recommendations. One of the goals of the study was to perform the demonstration assessment using the MESOPUFF II modeling system as developed for a personal computer (PC) system. This presented some significant limitations regarding the ability to follow the interim IWAQM recommendations. As an example, for a realistic assessment of multiple sources, the interim IWAQM recommendations require that two five-year MESOPUFF II modeling exercises be conducted; one run using all relevant sources to determine impacts to secondary NAAQS pollutants (secondary particulate matter) and AQRVs (visibility and deposition), and a second model run using only sources beyond 50 km from a receptor for SO_2 and NO_x (and primary PM_{10}). The MESOPUFF II results for SO_2 and NO_x are then to be added to results from a Gaussian model (such as **ISCST2**) for sources within 50 km of the receptor. In the MESOPUFF II modeling demonstration described in this report, only one run was performed (for three years) using sources beyond 50 km of Shenandoah National Park. The MESOPUFF II results (for one month) were added to **ISCST2** results to demonstrate the integration process.

STUDY APPROACH

In order to assess the impact of implementing the Phase 1 recommendations, and ultimately to improve the Phase 1 modeling system, the following tasks were carried out:

- The MESOPUFF II model and associated processors were tested using the example problem intended for Support Center for Regulatory Air Models bulletin board (SCRAM BBS) distribution.

- The SCRAM BBS example problem computer files were evaluated and some suggested improvements were implemented.

- A five-year meteorological data set suitable for input to the MESOPUFF II model was developed for a multi-state area surrounding Shenandoah National Park.

- A modeling protocol was developed that outlined the approach and procedures to be followed in the MESOPUFF II demonstration modeling assessments.

- Demonstration model simulations were performed for the assessment of visibility, acidic deposition, and PSD increments for a set of real sources in the states surrounding Shenandoah National Park.

- Model simulations were performed to test the sensitivity of concentrations to the distance between sources and receptors using a set of "pseudo" sources placed in successive rings around Shenandoah National Park.

- An assessment report was developed (this report), documenting the modeling process, and the results obtained.

Throughout the project, there has been coordination with IWAQM members and coworkers regarding implementation of the Phase 1 recommendations for assessing visibility and acidic deposition impacts in Federal Class I land associated with the Shenandoah National Park. IWAQM members representing FLMs (National Park Service, NPS; and National Forest Service, NFS), have provided assistance in modeling protocol related to the determination of visibility and acid deposition in Class I areas. The Virginia Department of Environmental Quality (VDEQ) and the EPA Region III office provided assistance and guidance regarding receptor locations, emission source data collection, and PSD source selection. The Office of Air Quality Planning and Standards (OAQPS) provided direct oversight of the project. The IWAQM members who participated in this study are listed in Appendix A.

This report documents the procedures followed to demonstrate the implementation of the Phase 1 recommendations for assessing the PSD and AQRV impacts at Class I area land associated with Shenandoah National Park. Section 2 describes the testing of the SCRAM BBS example problem and the improvements made to those files. Section 3 describes the development and application of the MESOPUFF II modeling system for assessing the impacts

of regional point sources on Shenandoah National Park. Section 4 describes the analysis performed to assess the relationship between distance of a source and impact at a receptor in the park. The study results are summarized in Section 5, including a discussion of what was learned during the modeling process.

The technical approach for this study is described briefly below:

Testing of the Example Problem

The MESOPUFF II software and documentation were retrieved from the SCRAM BBS, installed on a PC, and run for the example problem. The model output was compared with the sample output provided to ensure that the model was running properly on our system. Errors and/or omissions in the model documentation were identified.

A set of recommended improvements for the MESOPUFF II system and example problem were developed. The recommended improvements considered input files, documentation and user instructions, and modifications to the MESOPUFF II code. The recommended improvements were implemented and a revised version of the MESOPUFF II PC files were placed on the SCRAM BBS.

Demonstration Application of MESOPUFF II to Shenandoah National Park

MESOPUFF II was applied to the estimation of PSD and AQRV impacts at Shenandoah National Park as a demonstration of implementing the IWAQM interim (Phase 1) recommendations. The necessary data were collected and processed, including meteorological, emissions, receptor, and land use data. Data processing procedures were developed to prepare model inputs and for postprocessing of model output. The process involved in implementing the IWAQM Phase 1 recommendations was documented, including the identification and resolution of key modeling issues and the resources used to complete the application. The products of this application were: (1) an assessment of the experience in performing the modeling exercise, including suggestions for improving the Phase 1 recommendations, (2) a demonstration assessment of the impacts at Shenandoah National Park for a set of PSD sources surrounding the park, and (3) a five-year meteorological data set, to be made available for distribution.

Application of MESOPUFF II for Distance versus Impact Analysis

In addition to the application intended to demonstrate the use of MESOPUFF II to assess the impacts of real PSD sources on Shenandoah National Park, a second analysis was performed to provide some indication of the relationship between distance of a source and impact at a receptor in the park. MESOPUFF II was applied to assess the impacts of sources placed on rings at specific distances from Shenandoah National Park.

2 REVIEW OF THE SCRAM BBS FILES AND EXAMPLE PROBLEM

The Support Center for Regulatory Air Models bulletin board (SCRAM BBS) maintains a number of air quality models for distribution, including the MESOPUFF II modeling system. The SCRAM BBS MESOPUFF II modeling package consists of the model and processors, associated documentation, and an example problem. The initial task in evaluating the IWAQM Phase 1 recommendations regarding MESOPUFF II was to review these BBS distribution files and example problem, and suggest improvements to the package.

EVALUATION OF SCRAM BBS FILES

We were successful in locating and retrieving the MESOPUFF II modeling package and associated documentation from the SCRAM bulletin board. Downloading the four MESOPUFF II "zipped" files required approximately three hours (at 2400 baud rate). No problems were encountered in expanding the files and executing the test case. The test case output obtained on our system (PC/486) was identical to that provided with the model, and no problems were encountered in the actual mechanics of running the model. In addition, **WordPerfect** files for MESOPUFF II documentation were downloaded from SCRAM and printed. No problems were encountered with that operation.

It should be noted that no test case was provided for the first MESOPUFF II meteorological pre-processor, called **READ62**. Thus, this processor was not tested. **READ62** reads upper-air meteorological data from tape. Between the execution of **READ62** and the execution of **MESOPAC**, the user must fill in missing data by hand. This process is likely to cause more difficulties than the actual execution of the model. As will be described later in this report, a significant investment of manpower is necessary to create the input files for MESOPAC.

Some omissions were identified in the instructions provided for executing the test case that might cause confusion for new users. In addition, suggested improvements were made to the test case post-processing files. Each of these is described in detail below. During the testing process, one error in an input file supplied for the test case and one error in the model code itself were identified. These are also described below.

Instructions for Executing the Sample Problem (README.TXT)

The text file README.TXT was included in one of the MESOPUFF II "zipped" files. It begins with a discussion of how to "unzip" the files, which appears unnecessary since users who do not know how to unzip files will not be able to access README.TXT.

The next paragraph discusses disk space and memory requirements. We recommended that a statement be added that an 8087 math coprocessor or equivalent capability is required to run the model. Also, the total disk space required (12.65 MB) should be included. The disk space required for each of the unzipped files is listed, but the total disk space needed is larger, since the zipped and unzipped files must co-exist for at least a short time. It should be stated that an additional 2.57 MB are required to execute the test case, bringing the total disk space requirement to 15.22 MB.

The next section discusses documentation for the model and its application. The 1984 version of the User's Guide is cited, rather than the revised 1993 User's Guide. Since several changes have been made in the model and associated processors since 1984, we recommended that the 1993 Revised User's Guide be cited, and perhaps even included in the documentation available from SCRAM. (Key sections of the 1993 Revised User's Guide will be made available by EPA in the near future.)

The following sections describe how to execute the test case. A typographical error was found in the description of step 4, where it states that the user should type "MESOPAC" to run the model, rather than "MESOPUFF". Also, in that section it states that three output files are created, when actually four output files are created. The missing file is PUFF.LST. It might also be helpful to indicate that all output files with the .DAT extension are binary files, whereas those with .LST extensions are ASCII text files.

In step 6, the instructions for executing the **MESOFILE** post-processor are not provided. A line should be added stating that the user should type "FILE" to run the post-processor. If the user types "MESOFILE" rather than "FILE", an error message will result.

Error in Input File PUFF.INP

This file contains all non-meteorological parameters needed to run MESOPUFF II, including modeling domain definition, number of pollutants, and source and receptor information. Line 14 of this file contains chemistry parameters, including the background ozone concentration (CO3B) and the background ammonia concentration (CTNH3). For the test case, the value of CO3B is set to 80 ppb and the value of CTNH3 is set to 10 ppb. These are the default values specified for these parameters (Scire et al., 1984). However, these values were read by MESOPUFF II as 8.0 ppb and 1.0 ppb, respectively, because the decimal point was omitted in the input file. The values read by the model are echoed to the output file, PUFF.LST, which provided confirmation of the error.

The background O_3 value is not critical in the test case because hourly ozone values are provided. However, the background value is used to fill in for missing hourly data. The error in CO3B should be corrected because users are likely to copy the test case input file for use in other applications and may believe that they are using a value of 80 ppb rather than 8 ppb.

The total ammonia concentration, on the other hand, is critical to the test case results. CTNH3 is used to calculate the distribution of total nitrate between nitric acid (HNO_3) and aerosol nitrate (NO_3^-). The NO_3^- concentration is extremely sensitive to the specification of CTNH3. Changing CTNH3 from 1 ppb to 10 ppb results in a tenfold increase in NO_3^- in the test case.

Correction to the input file can be accomplished simply by moving the CO3B and CTNH3 values one place to the left, and adding decimal points after each value.

We recommended that further thought be given to the default values of CO3B and CTNH3. The value of 80 ppb for ozone on a regional scale is higher than the values assumed for other regional modeling applications, particularly in winter. A default value of 40-60 ppb may be more appropriate for CO3B. The background ozone level is used in the model to calculate the conversion rates of SO_2 to sulfate and NO_x to nitrate. The value of 10 ppb for CTNH3 also appears quite high for a regional background level. In fact, CTNH3 should not represent the total background ammonia since the model contains no background sulfate or nitrate for the sources not being simulated. It represents what could be termed "excess ammonia", the amount remaining after background sulfate and nitrate have been fully neutralized. Given this, 10 ppb is almost certainly an upper bound; hence, aerosol nitrate concentrations predicted by MESOPUFF II may represent upper bounds. A more representative value for the excess ammonia concentration in the eastern U.S. is between 0.5 and 3 ppb, depending on the season. For the test case, however, we recommended that the values of 80 ppb (for ozone) and 10 ppb (for ammonia) be retained, since they are the default values given in the existing documentation.

Error in MESOPUFF II Subroutine CHEMTF

The model code was not scrutinized in detail for this task. However, one error was found in the chemistry subroutine CHEMTF. In calculating the concentration of ammonia that is available to combine with nitric acid to form aerosol nitrate, the amount of ammonia taken up by sulfate is subtracted from the total ammonia:

```
CANH3 = CTNH3 - PPB(2)
```

The equation should read:

```
CANH3 = CTNH3 - 2.*PPB(2)
```

because ammonium sulfate contains two ammonium ions per sulfate ion.

Test Case Post-Processing Files

The test case input files for the **MESOFILE** postprocessor only calculate 24-hour average concentrations and deposition rates for a single species, SO_2. If the model is to be used for

visibility and acid deposition assessments, much more postprocessing will be required. **MESOFILE** is configured such that only one pollutant can be processed at a time. Thus, the user must either run a large number of small post-processing jobs for each MESOPUFF II simulation, or set up a file that will execute all desired **MESOFILE** runs in the appropriate order. A test case example would be helpful in demonstrating how such a file could be set up, and illustrating some of the additional features of **MESOFILE**.

We recommended that the test case postprocessing files be expanded to provide, at a minimum, 24-hour average concentrations and deposition rates for all five species. It might be desirable to calculate cumulative total (wet plus dry) deposition for total sulfur and total nitrogen. These calculations can be accomplished with the existing **MESOFILE** system. In order to calculate visibility parameters such as extinction, additional software development would be needed. Therefore it does not appear feasible at this time to expand the post-processing test case to include extinction calculations.

IMPLEMENTATION OF IMPROVEMENTS

Three recommended tasks were identified:

(1) Correct and expand the instructions for running the test case in README.TXT.

(2) Expand the test case post-processing files.

(3) Modify the PUFF.INP file to correct the format errors in CO3B and CTNH3, and modify the CHEMTF code to correct the CANH3 calculation.

The first task was implemented to correct and expand the instructions for running the test case. The README.TXT was updated, including editing the few typographical errors, and adding more detailed disk space information.

The second task, development of new post-processing software, was not included in the revised SCRAM BBS example files because sufficient documentation on the postprocessing program (**MESOFILE**), contained in the 1993 MESOPUFF II User's Guide, was not yet available on the SCRAM. However, for the distance versus impact analysis (see section 4 of this report), a post-processing procedure using MESOFILE was developed and applied.

The third task was approved and implemented. The SCRAM BBS files were revised to reflect the changes to PUFF.INP and the CHEMTF subroutine.

3 DEMONSTRATION OF THE PHASE 1 MODELING SYSTEM

The primary task of this research effort was to conduct a demonstration application of the MESOPUFF II modeling system, following the IWAQM Phase 1 recommendations (EPA, 1993). At the outset, the specific air quality setting that would dictate the use of the MESOPUFF II system was undefined. The focus of the project was to go through the process of gathering and processing data, exercising the models, and analyzing results, in order to identify issues and problems that users of the MESOPUFF II modeling system would inevitably confront. In addition, because the pre-processing of meteorological data is the most time-consuming step encountered during MESOPUFF II application, an important objective was to prepare a five-year set of MESOPUFF II meteorological inputs for a multi-state region surrounding Shenandoah National Park that would be suitable for future applications.

The first step in the demonstration application was the development of a modeling protocol. The EPA protocol for MESOPUFF II (EPA 1992a) and the interim IWAQM recommendations were consulted in development of the protocol. The first draft of this document was prepared in the form of an outline, and was used as a focus for discussion in initial meetings with the IWAQM. After several key issues were resolved, a more detailed modeling protocol was prepared. This document identified a proposed modeling domain and proposed approaches for development of inputs and processing of outputs. The issues presented in the modeling protocols, and the decisions that were ultimately made regarding modeling protocol, are presented in the remainder of this section.

In order for the results of the demonstration application to have some value, beyond simply demonstrating that the Phase 1 modeling system could be exercised, the IWAQM decided that the sources to be modeled should consist of existing sources subject to PSD requirements and located within 200 km of Shenandoah National Park.

The original modeling plan, as described in the protocol, was to:

- Prepare 5 years (1988-92) of meteorological data using **MESOPAC**, suitable for future applications in the region.

- Simulate 5 years (1988-92) with MESOPUFF II using a single set of PSD sources. The results would indicate the cumulative PSD increment and AQRV impacts due to all the modeled sources.

As the source data were being gathered, it became apparent that identification of "PSD sources" is not straightforward, that there are multiple triggering dates for PSD provisions for

major and minor sources and for differing locations, and that it might not be possible to identify and model all PSD sources. Some of these issues are described in Appendix B. These uncertainties diminished the possible relevance of the MESOPUFF II results but do not impair the objectives of the demonstration application.

Further discussions with IWAQM members led to the idea of reducing the scope of the PSD source application of MESOPUFF II and adding an additional analysis using hypothetical sources. A proposal was developed, whereby the original scope would be changed to:

- Prepare 5 years (1988-92) of meteorological data using **MESOPAC**, suitable for future applications in the region. This task would remain the same.

- Simulate 3 years (36 contiguous months selected from 5 year period 1988-92) using MESOPUFF II with selected PSD sources, using actual source data collected from EPA Region III states.

- Perform 24 additional MESOPUFF II simulations using hypothetical sources at varying distances from Shenandoah NP to provide some insight into the relationship between distance from Shenandoah NP and potential PSD and AQRV impacts.

This modified modeling approach still accomplished the original objectives of preparing 5 years of meteorological data for future applications, going through and documenting the modeling process for actual PSD sources, and using the modeling results to evaluate the long-term PSD and AQRV impacts (over a 3-year period, instead of 5 years). By modifying the scope in this way, the total number of MESOPUFF II simulations remained constant, and the additional effort to prepare the source ring data was not significant. Hence, we were able to obtain two useful modeling results instead of just one, and did not relinquish the original objectives of the demonstration modeling exercise.

The remainder of this section describes model input preparation and application for the PSD source analysis. This section is structured to provide discussions of issues, proposed approach (protocol), problems, and resolutions for each step of the modeling process. The impact versus distance analysis is described in Section 4.

MODELING DOMAIN DEFINITION

MESOPUFF II is suitable for simulating the mesoscale transport and dispersion of air pollutants from a source or group of sources, and estimating their impacts on remote receptors at distances of ten to hundreds of km downwind (Scire et al., 1984). The MESOPUFF II modeling system utilizes three modeling grids. The meteorological grid is the largest; the computational grid may be smaller than the meteorological grid or the same size, but must be of the same resolution. The sampling grid may be smaller than the computational grid and may be of higher resolution. The errors resulting from the projection of a curved surface onto a

rectangular grid become more pronounced for larger dimensions. Maximum recommended dimensions for the modeling domain of 1000 km in the east-west direction and 600 km in the north-south direction are suggested. Grid resolution is recommended to range from 10 to 50 km, based on the overall size of the domain and limitations in data storage.

Meteorological Domain

This domain is defined through inputs to the **MESOPAC** II meteorological preprocessor (hereafter referred to as **MESOPAC**), and is the basic reference frame for all spatially varying input data to MESOPUFF II. In the Phase 1 demonstration implementation of MESOPUFF II, PSD and AQRV impacts were estimated for receptors located in and around Shenandoah National Park (SNP) and James River Face Wilderness (JRFW) in Virginia. These Class I areas are 250-300 km west of the Atlantic Coast. Prevailing winds tend to be from the southwest but range from south through northwest. Considering the regional meteorology along with known PSD source emission distributions in the eastern U.S., we suggested in the protocol that the meteorological domain extend further to the west from SNP than it does to the east. Consequently, we developed a preliminary domain to cover a full 1000 by 700 km region, extending about 300 km to the north, east and south of SNP, and 500+ km to the west.

We then proposed two optional extensions to this domain. In the first option, the southern boundary of the preliminary domain could be extended southward by 100 km to encompass a larger potential source region, which could strongly impact the Shenandoah area under prevailing southwest flow conditions. In the second option, the northern boundary could similarly be extended 100 km northward, which would encompass the important source regions of northern Ohio as well as include all of EPA Region III.

Although both extensions would safely contain (within an ample number of buffer cells) all potential source areas to be modeled by future MESOPUFF II applications, we proposed implementing the preliminary 1000 by 700 km domain (without extensions) for the Phase 1 MESOPUFF II demonstration. This decision was primarily based on projected data and storage requirements and the fact that the longitudinal and meridional extents of the preliminary domain were at recommended limits. Beyond these issues, however, we felt that this grid represents the best balance between adequate geographical coverage and the performance limits of the MESOPUFF II model; i.e., sources located in regions beyond the boundaries of this grid would not be well modeled by MESOPUFF II as the model was not designed for travel distances beyond 500 km. Further, although application of MESOPUFF II will not necessarily utilize the full meteorological domain in this or future studies, it was desirable to generate relatively well resolved meteorological fields on a large regional domain so that we could establish a flexible meteorological database for future MESOPUFF II applications.

Recommended grid spacing for MESOPUFF II is 10-50 km. The IWAQM selected a grid spacing of 20 km for the demonstration study. To minimize storage and CPU requirements, grid spacing of 40 or 50 km could have been used, but may have degraded model estimates.

We had also recognized that future coordination with MM4 (to be used in Phase 2) modeling grid definition may have been desirable, although differences in mapping projections between the two models would have to be addressed.

Figure 3-1 displays the final meteorological domain selected for the Phase 1 demonstration. By specifying a grid size of 20 km, an array of 35 by 50 grid points covers the recommended 1000 km by 700 km domain within the 100 by 100 grid limit currently set in **MESOPAC** and MESOPUFF II. We had estimated in the protocol that the resulting five years of hourly meteorological data generated on this grid would require about 3.3 gigabytes of storage.

Computational Domain

All sources and receptors to be modeled must be contained within the computational domain. Puffs are not tracked after they leave this grid. Overall size of this domain can be set equal to the full dimensions of the meteorological domain, or specified to occupy a subset of the grid. All sources and receptors should be at least 20-50 km from the boundaries of this grid to avoid underestimating concentrations by immediately losing puffs from near-boundary sources and/or missing short-term recirculation events at near-boundary receptors. The size of the computational domain does not affect the volume of output produced, but does affect the CPU requirements of the modeling. Grid spacing must be the same as the meteorological domain.

For the demonstration study, sources were to be located as far as 200 km from SNP. Provision for a 4 grid (80 km) buffer zone on all sides of this source region yielded a computational domain of 30 by 30 grid points (Figure 3-1; dotted inset). We proposed using this smaller computational grid, rather than the entire meteorological domain, to minimize computing requirements while still giving an adequate representation of the sources to be studied. Future studies that include different source regions can use the same meteorological fields, but specify a computational domain appropriate to the application.

Sampling Domain

MESOPUFF II allows output concentrations and fluxes to be reported for both gridded and non-gridded receptors. Gridded receptors consist of all grid points within a user specified sampling domain. Non-gridded receptors can be located anywhere within the computational domain. Gridded receptor concentrations and fluxes can be used to produce spatial isopleth maps; as such, specification of a sampling grid is useful for general characterizations of an area.

The sampling domain may be specified as a subset of the computational domain, with a maximum of 40 by 40 grid points. Grid spacing may be smaller than on the meteorological and computational grids. This is accomplished by specifying an integral number of divisions of the computational grid spacing (usually 2). Note that an increase

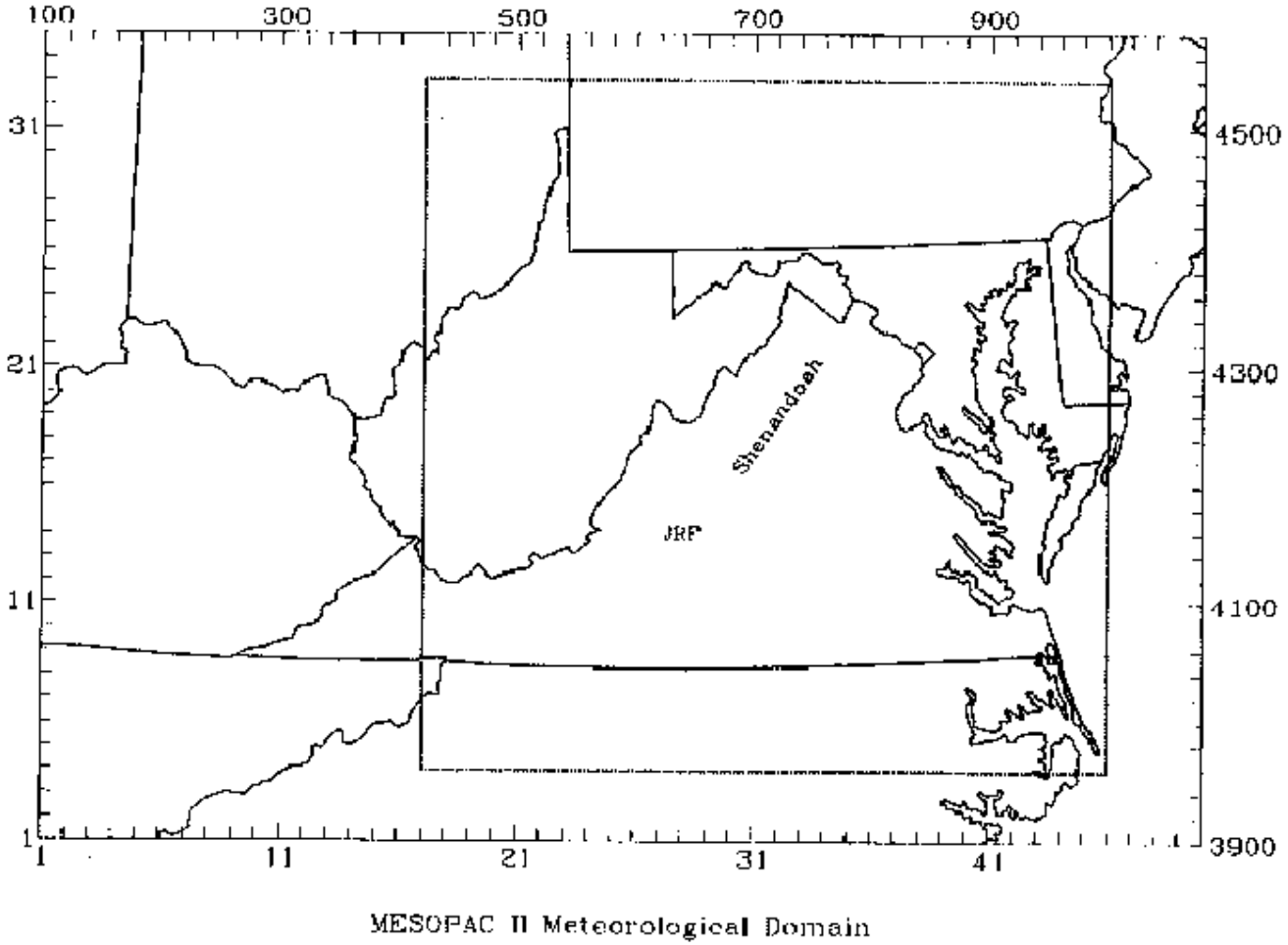

Figure 3-1. The MESOPAC II meteorological modeling domain. Dotted inset denotes the area covered by the MESOPUFF II computational domain. The approximate locations and extent of Shenandoah NP and James River Face W are displayed.

in the number of divisions reduces the overall coverage of the sampling domain when the maximum number of grid points are specified. Since the size/resolution of the sampling domain controls the amount of MESOPUFF II output produced, it should not be larger than absolutely necessary.

In preparing the Phase 1 demonstration protocol, we recognized that the use of gridded receptors greatly increases the amount of output produced by MESOPUFF II. In an effort to control MESOPUFF II computation time and the size of sampling output we did not anticipate using the sampling grid in the demonstration application of MESOPUFF II. Model concentrations and fluxes were calculated at non-gridded receptor locations only.

Non-Gridded Receptor Locations

As discussed in the protocol, receptor sites were to be located within SNP and JRFW. Receptor sites within SNP were to be distributed in a manner that represented the entire park, but not so densely that nearly identical results would be obtained at neighboring receptors. For a grid spacing of 20 km and sources located 50 to 200 km from the park, a spacing between receptors of 5-10 km was expected to be adequate. Additionally, we had planned to place several receptors outside SNP and JRFW, between the sources and the Class I area receptors. These were to be selected after the locations of sources to be modeled had been provided. Decisions on receptor selection for future MESOPUFF II applications should be made on a case-by-case basis.

Selection of Non-Gridded Receptors

We received UTM coordinates for 200 receptor locations in SNP and 67 receptor locations in JRFW from VDEQ (Browder, 1993). The specification of 267 non-gridded receptors within MESOPUFF II would have resulted in larger amounts of output than would have been optimal for post-processing. Furthermore, many of the receptors were located very close together, and the model was not expected to be able to resolve the differences between them. Therefore, we selected a subset of the receptors to be used in the MESOPUFF II demonstration modeling.

A simple approach was developed to estimate the minimum spacing for which concentration differences would be modeled. Since the sources were to be at least 50 km from the receptors, we examined downwind plume widths at 50 km using the Pasquill-Gifford-Turner dispersion curves. The plume width at 50 km for D stability is approximately 8 to 9 km. Half the expected plume width, or roughly 4 to 5 km, was used as a guideline in selecting non-gridded receptors for MESOPUFF II.

Figure 3-2(a) displays the entire MESOPUFF II computational domain, where the insets denote the placement and extent of the SNP and JRFW receptor areas shown in Figures 3-2(b) and 3-2(c), respectively. Figure 3-2(b) presents the array of receptors for SNP, and identifies those selected as MESOPUFF II receptors (denoted as circles). Receptors

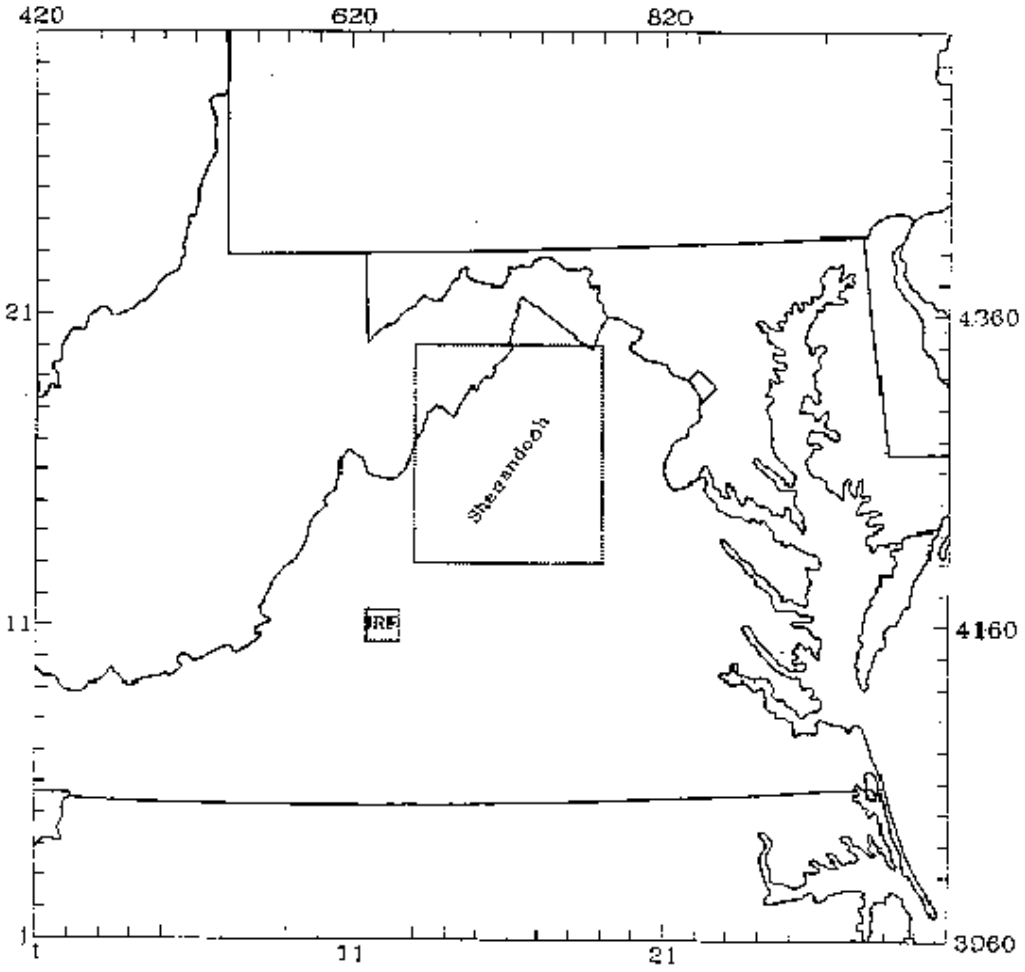

Figure 3-2(a). The MESOPUFF II computational domain. Dotted insets display the area covered by Figures 3-2(b) and (c).

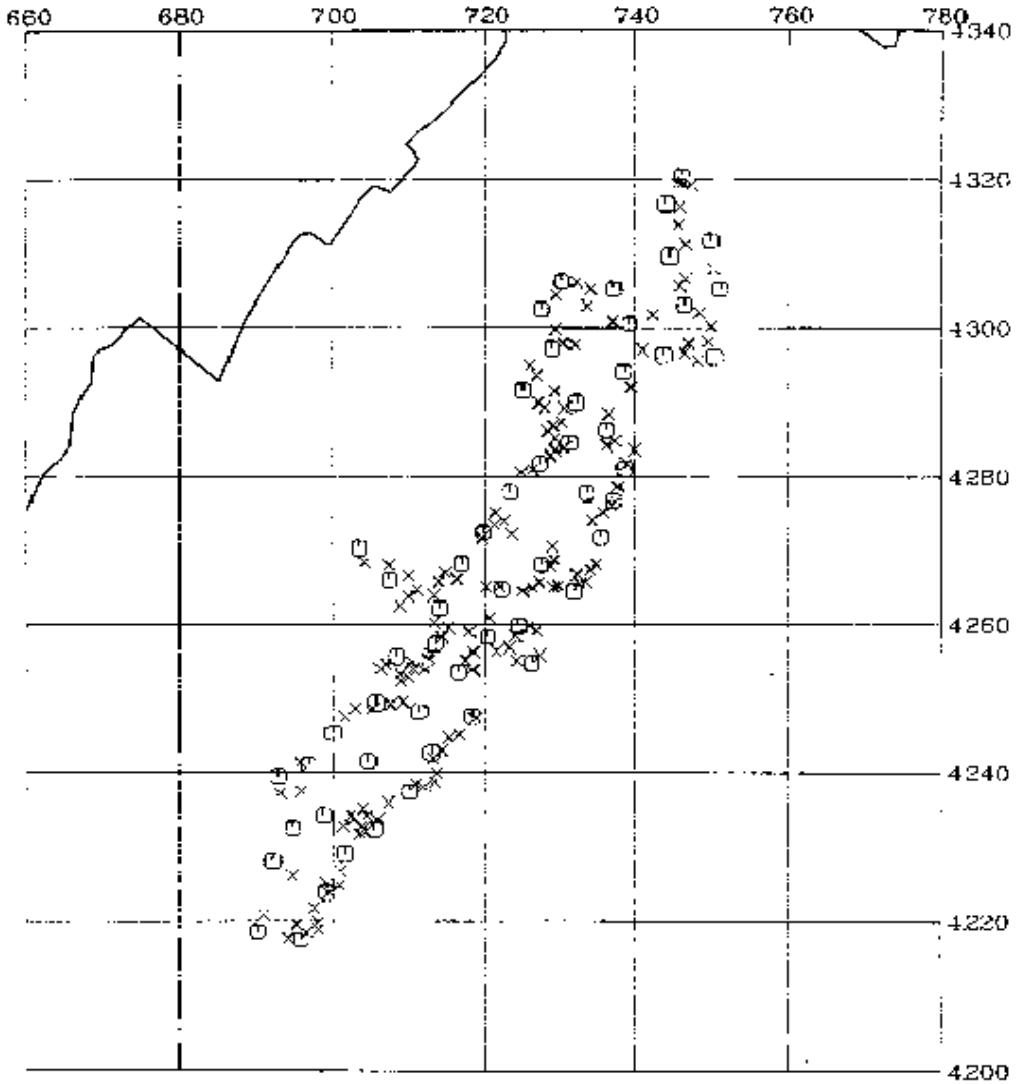

Figure 3-2(b). Non-gridded receptors located within Shenandoah NP. Circles denote receptor locations selected for the MESOPUFF II applications; the union of circles and crosses include all 200 original Shenandoah receptors. The 20 km computational grid lines are also shown.

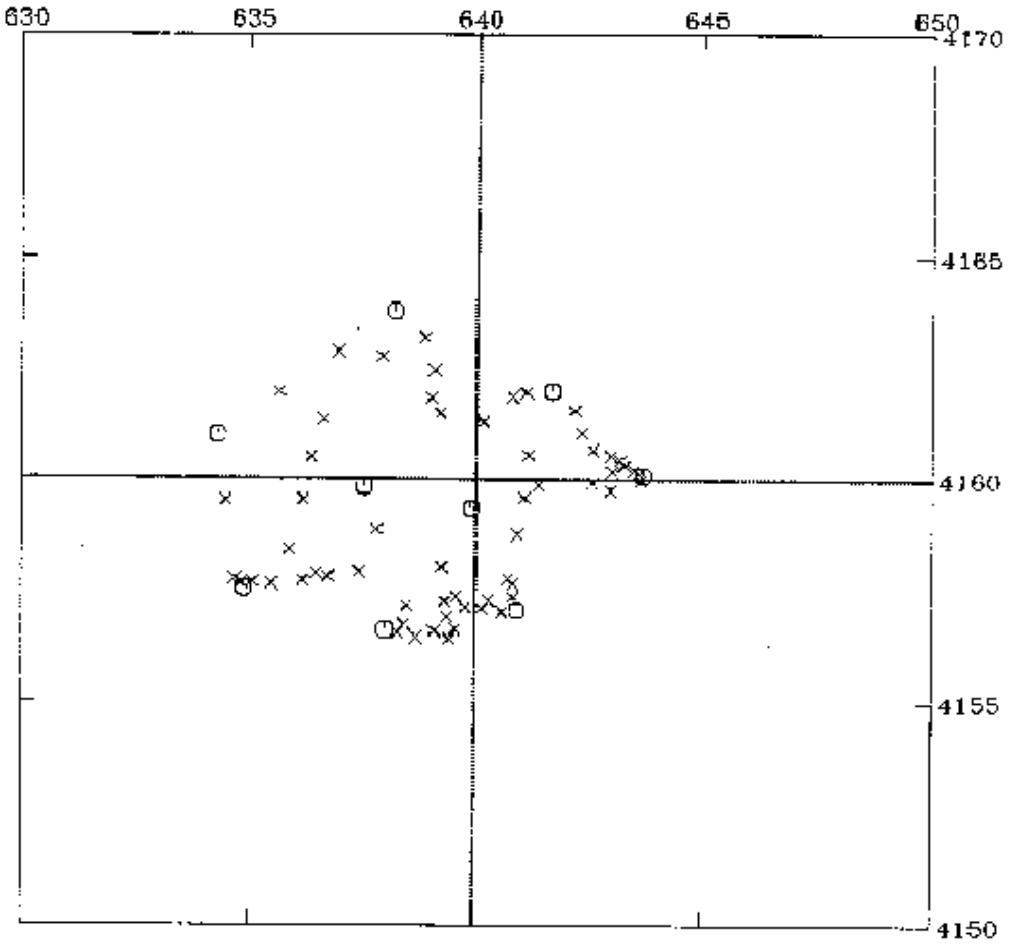

Figure 3-2(c). Non-gridded receptors located within James River Face W. Circles denote receptor locations selected for the MESOPUFF II applications; the union of circles and crosses include all 67 original James River Face receptors. The 20 km computational grid lines are shown dotted.

were selected to cover all boundaries of the park. In total, 55 of the 200 receptors were selected for modeling.

Figure 3-2(c) shows the array of receptors for JRFW, and identifies those selected as MESOPUFF II receptors (again denoted as circles). This is a much smaller region than SNP, extending less than 10 km in each direction. Nine of the 67 receptors were selected for use in MESOPUFF II.

Once receptors for the Class I areas were selected, however, no additional outside receptors were specified. Reduction in the number of PSD sources to be modeled, and consequent movement of resulting aggregated sources to average locations (to be discussed below), clouded the importance of monitoring concentrations between sources and receptors. When we considered the uncertain benefits from such an analysis, we found it difficult to justify the additional output and complications to postprocessing.

SOURCES TO BE MODELED

Selection of Sources: Issues and Protocol

MESOPUFF II can be used to simulate impacts from existing sources, proposed sources, or hypothetical sources. For the demonstration study, the IWAQM decided that existing sources that began operations since the beginning of the PSD program would be modeled. The IWAQM felt that this would provide a good foundation for future modeling in the area. In addition, since the PSD increments are expressed as the cumulative impact of all changes in emissions, it was of interest to assess how much of the available Class I PSD increments have already been "consumed" to date.

The IWAQM agreed to limit the sources to be modeled in the present study to those within EPA Region III, comprising the states of Delaware, Maryland, Pennsylvania, Virginia and West Virginia, and the District of Columbia. This decision was based upon practical considerations such as ease of communications between affected states. The IWAQM recognized from the outset that sources outside EPA Region III (located at distances further than 200 km from SNP, such as those in Ohio) also have the potential to impact air quality and deposition in SNP, and that therefore this demonstration application would not provide a complete answer of the impact of existing sources. For that reason, the meteorological modeling domain was specified to be large enough to encompass these sources and transport corridors. Sources located within EPA Region III and at a distance of between 50 km and 200 km from SNP became the focus of this study.

It was proposed that all PSD sources or a subset of sources would be modeled, depending upon the number of such sources and data availability. The identification of existing PSD sources includes the determination of a baseline date, i.e., the date after which any new construction or modification of existing sources will be considered as part of the accumulative PSD impact. A discussion of the issues involved in determining the various baseline dates (for

major and minor sources) to be applied for PSD impact analysis, determination of AQRV impacts, and the associated inventories needed for each analysis is presented in Appendix B (Cimorelli 1993).

Therefore, the actual number of sources to be modeled in the demonstration study was not specified in the modeling protocol. This caveat was also based upon recognition that the CPU time needed to run the model increases with the number of sources, and can become an important factor in the decision of number of sources to model. As originally configured, MESOPUFF II could treat up to 1000 point sources. Although MESOPUFF II can also be used for area sources, no area sources were to be modeled in this study. It is important to note that when multiple sources are included, only the cumulative effect is modeled -- individual source attribution is not possible.

For each source, the model requires location, stack parameters (height, diameter, temperature, flow rate), and emission rates of SO_2, sulfate, and NO_x. If primary non-sulfate aerosol is to be modeled, two MESOPUFF II simulations are needed, with the primary aerosol labeled "sulfate" in the second simulation. Primary non-sulfate aerosol was not to be modeled in the present study, as available resources did not allow for two sets of simulations, and since it was expected that the majority of visibility impacts due to PSD sources was to be captured by examining only sulfate and nitrate effects.

The Phase 1 recommendations state that, for sources within 50 km, MESOPUFF II should not be used to estimate PSD impacts but can be used to estimate visibility and deposition impacts. This means that in a situation where sources both closer and further than 50 km are to be modeled, two MESOPUFF II simulations would be needed, one with and one without sources within 50 km. In order to avoid the need for two model runs, it was decided that sources within 50 km of the park would not be modeled with MESOPUFF II in the demonstration study, but one or two would be modeled with **ISCST2**, in order to demonstrate the integration of MESOPUFF II and **ISCST2** results. We planned to follow the Phase 1 recommendations concerning application of **ISCST2**.

Subsequent to the development of the modeling protocol, the decision was made to conduct a parallel set of MESOPUFF II analyses using uniform idealized sources placed in rings at various distances from SNP. The ring source analysis is described in Section 4. The remainder of this section is devoted to the PSD source analyses.

Processing of PSD Source Data

For the demonstration application, source data were received from the states of Pennsylvania, Maryland, and Virginia. The data provided by Virginia also included some sources that are in the states of Maryland and West Virginia, but are traditionally included in Virginia PSD analyses. Therefore, some duplicate information was obtained for the state of Maryland. In processing these data for input to MESOPUFF II, the following operations were carried out:

1. Sources within 50 km of any SNP receptor were identified and removed. There were seven such sources, all in the state of Virginia.

2. Sources where two or more stacks are present at the same location were combined into a single source with emissions equal to the sum of the individual emissions, exit velocity equal to the average of the individual exit velocities, and stack diameters adjusted to give the appropriate total combined mass fluxes.

3. All information provided in English units were converted to metric units. Also, UTM coordinates provided in zone 18 were assigned zone 17 equivalents by first converting them to latitude-longitude and then converting back to UTM.

4. Small sources, with emissions of both SO_2 and NO_x less than 5 g/s, were excluded.

The resulting set of 27 sources is shown in Table 3-1; their locations are displayed in Figure 3-3 (indicated by crosses). Several issues arose during the processing of these sources. These issues, and our approach in resolving them, are described below:

1. Some emission totals were provided as both short-term and annual rates. In these cases, the short-term rates were used, since the model was to be used primarily to determine the highest short-term impacts. The resulting annual average impacts will overestimate the true annual average impacts.

2. There were some differences between the emission totals reported by Maryland and Virginia for several Maryland sources. In case of differences, the higher total was used.

3. In two cases, emission offsets were reported as negative emissions. Negative emissions cannot be input into MESOPUFF II. In one case, where the offset occurred at the same location as actual emissions, the offset was subtracted from the total emissions. In the other case, the offset was at a different location. This offset cannot be modeled in a single model run.

4. MESOPUFF II allows emissions of primary sulfate. The sulfur emissions data provided were in terms of SO_2 and did not specify emission levels of primary sulfate. For most fuel burning sources, primary sulfate emissions are roughly equal to 3 percent of SO_2 emissions (Cass, 1980). Therefore, for purposes of this demonstration, primary sulfate emissions of 3 percent (as sulfur) of the SO_2 emissions were included in the MESOPUFF II input file. Accounting for the difference in molecular weight between sulfate ($SO_4^=$) and SO_2, the SO_2 emission rates were multiplied by 0.045 to obtain the sulfate emission rates.

This set of 27 sources was presented to IWAQM as the set of sources to be modeled in the demonstration application. However, attempts to model these 27 sources with MESOPUFF II for the first month, January 1988, were unsuccessful. On an 386/25 MHz PC, 16 hours were required to process the first 76 hours of the simulation. Hour 77 consumed 38 CPU minutes alone. Although these CPU times would be reduced somewhat on the 486/50 MHz PC that was planned for use in the demonstration application, it would clearly be impossible to complete a full 60 months of MESOPUFF

TABLE 3-1. Original set of sources to be modeled in the MESOPUFF II demonstration application for Shenandoah NP and James River Face W.

Name	UTM-E (km)	UTM-N (km)	x[a]	y[a]	Dist from SNP (km)	Stk Ht (m)	Diam (m)	Ex Vel (m/s)	Temp (K)	SO_2 (g/s)	NO_x (g/s)
50 - 100 km from SNP											
PEPCO H[b]	806.1	4345.7	36.3	23.7	64	65	6.87	35.4	260	317.2	179.3
Warrier Run	693.6	4385.0	30.7	25.3	83	82	3.75	23.6	398	54.8	26.0
Ogden-Martin	826.9	4289.4	37.3	20.5	77	88	2.26	19.2	405	20.3	82.5
Patowmack	800.3	4330.9	36.0	22.5	54	30	5.49	37.2	854	31.0	51.1
SEI Birch	822.5	4241.6	37.1	18.1	90	123	4.72	0.3	339	27.7	69.4
N Branch	643.5	4346.9	28.2	23.3	95	109	3.96	15.1	444	102.2	60.3
100 - 150 km from SNP											
LG&E Altavista	653.2	4109.3	28.7	11.5	115	67	2.44	23.6	341	17.9	28.7
Multitrade	653.3	4107.8	28.7	11.4	117	53	3.84	19.1	472	6.8	13.9
Old Dominion	704.6	4082.6	31.2	10.1	135	134	6.77	14.4	323	145.2	309.1
Doswell	813.2	4191.4	36.7	15.6	107	58	5.03	11.2	389	74.7	68.7
Westvaco	588.6	4183.7	25.4	15.2	108	147	3.44	24.3	444	0.0	23.0
Cogentrix, Richmond	815.2	4151.0	36.8	13.6	134	76	2.64	16.8	339	49.2	113.5
Brandon	885.2	4346.3	40.3	23.3	140	187	6.71	27.3	413	1893.6	630.8
Chalk Pt.	875.6	4275.4	39.8	19.8	127	65	11.25	33.7	789	136.4	177.0
Mettiki Coal[c]	638.0	4353.0	27.9	23.7	103	43	2.90	27.4	333	9.9	23.3
P.H. Glatfelter[d]	853.5	4421.4	38.7	27.1	147	69	4.10	13.7	430	0	61.3

TABLE 3-1. Concluded.

Name	UTM-E (km)	UTM-N (km)	x[a]	y[a]	Dist from SNP (km)	Stk Ht (m)	Diam (m)	Ex Vel (m/s)	Temp (K)	SO_2 (g/s)	NO_x (g/s)
150 - 200 km from SNP											
Cogentrix, Dinwiddie	815.2	4121.2	36.8	12.1	152	76	2.64	16.8	339	49.2	94.6
LG&E Hopewell	829.5	4134.1	37.5	12.7	156	67	2.44	23.6	341	14.9	27.5
Mecklenburg Cogen	720.8	4053.3	32.0	8.7	166	84	3.51	22.8	339	49.4	116.0
Cambria Cogen	695.1	4482.2	30.8	30.1	170	76	2.74	27.7	422	133.3	77.5
Coal Dynamics	597.0	4413.5	25.9	26.7	171	31	2.74	25.6	478	28.5	14.0
Colver PP	686.4	4490.9	30.3	30.5	181	107	3.48	18.0	411	144.7	72.4
Ebensburg	690.8	4480.4	30.5	30.0	169	76	2.59	18.3	422	9.8	5.9
Harrisburg	850.6	4465.0	38.5	29.3	178	59	3.66	8.1	477	2.8	46.7
Lancaster	871.5	4444.6	39.6	28.2	176	93	2.82	19.4	405	4.1	40.1
Solar Turbine	869.0	4435.0	39.5	27.8	168	20	2.00	15.7	488	0	48.9
York Co.	865.6	4436.6	39.3	27.8	167	95	2.42	20.0	389	7.2	15.3

[a] Meteorological grid cell coordinates.
[b] Combined values for three units, and including an emission offset for NO_x
[c] Emission data from Maryland. Virginia lists emissions from this facility of 2.4 g/s SO_2 and 3.8 g/s NO_x.
[d] Combined values for two units.table 3-1 (cont)

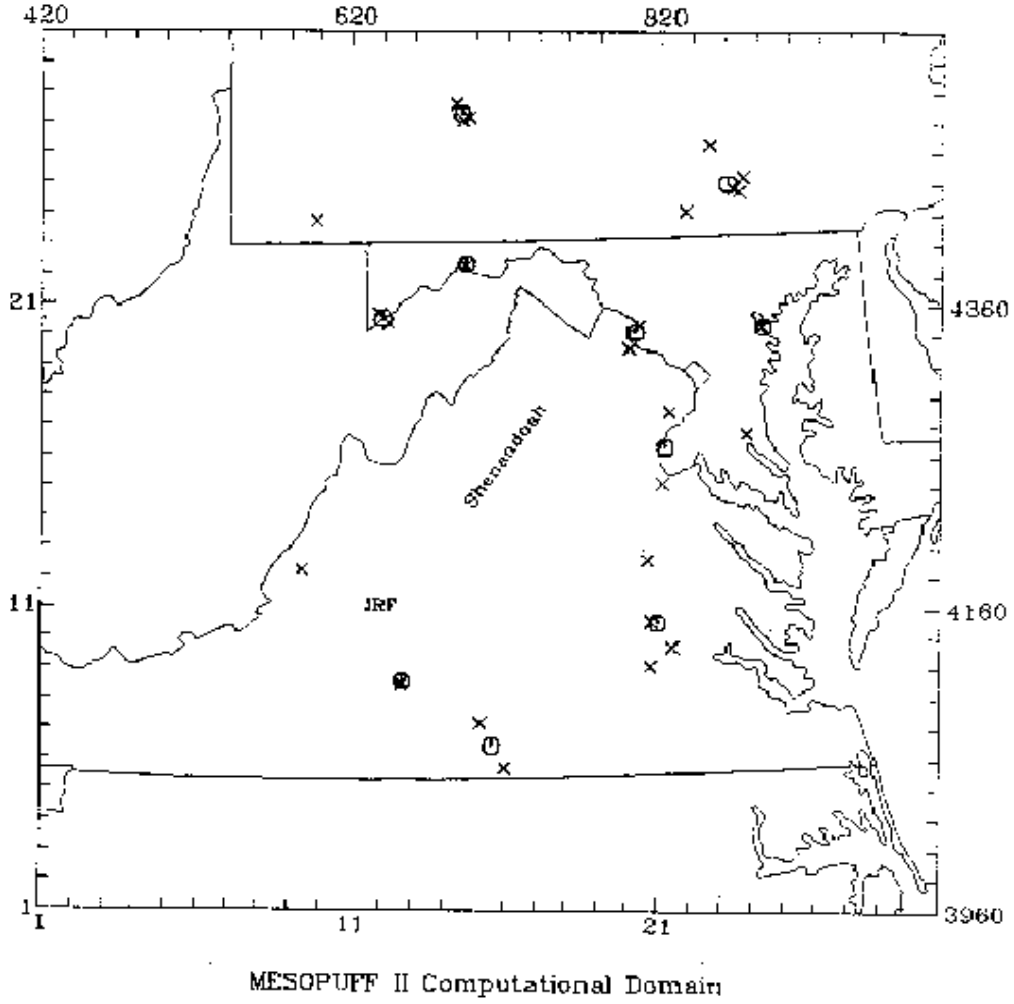

Figure 3-3. Display of the MESOPUFF II computational domain, showing positions of all PSD sources compiled for the MESOPUFF Phase I demonstration. Crosses represent all 27 original PSD sources, while circles denote the 10 final aggregated sources used for the PSD applications.

II simulations within the time frame of the project. A series of 24-hour test simulations was performed to determine which input parameters had the largest effect on CPU time. These simulations, described below, clearly demonstrated that the number of puffs was the key variable. They also suggested that the number of puffs must be reduced by a factor of 10 to achieve the needed reduction in CPU time.

The number of puffs is governed by the puff release rate and the number of sources. The puff release rate had been set at the default value of 4 puffs per hour. Although MESOPUFF II, as originally configured, allows up to 1000 point sources, it only allows for a total of 10,000 puffs. With 1000 sources and a puff release rate of 4 per hour, the limit on the number of puffs would be reached after 2.5 hours. With 27 sources and a puff release rate of 4 per hour, the original configuration for the demonstration application, the puff limit would be reached after 92 hours. In order to run MESOPUFF II in this configuration for one full month, therefore, it would be necessary to increase the maximum number of puffs substantially. This would require re-compiling MESOPUFF II and would increase the size of the executable code. Since the MESOPUFF II executable, at 3.3 MB, is near the limit for use on a PC with 4 MB memory, the maximum number of puffs might be a limiting factor even if CPU time considerations were not.

In order to reduce the number of puffs by a factor of ten and still preserve at least a portion of the original intent of the demonstration application, the puff release rate was reduced from 4 puffs per hour to 1 puff per hour. This deviates from the Phase 1 recommendations; however, because the output averaging interval used for the demonstration application was 3 hours rather than 1 hour, this change was considered acceptable. The number of sources was reduced from 27 to 18. Under these conditions, 25.8 CPU hours were required for the January 1988 simulation. Although this was a major improvement over the 27 source case, it was still too slow to allow completion of the project on schedule. Further reductions in the puff release rate were judged to be infeasible. Therefore, the number of sources was reduced further from 18 to 10. This reduced the CPU time to less than 12 hours for January 1988. This set of 10 sources was used for the demonstration application of MESOPUFF II.

In reducing the number of sources to be modeled, the goal was to retain as much as possible of the total emissions mass, and reduce the number of sources by consolidation of nearby sources rather than elimination of sources. In the condensation of the original 27 sources to 18 sources, sources within one grid cell of each other were consolidated. No sources were eliminated. In order to reduce the number of sources to 10, however, it was necessary to eliminate three small sources that were not located near other sources, and sources within 2-3 grid cells were consolidated. The consolidated sources were represented as point sources, with coordinates and stack parameters obtained as an arithmetic mean of the individual sources. The three sources eliminated, Westvaco, Chalk Pt., and Coal Dynamics, have total emissions of 165 g/s SO_2 and 214 g/s NO_x. This amounts to 5 percent of the total SO_2 emissions of the original 27 sources, and 8 percent of the total NO_x emissions. Table 3-2 shows the final set of 10 consolidated sources, the facilities that are included in each, and the location and emission parameters

TABLE 3-2. Final condensed set of sources modeled with MESOPUFF II for the SNP demonstration application.

	Sources Included	x[a]	y[a]	Stk Ht (m)	Diam (m)	Ex Vel (m/s)	Temp (K)	SO_2 (g/s)	$SO_4^=$ (g/s)	NO_x (g/s)
1	PEPCO H, Patowmack	36.2	23.1	48	8.77	36.3	557	348.2	15.7	230.4
2	Warrier Run	30.7	25.3	82	3.75	23.6	398	54.8	2.5	26.0
3	Ogden-Martin, SEI Birch	37.2	19.3	106	3.24	10.0	372	48.0	2.2	151.9
4	N Branch, Mettiki	28.0	23.5	76	4.69	21.3	389	112.1	5.0	83.6
5	LG&E Altavista, Multitrade	28.7	11.5	60	4.44	21.4	407	24.7	1.1	42.6
6	Mecklenburg, Old Dominion	31.6	9.4	109	7.11	18.6	331	194.6	8.8	425.1
7	Doswell, Cogentrix-Richmond, Cogentrix-Dinwiddie, LG&E Hopewell	37.0	13.5	70	5.35	14.0	352	252.1	11.3	426.4
8	Brandon	40.3	23.3	187	6.71	27.3	413	1893.6	85.2	630.8
9	Cambria Cogen, Colver PP, Ebensburg	30.5	30.2	86	5.08	21.3	418	287.8	13.0	155.8
10	P.H. Glatfelter, Harrisburg, Lancaster, Solar Turbine, York Co.	39.1	28.0	67	6.60	15.4	438	14.1	0.6	212.3

[a] Meteorological grid cell coordinates.

for each. Figure 3-3 also displays the locations of these sources in relationship to all 27 original PSD sources (indicated by circles).

Run Time as a Function of Number of Puffs

A series of 24-hour test simulations was performed to ascertain the dependence of MESOPUFF II execution time on input parameters including puff release rate, number of sources, number of receptors, ozone data specification and chemistry. The results of these simulations showed that decreasing the number of puffs, whether by decreasing the puff release rate or the number of sources, had a major effect on execution time. Changes in the other parameters had much smaller effects on CPU. Specifically, a 50 percent reduction in the number of puffs reduced CPU by 56 percent. A 50 percent reduction in the number of receptors reduced CPU by 6 percent. The use of a single default ozone value rather than hourly values at monitoring stations had virtually no effect on CPU. Even running the model in an inert mode (i.e. with all chemistry turned off) resulted in only an 8 percent reduction in CPU time.

These results show that there is a greater than linear dependence of CPU time on number of puffs, even within the first 24 hours of a simulation. The departure from linearity increases for longer simulations. Based on the CPU requirements for the month-long simulations, a simulation with 17 percent of the original number of puffs required only 6 percent of the CPU time.

MODELING EPISODE DEFINITION

Following the Phase 1 recommendations, a five-year period was to be modeled. In order to supply the MESOPUFF II modeling system with the most recent environmental input data, the IWAQM agreed to the five year period from 1988 through 1992. As planned, the **MESOPAC** meteorological preprocessor was run to generate MESOPUFF II input fields for this entire period. As discussed above, however, a decision was made to reduce the Phase 1 PSD demonstration to three years (1988-1990), with the remaining 24 months of MESOPUFF II integrations reserved for the ring source analyses.

The default value and Phase 1 recommended value for output averaging interval is one hour; however, substantial reductions in disk storage requirements can be achieved by increasing this interval. Based on the observation that the PSD increments and AQRV parameters are all based at a minimum on 3-hour averages, we judged that an averaging interval of 3 hours would be sufficient to produce each desired output.

It should be noted that this deviates somewhat from the Phase 1 recommendations, which state that visibility effects should be calculated using hourly concentrations and hourly relative humidities. The intent of this recommendation was to capture the diurnal effects and avoid calculating visibility on the basis of 24-hour averages. The use of 3-hour averages still allows for the determination of diurnal trends, and would seem to preserve the intent of the recommendation.

MESOPUFF II cannot simulate seasonal or annual time scales in a single model run, especially on a PC. One problem we had identified during review of the SCRAM BBS example problem at the start of the project was the demand put upon PC disk storage by **MESOPAC** and MESOPUFF II input/output (I/O). We had anticipated executing **MESOPAC** and MESOPUFF II in one-month intervals, using the MESOPUFF II restart option for all but the first month of each year. One month of **MESOPAC** output for the 50 by 35 grid point domain produced 50-55 megabytes of output. This is a manageable amount for the 200 MB PC hard drive systems we used; other potential users of the meteorological data are likely to have similar systems. Monthly MESOPUFF II output was significantly less (about 1 MB).

During the demonstration applications, we found that a single MESOPUFF II integration over several months would have also stressed MESOPUFF II memory requirements. This is related to simplistic puff accounting within MESOPUFF II, which continuously adds new puffs as they are emitted, yet does not purge old puffs that exit the computational grid. Particularly during stagnant conditions, the number of puffs quickly grows to the maximum dimension of the puff array, which slows MESOPUFF II considerably. This problem is discussed further in following sections.

DEVELOPMENT OF METEOROLOGICAL INPUTS

MESOPAC requires the following input meteorological data: (1) twice daily upper air temperature and wind soundings in NCDC TD-6200 format at up to 20 radiosonde stations; (2) scheduled airways surface observations in NCDC CD144 format, which include hourly winds, temperature, relative humidity, cloud cover and ceiling height at up to 100 stations; and (3) hourly precipitation data in NCDC TD-3240 format. The CD144 data sets are input directly into **MESOPAC**, whereas the upper air and precipitation data must be scanned for missing data and reformatted using several **MESOPAC** preprocessors. **MESOPAC** and its preprocessors expect the data in these specific NCDC formats.

Prior to the start of this project, SAI already possessed in-house upper air and hourly surface data for 1988 covering the entire U.S. However, we had to procure precipitation data for 1988-1992, and upper air and surface data for 1989-1992. At the time, we anticipated that some of the data sets we were to acquire would not necessarily fit the **MESOPAC** formats, and either the data would have to be reformatted for the processors, or the processors would have to be revised. Furthermore, the protocol called for the development of a procedure to fill in missing data in the upper-air soundings. We recognized that for a 5-year database, it would not be feasible to fill in missing data by hand. Consequently, we needed to develop a processor that uses a specified set of rules to automatically fill in missing data. Based upon the size of the proposed meteorological domain (see Figure 3-1), it was also expected that the **MESOPAC** limits on the number of surface and upper air sites would probably need to be increased.

Raw Data Processing for MESOPAC and Related Problems

Data Procurement

SAI managed to procure the remainder of the necessary raw meteorological data sets through the Western Regional Climate Center, Desert Research Institute (WRCC/DRI) of the University of Nevada, Reno. These nationwide data sets include TD-6201 upper air soundings and TD-3280 hourly surface observations for the years 1989-1992, and TD-3240 precipitation data for the years 1988-1992.

Two options were available for procuring meteorological data: to order through WRCC/DRI, or through the National Climatic Data Center (NCDC) in North Carolina. The least expensive format through DRI was to receive surface, upper air, and precipitation data sets in terms of annual files covering the entire U.S. Special processing to extract monthly data for the MESOPUFF II domain would have required extra charges for running their processors, and would have doubled or tripled processing time. DRI did not insist on prepayment, and was able to start delivering data within two weeks of the order. Data transfer was simplified by the fact that DRI processed all data on a SUN/Unix system and wrote to Exabyte 8 mm tape cartridges. This was a significant advantage since we expected to handle the large raw data sets on our Trace/Unix mainframe systems, which possess Exabyte tape drives. Finally, DRI subscribes to the Internet nationwide communications network, which enables data transfer from DRI to purchasers on Internet directly, removing mail time.

Alternatively, NCDC charges are based on the amount of data, not the amount of processing. To process the same surface, upper air, and precipitation data, but only within states covering the MESOPUFF II modeling domain, NCDC quoted SAI about a 25% higher cost than for the nationwide data sets from DRI. Hence, full nationwide data sets through NCDC would have been more than twice the DRI price. Further, NCDC requires payment for the total amount before they begin processing data, after which transfer of data tends to take about a month. Combining correspondence time between NCDC and SAI to request an estimate, time required to arrange for and transmit payment, and processing time at NCDC, we had estimated a wait of six or more weeks. Time constraints, along with the slightly higher cost, rendered this option infeasible. Realizing that breaking up nationwide data sets would demand more in-house labor and computer time than working with smaller regional data sets, we nevertheless decided to order through DRI.

Future users of the MESOPUFF II system may prefer to order raw meteorological data via NCDC if time constraints are not so crucial. **MESOPAC** front-end processing work may also be reduced substantially if data are requested for stations within a specific area for a particular time window. However, if a specific region is requested, NCDC requests a list of station identification (WBAN) numbers or a list of states to extract. Obviously, increased processing also escalates the time NCDC requires to process and deliver the data. NCDC writes all files to 9-track tape, and the purchaser must specify the exact tape format (variable vs. constant record length, byte density, blocking factors, etc.). In the future, it may also be possible to obtain the raw data on CD-ROM format.

Protocol for Raw Data Processing

Aside from the sheer volume of data to be processed, development of several new **MESOPAC** preprocessors was necessary for the following reasons. First, all data files were delivered in slightly modified formats from standard NCDC formats, such that long single station records were simply broken up to maintain 80-character width files to ease file transfer and quality assurance procedures. Further, each of the three data sets were delivered in several subfiles per year to facilitate transfer and handling. New processors were needed to read the altered formats, concatenate all subfiles for each year, and extract data for the time (monthly) and space windows of interest. Second, while all precipitation and upper air data we had on order and/or in-house were in the proper format for the **MESOPAC** preprocessors, it was necessary to convert all TD-3280 surface data to CD144 format before **MESOPAC** could be run. Finally, an automated system was required to scan and fill extracted surface and upper air data sets for missing values, and conduct simple quality assurance checks.

The first preprocessor that we had planned to develop was to reformat the TD-3280 surface data to CD144 format. It was expected that this would be a rather straightforward task, and should not have demanded much time. We planned to add provisions in the program to scan the data set for missing values and take appropriate steps to fill these gaps. At the time, we expected to simply linearly interpolate over time for periods of missing values of less than 6-12 hours. Linear interpolation over time is best for short periods (a few hours) but is increasingly inappropriate for longer periods since diurnal patterns, such as diurnal temperature waves, are eliminated. Therefore, a contiguous period of 12 hours was considered the maximum length of time considered for linear time interpolation. For sites with data missing for the bulk of an entire day or more, but with ample data coverage for the month, we proposed to spatially interpolate data from nearby sites to the station location using a distance-weighted average. For sites missing significant portions of data for a particular month (e.g., two or more weeks), the station was to be disregarded for that month.

We also planned to develop a processor for the upper air data that replaced manual editing between the **READ62** and **MESOPAC** programs. **READ62** only flags missing data within a sounding, or writes a warning message if an expected sounding is completely missing. The new processor was to read the **READ62** output; for missing data in the vertical, it would linearly interpolate between pressure levels. We realized that vertical interpolation is suitable only for relatively shallow portions of a sounding, since atmospheric conditions between two vertically distant levels are often decoupled. Therefore, if a large portion of a sounding was missing, or if a sounding was missing altogether, the program would spatially interpolate data from nearby sites to the station location using a distance-weighted average.

The revised MESOPUFF II user's guide (EPA, 1994) suggested simply replacing missing soundings with the nearest representative soundings. However, we felt that a better approach was to use spatial averaging, as upper air stations are typically separated by at least a few hundred kilometers, and no single sounding can properly represent a missing profile (particularly near the surface). Aloft, the scales of horizontal atmospheric motions are on the

order of 200-1000 km or larger (a distance that is well resolved by sounding data), so horizontal interpolation is acceptable above about 1000 m. Near the surface, this approach loses validity since local effects (1 km or less) dominate the vertical profile. However, we believe that averaging from several sites is far better than simply replacing a missing sounding with another.

Throughout the process of generating meteorological data input files for **MESOPAC**, we encountered a multitude of problems related to missing or substandard raw data. In developing a system of data extraction/filling/processing algorithms to work in tandem with existing **MESOPAC** preprocessors, we attempted to account for as many contingencies as possible. However, numerous unexpected patterns of missing data were flushed out during actual processing that required significant amounts of time in which to identify the problems and develop alternative programming approaches. As discussed below, many preprocessors had to be altered and rerun several times, which proved to be a very labor intensive process. The development and subsequent dissemination of a five year MESOPUFF II meteorological database was accomplished in part to alleviate this demanding step for future MESOPUFF II users. However, for those users who find it necessary to develop a new database, we present below a description of all meteorological preprocessing steps, along with a review of all significant problems we have encountered with the data and existing preprocessors.

Surface Data Processing

A preprocessor was developed that reformats the TD-3280 surface data to CD144 format. We added provisions in the program to scan the data for missing values and take appropriate steps to fill these gaps. A flow diagram showing the necessary steps to provide CD144 files to **MESOPAC** is shown below:

Concatenated Raw TD-3280 File

⇓

GETSTN/RESFC Tape Extraction Programs

⇓

Intermediate Monthly File

⇓

TOCD144 Data Reformatting/Filling Program

⇓

Monthly CD144 File

⇓

PARSE Station Splitting Program

⇓

Monthly CD144 Station Files

⇓

MESOPAC

The first two programs, **GETSTN** and **RESFC**, are used together to extract hourly surface data for a given time and space window from a single raw TD-3280 file. Because of file size and time required to operate the tape extraction programs, **GETSTN** and **RESFC** were run on our Trace Multiflow 14/300 Unix mainframe system.

As delivered to SAI, the TD-3280 data were broken down into many subfiles per year, arranged by station WBAN number. Since WBAN numbers are not necessarily ordered geographically, it was expected that all subfiles would have to be run through **RESFC** to ensure that all available surface data were extracted for the modeling domain. Hence, our original plan was to run **GETSTN**/**RESFC** programs on each raw annual subfile, and operate a rather complex concatenating procedure on the resulting intermediate monthly subfiles to obtain a single monthly intermediate file. For the 1988 surface data set this approach was satisfactory since only four subfiles existed for the year. Data sets for 1989-1992 were instead split into 13 subfiles per year.

Realizing that our original approach would be quite inefficient for the last four years, we decided instead to identify only those subfiles containing station data within our domain, and concatenate those raw TD-3280 subfiles together first and run **GETSTN**/**RESFC** for each single concatenated data set. In this way, we were able to disregard 5 of the 13 subfiles, and concatenated the remaining eight. The resulting raw files required about 250-300 MB of disk space per year. In terms of labor, about one-half hour was spent identifying which subfiles to concatenate, after which setting up and running the concatenating procedure required about an hour per year on our Unix mainframe system (yet very little CPU time).

GETSTN and **RESFC** already existed for previous in-house processing of meteorological data; however, CD144 format required slight modifications to **RESFC** to output different types of meteorological variables. The product of these two programs is an intermediate monthly surface data file for stations located within the meteorological modeling domain. These programs were run for all 60 months of 1988-1992, extracting data for a spatial window within the latitude/longitude ranges 34-42°N and 71-86°W, which resulted in hourly surface observations for up to 48 stations. Although **RESFC** required substantially more mainframe CPU time to process the larger annual concatenated files, significant labor was saved by removing **RESFC** setup time for all subfiles and removing the post-**RESFC** concatenating procedures. On the Unix system, processing of each month took between 20-30 minutes of mainframe CPU time (6 hours per year); about an hour of labor per year was spent setting up and executing **RESFC**, and inspecting output diagnostics and data files.

In order to reduce processing time further, we developed a process that screened stations within the intermediate surface file for missing data before running the **TOCD144** program. If a station was missing more than 50% of the data for a particular month, we deleted it from the file before running **TOCD144**. The process utilized rapid **awk**/**sed** editing (a Unix-based protocol), which requires very little time. For 1988, two surface stations had to be repeatedly deleted from all twelve months of data.

TOCD144 is a new PC preprocessor that reads the monthly intermediate files, fills missing values, and reformats the data into monthly files in CD144 format. The program was written to fill 1-6 hour intervals of missing data using linear interpolation over time. For longer periods of missing values, data from surrounding surface stations are used to spatially interpolate information to the station using an inverse-distance-squared weighting technique. A minimum of 2 stations and a maximum of 4 stations are used within 200 km of a station needing spatial interpolation. If all data for a particular station is missing for more than one week, the station is deleted from the database for that month. **TOCD144** was compiled using Microsoft (MS) FORTRAN 5.0; processing of each month took about 5 minutes of PC CPU time using an 486/66 MHz processor (this PC was used throughout all raw meteorological data preprocessing). Total labor and computer time required to run CD144 averaged about 1.5 hours per year.

We first encountered a problem with the 1988 TD-3280 surface data in that it did not contain a "present weather" field, which is needed in CD144 files to assign precipitation data as either liquid or frozen (for use in wet deposition calculations in MESOPUFF II). When the TD-3280 data was originally ordered, a decision was made to exclude present weather in the data set to reduce file size. Peculiarities of the present weather field format, along with complexities involved to map TD-3280 present weather descriptors to CD144 descriptors, would have necessitated the addition of highly complex logic structures to the **RESFC** program. After consulting one of the authors of MESOPUFF II, it was determined that **MESOPAC** uses input temperature to determine liquid/frozen precipitation states if present weather fields are missing from the CD144 data (Scire, 1993). Therefore, all present weather fields were set to missing values in the processed CD144 files.

It was eventually determined far into processing of surface data with **TOCD144** that pressure values were incorrect and appeared to be in wrong units. Upon further investigation, we realized that pressures read from the raw TD-3280 data set were station pressures in inches of mercury, rather than sea level pressure in millibars. Instead of restarting surface data processing from the raw TD-3280 level to extract the proper pressure field, we decided to convert station pressure to millibars and calculate a sea level pressure using the hypsometric equation (via station temperature and elevation) within **TOCD144**.

At the same time, we made a decision not to interpolate for missing cloud ceiling height fields, either in time or space, due to the often large temporal and spatial variations observed in cloud heights, and the potentially large and uncertain impacts on MESOPUFF II applications. **MESOPAC** requires cloud heights and cloud cover to adjust a daytime clear-sky solar insolation index, which is in turn used along with wind speed to estimate Pasquill-Gifford-Turner stability class. When cloud cover is less than 50 percent, **MESOPAC** ignores cloud height effects on solar insolation index. At night, only cloud cover and wind speed are used to determine stability class. For the most part, missing cloud heights occurred at night, as these observations are typically estimated visually; they only periodically occurred during daylight hours. In **TOCD144**, sky cover percentage was used to set cloud height: if sky cover was less than 50 percent, cloud height was set to an "unlimited" ceiling; if cloud cover was greater than

50 percent, cloud height was set to 5000 ft, a height which altered the classification of solar insolation within MESOPUFF II to "low cloud" values (refer to page 5-13 of the MESOPUFF II User's Guide; EPA, 1994). Our binary "all or nothing" methodology drastically simplified the procedure and only occasionally influenced the solar insolation index under daytime broken/overcast conditions.

A final simple processing program called PARSE was then written to split monthly CD144 files into numerous monthly station files, which are ready to be used directly by **MESOPAC**. Processing of single monthly files and splitting into separate station files just before running **MESOPAC** for each month simplified intermediate file management and provided faster meteorological data processing. Typically, data for 45-48 surface stations needed to be split into separate station files each month, taking just about 1 minute of PC CPU using MS FORTRAN 5.0, and virtually zero labor.

Upper Air Data Processing

Although TD-6201 upper air data were generally in the correct format for **READ62** (some minor modifications were necessary), the **READ62** program only flags missing data within a sounding, or writes a warning message if an expected sounding is completely missing. We therefore had to develop a processor that replaces manual editing between the **READ62** and **MESOPAC** programs with an automated procedure. A flow diagram showing the necessary steps to provide upper air data files to **MESOPAC** is shown below:

Raw TD-6201 File
⇓
REUPR2 Tape Extraction Program
⇓
Monthly TD-6200 File
⇓
FILLUPR Data Filling Program
⇓
Monthly Filled TD-6200 File
⇓
READ62 Program
⇓
Monthly MESOPAC File
⇓
PARSE Station Splitting Program
⇓
Monthly MESOPAC Station Files
⇓
MESOPAC

The first program (**REUPR2**) is a modified version of a program existing in-house for previous processing of upper air data. Its purpose is to extract 12-hourly upper air data for a given time

and space window from a single raw nationwide/annual TD-6201 file. It was modified to output TD-6200 format readable by **READ62**, as the previous version output a format useful for another meteorological model. Because of file size and time required to operate the tape extraction program, **REUPR2** was also run on our Unix mainframe system. Also, in order to reduce file sizes and expedite filling of missing data, **REUPR2** writes out sounding data between the surface and about 7000 m, and deletes non-mandatory levels if they have missing pressure. The resulting TD-6200 file contains intermediate monthly upper air data for stations located within the meteorological modeling domain. The program was run for all 60 months of 1988-1992, extracting data for a spatial window within the latitude/longitude ranges 34-42°N and 71-86°W, which resulted in upper air data from as many as 8 rawinsonde stations. **REUPR2** required about 15-20 minutes of mainframe CPU per month, yet very little labor was involved.

A new processor (**FILLUPR**) reads the intermediate TD-6200 file and scans the sounding data for missing values. The program linearly interpolates between pressure levels for data gaps less than 200 mb deep. If a significant portion of the sounding is missing (i.e., > 200 mb), or if the sounding is missing altogether, the program spatially interpolates data from nearby sites to the station location using a distance weighted average (at mandatory levels only). The value of 200 mb was a rather arbitrary choice; in the lower troposphere such a pressure depth is equivalent to about 2000 m. Vertical variations in hydrodynamic variables across this depth result from larger-scale atmospheric dynamics, and are thus better estimated via horizontal interpolation from other soundings. Vertical interpolation across large depths in a single sounding may overly simplify a sounding aloft.

We made the decision to use the program **FILLUPR** on the output of **REUPR2** instead of running the data through **READ62** first, which would flag the missing values or soundings. The main reason for this is that **READ62** eliminates non-mandatory sounding levels that may be important for performing a vertical interpolation on missing data. Since pressure is known for all levels up to 7000 m, only missing height, temperature, and winds are filled (in that order). **FILLUPR** follows the processing scheme outlined below:

(1) In a first pass through the data, the program finds the first level where there is a missing value (either height, temperature, or wind). The program proceeds up the sounding until a non-missing value is found. If this gap is greater than 200 mb deep, the mandatory levels within the missing block are flagged for spatial interpolation of this particular variable. If the gap is less than 200 mb deep, linear interpolation (using height, or log-pressure if height is not available) is performed for the variable at all levels (mandatory or otherwise) within the gap. For winds, interpolation is done for vector components.

(2) The program then proceeds farther up the sounding and repeats the procedure for data gaps aloft. If no valid data is found up to the top of the 7000 m sounding, and the data gap is greater than 200 mb, all mandatory levels above the level of good data are flagged for spatial interpolation. If the data gap to the top of the sounding is less than 200 mb, the data are extrapolated using the highest two levels with valid data (this saves on spatial interpolation time).

(3) Data for all soundings needing spatial interpolation are written to a temporary direct access file to ease memory requirements and quicken run time. In the second pass

through the data, a matrix containing the top 5 closest stations to each of the stations in the file is computed. Then the flags for missing data at mandatory levels are checked for spatial interpolation.

(4) When a mandatory level requiring spatial interpolation for a particular variable is identified, data from the closest 2 to 4 upper air stations within a radius of 500 km are used in an inverse-distance weighted average. Stations containing spatially interpolated values at the same mandatory level are not used in this calculation.

(5) After a temperature sounding has been completely filled via spatial interpolation, the resulting temperature gradients are checked against a slightly super-adiabatic lapse rate to insure thermodynamically realistic values. The limiting lapse rate specified was -0.15 K/m; this limit was violated only infrequently. When the violation did occur, the interpolated temperatures were adjusted to adhere to an adiabatic lapse rate (-0.01 K/m)

FILLUPR was compiled using MS FORTRAN 5.0, and took about 5 minutes PC CPU time per month. Labor and CPU time together required about two hours per year to process upper air data through **FILLUPR**.

In processing 1988 upper air data, many soundings were found at hours 6 and 18 supplementing or replacing the standard hour 00 and 12 soundings. Since **MESOPAC** expects only hour 00 and 12 soundings, these extra sounding data were deleted during the **FILLUPR** step. Upper air data for one particular station during August 1988 contained so many missing records that the resulting direct access file ran up against PC disk storage limits. Since so much data were missing, we decided to delete that station from the intermediate file and rerun **FILLUPR** for August 1988.

Several array overflows occurred during test extraction of 1989 upper air data. These were tracked to inadequate array dimensioning; array dimensions for the number of input sounding levels in **REUPR2** were increased from 100 to 150, and 1989 data were re-extracted. **FILLUPR** and **READ62** worked well for all of 1989 except for November. One of the stations was missing data for the entire last week of the month, causing **FILLUPR** to fail. Rather than alter **FILLUPR** to handle this situation, we simply deleted the station from the November 1989 intermediate data file and **FILLUPR** and **READ62** were rerun. We then discovered that extracted data for 1990 was unusable, due to an unexpected limitation in **REUPR2** that did not allow processing of as much data as it was supplied. This was apparently not a problem for previous years. **REUPR2** was revised and 1990 data were re-extracted.

When processing upper air data for 1991 and 1992, we found numerous stations commonly reporting at hours 11 and 23. Since **MESOPAC** cannot accept this, we elected to simply

relabel data at hour 11 to hour 12, and data at hour 23 to hour 00 on the following day. This presented a serious logistical problem for soundings at the end of each monthly file since they needed to be transferred to the beginning of the files for the following months. It was determined that such a task would be far too labor intensive; instead, the **REUPR2** extraction program was revised to find these incidences and properly relabel soundings before writing the monthly files to disk. Raw 1990-92 upper air data were then extracted once again using the modified version of **REUPR2**.

Data from only four upper air stations were available for August 1991. When attempting to process the data through **FILLUPR**, the program was unable to spatially interpolate data to the other four locations because of significant data gaps in the existing data. Additionally, upper air data for July 1992 contained only 2 stations. This leaves serious questions concerning the feasibility of using upper air data from August 1991 or July 1992 for future **MESOPAC**/MESOPUFF II applications. Nevertheless, all months of 1991 and 1992 were processed following the procedures outlined above.

The resulting filled monthly TD-6200 files were then processed through **READ62** to produce monthly upper air data files in **MESOPAC** input format. Although only about a minute of PC CPU time was required to run **READ62** per month, about one hour of labor was spent performing quality assurance checks on a year's worth of **READ62** output.

Finally, the PARSE station splitting program was run to provide monthly station upper air files for **MESOPAC**. Typically, eight separate upper air station files were generated by PARSE, taking only a few seconds of PC CPU time.

Precipitation Data Processing

The TD-3240 precipitation data was basically in the correct format for the **PXTRACT** preprocessor. No extra processing (e.g. data filling) was necessary for these data sets; it was therefore anticipated that processing precipitation information would be the most uncomplicated of our meteorological processing tasks. A flow diagram showing the necessary steps to provide precipitation data files to **MESOPAC** is shown below:

Raw TD-3240 File
⇓
PXTRACT Program
⇓
Monthly TD-3240 Station Files
⇓
PMERGE Program
⇓
Monthly MESOPAC File
⇓
MESOPAC

The **PXTRACT** preprocessor reads in an annual/national raw TD-3240 precipitation file and extracts a monthly TD-3240 file for each station within the specific states that cover the meteorological modeling domain. These monthly files are then read into **PMERGE**, which

processes the data into hourly precipitation rates, taking into account several data quality/accumulation flags, and merges all station data into a single file ready for use by **MESOPAC**.

Initial runs of **PXTRACT** for all 12 months of 1988 led to unreadable monthly output files. Although the raw TD-3240 precipitation data contained all information required by **PXTRACT** as outlined in the MESOPUFF II User's Guide, we found that these files were not in the exact format that **PXTRACT** was expecting. The raw data was reformatted using a Unix **awk** process (taking about 1.5 hours per year of combined computer and labor time), and **PXTRACT** was rerun for 1988. **PXTRACT** required about 10 minutes of PC CPU time per month; about 1 hour of labor per year was required to run **PXTRACT** and examine program diagnostics and output.

During processing of 1988 precipitation data, **PXTRACT** produced about 550 separate station files per month for the states covering the meteorological modeling domain. Although **PMERGE** is written to process any number of station files through repeated rerunning and merging, the sheer number of stations was rather unexpected. FORTRAN programs compiled with MS FORTRAN and operating in DOS environments only allow for 15-20 I/O files to be opened at one time, which would necessitate that **PMERGE** to be run 35-40 times per month. **PMERGE** was instead recompiled with Lahey 5.2 FORTRAN, which, if the PC is configured correctly, allows for up to about 250 I/O files to be opened at any one time.

A large percentage of the precipitation stations were located outside the meteorological domain. An intermediate program (run between **PXTRACT** and **PMERGE**) was written to flag those stations outside the domain for deletion from the precipitation database. The remaining stations within the modeling domain were further reduced in number by arbitrarily deleting every other precipitation station from the database (which still left a sufficient number of stations to adequately represent the spatial distribution of precipitation). The total number of precipitation stations was reduced in this way to just below 200. One **PMERGE** run per month processed each set of 200 files in just a few minutes; processing a full year took about half an hour, requiring about 2 hours per year of labor (mostly in QA).

We initially had many problems running **PMERGE**; each time we corrected for one type of data problem, **PMERGE** would stop on another. An extensive review of the code revealed that **PMERGE** did not allow for several possible combinations of data quality flags. We determined that it was easier to alter the **PMERGE** program to allow for all contingencies we had found within the precipitation data, rather than hand-edit or write yet another processor to handle the hundreds of monthly files.

The program **PMERGE** required modification in order to give it the capacity to handle effectively certain types of precipitation records it might encounter while processing TD3240 data. The data records in a TD3240 file may be flagged as 'M' (missing), 'A' (accumulation period), 'I' (incomplete), or 'D' (deleted). All of these files are expected to come in pairs. In other words, the first record flagged as 'A' signals the start of an accumulation period, and the next record with that flag signifies the end of that same type of period. When the **PMERGE** program was first run on the TD3240 data for the domain, it crashed because it was unable to process records flagged as 'I'. A few lines of code were added to enable the program to deal with records containing this flag. The program required

further modification to enable it to handle situations in which the beginning and end of accumulation periods (records flagged with 'A') were separated with missing, incomplete, or deleted periods of records. It was a common occurrence in the TD3240 data to have one or several pairs of deleted, missing, or incomplete data records sandwiched between valid accumulation period records, but the **PMERGE** program did not have the ability to deal with this structure. The same modification was required to enable the handling of missing record pairs being separated by incomplete or deleted periods of records. It appears that all contingencies are now handled by the revised **PMERGE** program.

We found during initial precipitation processing that the raw TD-3240 format did not contain any information about each station's physical location (i.e., latitude/longitude or UTM coordinates). TD-3240 format only contains station ID number, which includes a code denoting the state in which a particular station resides. The revised MESOPUFF II User's Guide (EPA, 1994) does not mention anything about where to obtain such information. Fortunately, we were able to download from WRCC/DRI an NCDC precipitation "Station History File" via Internet linkup. This file contains all station history and location information for the entire U.S. A program was written (**GRIDDIT**) to cross reference station identification numbers within each month's **MESOPAC**-ready precipitation data file with station numbers in the history file, and write out all station grid coordinates in the proper **MESOPAC** input format. This same program was used to calculate station grid coordinates for all surface and upper air stations from latitude/longitude information within respective intermediate files.

Development of Gridded Land Use for **MESOPAC**

Both **MESOPAC** and MESOPUFF II require a "typical" land use type to be specified for each grid point in order to determine surface characteristics (i.e. water vs. land) and to set default canopy resistances and surface roughness lengths. A single representative land use type for each grid point is designated within the **MESOPAC** user input file; from there, the user may wish to specify roughness lengths for each land use type, or have **MESOPAC** use default values. For the current study, default surface roughness values and canopy resistances were selected.

SAI has possessed a nationwide land use file in-house for many years; it was originally procured from a Geographical Information System (GIS) database maintained by the U.S. Geological Survey (USGS). This file contains the distribution of 11 land use categories over the entire U.S. at 1/4 degree longitude by 1/6 degree latitude resolution. The data were first mapped to the meteorological grid in terms of the percentage of each of the 11 categories in each cell, using the UAM preprocessing program **PRELND**. These land use categories,

however, do not agree with the categories required for MESOPUFF II. A new program was written to identify the dominant GIS land use category in each cell and map it into an appropriate MESOPUFF II category. The assumed mapping arrangement of GIS-MESOPUFF II land use categories is displayed in Table 3-3. All steps in developing a MESOPUFF II land use field were executed on our Unix mainframe, where the land use database and **PRELND** preprocessor reside.

For those future MESOPUFF II/**MESOPAC** users finding it necessary to develop gridded land use for some other modeling domain, there are several land use databases available. SAI has supplied the National Park Services (NPS) with the same land use file used in this analysis as part of the delivery of the NPS Air Quality Modeling System (Morris and Chang, 1992). Other common databases are available through the USGS, including the GIS database described above, and newer, higher resolution (200m) GIS databases covering most of the U.S.

MESOPAC Applications

Meteorological fields for all 60 months of the years 1988-1992 were generated for MESOPUFF II using the **MESOPAC** meteorological preprocessor. The operation demanded a high degree of file handling/transfer because of the large number of **MESOPAC** input files (as many as 58 total files), and the huge output files generated by **MESOPAC**. The following steps outline our approach to setting up **MESOPAC** for each month:

1. The appropriate **MESOPAC** input data files for the month were assembled (surface, upper air, and precipitation) into a common run directory; to maximize PC disk utilization, all **MESOPAC** input files were compressed together after preprocessing using the **PKZIP** utility. Assembling the appropriate files simply meant "unzipping" them from the compressed files.

2. The PARSE splitting program was run on the monthly surface and upper air files to split them into separate monthly station files, named appropriately for **MESOPAC** (CD1.DAT, CD2.DAT, etc., for surface data; UP1.DAT, UP2.DAT, etc., for upper air data).

3. The **GRIDDIT** station location processor was run to obtain gridded station locations for input surface, upper and precipitation data. It was necessary to run the program each month since the collection of station data changed month to month. The output from this program contains station locations, in terms of the meteorological grid location, in the proper format for the **MESOPAC** user input file (PAC.INP).

4. The **GRIDDIT** output file was concatenated onto a sample header of the PAC.INP file, and the resulting complete PAC.INP file was edited for the particular month to be run.

TABLE 3-3. Assumed correspondence between GIS land use categories and MESOPUFF II land use categories.

GIS Category	GIS Land use Type	MESOPUFF II Category	MESOPUFF II Land use Type
1	Urban	11	Metropolitan City
2	Agriculture	1	Cropland and Pasture
3	Rangeland	6	Subhumid Grassland and Semi-arid Grazing Land
4	Deciduous Forest	5	Ungrazed Forest and Woodland
5	Coniferous Forest	5	Ungrazed Forest and Woodland
6	Mixed Forest	5	Ungrazed Forest and Woodland
7	Water	12	Lake or Ocean
8	Barren Land	6	Subhumid Grassland and Semi-arid Grazing Land
9	Non-forested Wetland	10	Marshland
10	Mixed Ag-rangeland	2	Cropland, Woodland, and Grazing Land
11	Rocky Open Areas	8	Desert Shrubland

5. **MESOPAC** was run for the month with all appropriate input files.

During initial trial runs of **MESOPAC**, two small inconsistencies were found between the model and the input data. First, the new upper air preprocessors wrote the sounding height field in six characters, rather than the original five. The appropriate READ statement within **MESOPAC** was altered to allow for this. Second, unlimited ceiling heights are recorded with a series of X's in standard CD144 format; in **MESOPAC**, a quality assurance routine was checking for dash characters (-) rather than X characters. **MESOPAC** was altered to check for the appropriate character.

MESOPAC contains two date/time routines specific to the Lahey FORTRAN compiler. **MESOPAC** was therefore recompiled using Lahey FORTRAN 5.2; processing a single month of meteorological fields required 60-70 minutes of CPU time on a 486DX50 (50 MHz) PC for the 50×35 grid meteorological domain.

The 486/50 MHz PC used for **MESOPAC** contained a 340 MB hard drive, of which about 220 MB were available for data processing. Since **MESOPAC** produced 50-55 MB of binary output per month for this particular meteorological domain, and required about 5 MB per month of input data, only four months could be processed by **MESOPAC** at a time. Obviously, mass off-line storage became a key importance. As **MESOPAC** was run for each year, meteorological data files were generated on the PC four at a time, and transferred via FTP (a network file transfer protocol) to one of the Unix mainframe disks (with a volume of nearly 1 gigabyte). After an entire year was completed and transferred (600 MB total), all data were backed up to magnetic 8 mm tape cartridge via the mainframe Exabyte drive.

DEVELOPMENT OF BACKGROUND AIR QUALITY INPUTS

Protocol for Developing Air Quality Inputs

MESOPUFF II requires input values for background ozone and ammonia. Initial or boundary concentration data are not supplied. Background ozone can be specified as a single time-invariant region-wide default value of 80 ppb, or the default value may be overridden by designating some other value within the MESOPUFF II input file. MESOPUFF II also optionally accepts hourly ozone observations for a large number of monitoring sites via the OZONE.DAT input file. MESOPUFF II uses the ozone values to calculate chemical conversion rates for NO_x and SO_2.

Following the Phase 1 recommendations, we planned to develop hourly ozone input fields. This option was chosen for the current study in order to provide both spatially and temporally improved estimates of sulfate and nitrate production over the single background level approach. Complete ozone data for the years 1988 through 1991 from all stations reported to the Aerometric Information Retrieval System (AIRS) database were available in-house at the start of the project. We planned to obtain 1992 ozone data from the AIRS network. We realized that it was necessary to pre-process the data to obtain the format needed for input into MESOPUFF II.

MESOPUFF II can accept data from up to 50 ozone sites as originally configured. Most AIRS monitors are clustered in urban areas. We anticipated that in some cases there may be multiple sites within one 20-km grid cell. In such cases, we considered averaging the hourly values for all monitors within a grid cell. Since MESOPUFF II uses the nearest monitor to each puff, we optionally considered the addition of "pseudostations" with background ozone values in some rural locations to prevent urban ozone values from being used in those areas. Fortunately, several AIRS monitors are located either within, or very near, SNP. These were expected to allow a good estimate of rural ozone levels in the area of interest.

MESOPUFF II's default background ammonia concentration is 10 ppb. At the start of the project, we recognized that this value was likely to be too high for the eastern United States, but would provide an upper bound for aerosol nitrate. This would also result in a conservative (high) estimate of PM_{10} and visibility impacts. However, we noted that such an approach would not provide a conservative estimate of deposition impacts, since overestimating aerosol nitrate means that nitric acid would be underestimated, and nitric acid deposits more rapidly than aerosol nitrate. Nevertheless, we planned to maintain background ammonia levels at the default 10 ppb level.

Development of Ozone Input Files

During the course of the Phase 1 Demonstration, SAI procured (independently from this project) hourly ozone data for the entire U.S. for the years 1970-1992. The data were extracted from EPA's Aerometric Information Retrieval System (AIRS) in AMP-350 data work file format. Existing programs were used to withdraw hourly ozone data from 1988-1992 annual files into 60 monthly files for a spatial window covering the entire **MESOPAC** meteorological domain. A new processor was developed (**AIR2MESO**) that reformats the hourly data into OZONE.DAT format, and produces a separate file containing grid coordinates for each AIRS monitor location. The coordinates file was then easily inserted into the MESOPUFF II input file as necessary when supplying an OZONE.DAT file to the model. In order to simplify processing, we did not average multiple stations within the same grid cell. A casual inspection of the data revealed a fairly high degree of uniformity in ozone levels for much of the year. Further, we did not add pseudo stations with background ozone. The total number of ozone monitoring sites within the meteorological domain depended highly on season, ranging from about 50 or 60 in the winter, to around 150 in the summer. Hence, the maximum allowable number of ozone stations in MESOPUFF II was increased from 50 to 200.

MESOPUFF II identifies missing data within the OZONE.DAT file and fills it with either the default (80 ppb) or user-specified background ozone concentration. Since 80 ppb is a rather high value to represent daytime-average background concentrations for the entire year, and since such a high value would likely produce relatively large "spikes" in observed ozone time-series (particularly in the wintertime), a background ozone level was supplied for each month. The **AIR2MESO** program was written to calculate daytime/domain average ozone concentrations for each month; these values, rounded to the nearest 5 ppb, were supplied to each monthly MESOPUFF II input file to specify background ozone levels.

MESOPUFF II APPLICATION

MESOPUFF II was integrated over all 36 months of the years 1988-1990 on the same 486/50 MHz PC as used in **MESOPAC** processing. Each monthly MESOPUFF II run required disk space for a 50-55 MB input meteorological data file, the 3.3 MB MESOPUFF II executable file itself, and 1.5-1.8 MB of output -- a total of about 60 MB. Again, due to the 200 MB disk storage limit, MESOPUFF II was run for only 3 or 4 months before another set of meteorological input files were transferred to the PC from off-line storage.

After MESOPUFF II was revised to correct a chemistry routine (during the review of the BBS example problem) and to increase the maximum number of ozone sites, it was recompiled using Lahey FORTRAN 5.2. This version of the Lahey compiler combines extended and virtual (disk swapping) memory managers into the program executable file. This alleviated the necessity of running the 3.3 MB MESOPUFF II executable in a Windows environment, and in fact required execution from standard DOS. We found that some applications loaded into memory via the AUTOEXEC.BAT led to runtime problems for MESOPUFF II. In particular, the PC had to be rebooted without **SMARTDRIVE** (a hard disk drive utility), **PREDIR**, and **SHARE** (network application sharing software). It is suspected that MESOPUFF II overloaded **SMARTDRIVE** by filling I/O buffers too quickly for **SMARTDRIVE** to handle.

MESOPUFF II has a restart option that allows puffs from the end of a previous simulation to carry over to the beginning of a new simulation. To limit the number of puffs carried over into each monthly integration, two days were assumed adequate to supply a reasonable amount of puff mass to the system from a zero background state. A monthly MESOPUFF II application therefore involves two steps: (1) "cold starting" MESOPUFF II from a zero background state (no restart) two days before the end of the previous month, and running the model for a two-day "spin-up" period; and (2) restarting MESOPUFF II at the beginning of the current month and integrating for the entire month. MESOPUFF II was "cold started", however, from a zero background state for each January. Depending on environmental conditions, particularly in regards to the frequency and duration of stagnation events, CPU requirements for monthly MESOPUFF II integrations varied substantially. In general, months in the winter and spring ran fastest, while the summer and fall months were markedly slower. Monthly runtimes ranged from about 45 to 120 minutes on the 486/50 MHz PC.

All input data and parameters specified within the MESOPUFF II user input file (PUFF.INP), except for background ozone concentration and averaging interval, were set at default or recommended values, as outlined in Appendix A of the Phase 1 recommendations. The concentration/deposition averaging time, as stated above, was set to three hours.

DATA ANALYSIS

PSD and AQRV Issues and Protocol

The MESOPUFF II model produces concentrations, wet fluxes, and dry fluxes for each sampling grid point and for each non-gridded receptor for each of the following species: SO_2, sulfate, NO_x, nitric acid, and aerosol nitrate. As stated in the working protocol, since PSD increments represent incremental concentration totals for specified averaging periods, these values could be calculated with the existing MESOPUFF II post-processor **MESOFILE**. Averaging times for each species should correspond to PSD requirements and associated standards. The pollutants covered by the PSD regulations, the averaging time for each pollutant, calculation method and allowable PSD increment are summarized in Table 3-4.

For this study, PM_{10} increments were to be calculated as described in the Phase 1 recommendations. Modeled concentrations of sulfate and aerosol nitrate were to be converted to ammonium sulfate and ammonium nitrate, and summed to estimate PM_{10} increments. The PSD increments were to be calculated for each non-gridded receptor, and the highest values within SNP and JRFW were to be identified.

Since there are no standards or mandated increments for AQRVs, it was necessary to define AQRV criteria before postprocessing could begin. The measures for visibility and deposition agreed to by the IWAQM are summarized in Table 3-4. For visibility, incremental extinction coefficients were to be computed from 3-hour average modeled PM_{10} concentration increments using relative humidity data and the equation provided in Appendix B of the Phase 1 recommendations. The equation to estimate extinction was to be used for both sulfate and aerosol nitrate, and no other contributors to visibility were to be considered. This calculation required the development of a MESOPUFF II visibility post-processor that reads the 3-hour average concentrations and relative humidity, and calculates the incremental extinction.

The maximum incremental 3-hour extinction over all receptors was to be compared to measured total extinction from the SNP IMPROVE monitoring site. The number (and percentage) of 3-hour periods for which the maximum incremental extinction represents 10 percent or more of the measured extinction for the 90th percentile cleanest day was to be reported.

Deposition impacts were to be calculated for each non-gridded receptor for total sulfur (SO_2 plus sulfate, expressed as S) and total nitrogen (NO_x plus HNO_3 plus nitrate, expressed as N). Deposition impacts were to be expressed as the cumulative annual sum of wet and dry deposition, in units of kg/hectare. At the time the protocol was written, a level of concern (analogous to the 10 percent increase in the 90th percentile cleanest day for visibility) had not been identified for deposition.

TABLE 3-4. PSD and AQRV parameters to be calculated from MESOPUFF II output.

Parameter	Averaging Period	Calculation Method	Allowable Class I Increment ($\mu g/m^3$)
		PSD Increments	
SO_2	Annual	Highest annual average for each year	2
	24-hour	Highest 2nd-high 24-hour average for each year[a]	5
	3-hour	Highest 2nd-high 3-hour average for each year[b]	25
NO_x	Annual	Highest annual average over each year, expressed as NO_2	2.5
PM_{10}	Annual	Highest annual average; sum of ammonium sulfate and nitrate	4
	24-hour	Highest 2nd-high 24-hour average; sum of sulfate and nitrate	8
		Visibility	
Extinction	3-hour	Maximum 3-hour extinction (sulfate plus nitrate), added to 90th percentile cleanest day extinction. Calculate number (%) of 3-hour periods for which extinction is increased by more than 10%	
		Deposition	
Total S	Annual	Highest cumulative annual deposition, sum of wet and dry, SO_2 plus $SO_4^=$, expressed as S	
Total N	Annual	Highest cumulative annual deposition, sum of wet and dry, NO_x plus HNO_3 plus NO_3, expressed as N	

[a] Defined as follows: calculate 2nd-highest value for each receptor for each year, then find the highest value among all receptors.

[b] 3-hour averages are fixed interval averages, not running averages.

Processing MESOPUFF II Output Into PSD and AQRV Measures

MESOFILE was developed to allow for a great deal of flexibility; as such, it requires a user to construct complex command streams in order to identify the desired pollutant, perform the desired function, and output the desired quantity. Unfortunately, as the requested output quantity becomes more complex (e.g., total sulfur deposition) it is necessary to expand the **MESOFILE** command streams into highly complicated structures.

We had become familiarized with the **MESOFILE** postprocessor during review of the SCRAM BBS sample application and associated dissemination files. To become adept at utilizing **MESOFILE**, as well as to further test the postprocessor, we decided to improve the sample **MESOFILE** runstream to calculate, from the same sample MESOPUFF II output, 24-hour average/sums of concentrations/deposition for all species, rather than just for SO_2.

We found the task to develop expanded **MESOFILE** output for the sample application to be overly tedious and complicated, and resulting file manipulation (of both MESOPUFF II output and **MESOFILE** intermediate files) to be burdensome. Clearly, developing a similar **MESOFILE** process to generate averages and sums over an entire year, as required by PSD and AQRV measures, would be difficult and inefficient. Furthermore, **MESOFILE** does not produce second highs needed for PSD analysis. Since development of a new program was necessary to calculate visibility parameters from MESOPUFF II output anyway, we decided to include all PSD and AQRV calculations into a single new postprocessor.

The single postprocessor approach, designated **PSDPOST**, allowed for quick and efficient calculations of the specific PSD and AQRV impacts as described in Table 3-4, without intermediate computations and file management. AQRV computations include the calculation of aerosol extinction, which in turn is dependent on relative humidity. Relative humidity data is contained within the large 50 MB **MESOPAC** output files, only a few of which can fit onto the PC hard drive. The objective of **PSDPOST**, however, was to operate on all 12 months of each year continuously. Therefore, it was necessary to write another processor (**RHPOST**) to extract hourly relative humidity data at each surface station from **MESOPAC** files, and output 3-hour average relative humidity at each receptor location to a much smaller file for **PSDPOST**.

PSDPOST requires 12 months of binary MESOPUFF II output files and 12 monthly **RHPOST** output files for each year. The program calculates all concentration averages and deposition sums outlined in Table 3-4. As discussed in the protocol, **PSDPOST** then determines humidity-dependent extinction coefficients resulting solely from ammonium sulfate and ammonium nitrate. This calculation specifically follows the procedure outlined in Appendix B of the IWAQM Phase 1 recommendations. Visibility impacts are then reported as the amount of time (both in terms of the absolute number of 3-hour periods and percent of each year) the calculated maximum extinction over all receptors is more than 10 percent higher than the cleanest observed extinction. The cleanest observed extinction was taken to be the

90th percentile extinction over all years in which statistical analyses of IMPROVE monitoring data are available at SNP (1987 through 1991). From Sisler et al. (1993), the 90th percentile particulate extinction for this period at the Shenandoah monitor was 0.005 km^{-1}. This was combined with a Rayleigh (pure air) scattering extinction of 0.010 km^{-1} to obtain a total observed cleanest extinction of 0.015 km^{-1}.

Since both MESOPUFF II and **MESOPAC** were compiled using Lahey FORTRAN 5.2, both **PSDPOST** and **RHPOST** had to be compiled with the same in order to read the binary model output files. **RHPOST** required just a few minutes of CPU time per month (on the 486/50 MHz PC) to extract relative humidity data from **MESOPAC** output files. Again, humidity files could only be extracted from 3 or 4 **MESOPAC** output files before more **MESOPAC** files could be transferred from off-line storage. **PSDPOST** required about 10 minutes of PC CPU per month.

RESULTS

Note: The modeling results presented below are for a partial list of relevant PSD sources.

Table 3-5 displays a summary of **PSDPOST** calculations from three years of MESOPUFF II output (1988-1990). Results are given for receptor groups in both SNP and JRFW. All PSD and AQRV measures for JRFW are markedly lower than for SNP; this may be caused by the relative isolation of JRFW from the bulk of modeled PSD sources, in combination with the fact that the small number of receptors within JRFW are spatially compact. As for concentrations of criteria pollutants, annual averages of SO_2, NO_x, and modeled PM_{10} in both Class I areas were predicted to be small fractions of the total allowable Class I increments for all years modeled. Short-term concentration increments were predicted to approach the allowable Class I increments, particularly at SNP. The 2nd highest 3-hour and 24-hour average SO_2 concentrations approach or exceed the allowable Class I increments, while the 2nd highest 24-hour average modeled PM_{10} is between an eighth and one-half the allowable limit. Also note that whereas summer 1988 was characterized by widespread high pollution levels throughout the eastern U.S. (particularly for ozone), all concentration, extinction, and deposition predictions were distinctly higher during 1989 than during the other two modeled years at both Class I areas.

The extinction measure reported in Table 3-5 corresponds to the percent of each year in which calculated incremental modeled PM_{10} (sulfate plus nitrate) concentrations lead to incremental extinction levels more than 10 percent above clean background levels for SNP. According to these calculations, it is predicted that secondary particulate matter from the PSD sources modeled in this analysis lead to such conditions between 20 and 28 percent of the year for SNP, and about 7 to 8 percent of the year at JRFW. At SNP, maximum 3-hour extinction for the years 1988, 1989, and 1990, were 0.0507, 0.3348, and 0.1345 km^{-1}, respectively. Using a simple standard estimation procedure for clear-sky visual range (3.0 divided by extinction in km^{-1}), the extinction increments at SNP

TABLE 3-5. PSD and AQRV parameters calculated from MESOPUFF II output.

Parameter	Averaging Period	Shenandoah NP 1988	Shenandoah NP 1989	Shenandoah NP 1990	James River Face W 1988	James River Face W 1989	James River Face W 1990	Allowable Class I Increment
			PSD Increments					
SO_2	Annual ($\mu g/m^3$)	0.23	0.32	0.21	0.08	0.10	0.06	2
	24-hour ($\mu g/m^3$)	3.92	5.03	3.15	1.39	2.93	1.61	5
	3-hour ($\mu g/m^3$)	16.56	19.62	9.55	5.38	7.35	3.65	25
NO_x	Annual ($\mu g/m^3$)	0.12	0.15	0.13	0.05	0.07	0.04	2.5
PM_{10}	Annual ($\mu g/m^3$)	0.08	0.12	0.07	0.05	0.07	0.04	4
	24-hour ($\mu g/m^3$)	1.24	3.32	1.31	0.85	1.25	1.31	8
			Visibility					
Extinction	3-hour (% of year)[a]	19.9	27.9	22.4	7.3	8.2	6.8	
			Deposition					
Total S	Annual (kg/Ha)	0.38	0.36	0.28	0.11	0.15	0.08	
Total N	Annual (kg/Ha)	0.09	0.12	0.07	0.04	0.16	0.03	

[a] Percent of 3-hour periods for which incremental extinction is greater than 10 percent of clear-day extinction levels.

translate to minimum visual ranges of 59, 9, and 22 km, for each year modeled. The maximum extinction increments are quite high when one considers that these estimates were calculated solely as a result of the secondary particulate matter generated by these emission sources alone, and that other SO_2 and NO_x sources, and natural/anthropogenic sources of organics and dust, were not taken into account.

The extinction coefficient, as defined in these analyses, results from the product of 3-hour average modeled PM_{10} concentrations and a logarithmic humidity-dependent extinction efficiency (ranging from 3.0 m^2/g at less than 30 percent relative humidity to 48 m^2/g at 98 percent relative humidity). High levels of extinction (visibility degradation) are expected to occur when a highly concentrated plume of secondary particulate matter is advected into a Class I area, coinciding with maximum relative humidity conditions. The logarithmic humidity-dependent approach for calculating extinction, however, can yield large extinction coefficients for even modest particulate levels if relative humidity is maximized. For purposes of this study, we attempted to reduce the uncertain influence of particulate extinction under the highest humidities by limiting relative humidity in **PSDPOST** to 95 percent (corresponding to an extinction efficiency of 33.8 m^2/g).

On the other hand, the potential certainly exists for very high incremental modeled PM_{10} concentrations to be supplied to **PSDPOST**. Maximum 3-hour average modeled PM_{10} concentrations (sulfate plus nitrate) determined by **PSDPOST** (but not required for PSD analyses) for these years were 6.5, 17.6, and 6.9 $\mu g/m^3$, respectively. At these levels, high humidity is not necessary to generate large extinction numbers. During screening of the SCRAM BBS example MESOPUFF II problem, we identified that the default value of background ammonia (10 ppb) supplied to MESOPUFF II via the user input file was much higher than typically observed. In view of the fact that there is no background SO_2 or sulfate specified (from non-modeled sources), the background ammonia concentration is probably far too high for annual particulate nitrate calculations. In the eastern U.S., particulate mass is generally dominated by sulfate and organic species, with much smaller contributions from nitrate. We anticipated that 10 ppb of ammonia would consistently produce the maximum potential (i.e. conservative) ammonium nitrate concentrations. Although separate 3-hour average sulfate and nitrate levels were not analyzed by **PSDPOST**, it is likely that maximum 3-hour average modeled PM_{10} concentrations would be lower if the input ammonia level is reduced to more realistic levels.

Predicted maximum accumulated sulfur and nitrogen deposition for both sets of receptors is a small percentage of commonly observed deposition loadings for the area. As reported by Olsen (1988), annual sulfur deposition in the area around Virginia and West Virginia in 1986 ranged from 25 to 30 kg/ha, while nitrogen deposition ranged between 15 and 20 kg/ha. Predicted annual sulfur and nitrogen deposition within SNP from the PSD sources modeled in this study is typically about 10 percent and 5 percent of these observations, respectively. Predicted annual deposition loadings for JRFW are about 1/3 lower than the SNP numbers.

ISCST2 Application and Integration

The IWAQM Phase 1 recommendations (EPA, 1993) require the use of a steady-state Gaussian model for evaluating the incremental impacts of PSD sources within 50 km of a receptor. These impacts should be added to the MESOPUFF II results for sources farther than 50 km from the receptors. The **ISCST2** Gaussian model was applied in order to demonstrate the reconciliation of the **ISCST2** and MESOPUFF II results.

The **ISCST2** model is described in detail elsewhere, including instructions for its application (EPA, 1992b), so no description of the model will be presented here. The **ISCST2** model was used to simulate the 3-hour average concentrations of SO_2 and NO_x at each of the MESOPUFF II receptors corresponding to one of the months modeled with MESOPUFF II. Seven of the sources considered for MESOPUFF II application were within 50 km of a SNP receptor. Of the seven, the largest NO_x and second largest SO_2 emission source, Wampler-Longacre, is situated 13 km from the western tip of SNP (see Figure 3-4). This source was modeled with **ISCST2** for the month of July 1990.

The objective of the **ISCST2** application was to generate output files that provided the same PSD measures that were created by the MESOPUFF II demonstration application. The **ISCST2** results and MESOPUFF II results would then be combined. A postprocessing program, **ISCMPF**, was developed by VDEQ that we would use for combining the model results (Browder, 1994). This program was designed to read from a single binary hourly MESOPUFF II output file (for up to five species) and four separate binary **ISCST2** output files for each species (SO_2 and NO_x) modeled; hourly concentrations, three-hour averages, 24-hour averages, and annual averages. Since each MESOPUFF II output file generated during the demonstration exercise was for a single monthly period and the concentrations were output as three-hour averages, **ISCMPF** could not be exercised for one-hour or for annual average data. Therefore, **ISCST2** was used to produce three-hour and 24-hour average output only.

Surface and upper air meteorological data for Richmond, Virginia were obtained from the SCRAM BBS for use in **ISCST2** modeling. **ISCST2** input files were constructed with the following data (separate runs are required for SO_2 and NO_x):

Source
Wampler-Longacre

Location
UTM coordinates: 692.8 E, 4278.0 N, zone 17

Emission rates
SO_2: 30.2 lbs/hr (3.81 g/s)
NO_x: 98.4 tpy (2.8 g/s)

Stack Parameters
base elevation: 1020 ft (310.9 m)
stack height: 45 ft (13.7 m)

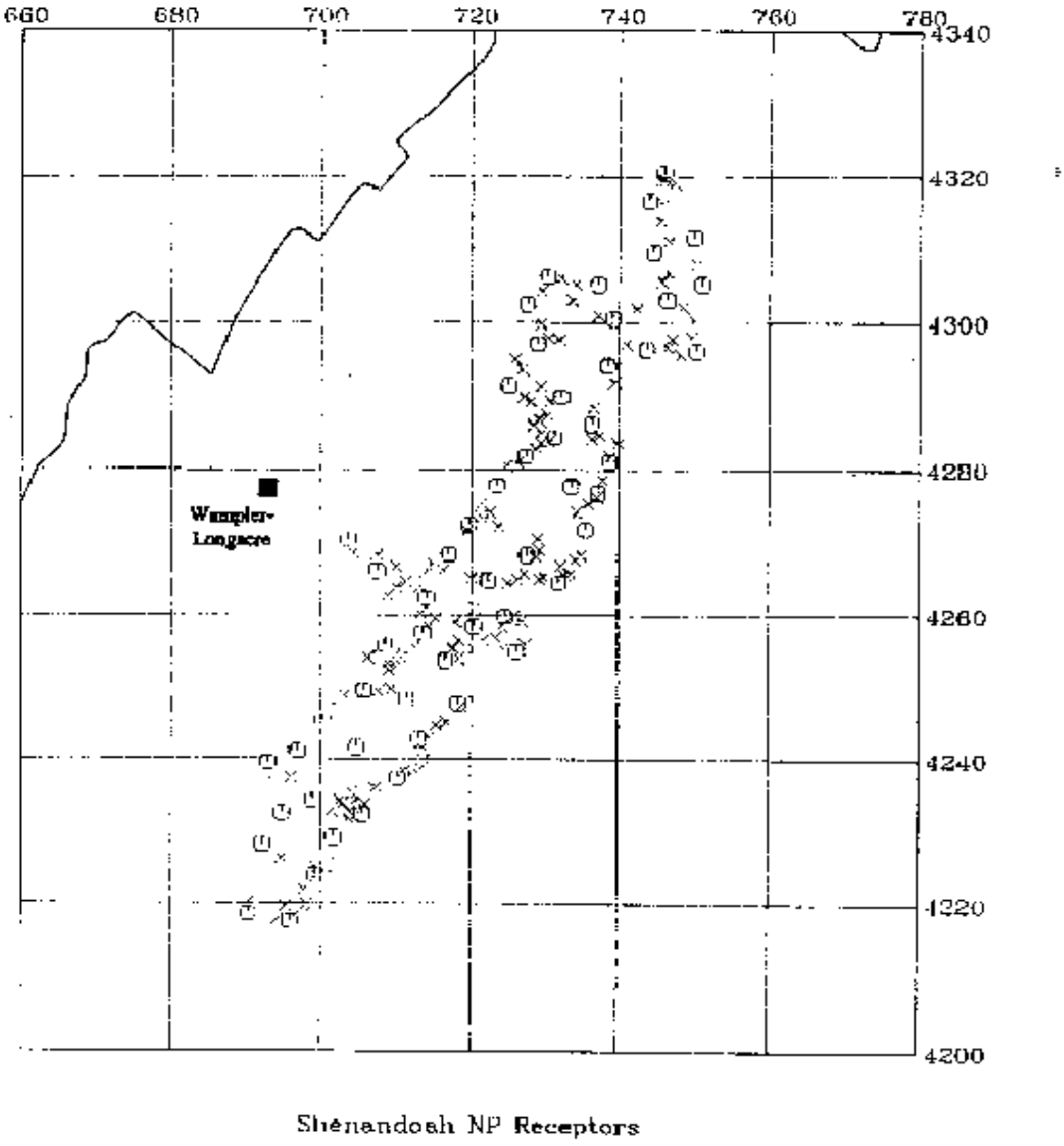

Figure 3-4. Location of Wampler-Longacre, source modeled with ISCST2.

temperature: 400 F (477 K)
velocity: 3720 fpm (18.9 m/s)
diameter: 2 ft (0.61 m)

Receptors
64 discrete receptors, located as shown in Figure 3-2(b,c)

The **ISCST2** model runs also produced ASCII output files. Two tables from these output files, showing the highest second high three-hour average SO_2 and NO_x concentrations, are reproduced in Appendix D. As expected, the peak impacts from Wampler-Longacre were predicted to occur at the closest SNP receptor (located at UTM 703.58 E, 4270.24 N). Examination of the **ISCST2** results show that the highest second high three-hour average concentrations (during July 1990) were 8.16 $\mu g/m^3$ for SO_2, and 6.00 $\mu g/m^3$ for NO_x. The modeled peak impacts from this one nearby source was comparable in magnitude to the cumulative impacts from the set of PSD sources that were modeled with MESOPUFF II, although the impacts were at different times and receptor locations. For example, the maximum three-hour average SO_2 concentration during July 1990 for MESOPUFF II sources was about 10.5 $\mu g/m^3$ (in the northeast corner of SNP), whereas the maximum three-hour average SO_2 concentration from **ISCST2** for just Wampler-Longacre was 11.4 $\mu g/m^3$ (at the receptor closest to the source).

Following execution of **ISCST2**, the results from **ISCST2** and MESOPUFF II were merged using **ISCMPF**. (Note: In order to have compatible binary file formats, **ISCMPF** must be compiled with the same compiler, e.g., Lahey 5.0, that was used to compile the MESOPUFF II and **ISCST2** programs.) The **ISCMPF** program adds the SO_2 and NO_x results from **ISCST2** and MESOPUFF II, but summarizes the results for all five MESOPUFF species. Only MESOPUFF II is capable of modeling secondary species and providing results for species other than SO_2 and NO_x. For the secondary species, the statistical summary from **ISCMPF** only includes the PSD increment measures (see Table 3-4), whereas the results from **PSDPOST** include the estimation of the AQRV parameters for extinction and deposition. For this reason, the **PSDPOST** output is preferred over the **ISCMPF** output for these species. In addition, **PSDPOST** was designed to read 12 monthly input files per year in order to compute annual PSD and AQRV statistics. Since the MESOPUFF II output files were monthly, **ISCMPF** could not be used for annual statistics. To provide annual statistics, it would be necessary to either (1) edit the **ISCMPF** program to accept 12 monthly files instead of one annual file, (2) combine all the binary MESOPUFF II monthly output files into one binary annual file for input to **ISCMPF**, or (3) run MESOPUFF II for an entire year.

The results of the model output integration indicate that the highest second high three-hour average SO_2 concentration (during July 1990) for all sources was 10.44 $\mu g/m^3$. Since this occurred during the same hour as the highest second high from **ISCST2**, the contribution during this hour from MESOPUFF II sources (sources other than Wampler-Longacre) can be computed as 2.28 $\mu g/m^3$ (10.44 - 8.16). Similarly, the highest second high three-hour average NO_x concentration for all sources was 6.24 $\mu g/m^3$. This also occurred during the same hour as the highest second high from **ISCST2**, so the contribution during this hour from only MESOPUFF II sources can be computed as 0.24 $\mu g/m^3$ (6.24 - 6.00).

The results of this exercise demonstrate that it was possible to combine the SO_2 and NO_x results from MESOPUFF II and **ISCST2** using the **ISCMPF** program. Some concerns were raised regarding the **ISCMPF** program, however. The program could be more general. Currently, the program is hardwired into accepting only annual average MESOPUFF II output, and the user must provide **ISCST2** output files for four averaging times (1-hour, 3-hour, 24-hour, and annual). If, for example, only 1-hour **ISCST2** output were available, then the program should be flexible enough to compute the data for the other averaging periods (as it does for the MESOPUFF II data). In this case, since we only had 3-hour output from MESOPUFF II, it was necessary to alter the **ISCMPF** program to accept and process 3-hour data. Additionally, the program has the ability to produce tables of maximum concentrations and second high concentrations for each receptor, and a table of N-maximum concentrations (these three **ISCMPF** output tables corresponding to 3-hour average SO_2 concentrations are shown in Appendix D). However, the PSD increment parameters required for SO_2 are the highest second high (3-hour and 24-hour averages) concentrations (see Table 3-4). The N-maximum table does not provide this result, so one is forced to find the highest value on the table of second high concentrations in order to ascertain this required PSD increment parameter. It is recommended that the **ISCMPF** program be revised in order to be more flexible regarding input files, and that it be able to readily display the necessary PSD increment parameters.

An additional minor difficulty in using the **ISCMPF** results is that the coordinate locations for the discrete receptors are input from the MESOPUFF II output file in grid cell units. These grid cell coordinates are later scaled into meters, however, the appropriate UTM coordinate of the modeling grid origin needs to be added to convert the locations into proper UTM coordinates. The receptor coordinates shown in the output file (see Appendix D) are almost meaningless. Since the receptor numbers (indices) were also provided, it was necessary to refer to the discrete receptor list from **ISCST2** in order to determine the actual locations.

For future users of MESOPUFF II and **ISCST2**, one option for integration of results would be to obtain the **ISCMPF** program (it may be made available on the SCRAM BBS), and edit the program to match the MESOPUFF II output structure (i.e., monthly files, 3-hour data). A second (probably simpler) option would be to revise the **PSDPOST** program to read an entire year of **ISCST2** 3-hour averages and add them to the MESOPUFF II (SO_2 and NO_x) 3-hour average concentration results before processing as before.

4 SOURCE IMPACTS AS A FUNCTION OF DISTANCE

A set of 24 MESOPUFF II simulations were performed with sources at varying distances from Shenandoah National Park (SNP) to provide some insight into the relationship between distance from SNP and potential PSD and AQRV impacts. Four months of one year (representing each season of one of the years simulated with the PSD sources) were modeled under six different source scenarios. Each source scenario included a number of identical hypothetical point sources placed on a ring at a constant distance from the park. The number of sources was proportional to the ring circumference; in other words, the linear density of sources was held as constant as possible.

This section describes the preparation of input data for this "ring source" analysis, the application of MESOPUFF II, and analysis of modeling results. This exercise provided an opportunity to utilize the MESOPUFF II post-processor, **MESOFILE**, which was not used in the PSD source analysis described in the previous section. The results are presented as maximum impacts as a function of distance, and as maximum impacts normalized to the emission strength and number of sources.

INPUT DEVELOPMENT

For the ring source analysis, the modeling domain, meteorological input files, land use, and air quality input files were identical to those described in Section 3 for the PSD source analysis. The modeling episode for the ring source analysis included the months of January, April, July, and October of 1988. The months were selected to include one representative month from each season.

Development of Ring Source Data

Six non-circular rings of hypothetical point sources were developed to encompass SNP at a range of distances from the SNP "spine". The park's spine was defined as a line segment connecting the most northeastern and most southwestern modeling receptors. The source rings were established at 50, 100, 125, 150, 175, and 200 km from the spine. Each ring consisted of two semicircles connected by two line segments, the segments being identical in length and parallel to the SNP spine (Figure 4-1).

The distribution of hypothetical point sources around each ring was determined in the following manner. First, SO_2 and NO_x emission rates for all available PSD point sources between 50 and 200 km of Shenandoah NP (see Table 3-2) were summed to obtain total

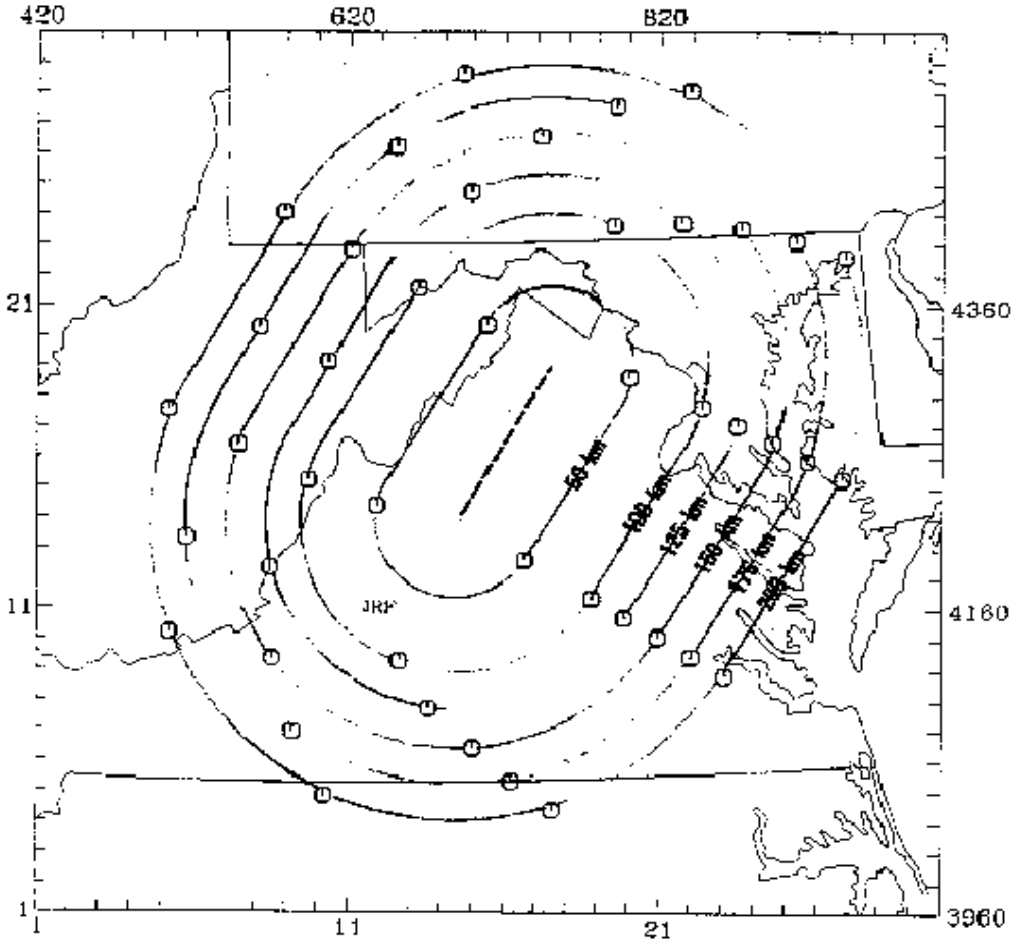

FIGURE 4-1. MESOPUFF computational domain for ring source analyses, showing the location of the ring sources. The dashed line at the center of the rings represents the SNP spine.

SO_2 and NO_x emission rates of 3330 g/s and 2480 g/s, respectively. Based on these total emissions and the total area covered by the PSD sources in Table 3-2, an average emission density (emission rate per unit area) was determined. For each ring, this emission density was multiplied by the area of an annulus extending ±25 km from the ring to determine the total emission rates for the ring.

The next step was to determine how many individual sources to place on each ring. In order for the results to be somewhat representative of typical PSD sources, average SO_2 and NO_x emission rates were calculated for the PSD sources in Table 3-2. The average emission rates were 123 g/s for SO_2 and 92 g/s for NO_x, although the emission rates varied over two orders of magnitude. In order to obtain a 1-source increase per 25 km increase in ring distance from SNP, slightly higher emission rates of 181 g/s for SO_2 and 135 g/s for NO_x were selected for the hypothetical sources.

The emission rates and stack parameters used for the hypothetical sources are summarized in Table 4-1. The stack parameters are average values from the PSD source data in Table 3-2. Emission rates of primary sulfate were specified at 3 percent of SO_2 rates, with an additional 1.5 factor to account for the larger sulfate molecular weight. Source characteristics of each ring are summarized in Table 4-2; the locations of the sources are shown in Figure 4-1.

Non-gridded Receptors for the Ring Source Analysis

The ring sources were arranged in concentric ovals around Shenandoah NP. Thus, only the SNP non-gridded receptors, and not those at JRFW, were used to assess impacts. For the July and October ring source simulations, only the 55 SNP receptors were included in the MESOPUFF II input files. The locations of the SNP receptors were the same as those described in Section 3. For the January and April ring source simulations, the JRFW receptors were inadvertently included in the input files, but were excluded in the analysis of results.

APPLICATION OF MESOPUFF II FOR RING SOURCES

A total of 24 MESOPUFF II input files were constructed for the ring source analysis, corresponding to six distances for each of the four months. MESOPUFF II ring source simulations were performed in batches of six over weekends on a 386/25 MHz PC with a 100 MB disk drive. The **MESOPAC** output file for each month, needed as input to MESOPUFF II, required 53 MB of disk storage space, the MESOPUFF II executable required 3.3 MB, and the output from each simulation required 1.5 MB. Thus, the total disk space requirements for one set of six ring simulations was 65 MB.

The large size of the MESOPUFF II executable file also required some adjustments to the PC. Although the PC used for this exercise was equipped with 4 MB of memory, applications such as Windows and network software typically consume a large portion of the 4 MB. In order to run MESOPUFF II, the PC was re-booted from a floppy disk in a

TABLE 4-1. Emission rates and stack parameters for idealized sources.

Stack Parameters	Value for Idealized Source
SO_2 Emission Rate (g/s)	181.0
SO_4 Emission Rate (g/s)	8.1
NO_x Emission Rate (g/s)	135.0
Stack Height (m)	81.0
Stack Diameter (m)	3.97
Stack Exit Velocity (m/s)	20.7
Stack Exit Temperature (K)	425.0

TABLE 4-2. Source ring characteristics

			Total Emissions (g/s)	
Ring Distance from SNP	Number of Sources	Distance Between Sources	SO_2	NO_x
50 km	4	138 km	724	540
100 km	6	144 km	1086	810
125 km	7	146 km	1267	945
150 km	8	148 km	1448	1080
175 km	9	149 km	1629	1215
200 km	10	150 km	1810	1350

stripped-down mode without applications. The consequences of this were that it was not possible to run MESOPUFF II from Windows, which would allow the model to run in a background mode. Instead, the MESOPUFF II runs were performed overnight and over weekends when dedicated use of the PC was possible. The size of the MESOPUFF II executable varies with parameters such as the number of surface and upper air meteorological stations, ozone stations, sources, and receptors. The parameters used for the applications described here, both the PSD and ring applications, pushed the executable close to the maximum size that could be executed on a machine with 4 MB of memory.

For the months of January, April, and October, CPU times on the 386 were approximately one hour per source per month simulated. For July, the CPU times were approximately twice as large as the other months. The reason for this increase in CPU was not investigated, but may be due to lower wind speeds in July which kept puffs in the modeling domain for a longer period of time. Based on CPU times for the PSD source analysis (Section 3), CPU times would be decreased by a factor of 5 to 10 on a 486 PC.

MESOPUFF II output for the ring source analysis consisted of 3-hour average concentrations and wet and dry fluxes of all species. The results were processed using the **MESOFILE** postprocessor.

APPLICATION OF MESOFILE FOR RING SOURCES

The **MESOFILE** postprocessor was used to obtain 24-hour average and monthly average concentrations and monthly cumulative deposition for the ring source simulations. Because **MESOFILE** only processes a single species during each run, batch files were set up to execute a series of ten consecutive **MESOFILE** runs for each ring scenario. As a result, a total of 240 **MESOFILE** input and output files were generated for the ring source analysis.

MESOFILE requires the input files to be named infile1.dat and infile2.dat, and creates a single output file called file.lst. Thus, batch files are needed to rename the MESOPUFF II output files, execute **MESOFILE**, and rename the **MESOFILE** output.

MESOFILE can perform two basic operations: averaging and summing. Averages can be specified over any integral number of output intervals. Values can also be scaled by a constant prior to averaging or summing. This feature is useful for converting sulfate and nitrate concentrations to ammonium sulfate and ammonium nitrate in the modeled PM_{10} calculation.

MESOFILE also creates a binary file called file25.dat. Results from a previous **MESOFILE** run can be accessed through this file. This allows for the calculation of parameters involving more than one species at a time, such as the combination of sulfate and nitrate into modeled PM_{10} and the calculation of total S and total N deposition.

The values calculated for the ring source analysis were based on the PSD and AQRV indicators in Table 3-4. For SO_2, **MESOFILE** was set up to report 3-hour, 24-hour, and monthly averages. For NO_x, nitric acid, sulfate ($SO_4^=$), nitrate (NO_3^-) and modeled PM_{10}, 24-hour averages and monthly averages were produced. $SO_4^=$ and NO_3^- concentrations output by MESOPUFF II were multiplied by factors of 1.38 and 1.29 to convert to ammonium sulfate ($(NH_4)_2SO_4$) and ammonium nitrate (NH_4NO_3), respectively. Following the Phase 1 recommendations, the sum of ammonium sulfate and ammonium nitrate was reported as modeled PM_{10}. Total sulfur deposition was calculated by summing wet and dry deposition fluxes for SO_2 and $SO_4^=$ over the month. Conversion factors were applied to convert SO_2 and $SO_4^=$ to a sulfur basis, and to convert 3-hour average fluxes to 3-hour cumulative deposition. Total nitrogen deposition was calculated by summing wet and dry deposition fluxes for NO_x, HNO_3, and NO_3^- over each month. Conversion factors were applied to convert NO_x, HNO_3, and NO_3^- to a nitrogen basis, and to convert 3-hour average fluxes to 3-hour cumulative deposition.

Other input files required by **MESOFILE** are the MESOPUFF II output files for concentration and wet and dry deposition. The total disk space required for MESOPUFF II output files from the ring simulations is 24 MB (1 MB per simulation). **MESOFILE** output files also occupied 1 MB for each of the 24 scenarios. Individual **MESOFILE** runs were very fast; each set of ten runs required only about 5 minutes of elapsed time on the 386 PC. Also, the **MESOFILE** executable code occupies only 1.3 MB, and thus can be run without any of the special set-up needed for the MESOPUFF II runs.

MESOFILE output is in the form of text files that contain the averaged concentrations or cumulative fluxes for each receptor. Note that **MESOFILE** can produce isopleth plots for gridded receptors, but not for non-gridded receptors. **MESOFILE** also identifies the highest value among all receptors for a given averaging period. However, it does not calculate the highest value among a set of highest values. For example, in this application, **MESOFILE** provided 30 or 31 sets of 24-hour averages for each species (per month modeled). In order to find the highest 24-hour average that occurred during the month, it was necessary to scan the output file manually to locate the highest value from among the 30 or 31 daily maximum values. This was somewhat time-consuming. It is virtually impossible to use **MESOFILE** to identify the highest second-high value, as defined for PSD analyses.

The calculation of 4-month averages from the monthly averages was also very time-consuming. This was accomplished by importing the sections of the **MESOFILE** output text files containing monthly averages for each receptor into PC spreadsheets, re-arranging the data into columns, averaging, and locating the maximum. For each species, 24 blocks of text had to be imported and re-arranged.

RESULTS FROM RING SOURCE SIMULATIONS

The results obtained with **MESOFILE** were input into PC spreadsheets to produce the graphs shown in Figures 4-2 through 4-22. The results are presented as the highest value among all SNP non-gridded receptors, as a function of source distance from SNP. In the following

discussion, for comparison purposes, the impacts are examined relative to the allowable Class I PSD increments listed in Table 3-4. In these comparisons, it is important to bear in mind that the sources do not represent actual sources.

Concentration Impacts as a Function of Distance

SO_2 Concentrations

Figure 4-2 shows the highest 3-hour average SO_2 concentration for each of the four months as a function of source distance from SNP. As might be expected for a primary pollutant, the highest impacts occur for the 50-km source ring. The highest 3-hour average concentration is 20 $\mu g/m^3$, close to the allowable Class I PSD increment of 25 $\mu g/m^3$. The simulated 3-hour average SO_2 concentrations decrease by up to a factor of four between the 50 and 100 km rings, but then increase between the 100 and 125 km rings for two of the months. This increase occurs because the sources on each ring are located in different positions relative to SNP (see Figure 4-1). If a larger number of smaller sources were used, a smoother decrease in concentration with source distance would likely result.

There is no consistent trend for the highest 3-hour average SO_2 concentrations to be higher in any particular month of the year, although the lowest values were simulated for July for five of the six rings. Modeled conversion of SO_2 to sulfate and SO_2 deposition are both maximized in July. These two effects may account for the lower SO_2 concentrations simulated for July.

The ratio of concentration to source strength is commonly termed χ/Q, and represents a tool for estimating impacts based on source strengths. In the ring source application, 3-hr impacts are likely to be primarily the result of a single source, rather than the total source strength of the source ring. Dividing the maximum 3-hr SO_2 concentrations by the single-source SO_2 emission rate of 181 g/s (1437 lbs/hr) gives χ/Q values of 0.11, 0.038, and 0.014 for the 50 km, 125 km, and 200 km rings, respectively, where the units are $(\mu g/m^3)/(g/s)$. In units of $(\mu g/m^3)/(lbs/hr)$ the corresponding χ/Q values are 0.88, 0.30, and 0.11.

Figure 4-3 shows the highest 24-hour average SO_2 concentrations for each month as a function of source distance from SNP. Again, the greatest impacts occur for the 50-km ring, although the decrease from the 50-km to the 100-km ring is not as pronounced as for the 3-hour impacts. The highest 24-hour average concentration of 2.8 $\mu g/m^3$ is slightly more than half the allowable Class I PSD increment of 5 $\mu g/m^3$. The highest concentrations at each source distance generally are simulated for October and January, with the lowest concentrations generally simulated for July.

For the 24-hour impacts, it is not possible to determine whether the 24-hour impacts are the result of a single source, or the confluence of puffs from two or more sources. Thus, it is difficult to select the most appropriate source strength to use in calculating χ/Q.

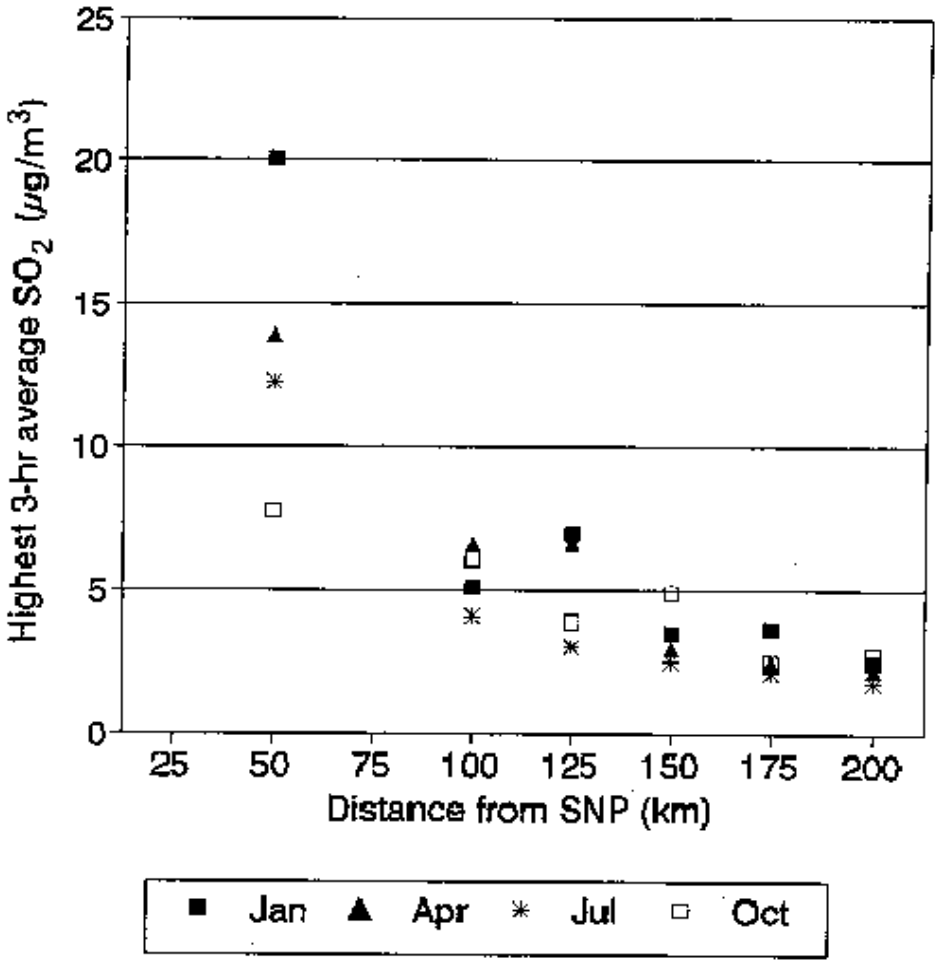

FIGURE 4-2. Highest simulated 3-hour average SO_2 concentrations ($\mu g/m^3$) from ring sources for January, April, July, and October, 1988.

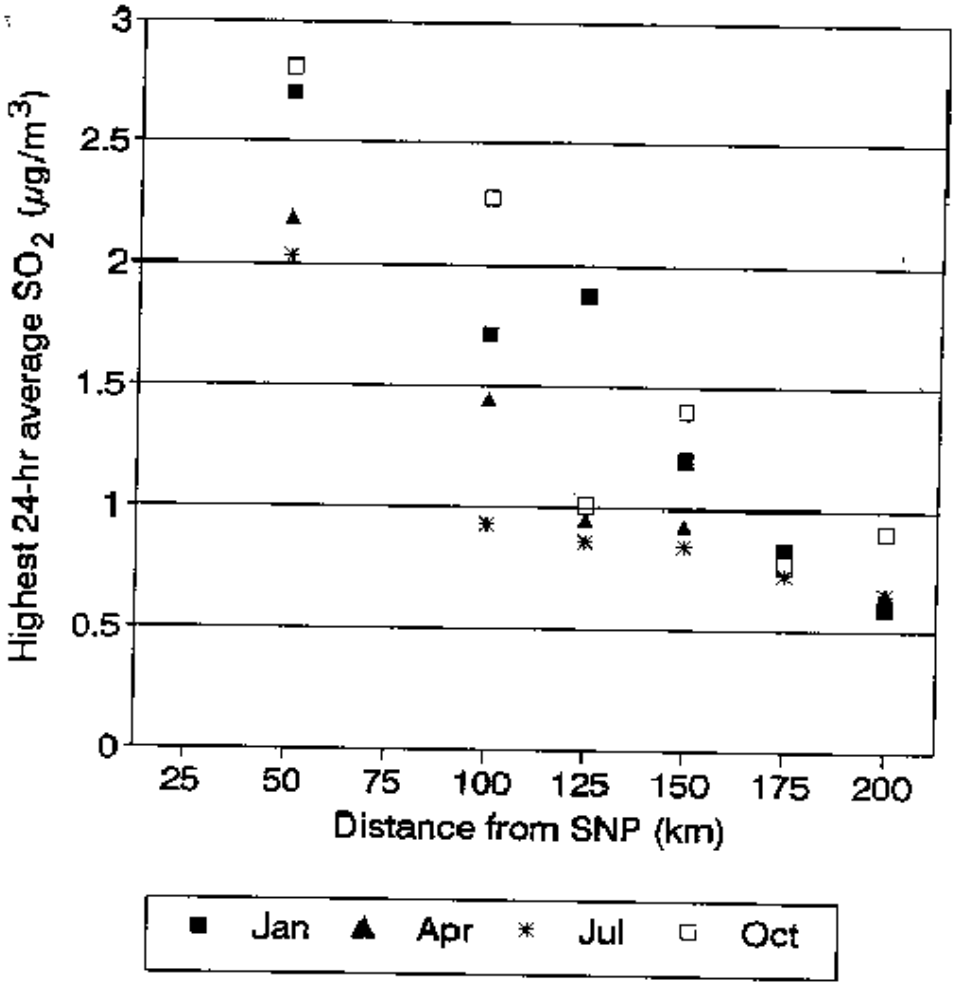

FIGURE 4-3. Highest simulated 24-hour average SO_2 concentrations ($\mu g/m^3$) from ring sources for January, April, July, and October, 1988.

Using the total source strength for the ring would seriously underestimate χ/Q, whereas using the source strength from a single source might result in an overestimate.

Figure 4-4 shows the highest monthly average SO_2 concentrations. Note that because each point represents a different receptor, the highest 4-month average is not determined as the average of the four points for each source distance in Figure 4-4. Figure 4-5 shows the highest 4-month average SO_2 concentrations. Since one month from each season was modeled, the 4-month averages may be used to approximate an annual average. The highest 4-month average SO_2 concentration is 0.34 $\mu g/m^3$, about one-sixth of the allowable PSD increment for the SO_2 annual average.

Comparison of Figures 4-2 through 4-5 shows that the decreasing trend in peak SO_2 concentration with distance is less pronounced as averaging time increases. Recall that the total emissions from each source are constant, but that the total emissions for each ring increase proportionally to ring circumference. Short-term impacts are generally the result of only one source at a time. Since the ring sources are all the same size, the 3-hour impacts would be expected to decrease as the inverse of the distance from SNP (1/distance). However, the longer-term impacts are the cumulative impacts of all the sources. For longer-term impacts, therefore, the concentrations normalized by the number of sources would be expected to decrease as the inverse of the distance.

Figure 4-6 shows the per-source highest 4-month average SO_2 impacts. Whereas the absolute impact decreased by a factor of two from the 50 km ring to the 200 km ring, the normalized impact decreased by more than a factor of four. Thus, the normalized impact decreased at greater rate than 1/distance. This is likely to reflect additional losses of SO_2 due to reaction and deposition at the greater distances.

These results for SO_2 suggest that 3-hour impacts are the limiting consideration for sources located 50 km from SNP. For sources of the size used in this analysis, sources located further than 200 km are likely to have small 3-hour SO_2 impacts by comparison to sources located closer in. However, it is not possible from this analysis to make a blanket statement that all sources located further than 200 km can be considered negligible in terms of 3-hour SO_2 impacts. The largest source in the PSD analysis (see Table 3-2) has SO_2 emissions that are ten times as large as the per-source emissions used in the ring analysis. For sources that size or larger, 3-hour SO_2 impacts at 200 km or greater distances may approach the allowable increment.

For sources located 100 km or further from SNP, these results suggest that 24-hour impacts may be the limiting consideration. Sources located at 100 km from SNP with emissions double those used in this analysis would produce maximum simulated 24-hour SO_2 concentrations near the allowable increment. Simulated 4-month average SO_2 concentrations were sufficiently low that the annual average PSD increment for SO_2 does not appear to be a limiting consideration at any distance for the range of source strengths addressed in this analysis.

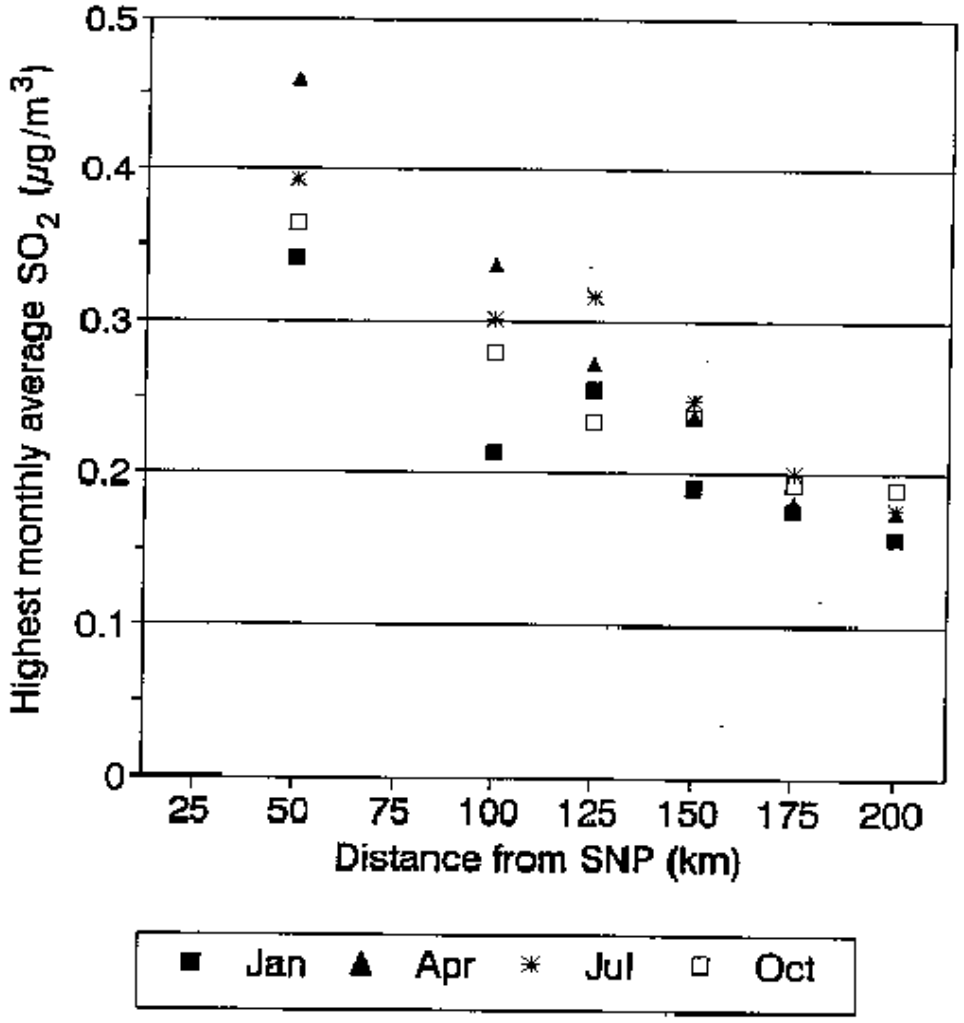

FIGURE 4-4. Highest simulated monthly average SO_2 concentrations ($\mu g/m^3$) from ring sources for January, April, July, and October, 1988.

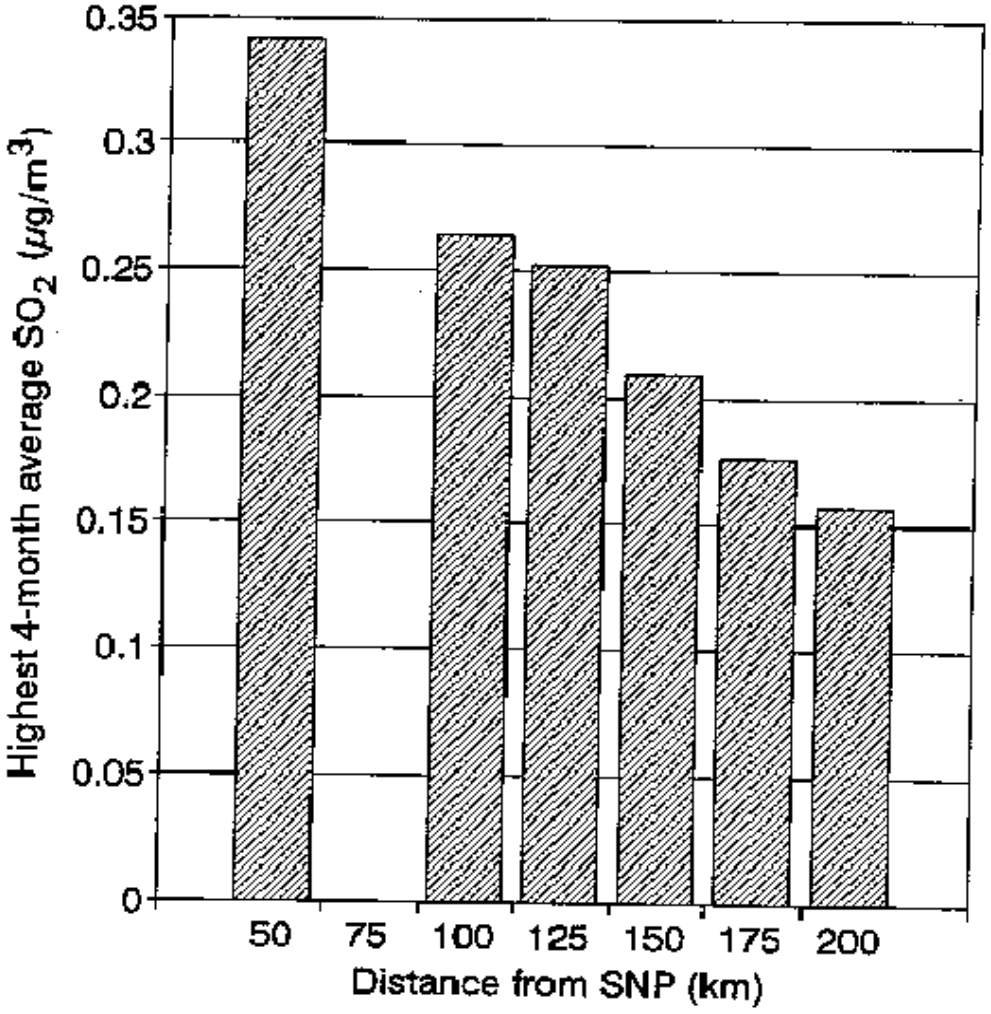

FIGURE 4-5. Highest simulated 4-month average SO_2 concentrations ($\mu g/m^3$) from ring sources for 1988.

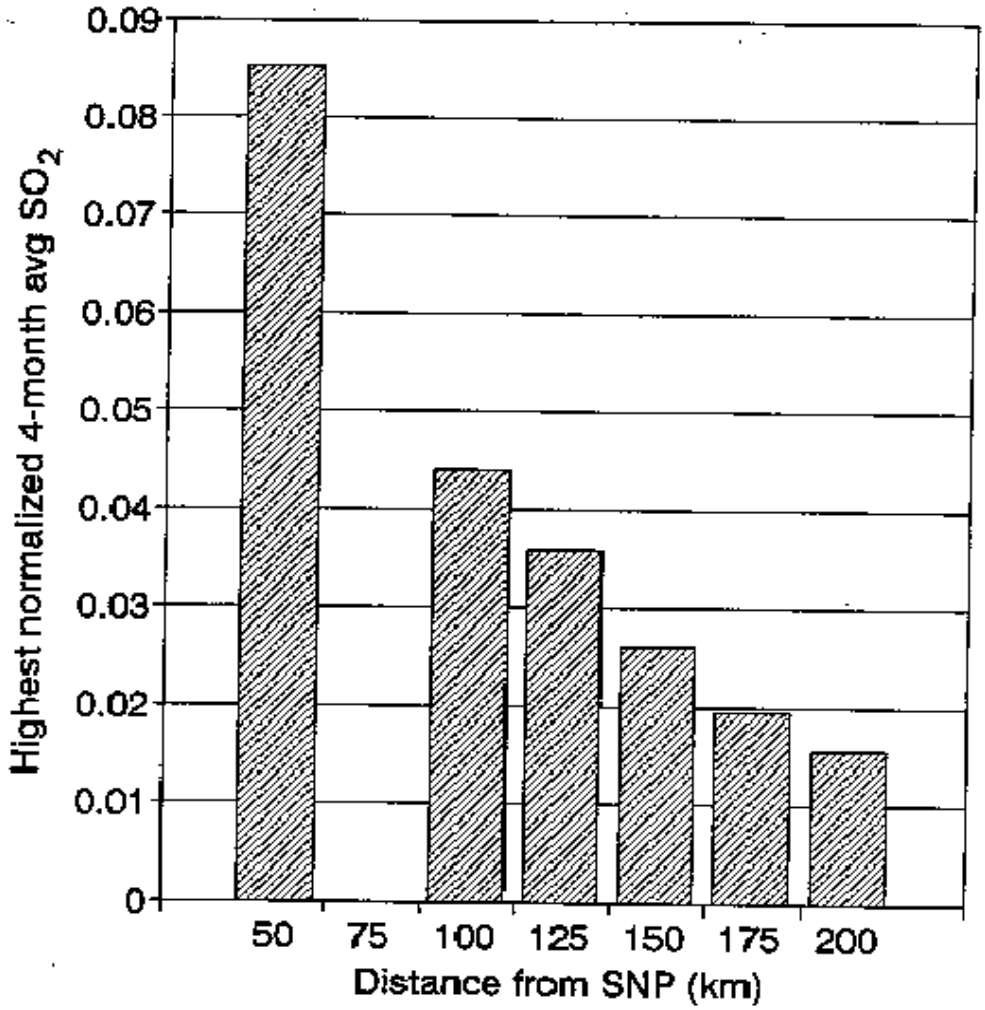

FIGURE 4-6. Highest simulated per-source 4-month average SO_2 concentrations from ring sources for 1988.

No_x Concentrations

Figure 4-7 shows the highest monthly average concentrations for NO_x. (Plots of shorter-term NO_x concentrations were not prepared because there are no short-term PSD standards for NO_x.) Comparison of Figure 4-7 to Figure 4-4 for monthly average SO_2 illustrates the faster rate of chemical decay for NO_x. At 50 km, NO_x concentrations are generally on the order of 60 percent of the SO_2 concentration for January, April, and October, reflecting the ratio of the emission strengths of SO_2 and NO_x in the ring source input files. NO_x concentrations at 50 km are 40 percent of SO_2 concentrations for July, because NO_x reacts much more rapidly than SO_2. At 200 km, NO_x concentrations are on the order of 50 percent of the SO_2 concentration for January, April, and October, and 30 percent of SO_2 concentrations for July.

The highest monthly average NO_x concentration was slightly less than 0.3 $\mu g/m^3$, or about 11 percent of the allowable increment of 2.5 $\mu g/m^3$ for NO_x annual average in Class I areas. The annual average will be lower than the highest monthly average. Thus, much greater NO_x source strengths than those used in this analysis would be needed for NO_x concentrations to approach the allowable increment.

PM_{10} Concentrations

As discussed in Section 3, the only PM_{10} constituents modeled by MESOPUFF II are sulfate and nitrate. In the remainder of this section, modeled PM_{10} refers to the sum of ammonium sulfate and ammonium nitrate, and includes both primary and secondary sulfate. Typical sources may emit other primary PM_{10} components that are not included in this analysis.

Figure 4-8 provides the highest 24-hour average modeled PM_{10} concentrations as a function of source distance from SNP. These impacts show a completely different pattern than SO_2 or NO_x. The highest 24-hour average modeled PM_{10} concentration of 0.7 $\mu g/m^3$ occurs for July for the 175 km ring. This represents less than one-tenth of the allowable PSD increment of 8 $\mu g/m^3$ for PM_{10} in Class I areas. There are no clear trends in the 24-hour average modeled PM_{10} concentrations with source distance from SNP. For the months of January, April, and October, a weak decrease in maximum concentration with distance was simulated. July modeled PM_{10} concentrations show a minimum at 125 km and are roughly equal for the 50 km and 200 km rings. At the greater distances, July modeled PM_{10} concentrations are much higher than those from the other seasons.

Figure 4-9 presents the highest monthly average modeled PM_{10} concentrations as a function of source distance from SNP. The highest impact occurred for July for the 150 km ring. The seasonal effect is very pronounced for the monthly average modeled PM_{10}, with July concentrations more than twice those in January, and April and October falling somewhere between the two.

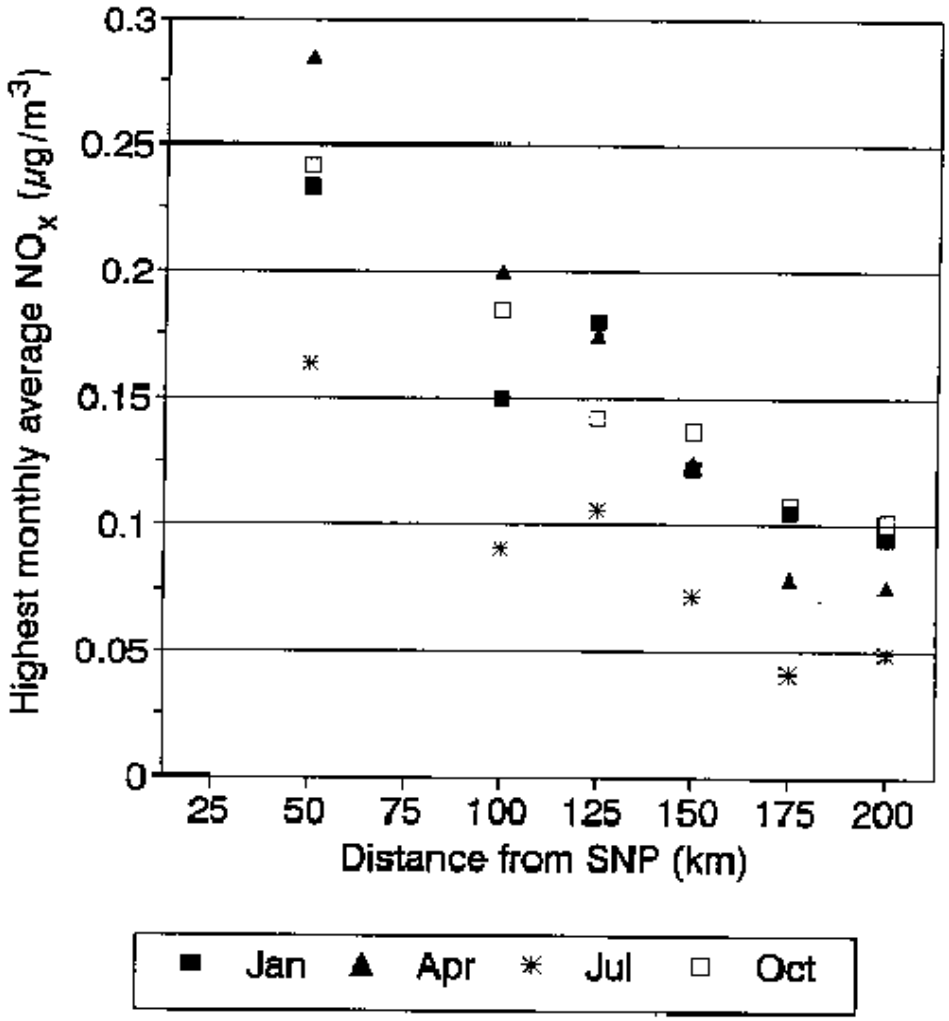

FIGURE 4-7. Highest simulated monthly average NO_x concentrations ($\mu g/m^3$) from ring sources for January, April, July, and October, 1988.

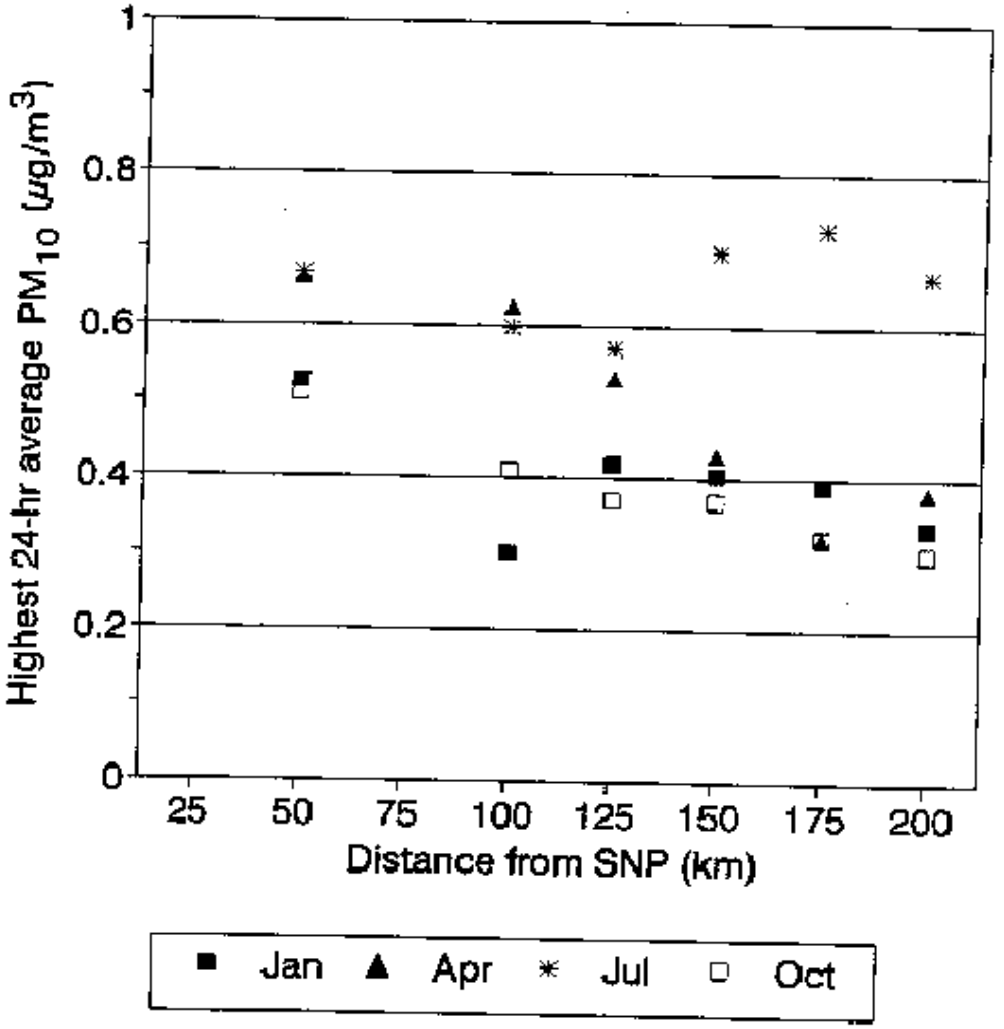

FIGURE 4-8. Highest simulated 24-hour average PM_{10} concentrations ($\mu g/m^3$) from ring sources for January, April, July, and October, 1988. For this exercise, PM_{10} is defined as the sum of ammonium sulfate and ammonium nitrate.

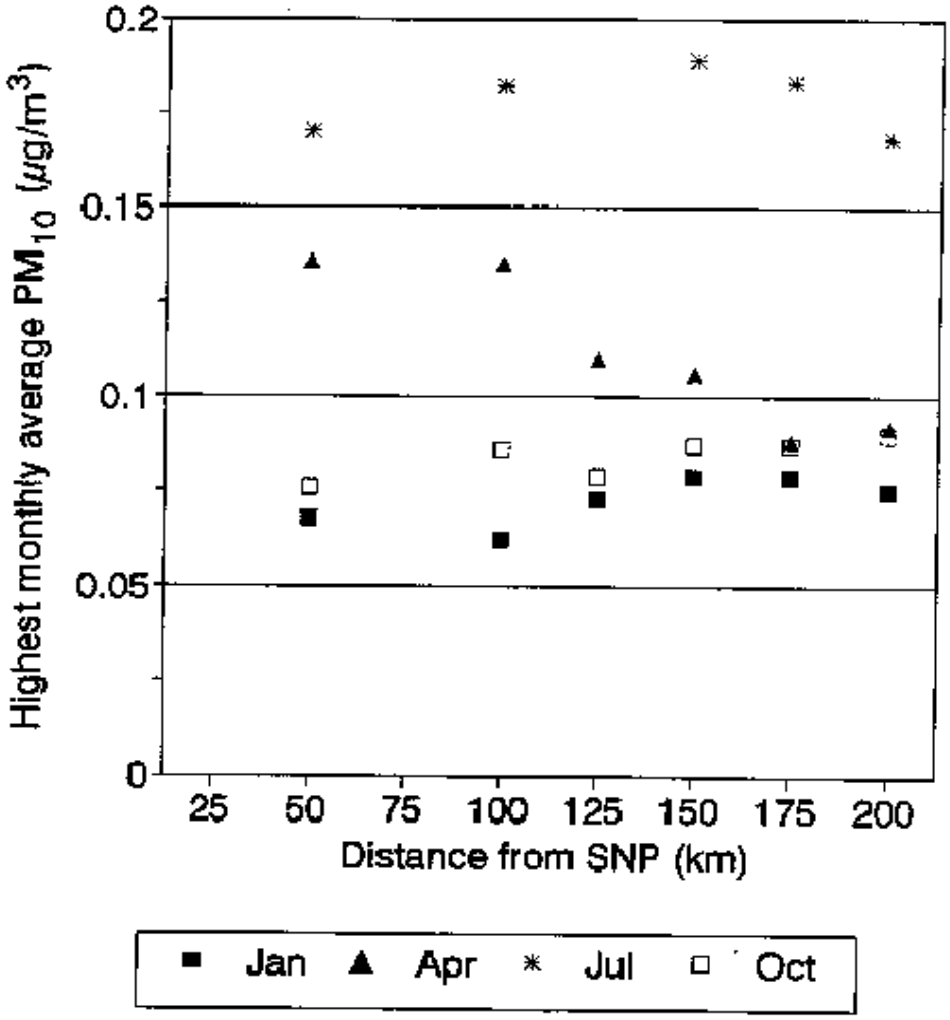

FIGURE 4-9. Highest simulated monthly average PM_{10} concentrations ($\mu g/m^3$) from ring sources for January, April, July, and October, 1988. For this exercise, PM_{10} is defined as the sum of ammonium sulfate and ammonium nitrate.

In Figure 4-10, the seasonal dependence of modeled PM_{10} concentrations is illustrated for the 125 km ring. Figure 4-10 clearly shows that sulfate formation is maximized in July in the MESOPUFF II model, whereas modeled nitrate concentrations are relatively constant year round. Modeled sulfate and nitrate concentrations were nearly equal for all months but July. This is contrary to measured PM_{10} data for SNP and other locations in the eastern U.S., where sulfate concentrations are typically three times as large as nitrate concentrations. Two factors are likely to be responsible for this apparent inconsistency. The high background ammonia concentration of 10 ppb used as a default value in MESOPUFF II will result in an overestimate of aerosol nitrate concentrations. However, the lack of a parameterization of rapid in-cloud sulfate formation in MESOPUFF II may lead to an underestimate of sulfate concentrations.

Figure 4-11 presents the highest 4-month average modeled PM_{10} concentrations. The 4-month average peaks for the 125 km ring. The peak value of 0.11 $\mu g/m^3$ is only 3 percent of the allowable PSD increment for annual average PM_{10} concentrations in Class I areas. Comparison of Figure 4-11 to Figure 4-5 for SO_2 shows that, at a distance of 50 km, 9 percent of the modeled total sulfur is in the form of sulfate. At 200 km, 16 percent of the modeled total sulfur is in the form of sulfate.

It is important to recognize that there is a primary component to the modeled PM_{10} concentrations shown in Figures 4-8 through 4-11, since primary $SO_4^=$ emissions equal to 3 percent of SO_2 emissions (as sulfur) were assumed. Although it is not possible to distinguish the primary sulfate from the secondary sulfate, an estimate of the magnitude of the primary contribution can be obtained from the SO_2 concentration at the same receptor over the same averaging period. For the highest monthly average modeled PM_{10} concentrations (Figure 4-9), up to 50 percent of the sulfate at 50 km is estimated to be primary. At 200 km, approximately 25 percent of the monthly average sulfate is primary. Primary sulfate is less of a contributor to the 24-hour averages, contributing 15 percent or less of the highest 24-hour average sulfate concentrations at 50 km.

Figure 4-12 shows the normalized, per-source, 4-month average modeled PM_{10} concentrations. When the modeled PM_{10} concentrations are normalized in this manner, a decreasing trend in modeled PM_{10} concentration with source distance is observed. Normalized 4-month average modeled PM_{10} concentrations at 200 km are 37 percent of those at 50 km.

These results suggest that 24-hour average PM_{10} impacts, rather than the annual averages, are the limiting consideration for PSD purposes. However, considerably greater source strengths than those used here would be needed for modeled PM_{10} concentrations to approach the allowable increment for Class I areas. At 175 km, roughly ten times the source strength used here would produce 24-hour average impacts near the allowable increment. (According to Table 3-2, at least one source of that size is located at roughly 175 km from SNP). Because distances of only 200 km were used in this analysis, it is difficult to draw firm conclusions about the modeled PM_{10} impacts. The cumulative impacts from numerous sources both closer and further than 200 km from SNP might well be considerably greater than the ring source impacts modeled in this analysis.

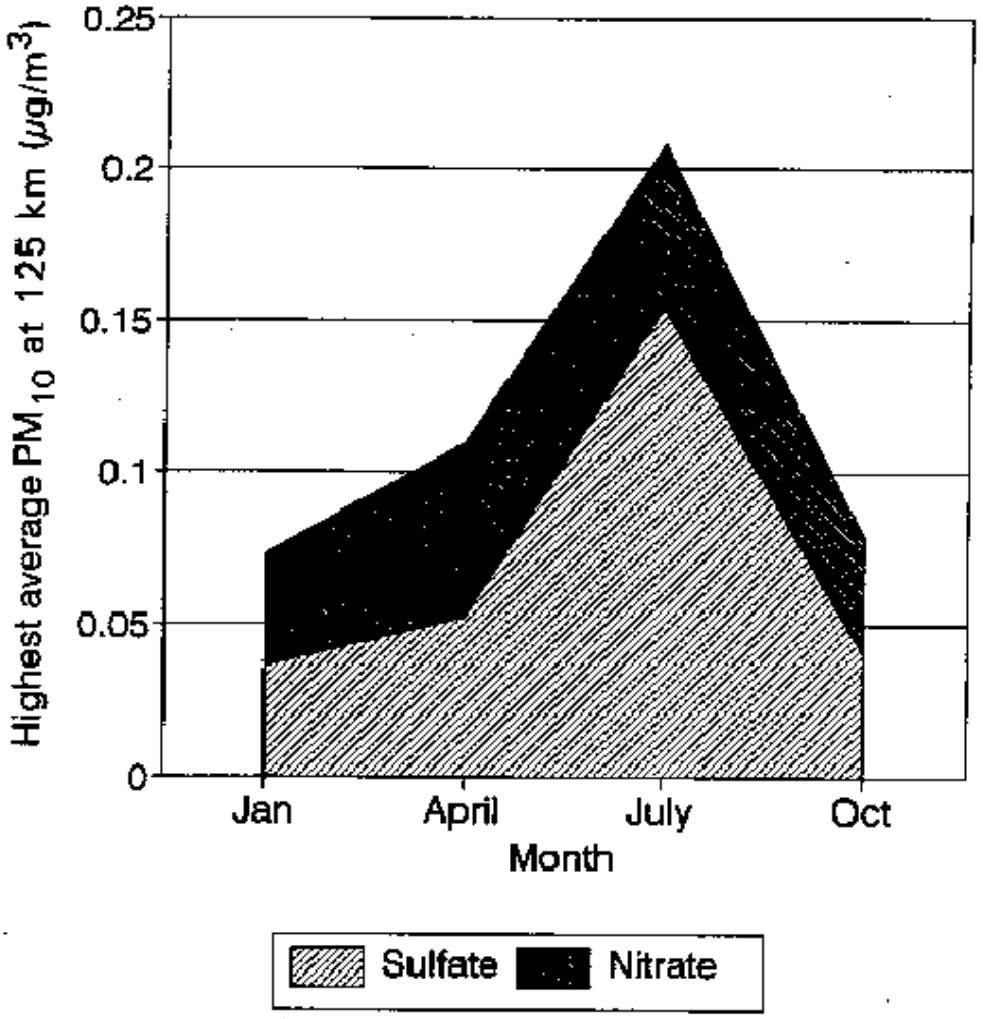

FIGURE 4-10. Seasonal effects for sulfate, nitrate and total PM_{10} monthly average concentrations ($\mu g/m^3$) for the 125 km ring for 1988. For this exercise, PM_{10} is defined as the sum of ammonium sulfate and ammonium nitrate.

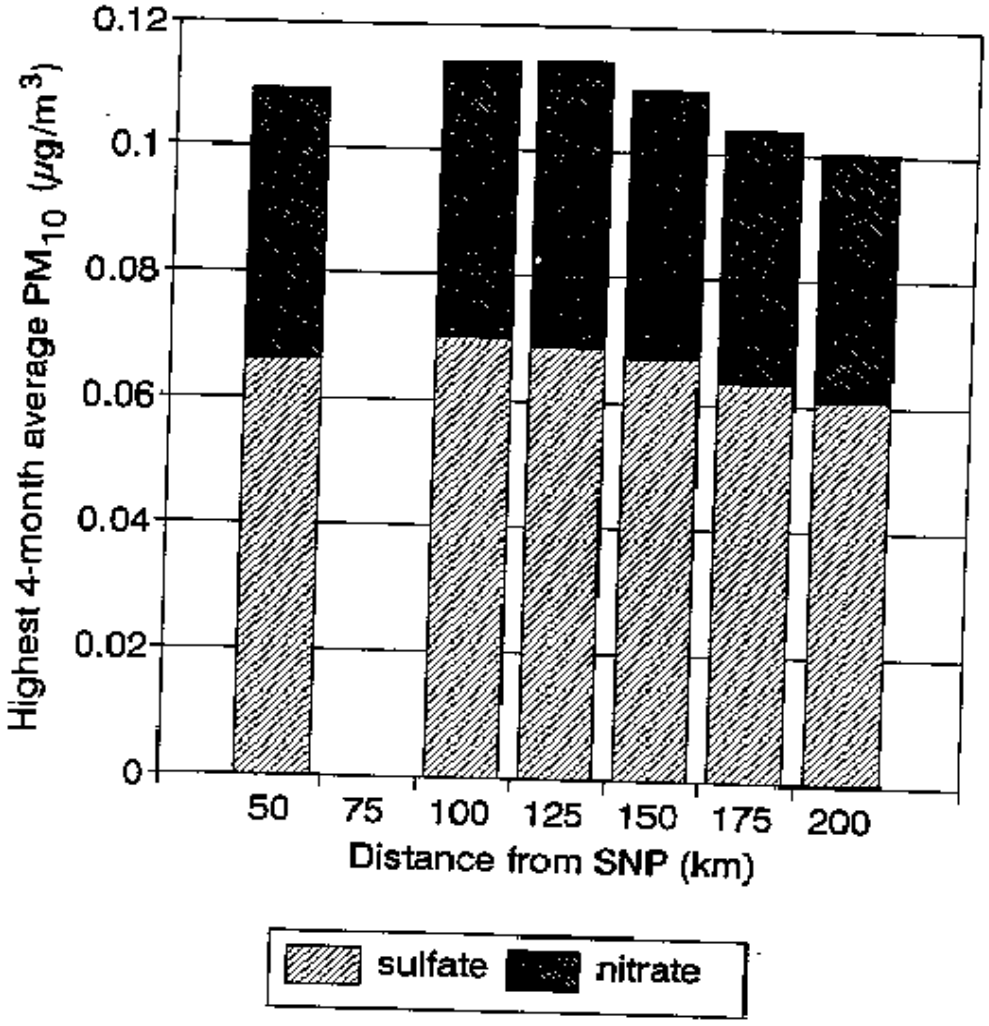

FIGURE 4-11. Highest simulated 4-month average PM_{10} concentrations ($\mu g/m^3$) from ring sources for 1988. For this exercise, PM_{10} is defined as the sum of ammonium sulfate and ammonium nitrate.

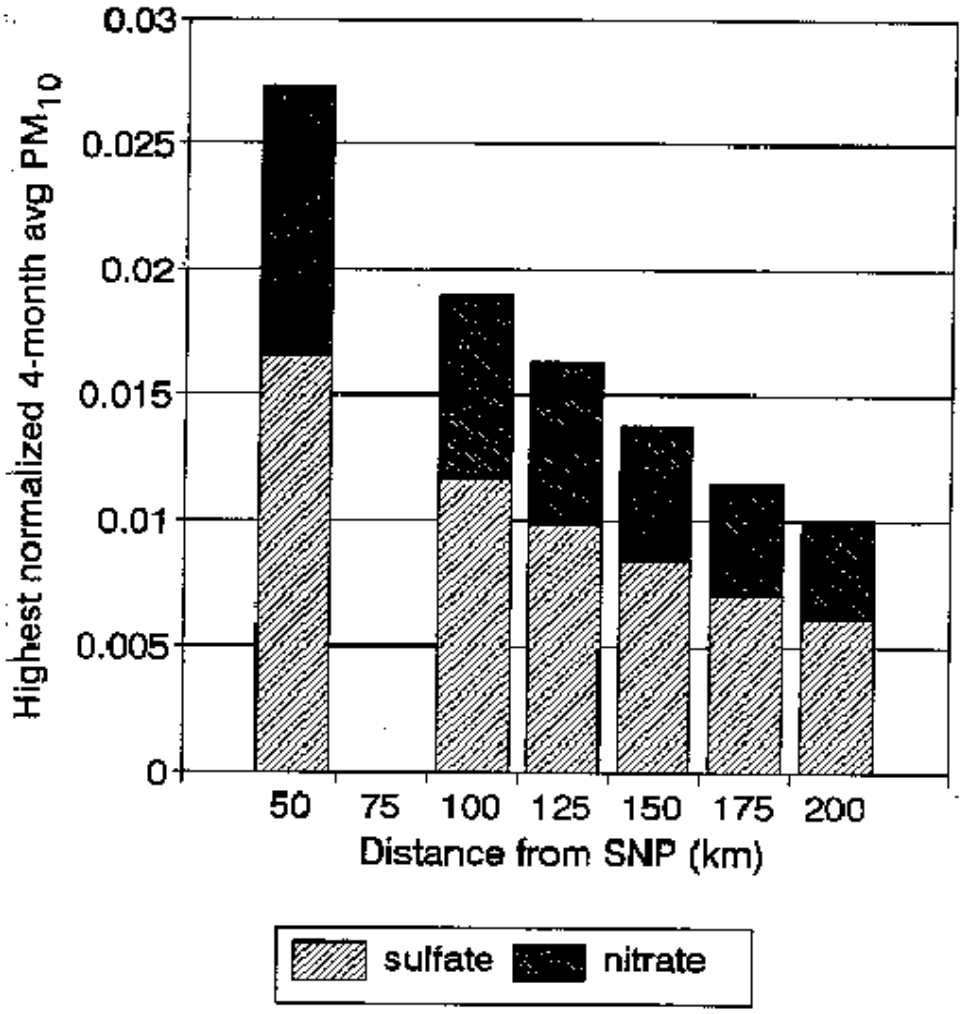

FIGURE 4-12. Highest simulated per-source 4-month average PM_{10} concentrations from ring sources for 1988. For this exercise, PM_{10} is defined as the sum of ammonium sulfate and ammonium nitrate.

An important AQRV associated with PM_{10} is visibility. **MESOFILE** is not capable of producing visibility estimates as outlined in the Phase 1 recommendations, where extinction is a function of relative humidity. Thus, visibility impacts were not assessed for the ring source analysis.

Deposition Impacts as a Function of Distance

S Deposition

Figure 4-13 shows the highest monthly cumulative S deposition. The highest monthly total S deposition of nearly 0.05 kg/hectare occurred for July for the 50 km ring. Modeled S deposition decreased with source distance from SNP, although the decreasing trend was very weak for October. At all distances, the highest S deposition occurred in July, and the lowest in January.

Figures 4-14 through 4-17 show the contributions of the four components of total S deposition (wet and dry deposition of SO_2 and $SO_4^=$) for each month. Dry SO_2 deposition accounts for most of the modeled S deposition in all months. Deposition of $SO_4^=$ is small for all months except July. The main reason for this is that most of the total sulfur remains in the form SO_2 at all distances modeled. Thus, although deposition velocities for $SO_4^=$ may be higher than those for SO_2, deposition fluxes are higher for SO_2.

Wet deposition shows greater random variability than dry deposition. This makes sense, as wet deposition requires both a puff and precipitation to be present at the same time at a given receptor. Thus, trends in wet deposition with source distance are somewhat obscured by the random variability.

N Deposition

Figure 4-18 shows the highest monthly cumulative N deposition. The highest monthly total N deposition of 0.013 kg/hectare occurred for the 50 km ring for July. Modeled N deposition decreased slowly with source distance from SNP. At all distances, the highest N deposition occurred in July, and the lowest in January. Total N deposition was less than half the modeled total S deposition for all months and distances.

Figures 4-19 through 4-22 show the contributions of the five components of total N deposition (wet and dry deposition of HNO_3 and NO_3^-, and dry deposition of NO_x) for each month. MESOPUFF II assumes zero wet deposition for NO_x. The majority of modeled N deposition in July is due to dry deposition of HNO_3. In the other months, NO_x dry deposition is important, and NO_3^- deposition can be important as well. Considering the high aqueous solubility of HNO_3, the modeled wet deposition of HNO_3 appears surprisingly low.

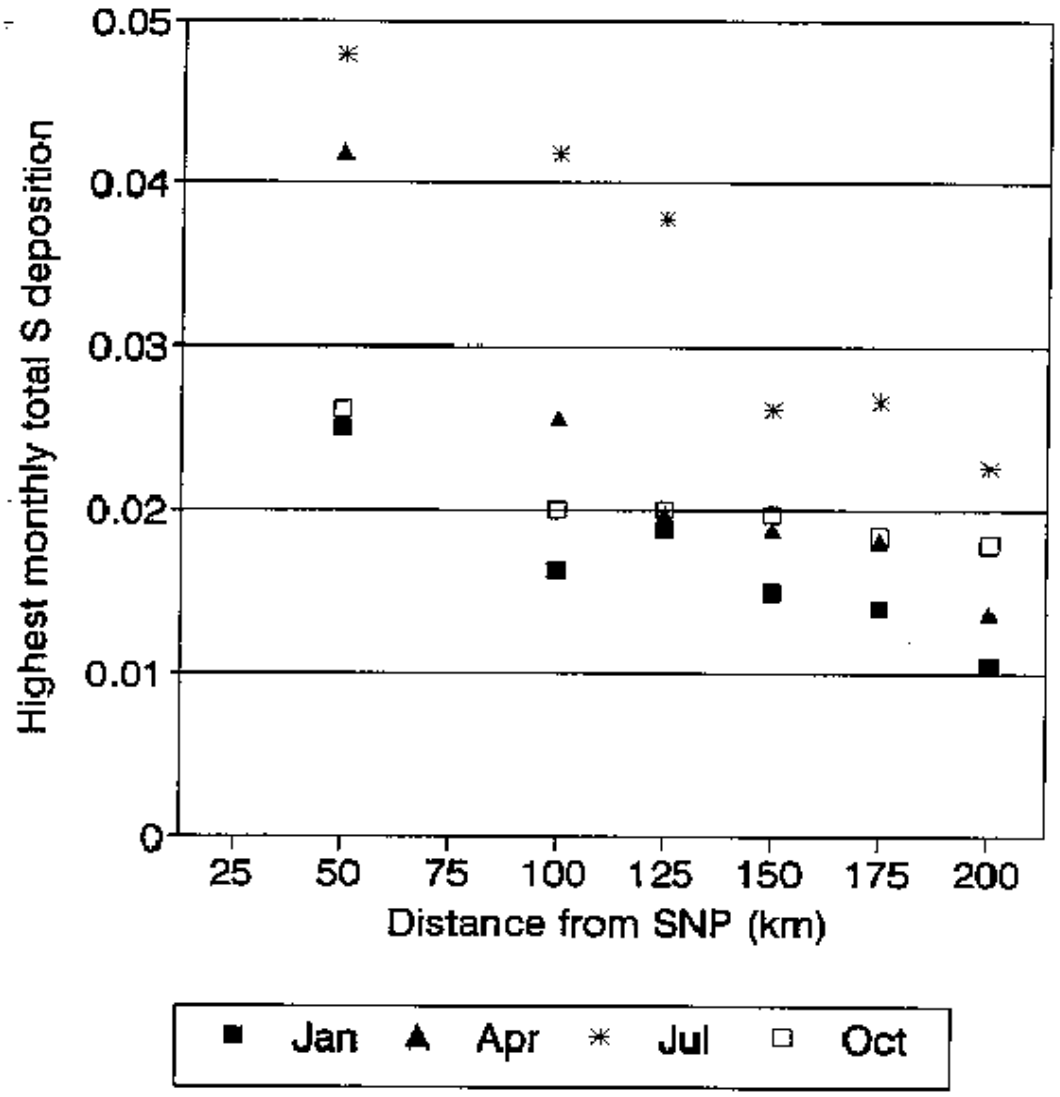

FIGURE 4-13. Highest simulated monthly cumulative total S deposition (kg/hectare) from ring sources for January, April, July, and October, 1988.

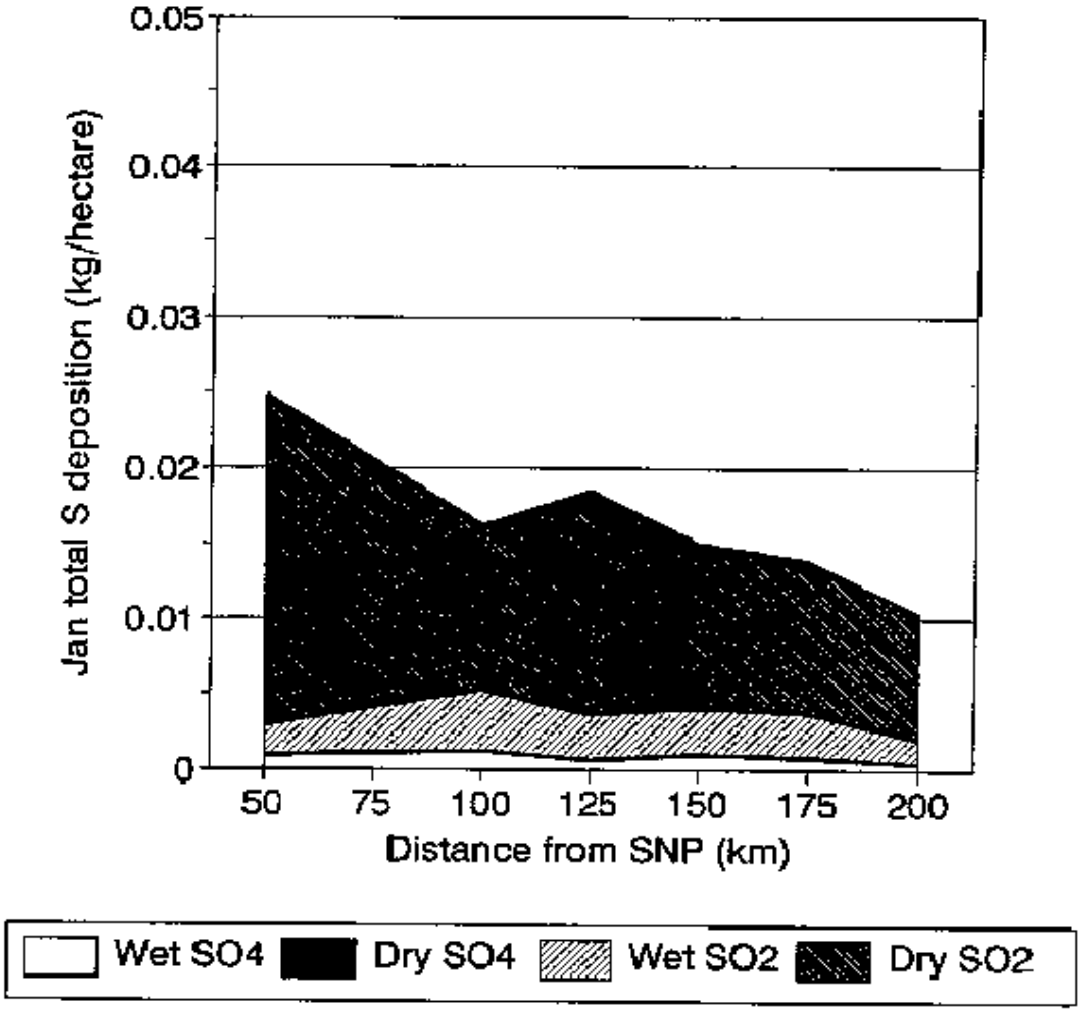

FIGURE 4-14. Components of simulated January 1988 total S deposition from ring sources.

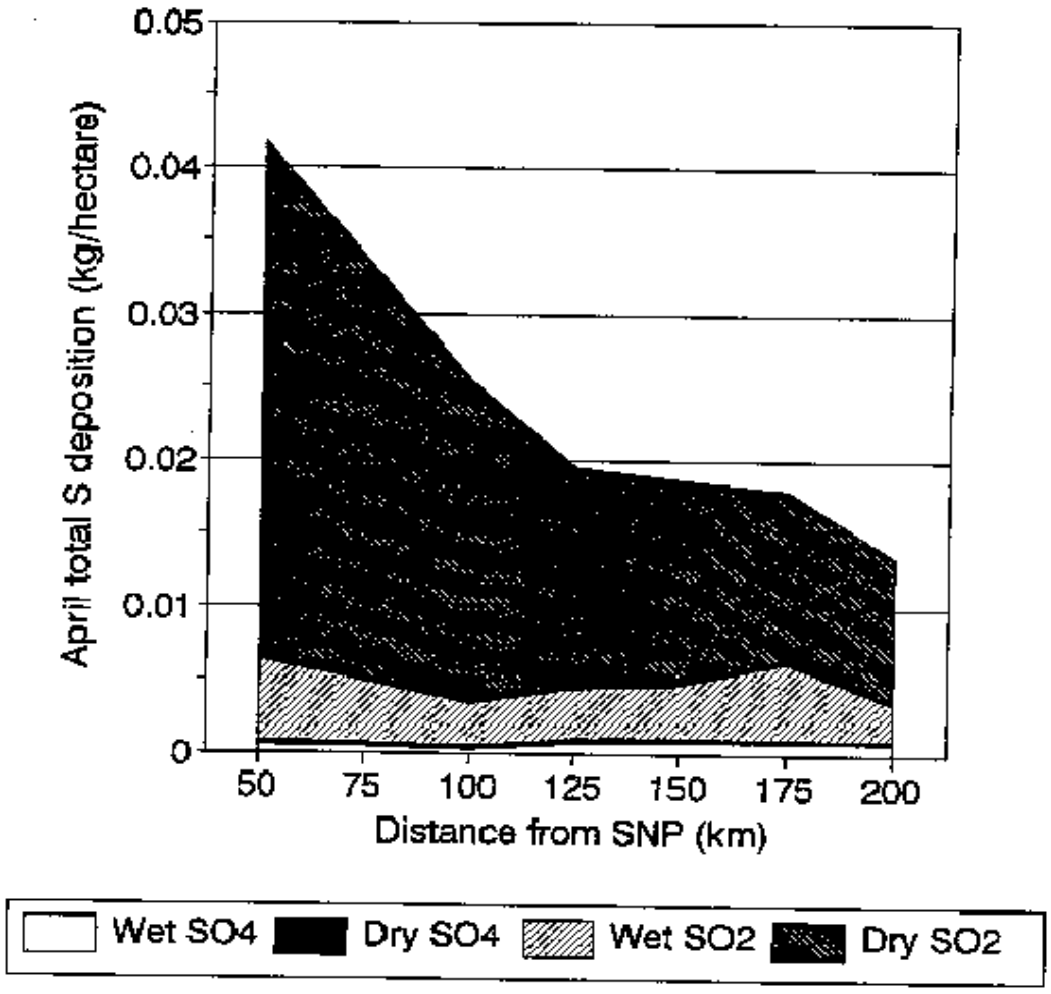

FIGURE 4-15. Components of simulated April 1988 total S deposition from ring sources.

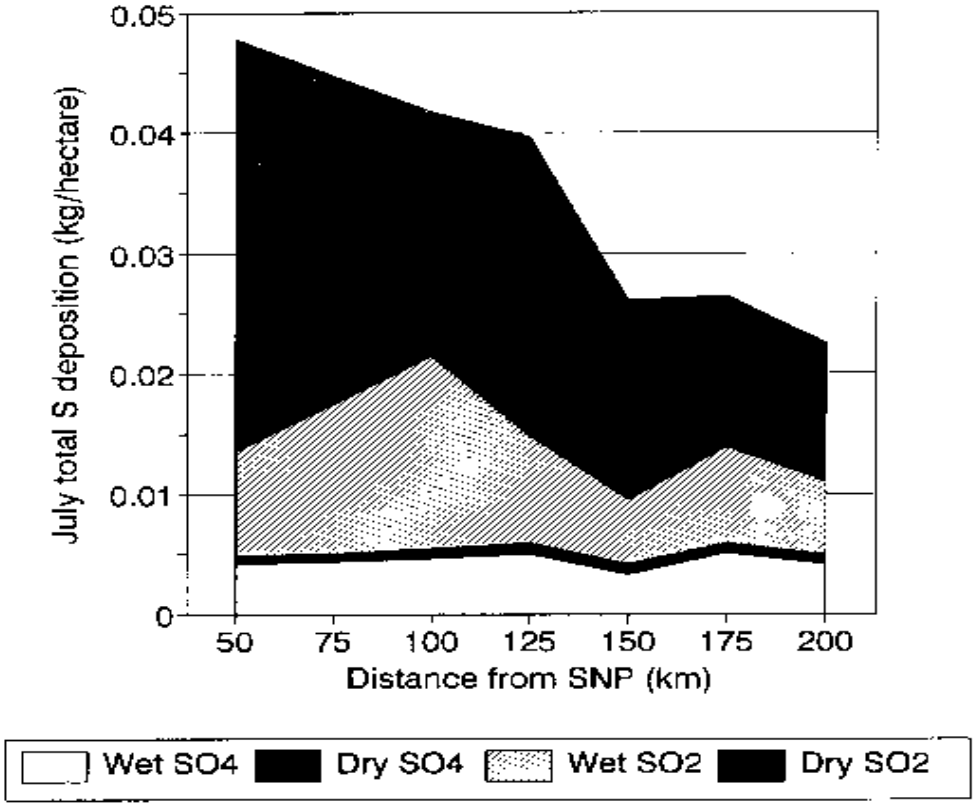

FIGURE 4-16. Components of simulated July 1988 total S deposition from ring sources.

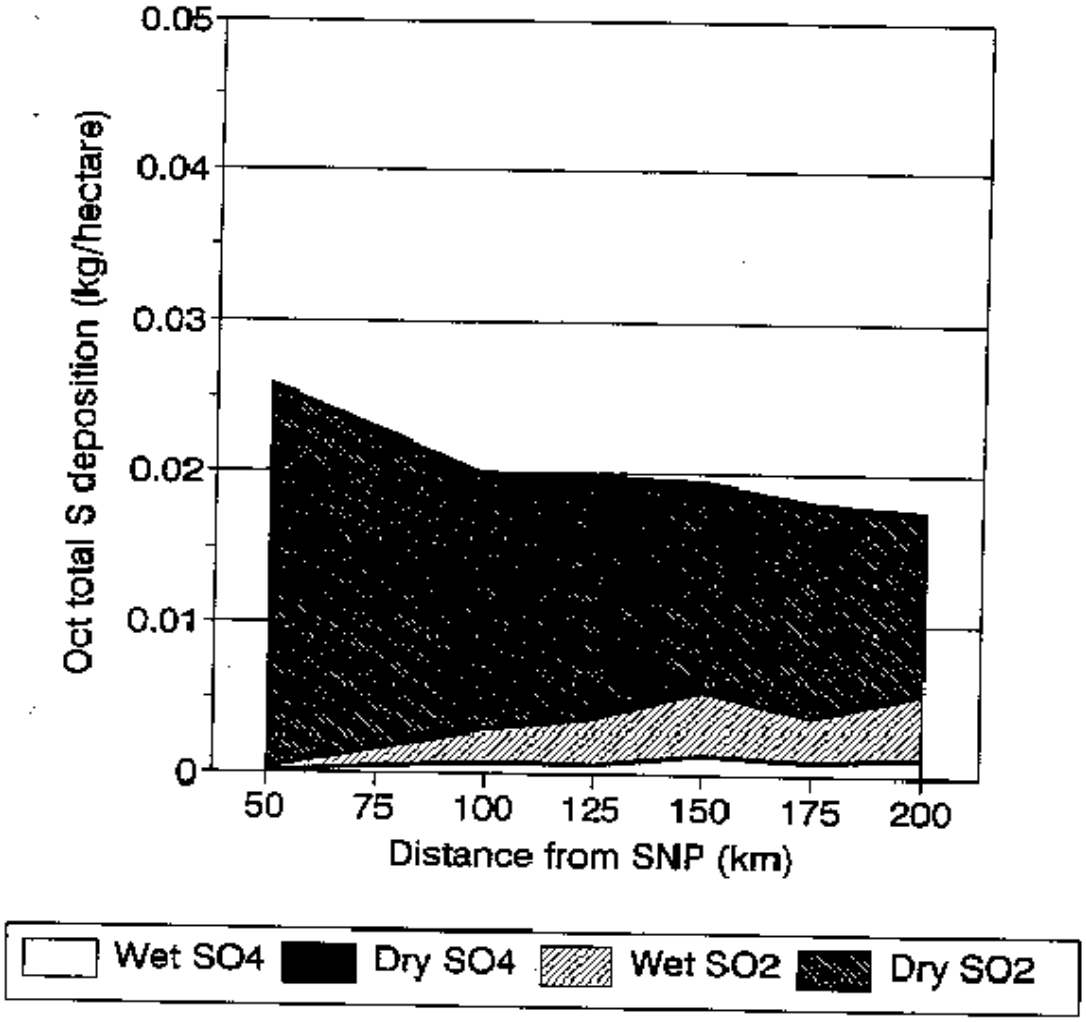

FIGURE 4-17. Components of simulated October 1988 total S deposition from ring sources.

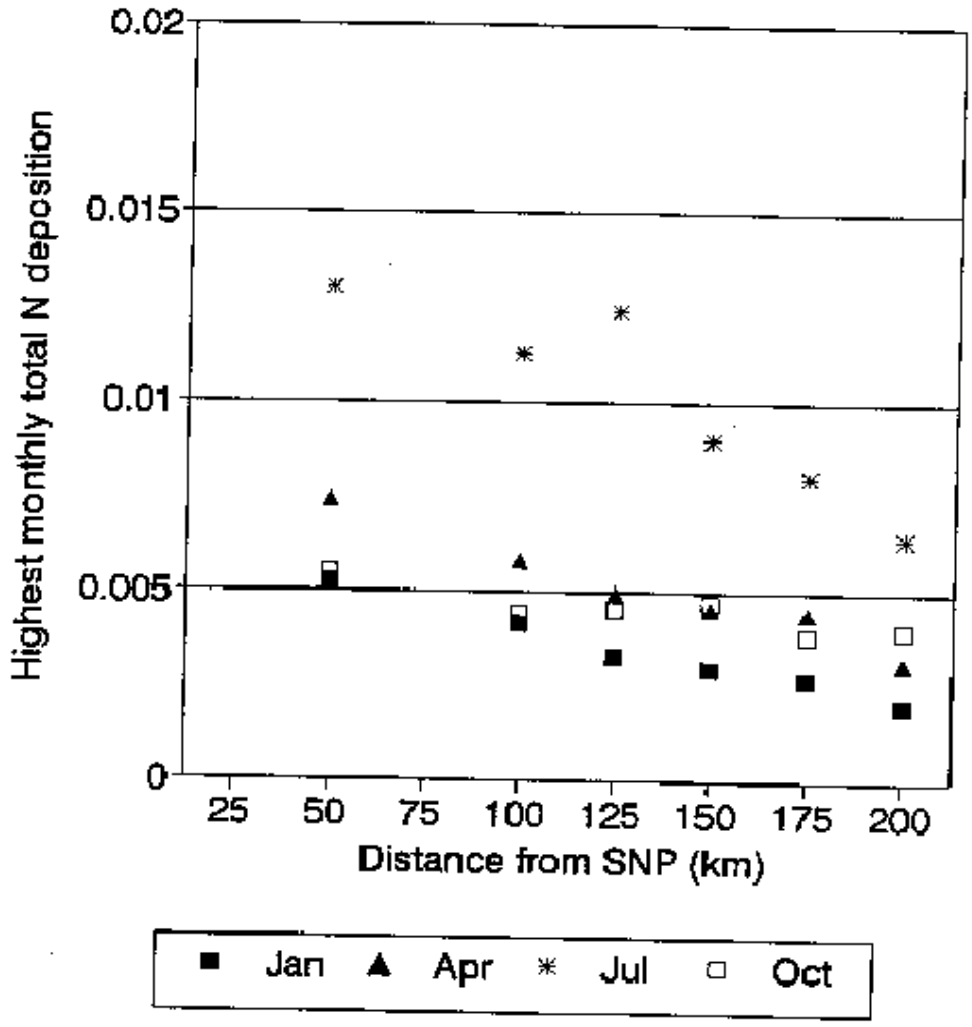

FIGURE 4-18. Highest simulated monthly cumulative total N deposition (kg/hectare) from ring sources for January, April, July, and October, 1988.

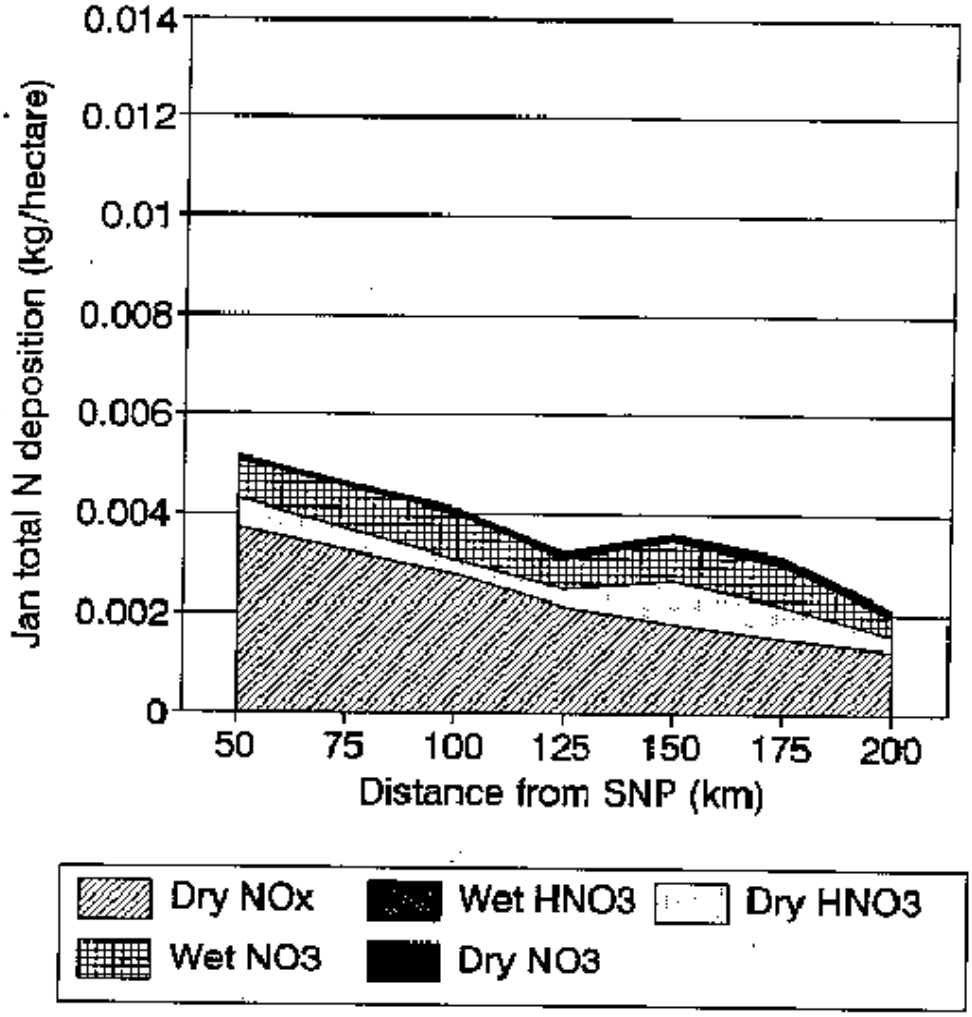

FIGURE 4-19. Components of simulated January 1988 total N deposition from ring sources.

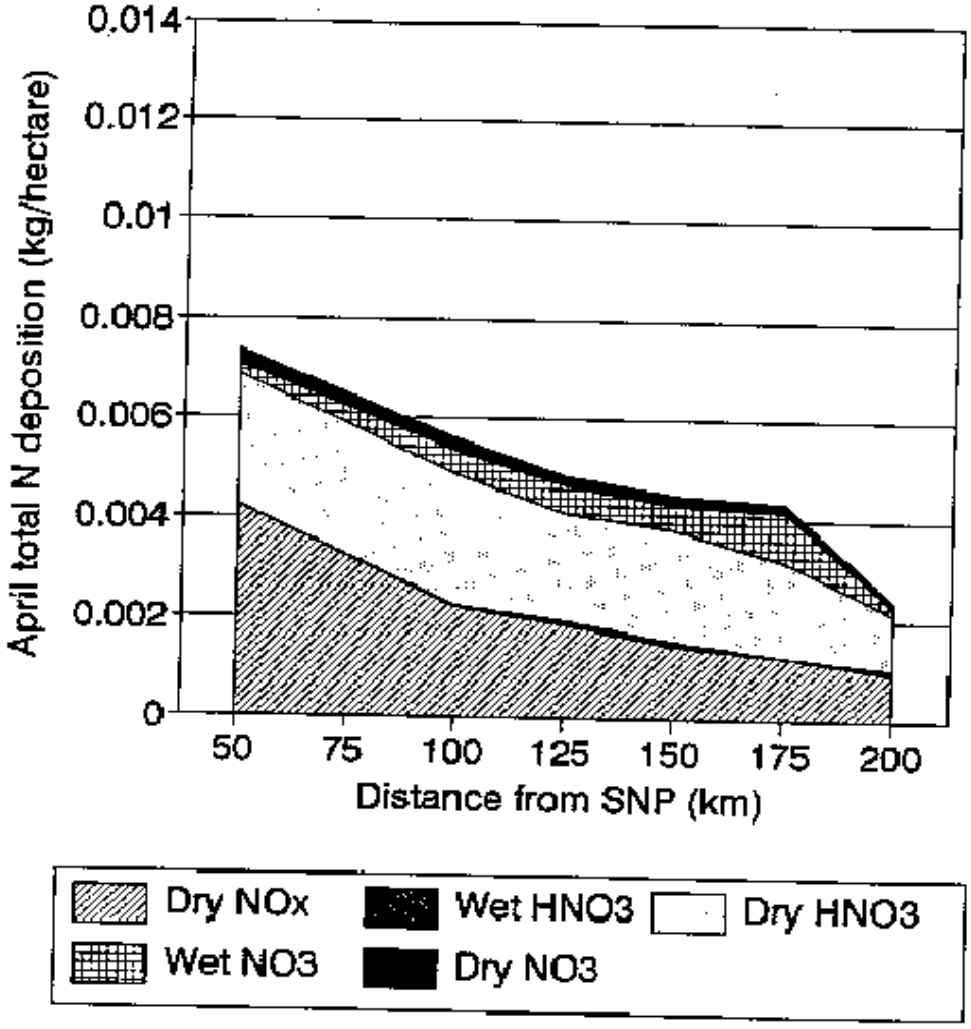

FIGURE 4-20. Components of simulated April 1988 total N deposition from ring sources.

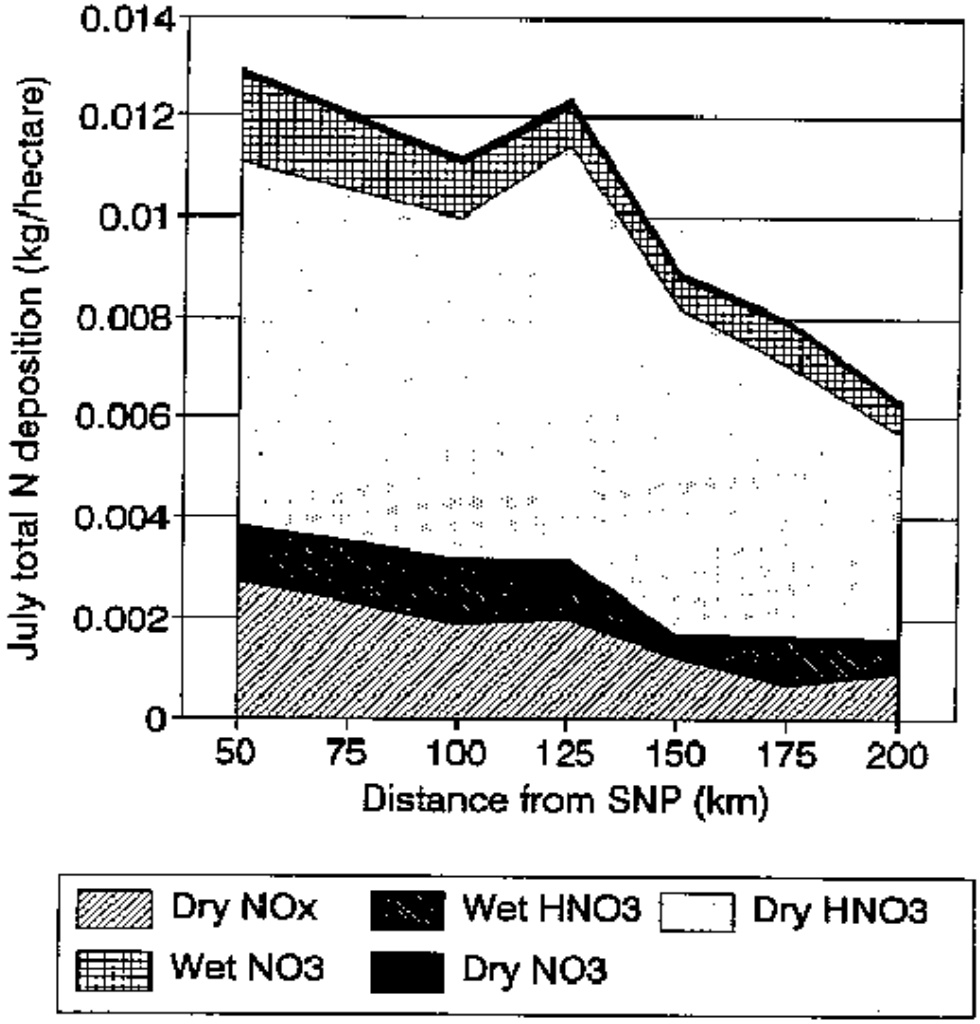

FIGURE 4-21. Components of simulated July 1988 total N deposition from ring sources.

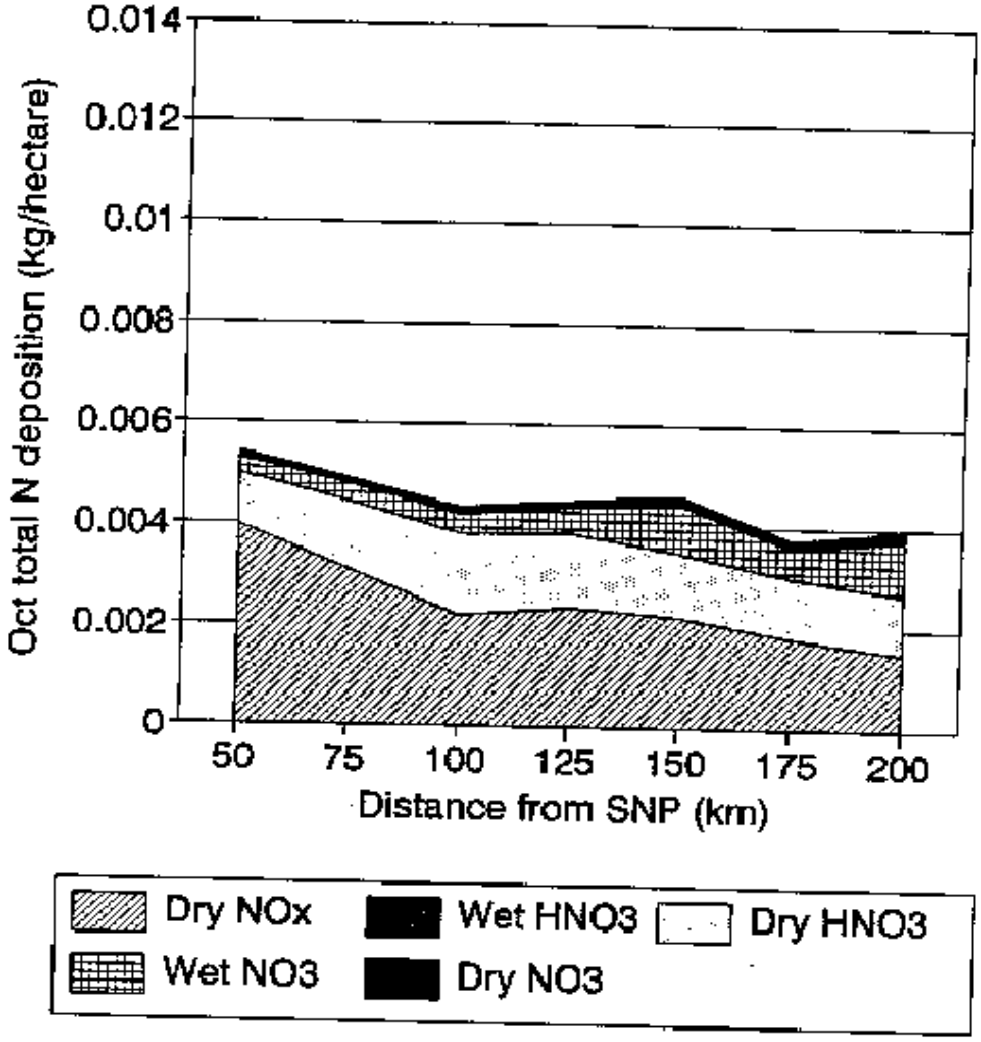

FIGURE 4-22. Components of simulated October 1988 total N deposition from ring sources.

The equilibrium between HNO_3 and NO_3^- affects the results presented here, both for the modeled PM_{10} concentrations and the nitrogen deposition. The ring source analysis utilized the default value for background ammonia of 10 ppb. This value is likely to be too high, especially for winter. When ammonia concentrations are high, the nitrate equilibrium favors the formation of aerosol nitrate. As a result, modeled aerosol nitrate values may be too high. For N deposition, it is less clear what the effect of high background ammonia would be. Dry deposition is faster for HNO_3 than it is for NO_3^-, but wet deposition is faster for NO_3^-. In particular, snow is assumed in MESOPUFF II to scavenge particles but not gases. Therefore, if background ammonia is high, NO_3^- deposition will be overestimated and HNO_3 deposition will be underestimated. The net effect on N deposition may be small.

PROBLEMS ENCOUNTERED

Although **MESOFILE** is flexible, it cannot provide results in the form needed for the PSD/AQRV impact analyses as described in Table 3-4. It is not set up to identify second-highest impacts, and cannot calculate visibility impacts according to the formula outline in the Phase 1 Recommendations.

A minor error in the **MESOFILE** code was noted when we attempted to obtain average concentrations for a time period other than the full month simulated. The problem occurs with the specification of the day and hour. Apparently, the start day must be specified as the start day of the MESOPUFF II simulation, regardless of what day **MESOFILE** is to be run for. For example, in order to obtain an average concentration for day 3 of a simulation that began on day 1, hour 0, and continued for one month, one must specify the day as 1 and the hour as 48. Specifying the **MESOFILE** start date as 3 and the start hour as 0 will result in an error message. The **MESOFILE** code was not modified to alleviate this problem.

CONCLUSIONS

The ring source analysis illustrates some of the effects of source-receptor distance on air quality and deposition impacts. For the primary species, SO_2 and NO_x, peak impacts drop off rapidly with distance. MESOPUFF II results suggest that sources of the size used for this analysis (183 g/s SO_2), located 50 km from SNP, are capable of producing 3-hour SO_2 impacts close to the allowable PSD Class I increment. For the secondary species, $SO_4^=$ and NO_3^-, impacts did not show a decreasing trend for sources between 50 km and 200 km from SNP. The 4-month average modeled PM_{10} peaked at 125 km and was slightly lower at 200 km than it was at 50 km. Although modeled PM_{10} concentrations were well below allowable PSD Class I increments for all rings, the lack of a clear trend suggests that sources beyond 200 km may need to be considered in some cases in order to assess the impact upon PM_{10} and related parameters, such as visibility.

5 SUMMARY

STATUS OF THE MESOPUFF II MODELING SYSTEM

This project began with the retrieval of the MESOPUFF II modeling system from the EPA SCRAM electronic bulletin board. As discussed in Section 2, two minor changes to these files were made as a result of execution of the test case. The updated files have been released to the SCRAM bulletin board.

In order to run MESOPUFF II for the demonstration application, several other modifications were made to the modeling system. These changes primarily relate to formats and the ability of the models to read and process input data. None of these changes are required to execute the test case, however these MESOPUFF II modifications are necessary for future applications with the SNP modeling domain. These model changes were all presented and discussed in Section 3; they are summarized below:

PMERGE

- Several changes were made to accommodate two additional data quality flags that were present in the data but were not understood by **PMERGE**.

MESOPAC

- The format designator for the statement reading the upper air height field was changed from a length of 5 characters to 6 characters, as all preprocessing carried 6 characters.

- A quality assurance routine was changed to check for X characters rather than dash (-) characters to indicate unlimited ceiling heights, because standard CD144 format supplies X characters rather than dashes.

MESOPUFF II

- The format designator for the statement reading ozone data was changed to accommodate 200 ozone stations rather than 50.

- In the PARAMS.PUF file, the maximum number of ozone stations was increased to 200, and several other changes were made to optimize the parameters for this application. Changes to the PARAMS file require recompilation of the model source code.

DEMONSTRATION APPLICATION

A demonstration application of the MESOPUFF II modeling system was conducted for Shenandoah National Park and James River Face Wilderness. For this application, a five-year data set (1988-1992) of MESOPUFF II meteorological inputs was developed. MESOPUFF II was applied for the years 1988-1990 for a condensed set of existing PSD sources located within 200 km of SNP.

The primary purpose of this exercise was to document the implementation process rather than to obtain a set of modeling results. As described in detail in Section 3, a number of problems were encountered and resolved during the model application process. Additional processors were developed to streamline data preparation, modeling, and postprocessing systems.

Resources Consumed

For this project, five years of raw meteorological data, including surface, upper air, and precipitation data, were acquired. Five years of ozone data were also needed, but much of that data were already available in-house. Identifying data suppliers and ordering the needed data consumed about 20 labor hours. The total cost of the data was under $3,000. The data were supplied on 8-mm tape cartridges within 2 weeks of placing the order. These tapes were read onto our TRACE/Unix mainframe computer.

Development of the five-year set of meteorological inputs consumed 460 labor hours over four months. During much of this time, two 486 PCs were dedicated for use in the meteorological data processing. In addition, several data processing steps were not feasible on a PC and were conducted on a mainframe computer. The mainframe computer was also used for temporary storage of the 3.2 gigabytes of output produced by **MESOPAC** and for transferring the output to 8 mm tape cartridges.

Application of MESOPUFF II was much less resource-intensive than application of **MESOPAC**. Exercise of MESOPUFF II for three years required 45 labor hours and three weeks of dedicated usage of one 486 PC. Again, the mainframe computer was needed for temporary storage of the **MESOPAC** output files.

Processors Developed

Six pre-processors and two post-processors were developed for this project. The names and functions of each are summarized below.

Two pre-processors extract information from raw data files:

- **RESFC** reads TD-3280 hourly surface data and extracts data for a given space/time window.

- **REUPR2** reads TD-6201 upper air data and extracts data for a given space/time window.

Additional pre-processors are used to prepare data:

- **TOCD144** reformats TD-3280 surface data into CD144 format and fills in missing data.

- **FILLUPR** reads the upper air data output by **REUPR2** and fills in missing data according to a specified set of rules (see Section 3).

- **PARSE** splits the surface and upper air data into separate files for each station, as required by **MESOPAC**.

- **GRIDDIT** calculates and formats station grid coordinates for surface, upper air, and precipitation stations.

Two post-processors generate air quality summaries from MESOPUFF II results:

- **RHPOST** extracts relative humidity data from the **MESOPAC** output file and prepares 3-hour averages for input to **PSDPOST**.

- **PSDPOST** calculates specific PSD and AQRV parameters for one year of MESOPUFF II output for non-gridded receptors.

These processors will be made available to future MESOPUFF II users via the SCRAM BBS. A description of each program and a guide for application are presented in Appendix C. The use of these processors, combined with review of the demonstration MESOPUFF II application, will greatly facilitate future MESOPUFF II applications.

Data Files Created

For future applications utilizing the same modeling domain, none of the meteorological pre-processing steps described here need be repeated. MESOPUFF II can be run with different sources and/or receptors using the **MESOPAC** output files and the ozone data files developed for this demonstration modeling exercise. However, the **MESOPAC** output files are rather large, so it may be a simpler process to start with the **MESOPAC** input files (processed surface, upper air, and precipitation data) constructed for this domain, and then run **MESOPAC** and MESOPUFF II for each modeling period.

Deviations From Phase 1 Recommendations

A number of deviations from the IWAQM recommended approach were used for this demonstration MESOPUFF II application. Many of these deviations were made due to the limited resources available for conducting the demonstration modeling effort. For example, since the MESOPUFF II model was applied on a PC, it was necessary to perform monthly

runs (for a subset of the PSD source inventory), for which data handling was cumbersome. If a faster computer system were used, the runtime could be reduced, enabling multiple runs, more sources to be modeled, or a higher puff release rate. If a larger computer system were used, storage concerns could be minimized, which might eliminate the need to perform monthly runs (i.e., an entire year could be run at once). A PC-based system with one to two gigabyte hard drives and a removable optical drive may lessen many of the obstacles that were encountered.

The deviations from the interim IWAQM recommendations are identified below:

In order to reduce the volume of MESOPUFF II output, 3-hour average concentrations and fluxes were output rather than 1-hour averages, as required by the IWAQM interim recommendations. However, the minimum averaging time necessary to compute the desired PSD and AQRV impact measures (see Table 3-4) is three hours.

To reduce CPU time and the size of the MESOPUFF II executable code, a puff release rate of 1 puff per hour rather than 4 puffs per hour was used. If possible, a realistic assessment (following the interim IWAQM recommendations) should use 4 puffs per hour. However, if CPU time is limited, a release rate of one puff per hour should be adequate (i.e., will produce similar results), especially for the long travel times associated with secondary air pollutants.

Both of these parameters (output averaging period and puff release rate) are specified in the MESOPUFF II user input file and can be changed by future users. However, the **RHPOST** and **PSDPOST** processors are configured for 3-hour averages; **PSDPOST** cannot be used with any other averaging interval without modification. In addition, if the puff release rate is increased beyond 1 puff per hour, the maximum allowable number of puffs may be exceeded. This would necessitate changes to the PARAMS.PUF file, which would in turn require recompilation of the MESOPUFF II executable code.

The collected source data represents only a subset of the actual set of sources that would be required in order to properly assess the PSD impacts on SNP. As was discovered, multiple triggering dates apply to various types of sources in each of the states surrounding a particular receptor. In addition, different inventories are needed to assess PSD increments than those required for AQRV impact analysis (see Appendix B). For future MESOPUFF II applications, it will be necessary to identify the multiple inventories necessary for assessment, and then apply the MESOPUFF II model for each inventory. In addition, for the demonstration modeling exercise, many sources were consolidated (to reduce computer time). In order to follow the interim IWAQM recommendations, all sources must be modeled individually (i.e., consolidating sources would not be an acceptable approach for future regulatory MESOPUFF II applications).

A large set of receptors was obtained from the state of Virginia for SNP and JRFW. A subset of these receptors were used for the demonstration modeling exercise. A number of the receptors were spatially close together, so there is arguably justification for removing some of these, however, this reduction of receptors was done largely to make the size of output files

more manageable. All sensitive receptors (as defined by the FLMs responsible for the Class I area in question) should be included in future regulatory MESOPUFF II applications.

For assessments of multiple sources, the interim IWAQM recommendations require that two five-year MESOPUFF II modeling exercises be conducted; one run using all sources to determine impacts to secondary NAAQS pollutants (secondary particulate matter) and AQRVs (visibility and deposition), and a second model run using only sources beyond 50 km from a receptor for SO_2 and NO_x. To simplify the analysis (and reduce resources required), only one run was performed for the demonstration modeling exercise (for three years) using sources beyond 50 km of Shenandoah National Park for all pollutants.

Primary sulfate emissions are allowed in the MESOPUFF II modeling system, however these emission rates are generally not well documented and most emission inventories do not include primary sulfate emission rates. For the demonstration modeling exercise, it was assumed that primary sulfate emissions were 3 percent of the SO_2 emissions. The interim IWAQM recommendations do not specifically address this issue.

Another issue that is not specifically addressed in the interim IWAQM recommendations is the procedure for filling in missing meteorological data. The approach developed for the demonstration modeling exercise (and applied in the preprocessing programs; see Appendix C) represents sound engineering practice for filling in missing data. Other approaches are possible, including various other interpolation schemes.

For the demonstration modeling exercise, background ozone data were prepared to represent the seasonal variation in observed background concentrations. MESOPUFF II uses a default concentration (80 ppb), however users may supply their own data. The interim IWAQM recommendations do not specify whether the default is acceptable, however it was our determination that seasonal observations should be used instead. This decision was supported by IWAQM.

As a practical consideration, relative humidities (used to estimate extinction) were limited to 95 percent. The extinction efficiency/relative humidity relationships that were employed are not valid at such high relative humidities. Relative humidity is not typically measured accurately above 95 percent. In addition, such high relative humidity conditions are likely to involve sufficient water condensation for cloud formation, and light extinction (and hence, visibility) in the presence of obscuring clouds is generally not regulated. This adjustment was made to improve the relationship between concentration and visibility impacts, however the interim IWAQM recommendations do not include this adjustment.

Finally, the **ISCST2** model was only exercised for one month in order to demonstrate the process of integrating the **ISCST2** results with MESOPUFF II results. The IWAQM interim recommendations require that 5 years be simulated with MESOPUFF II, and that the Gaussian model (**ISCST2**) be modeled for the same 5-year period. The **ISCST2** and MESOPUFF II model results for all periods simulated are to be integrated.

Process Review

During the course of performing the demonstration application, the project team received considerable guidance and technical review from members of the IWAQM. An initial work assignment was developed by EPA OAQPS that called for review and testing of the MESOPUFF II system, followed by development of a demonstration modeling exercise. A modeling protocol was developed after consultation with the IWAQM team, in which issues such as modeling domain, period to be modeled, receptor locations, and sources to be modeled, were presented, discussed and resolved. The IWAQM members who represent Federal Land Managers (NPS and NFS) provided technical guidance with respect to interpreting model results, i.e., determining the parameters to be used to measure PSD and AQRV impacts at Class I areas. The IWAQM representatives from EPA Region III were contacted for assistance in collecting source data. Each of the individual states within Region III were asked by Region III to supply emission source data (we were able to receive source data from all but one state within about six weeks). The IWAQM representatives from the Virginia Department of Environmental Quality provided the receptor locations for Shenandoah National Park and James River Face Wilderness (and the source data for Virginia).

The IWAQM group assisted the project team in defining the scope of the demonstration analysis. It was the primary objective of the work assignment to carry out an analysis using the IWAQM Phase 1 Recommendations in order to demonstrate and improve the modeling system. The IWAQM group's original intent was to exercise the model in the most realistic manner as possible in order to discover any and (hopefully) all the problems that would be faced by potential future users of the system. Therefore it was decided that we would attempt to perform a meaningful analysis with the demonstration modeling exercise. An analysis that would consider the impacts from all PSD sources impacting SNP and JRFW would be informative, in that the results would indicate the total amount of the allowable PSD increment that has been consumed by sources that were either constructed or modified since the enactment of the PSD rules in 1977. However, it was soon readily apparent, after discussions with officials responsible for PSD regulations, that the determination of PSD sources is not straightforward; there are multiple triggering dates that are applicable for various classes of sources, and furthermore, AQRV analyses should consider a separate group of sources. The scope of the analysis was modified so that the demonstration modeling exercise would evaluate the PSD and AQRV impacts of an arbitrary group of PSD sources, consisting of most or all sources for which data were made available.

Because the demonstration modeling scope was altered in this way, the IWAQM group welcomed an additional change in project scope whereby the 60 monthly MESOPUFF II simulations were reduced to 36 simulations. Since the resources had been allocated for 60 months of simulations, the remaining 24 monthly simulations were used in an additional analysis to examine the potential for PSD and AQRV impacts as a function of source distance.

Numerous technical memoranda were distributed to the IWAQM members seeking input and approval regarding modeling issues, including results of the review of the example problem,

recommendations for improvements to example problem distribution files, plans for meteorological data collection and preparation, receptor selection, source selection, development of the modeling plan for the distance vs. impacts analysis, and processing of the model output. The IWAQM representative from EPA OAQPS acted as the EPA work assignment manager for the project, overseeing the technical and administrative details of the work, and coordinating the communication between the project team and the IWAQM membership.

For future applications of MESOPUFF II using the IWAQM Phase 1 recommendations, the first step is to define the scope of modeling work by specifying the sources to be analyzed and the receptors of interest. It is necessary to determine what technical questions are being asked of the regional air quality model and how regulations might dictate the objective of the model's application. It will be necessary to consult with the FLMs and/or other applicable regulatory authorities, such as local State or regional EPA representatives, to establish the recommended procedure for selecting sources and receptors for the given application (i.e., PSD permit application, AQRV analysis, etc.). The allowable cumulative PSD increments for Class I areas have been established (see Table 3-4, for example), however the acceptable levels for AQRV impacts have not been identified. It may be sufficient to assess the incremental impacts from a single new (or modified) source in the context of current conditions, or it may be necessary to evaluate the cumulative impact of all sources. Guidance from the FLMs will therefore be required to determine how to evaluate the AQRV impacts from a new (or modified) source in Class I areas.

If the modeling domain coincides with the domain constructed for this demonstration modeling exercise, then it would be advisable, if possible, to utilize the five-year (1988-92) meteorological data set prepared for the current analysis because development of those data was particularly resource intensive and difficult. Once the sources, receptors, modeling domain and modeling period have been selected, the regional impact analysis should be conducted by following the IWAQM Phase 1 Recommendations, and through the use of this report as a demonstration of the modeling process.

IMPACTS AS A FUNCTION OF DISTANCE

In addition to the PSD analysis, a separate investigation of the impacts of hypothetical sources as a function of distance was conducted on the same modeling domain. In this investigation, uniform hypothetical sources were placed in rings of constant distance from SNP, ranging from 50 km to 200 km. Four months were simulated, each representing one season of the year 1988.

The results from this investigation showed that impacts from primary species such as SO_2 and NO_x decreased with source distance from SNP. Short-term impacts decayed with source distance in a manner consistent with the hypothesis that they are the result of a single source. Long-term impacts decayed with source distance as though they were the result of the entire ring of sources. Specifically, maximum 3-hour SO_2 impacts decreased by 86 percent between the 50 km and 200 km source rings. For the maximum 24-hour SO_2 impacts, the decrease was

68 percent. Maximum monthly average SO_2 levels decreased by 58 percent; when the concentrations are normalized by the number of sources on each ring, the decrease was 83 percent. For NO_x, the maximum monthly average concentration decreased by 65 percent between the 50 km and 200 km source rings, and the normalized maximum monthly average concentration decreased by 86 percent.

The trend in simulated PM_{10} (defined here as the sum of ammonium sulfate and ammonium nitrate) with source distance was very different from the trend in SO_2 and NO_x. Maximum modeled PM_{10} impacts occurred at the intermediate distances (125 to 175 km).

Modeled sulfur deposition was dominated by SO_2 deposition at all distances and for all seasons, although sulfate deposition peaked in July. Therefore, sulfur deposition showed a similar trend with distance as did the long-term SO_2 concentrations. Modeled nitrogen deposition was dominated by HNO_3 deposition in summer and NO_x deposition in the other seasons.

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APPENDIX A

INTERAGENCY WORKGROUP ON AIR QUALITY MODELING (IWAQM)

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APPENDIX B

BASELINE DETERMINATION

The following notes are a summary of a telephone conference held on November 2, 1993, between the project team, IWAQM members, and Dan deRoeck (responsible for new source review at EPA OAQPS). The topics of the conversation were (1) how to select sources that should be included as PSD sources for the demonstration modeling analysis, (2) the relationship between PSD increments and AQRVs, and (3) a summary of emission inventory needs for each proper analysis. An important issue for PSD source determination was the triggering dates for various classes of emission source.

As a result of this conversation, it was discovered that more than one emission inventory would be needed and that the MESOPUFF II model would have to be exercised for each inventory separately to determine the impacts from each grouping of sources. Because these additional model runs were not possible within our resources, we decided to restrict the scope of the demonstration modeling exercise to determine the PSD and AQRV impacts at Class I areas (Shenandoah NP and James River Face W) from to an arbitrary group of PSD sources.

The following notes were received from Al Cimorelli, EPA Region III, on November 3, 1993:

BASELINE DETERMINATION

- Baseline determination is no different for Class I areas than it is for Class II.
    - Baseline is determined individually for Section 107 areas (i.e., attainment and unclassified areas). This means that for Class I areas as large as Shenandoah baseline dates may be different for different parts of the park.
    - There are 2 dates that are important: MAJOR source baseline date and MINOR source baseline date.
        - Major Source Baseline Date: Established by the Statute (1/6/75 for SO2 and Particulate) - All major sources whose emissions have changed, as a result of construction activities, after 1/6/75, effect increment. However, only the emission changes effect increment (major source is defined as 100 tons/yr for the 28 categories listed in the PSD regs and 250 tons/yr for all other sources.

- Minor Source Baseline Date: Established by first complete PSD application either locating in 107 area or whose emissions significantly impact the 107 area. After the Minor Source Baseline date all actual emission changes from any source for any reason effect increment.

- Therefore, proper construction of the increment effecting inventory must consider both dates.

- For the Demo project we did not ask for an inventory of this type. We asked simply for the increment effecting inventory. We decided not to go back to the states and clarify, we will see what we get back and discuss at the 11/30 meeting. At that meeting we may request the states to develop the appropriate inventory by say the end of the year.

AQRV's

- We discussed AQRVs and their relationship to Increment:

  - Dan explained that he believed that AQRVs should be viewed in a way similar to NAAQS not Increment. That is, they should be viewed from an absolute air quality point of view not relative to some baseline. However, he indicated that there may be others in the program with a different view. For example, AQRVs could be evaluated in the same way as increment.

  - However adverse impacts on AQRVs, unlike NAAQS, should represent what is actually occurring not what could occur if all sources were operating at their allowable emissions.

  - Therefore, to properly evaluate AQRVs we either must rely on measured data or model using an inventory of actual emissions from ALL presently existing sources which have a meaningful impact in the Class I area. It is against this measurement or prediction which we compare the modeled incremental impacts of an applicant source.

- In designing the Demo Project we did not follow this interpretation of AQRVs. We plan to calculate the AQRVs using the increment effecting inventory we requested from the states. If we continue along this line we must be careful in explaining what we have done, what it means & how it relates to properly constructed analysis.

EMISSION INVENTORIES

In summary, a proper Class I area analysis would require the development of three separate inventories.

i. For PSD Increment:

(1) The change in emissions that have occurred as a result of construction at any major sources, if that construction occurred after the Major Source Baseline date.

(2) All actual emission changes, from any source, which occurred after the Minor Source Baseline Date.

ii. For AQRVs:

Actual present day emissions from all sources

iii. For NAAQS:

Allowable emissions from all sources.

APPENDIX C

DESCRIPTION AND USER'S GUIDE FOR NEW MESOPUFF II PRE- AND POSTPROCESSORS

The MESOPUFF II program system is divided into three basic processors: the **MESOPAC II** meteorological preprocessor, the MESOPUFF II Lagrangian puff model, and the **MESOFILE** receptor concentration postprocessor. The MESOPUFF II system also contains several programs that prepare raw meteorological data for the **MESOPAC** preprocessor, including **READ62**, **PMERGE**, and **PXTRACT**. These programs, as well as **MESOPAC**, require raw data in specific formats, which are available through the National Climatic Data Center.

Before the demonstration study, internal array dimensions within all programs were set to values that were assumed to allow for a large degree of flexibility over the range of potential model applications. During the demonstration study, however, we found that several array dimensions were inadequately small, and that others were too large (leading to unnecessarily large memory requirements). The table below presents a comparison between the original array dimensions and those currently set in the programs. The new values were selected to tailor the codes for the quantity of raw data, emission sources, and receptors required in the demonstration study, and are adequate for most future applications on this domain. It is by no means meant to be optimum for all future applications in other areas. We recommend, however, that dimensions for the number of point sources and total puffs should not be increased significantly above the current settings, as MESOPUFF II speed is non-linearly dependent on the number of sources and puffs modeled.

Table C-1. Comparison of array dimension parameters between "original" and "demonstration" versions of the **MESOPUFF II** modeling system.

Parameter	Original Value	Demonstration Study Value	Description
MXNX	100	50	Maximum cells in x direction
MXNY	100	35	Maximum cells in y direction
MXSS	100	50	Maximum surface stations
MXUS	20	10	Maximum upper air stations
MXPS	100	200	Maximum precipitation stations
MXPUFF	10,000	20,000	Maximum active puffs on the grid
MXREC	1,000	100	Maximum non-gridded receptors
MXPTS	1,000	20	Maximum point sources
MXARS	200	1	Maximum area sources
MXOZ	50	200	Maximum ozone stations

Besides meteorological data requirements, **MESOPAC** and MESOPUFF II require gridded land use information, and optionally, hourly observed ozone concentrations at an array of monitoring sites within the modeling domain. The original MESOPUFF II system does not contain programs to prepare these input data. Further, we were not able to procure raw meteorological data in the exact formats required by **MESOPAC**, and were not able to use **MESOFILE** to calculate concentration, deposition, and visibility increments on seasonal to annual time scales. Therefore, additional pre- and postprocessors were developed to prepare the input and output data for the demonstration modeling study. These processors have been packaged for the SCRAM BBS, where they will be available for public use. The processors are grouped into the following categories:

- Surface data processing
- Upper air data processing
- Meteorological station programs
- Gridded land use data processing
- Ozone data processing
- Postprocessing programs

A description of each program and a guide for application are presented on the following pages.

GETSTN/RESFC Tape Extraction Programs

GETSTN and **RESFC** are used together to extract hourly surface data for a given time and space window from a single raw TD-3280 file. The product of **GETSTN** and **RESFC** programs is an intermediate monthly surface data file for stations located within the meteorological modeling domain. These programs were run for all 60 months of 1988-1992, extracting data for a spatial window within the latitude/longitude ranges 34-42°N and 71-86°W, which resulted in hourly surface observations for up to 48 stations.

RESFC can be run on each single raw TD-3280 file and its output combined into a single monthly intermediate file (a rather cumbersome process if many raw files exist for a particular year), or, as is recommended in Section 3, the raw data can be first concatenated and **RESFC** run on the combined raw file. Although **RESFC** requires substantially more mainframe CPU time to process the larger annual concatenated files, significant labor can be saved by removing **RESFC** setup time for all subfiles and removing the post-**RESFC** combining procedures.

Because of file size and time required to operate the tape extraction programs, **GETSTN** and **RESFC** were run on our Trace Multiflow 14/300 Unix mainframe system. On the Unix system, processing of each month took between 20-30 minutes of mainframe CPU time (6 hours per year); about an hour of labor per year was spent setting up and executing **RESFC**, and inspecting output diagnostics and data files.

Raw TD-3280 data does not contain information about each station's geodetic coordinates, so location information must be obtained from a separate source. The ASCII WBAN master list file, obtained from DRI along with the raw TD-3280 surface data, catalogs (in numerical order) all WBAN weather station identification numbers within the U.S. and its territories along with station names, latitude/longitude coordinates, period of operation, and types of services each station offered. Often, one WBAN station number is repeated for several sites if a particular station has moved; dates of operation at each site location are given in the file with the most current coordinates for active stations reported first (current locations are valid as of 1987). Usually, station sites are moved by no more than 1 kilometer, but there are some instances when an old WBAN number for a non-operational site has been recycled for a new station much farther away. Under these circumstances, the most current location for a particular WBAN number may not be reported first.

GETSTN reads the WBAN master list file and extracts all station information for those sites within a specified latitude/longitude range. The output file generated by **GETSTN** is used by **RESFC** to assign latitude/longitude coordinates to the surface station data. Once **GETSTN** has been run, the output file should be checked to ensure that the most current position for each active WBAN number is reported first. **GETSTN** reads input parameters from the standard input unit. This can be accomplished using a free-format run stream, an example of which is presented below:

```
%/bin/time -i getstn << ieof
```

```
wbanmst1.lst      |master WBAN station file name
all.station.lst   |GETSTN output file name
34.,42.,71.,86.   |latitude/longitude minima & maxima
ieof
```

After running **GETSTN**, **RESFC** can be run on a concatenated TD-3280 file or individual sub-file. As the program processes the raw surface data and comes upon a new station, it will search through the output of **GETSTN** for the first record containing the current WBAN number and assign those coordinates. The following is an example Unix run command for **RESFC**:

```
%/bin/time -i resfc
```

RESFC requires an input parameter file labelled "resfc.in", which contains information about the input file names, period over which to extract surface meteorological data, coordinate type, and time zone. A sample free-format **RESFC** parameter file for December 1990 is displayed below:

```
all.station.lst   |GETSTN output file name
1990sfc.all       |Concatenated raw TD-3280 file name
sfcdec.90         |monthly RESFC output data file name
12 01 12 31       |Start month/day, end month/day
0 5               |Coordinates (lat/lon), time zone (EST)
```

where coordinate and time zone codes are given by:

Code	Coordinates
0	Lat/lon
>0	UTM
<0	Local grid units

Code	Time zone (standard time)
5	Eastern
6	Central
7	Mountain
8	Pacific

TOCD144 Data Reformatting/Filling Program

TOCD144 reads the monthly intermediate files, fills missing values, and reformats the data into monthly files in CD144 format. The program was written to fill 1-6 hour intervals of missing data using linear interpolation over time. For longer periods of missing values, data from surrounding surface stations are used to spatially interpolate information to the station using an inverse-distance-squared weighting technique. A minimum of 2 stations and a maximum of 4 stations are used within 200 km of a station needing spatial interpolation. If all data for a particular station is missing for a significant portion of a month, the station should be deleted from the database for that month.

TOCD144 was compiled using Microsoft (MS) FORTRAN 5.0; processing of each month took about 5 minutes of PC CPU time using an 486/66 MHz processor (this PC was used throughout all raw meteorological data preprocessing). Total labor and computer time required to run **TOCD144** averaged about 1.5 hours per year.

Since **MESOPAC** uses input temperature to determine liquid/frozen precipitation states if present weather fields are missing from the CD144 data, all present weather fields are set to missing values in the processed CD144 files. Sea level pressure in millibars is calculated from station pressure in inches of mercury using the hypsometric equation (via station temperature and elevation) within **TOCD144**. **TOCD144** does not interpolate for missing cloud ceiling height fields, either in time or space, due to the often large temporal and spatial variations observed in cloud heights, and the potentially large and uncertain impacts on MESOPUFF II applications. For the most part, missing cloud heights occur at night, as these observations are typically estimated visually; they only periodically occur during daylight hours. In **TOCD144**, sky cover percentage is used to set cloud height: if sky cover is less than 50%, cloud height is set to an "unlimited" ceiling; if cloud cover is greater than 50%, cloud height is set to 5000 ft, a height which alters the classification of solar insolation within MESOPUFF II to "low cloud" values (refer to page 5-13 of the MESOPUFF II User's Guide; EPA 1994).

TOCD144 is run at the DOS prompt by typing the program name and the name of the input parameter file as an argument:

```
C:\>TOCD144 APR92.PRM
```

The parameter file contains the names of the monthly surface data file generated by **RESFC**, the new "filled" and reformatted CD144 output file, and a diagnostic message file. A sample for April 1992 is given below:

```
apr92.sfc      |monthly surface data file name from RESFC
sf92_apr.fll   |monthly filled CD144 file name
apr92.msg      |message file name
```

UPPER AIR DATA PROCESSING

REUPR2 Tape Extraction Program

REUPR2 extracts 12-hourly upper air data for a given time and space window from a single raw nationwide/annual TD-6201 file. To reduce file sizes and expedite filling of missing data, **REUPR2** writes out sounding data between the surface and about 7000 m, and deletes non-mandatory levels if they have missing pressure. The resulting TD-6200 file contains intermediate monthly upper air data for stations located within the meteorological modeling domain. Because of file size and time required to operate the tape extraction program, **REUPR2** was also run on our Unix mainframe system. The program was run for all 60 months of 1988-1992, extracting data for a spatial window within the latitude/longitude ranges 34-42°N and 71-86°W, which resulted in upper air data from as many as 8 rawinsonde stations. **REUPR2** required about 15-20 minutes of mainframe CPU per month, yet very little labor was involved.

A sample Unix run command for **REUPR2** is provided below:

```
%/bin/time -i reupr2
```

REUPR2 requires an input parameter file called "reupr.in" that contains the longitude/latitude range, date range, name of the raw nationwide TD-6201 data file, and name of the **REUPR2** output file. A sample for December 1992 is presented below:

```
    71.0     86.0     34.0     42.0
1130 1231          |Beginning month/day, ending month/day
1992upr.all            |Input raw TD-6201 file name
up92_dec.dat           |Output upper air data file
```

The first record format is (4f10.1); the second record is free-format. It is generally good practice to specify an extra day before and after the month of interest when extracting 12-hourly upper air data, particularly if time-interpolation is required in later processing (which was not done in the current study).

FILLUPR Data Filling Program

FILLUPR reads the intermediate TD-6200 file and scans the sounding data for missing values. The program linearly interpolates between pressure levels for data gaps less than 200 mb deep. If a significant portion of the sounding is missing (i.e., > 200 mb), or if the sounding is missing altogether, the program spatially interpolates data from nearby sites to the station location using a distance weighted average (at mandatory levels only). **FILLUPR** follows the processing scheme outlined below:

(1) In a first pass through the data, the program finds the first level where there is a missing value (either height, temperature, or wind). The program proceeds up the sounding until a non-missing value is found. If this gap is greater than 200 mb deep, the mandatory levels within the missing block are flagged for spatial interpolation of this particular variable. If the gap is less than 200 mb deep, linear interpolation (using height or log-pressure) is performed for the variable at all levels (mandatory or otherwise) within the gap. For winds, interpolation is done for vector components.

(2) The program then proceeds farther up the sounding and repeats the procedure for data gaps aloft. If no valid data is found up to the top of the 7000 m sounding, and the data gap is greater than 200 mb, all mandatory levels above the level of good data are flagged for spatial interpolation. If the data gap to the top of the sounding is less than 200 mb, the data are extrapolated using the highest two levels with valid data (this saves on spatial interpolation time).

(3) Data for all soundings needing spatial interpolation are written to a temporary direct access file to ease memory requirements and quicken run time. In the second pass through the data, a matrix containing the top 5 closest stations to each of the stations in the file is computed. Then the flags for missing data at mandatory levels are checked for spatial interpolation.

(4) When a mandatory level requiring spatial interpolation for a particular variable is identified, data from the closest 2 to 4 upper air stations within a radius of 500 km are used in an inverse-distance weighted average. Stations containing spatially interpolated values at the same mandatory level are not used in this calculation.

(5) After a temperature sounding has been completely filled via spatial interpolation, the resulting temperature gradients are checked against a slightly super-adiabatic lapse rate to insure thermodynamically realistic values. The limiting lapse rate specified was -0.15 K/m; this limit was violated only infrequently. When the violation occurs, the interpolated temperatures are adjusted to adhere to an adiabatic lapse rate (-0.01 K/m)

FILLUPR was compiled using MS FORTRAN 5.0, and took about 5 minutes PC CPU time per month. Labor and CPU time together required about two hours per year to process upper air data through **FILLUPR**.

Like **TOCD144**, **FILLUPR** is run at the DOS prompt; it is supplied with the name of the input parameter file as an argument:

C:\>FILLUPR APR.PRM

The parameter file contains the name of the extracted TD-6200 data from **REUPR2**, the name of a temporary direct access file for intermediate processing, the name of the "filled" output TD-6200 data file, the name of a message file, and the date/time of the sounding preceding the first sounding of the month. A sample parameter file for April 1992 is presented below:

```
up92_apr.dat        |Input monthly upper air data file name
dummy.out           |Temporary direct access file name
up92_apr.fll        |"Filled" output file name
apr92.msg           |Message file name
3 31 12             |Month/day/hour of preceding sounding
```

In the last record, the free format string "3 31 12" represents the March 31 1200Z sounding, whereas the first sounding in the "up92_apr.dat" file is April 1 0000Z.

PARSE Station Splitting Program

PARSE was written to split monthly surface CD144 files and TD-6200 upper air files into numerous monthly station files, which are ready to be used directly by **MESOPAC**. Processing of single monthly files and splitting into separate station files just before running **MESOPAC** for each month simplified intermediate file management and provided faster meteorological data processing. Typically, data for 45-48 surface stations needed to be split into separate station files each month, taking just about 1 minute of PC CPU using MS FORTRAN 5.0, and virtually zero labor. Up to eight separate upper air station files were generated by **PARSE**, taking only a few seconds of PC CPU time.

PARSE is run separately for surface and upper air data files. The program must be told which type of file it is supplied by specifying a flag as an argument. For example, the following command at the DOS prompt will split surface data for April 1992 into 45 separate station files:

```
C:\>PARSE SF92_APR.FLL S
```

where the "S" denotes surface data, and the file name is the "filled" CD144 format data file generated by **TOCD144**. Similarly for upper air data in the same month, **PARSE** will produce 7 upper air station data files:

```
C:\>PARSE R6APR_92.DAT U
```

where the "U" denotes upper air data, and the file name is the file generated by **READ62**, which operates on output from **FILLUPR**.

GRIDDIT Station Location Processing Program

GRIDDIT calculates surface, upper air, and precipitation station meteorological grid coordinates from latitude/longitude data. The program generates one file containing grid coordinates and other information for all stations on the **MESOPAC** grid, which is then ready to be concatenated into a **MESOPAC** input control file (PAC.INP). Since the number of stations reporting each month vary, **GRIDDIT** must be run for each month to ensure that the proper station locations are supplied to **MESOPAC**.

For surface and upper air stations, the latitude/longitude position coordinates are stripped from their respective monthly intermediate files (i.e., those files output by **RESFC** and **REUPR2**, respectively). The **MESOPAC** input file PAC.INP also requires that surface station grid locations include representative surface roughness values. Therefore, **GRIDDIT** must be supplied with the MESOPUFF II land use file so that once surface station locations are determined within the **MESOPAC** domain, appropriate surface roughnesses can be assigned to each station. Since no coordinate information is available with the TD-3240 precipitation data, the program cross-references identification numbers within each month's **MESOPAC**-ready precipitation data file with station numbers in a "precipitation station history file" that SAI obtained from DRI.

For the upper air data, we extracted the first 18 columns from each record of the intermediate monthly TD-6200 files output by **REUPR2** (this file is formatted such that one record contains an entire sounding) and wrote them to monthly radiosonde station location files. An example of these files is given below:

```
 38603822  8233
137233605  7957
        •
        •
        •
    Continued for all radiosonde stations
```

The order of each record is station WBAN number (column 1-8), latitude degrees (column 9-10), latitude minutes (columns 11-12), longitude degrees (column 13-16), and longitude minutes (column 17-18). The format is (i8,2i2,i4,i2).

For the surface data, the station header records were stripped from the monthly **RESFC** output files and written to monthly surface station location files. An example of these files is given below :

```
3812 ASHEVILLE/      82.483   35.433   638.0   0 768   5
3860 HUNTINGTON      82.550   38.367   255.0   0 768   5
                        •
                        •
                        •
```

Continued for all surface stations

The order of each record is station WBAN number (columns 1-6), longitude in decimal degrees (columns 20-30), latitude in decimal degrees (columns 30-40), and station elevation in meters (column 40-50). The format is (i6,14x,f7.3,3x,f7.3,2x,f6.1).

GRIDDIT requires an input parameter file, which is read from the standard input file unit, and writes diagnostic messages to the standard output file unit. It is easiest to develop an input parameter file and execute **GRIDDIT** using the following DOS command:

```
C:\>GRIDDIT < GRIDDIT.INP > GRIDDIT.OUT
```

In the example above, **GRIDDIT** writes diagnostic output to the file GRIDDIT.OUT instead of the screen. The input parameter file (GRIDDIT.INP) contains the **MESOPAC** station location file name to be generated by **GRIDDIT**, the input surface station location file name, the input MESOPUFF II land use file name, the input radiosonde station location file name, the **MESOPAC**-ready precipitation file name, the precipitation station history file name, and some grid parameters. An example input file for December 1988 is given below:

```
dec88.stn              |MESOPAC station location file name
dec88.sfc              |Surface station location file name
landuse.mesopuff       |MESOPUFF II landuse file name
dec88.upr              |Upper station location file name
pmerge.dec             |MESOPAC precipitation file name
shfmst92.cat           |Station history file name
100. 3900. 17 20. 50 35 |Grid parameters
```

In this example, the grid parameters are read in free format, and include the UTM easting coordinate for the meteorological grid origin (southwest corner, km), the UTM northing for the grid origin (km), the UTM zone, the grid cell size (km), and the number of grid cells in the east-west and north-south directions, respectively.

GRIDDED LAND USE PROCESSING

PRELND Data Extraction Program

Land use data are supplied in the form of Geographical Information System (GIS) database files. The GIS file that **PRELND** requires contains the distribution of 11 land use categories over the entire U.S. at 1/4 degree longitude by 1/6 degree latitude resolution. This file (called "gis.dat") was made available to the National Park Service with delivery of the National Park Service Air Quality Modeling System. **PRELND** maps land use data from this file to the meteorological grid in terms of the percentage of each of 11 UAM categories in each cell.

PRELND was run on our Unix mainframes. A sample Unix run command is shown below:

```
%/bin/time -i prelnd2
```

PRELND requires an input parameter file called "plnd.in" that contains information about I/O file names and grid information:

```
gis.dat              |Raw GIS database file name
prelnd2.out          |Output ASCII message file name
landuse.gis          |Output binary landuse file name
    100.    3900.      17       20       50       35
```

The last record of "plnd.in" contains the grid UTM origin (km), UTM zone, grid cell size (km), and the number of cells in the east-west and north-south direction, respectively. The format is (2f10.0,4i10).

UAM2MESO Landuse Mapping Program

The UAM land use categories output by **PRELND** do not match those required by MESOPUFF II. The program **UAM2MESO** identifies the dominant GIS land use category in each cell and maps it into an appropriate MESOPUFF II category. The assumed mapping arrangement between UAM and MESOPUFF II land use categories is displayed in Table 3-3 (Section 3). All steps in developing a MESOPUFF II land use field were again executed on our Unix mainframe because of the necessity to read binary output from **PRELND**.

UAM2MESO is designed to read input information from the standard input file unit; an example of the Unix run stream for **UAM2MESO** is given below:

```
%/bin/time -i uam2meso << EOF
 landuse.gis              |Binary landuse file name from PRELND
 landuse.mesopuff                                  |ASCII MESOPUFF II-ready landuse file
                                                   name
 EOF
```

OZONE DATA PROCESSING

EXTRACT Data Extraction Program

EXTRACT withdraws hourly ozone data from files written in EPA Aerometric Information Retrieval System (AIRS) AMP-350 data work file format. The program produces monthly files for a spatial window covering the entire **MESOPAC** meteorological domain.

EXTRACT was run on our Unix mainframe. A sample Unix run stream for June 1992 is provided below:

```
%/bin/time -i extract << ieof
 rawairs.meso92.o3.dat    |Raw AIRS AMP-350 work file name
 1                        |Old/new data flag: should be "1"
 o3jun92.raw              |Output work file name
 o3jun92.out              |Message file name
 6 92                     |Month/Year of data to extract
 17                       |UTM zone
  100. 1100.              |Min/Max UTM easting coordinates
 3900. 4600.              |Min/Max UTM northing coordinates
 ieof
```

AIR2MESO Reformatting Program

AIR2MESO reformats the hourly ozone data into MESOPUFF II OZONE.DAT format, and produces a separate file containing grid coordinates for each AIRS monitor location. The coordinates file is then easily inserted into the MESOPUFF II input file (PUFF.INP) as necessary when supplying an OZONE.DAT file to the model. In order to simplify processing, **AIR2MESO** does not average multiple stations within the same grid cell. Also, the program does not add pseudo stations with background ozone in areas lacking data coverage. The total number of ozone monitoring sites within the meteorological domain depends highly on season, ranging from about 50 or 60 in the winter, to around 150 in the summer.

MESOPUFF II identifies missing data within the OZONE.DAT file and fills it with either the default (80 ppb) or user-specified background ozone concentration. The **AIR2MESO** program was written to calculate daytime/domain average ozone concentrations for each month to assist the user in supplying MESOPUFF II with a specific background ozone concentration for each application.

A sample Unix run stream for the June 1992 **AIR2MESO** run is shown below:

```
%/bin/time -i air2meso << EOF
 92 6                  |Year/Month
 100. 3900. 20.        |Grid UTM origin, cell size (km)
 o3jun92.raw           |Input work file name from EXTRACT
 o3jun92.dat           |Output OZONE.DAT file name
 o3jun92.inp           |Output monitor location file name
 EOF
```

POSTPROCESSING PROGRAMS

RHPOST Humidity Extraction Program

AQRV computations include the calculation of aerosol extinction, which in turn is dependent on relative humidity. Relative humidity data is contained within the large 50 MB **MESOPAC** output files, only a few of which can fit onto the PC hard drive. The objective of **PSDPOST**, however, was to operate on all 12 months of each year continuously. Therefore, **RHPOST** was developed to extract hourly relative humidity data at each surface station from **MESOPAC** files, and output 3-hour average relative humidity at each receptor location to much smaller files for subsequent input to **PSDPOST**.

Since **MESOPAC** was compiled using Lahey FORTRAN 5.2, **RHPOST** had to be compiled with the same in order to read the binary **MESOPAC** output files. **RHPOST** required just a few minutes of CPU time per month (on the 486/50 MHz PC) to extract relative humidity data from **MESOPAC** output files. Again, humidity files could only be extracted from 3 or 4 **MESOPAC** output files before more **MESOPAC** files could be transferred from offline storage.

RHPOST reads input parameters from the standard input file unit and outputs diagnostic messages to the standard output file unit. The easiest way to supply the program with the required input parameters is to edit an input file (e.g., called RHPOST.INP) and type the following command at the DOS prompt:

C:\>RHPOST < RHPOST.INP >RHPOST.OUT

In the above example, diagnostic messages will be sent to the file RHPOST.OUT instead of the screen. The input parameter file contains the name of the monthly **MESOPAC** output file from which to extract humidity data, the name of the monthly output humidity file, the number of receptors for which to assign humidity values, and a list of all non-gridded receptor locations (in terms of grid units). An example RHPOST.INP file is shown below:

```
jul90.out              |MESOPAC binary output file name
rh_jul90.dat           |Output binary humidity file name
64                     |Number of non-gridded receptors
   27.715   14.049     |Grid coordinates of receptors
   27.744   13.878     |(Free format)
   27.877   13.992
   27.901   13.831
   27.910   14.189
   27.995   13.969
        •
        •
        Continued for 64 receptor locations
```

PSDPOST Postprocessing Program

PSDPOST allows for quick and efficient calculations of the specific PSD and AQRV impacts (concentration averages and deposition sums), as described in Table 3-4 (Section 3). **PSDPOST** requires 12 months of binary MESOPUFF II output files and 12 monthly **RHPOST** binary output files for each year. **PSDPOST** then determines humidity-dependent extinction coefficients resulting solely from modeled PM_{10} (ammonium sulfate and ammonium nitrate). This calculation specifically follows the procedure outlined in Appendix B of the IWAQM Phase 1 recommendations. Visibility impacts are reported as the amount of time (both in terms of the absolute number of 3-hour periods and percent of each year) the calculated maximum extinction over all receptors is more than 10% higher than the cleanest observed extinction. The cleanest observed extinction was taken to be the 90th percentile extinction over all years in which statistical analyses of IMPROVE monitoring data are available at SNP (1987 through 1991). From Sisler et al. (1993), the 90th percentile particulate extinction for this period at the Shenandoah monitor was 0.005 km^{-1}. This was combined with a Rayleigh (pure air) scattering extinction of 0.010 km^{-1} to obtain a total observed cleanest extinction of 0.015 km^{-1}.

Since MESOPUFF II and **RHPOST** were compiled using Lahey FORTRAN 5.2, **PSDPOST** had to be compiled with the same in order to read the binary model output files. **PSDPOST** required about 10 minutes of PC CPU per month (on the 486/50 MHz PC).

Like **RHPOST**, **PSDPOST** reads an input parameter file from the standard input file unit, and outputs diagnostic messages to the standard output file unit. **PSDPOST** will generate a file called "PSDPOST.DAT", which will contain PSD increments and statistics for each non-gridded receptor and an overall summary. Again, it is easiest to execute **PSDPOST** using the following DOS command:

```
C:\>PSDPOST < PSDPOST.INP > PSDPOST.LST
```

In this example, diagnostic messages will be routed to PSDPOST.LST rather than to the screen. **PSDPOST** is meant to calculate certain measures for an entire year's worth of MESOPUFF II output. The input parameter file (PSDPOST.INP in this example) is therefore rather lengthy. For each run, the input file specifies the number of non-gridded receptor groups over which to calculate PSD increments, and the receptor index ranges for each group. Then for each month, the input file specifies the names of the binary MESOPUFF II output concentration, dry deposition, and wet deposition files, along with the name of the monthly relative humidity files generated by **RHPOST**. A sample input file for the 1989 MESOPUFF II run is presented below:

```
2                |Number of receptor groups
1 9 10 64        |Start/end indices (1-9,10-64)
jan89.dat        |Concentration file name
jan89.dry        |Dry dep file name
jan89.wet        |Wet dep file name
rh_jan89.dat     |Humidity file name
1                |Humidity flag
feb89.dat
```

feb89.dry
feb89.wet
rh_feb89.dat
1
mar89.dat
mar89.dry
mar89.wet
rh_mar89.dat
1
apr89.dat
apr89.dry
apr89.wet
rh_apr89.dat
1
may89_a.dat
may89_a.dry
may89_a.wet
rh_may89.dat
0
may89_b.dat
may89_b.dry
may89_b.wet
1
jun89.dat
jun89.dry
jun89.wet
rh_jun89.dat
1
jul89.dat
jul89.dry
jul89.wet
rh_jul89.dat
1
aug89.dat
aug89.dry
aug89.wet
rh_aug89.dat
1
sep89.dat
sep89.dry
sep89.wet
rh_sep89.dat
1
oct89.dat
oct89.dry
oct89.wet
rh_oct89.dat
1
nov89.dat

nov89.dry
nov89.wet
rh_nov89.dat
1
dec89.dat
dec89.dry
dec89.wet
rh_dec89.dat

Note that beginning with the second group of input file names (February), a flag must be given to signal whether a relative humidity file is to be opened for that group. A value of "1" indicates that a humidity file is to be opened, while a value of "0" will keep the current humidity file open for subsequent processing. This allows for cases in which a particular month was split into 2 or more MESOPUFF II runs (i.e., due to program crash, system problem, or planned separation). This was the case for May 1989, where in the above example, the MESOPUFF II application was split into "a" and "b" runs; for the "b" group, no humidity file is specified. **PSDPOST** attempts to resynchronize the humidity file with the current date/time that the program reads from the MESOPUFF II output files.

APPENDIX D

ISCST2 MODEL RESULTS AND INTEGRATION WITH MESOPUFF II RESULTS

The tables on the following pages are portions of output files from the **ISCST2** model runs and the **ISCMPF** integration program:

(1) page 9 of **ISCST2** output file for SO_2

(2) page 9 of **ISCST2** output file for NO_x

(3) page 1 of **ISCMPF** output file (MESOPUFF II header)

(4) **ISCMPF** output file table corresponding to maximum 3-hour average SO_2 concentrations

(5) **ISCMPF** output file table corresponding to second high 3-hour average SO_2 concentrations

(6) **ISCMPF** output file table corresponding to top 10 3-hour average SO_2 concentrations

*** MODELING OPTIONS USED: CONC RURAL DFAULT

*** THE SUMMARY OF HIGHEST 3-HR RESULTS ***

** CONC OF SO2 IN (MICROGRAMS/CUBIC-METER) **

GROUP ID		AVERAGE CONC	DATE (YYMMDDHH)	RECEPTOR (XR, YR, ZELEV, ZFLAG)	OF TYPE	NETWORK GRID-ID
ALL	HIGH 1ST HIGH VALUE IS	11.41345	ON 90070503:	AT (703580.00, 4270240.00, 0.00, 0.00)	DC	
	HIGH 2ND HIGH VALUE IS	8.16474	ON 90072624:	AT (703580.00, 4270240.00, 0.00, 0.00)	DC	

*** RECEPTOR TYPES: GC = GRIDCART
GP = GRIDPOLR
DC = DISCCART
DP = DISCPOLR
BD = BOUNDARY

*** MODELING OPTIONS USED: CONC RURAL DFAULT

*** THE SUMMARY OF HIGHEST 3-HR RESULTS ***

** CONC OF NOX IN (MICROGRAMS/CUBIC-METER) **

GROUP ID		AVERAGE CONC	DATE (YYMMDDHH)	RECEPTOR (XR, YR, ZELEV, ZFLAG)	OF TYPE	NETWORK GRID-ID
ALL	HIGH 1ST HIGH VALUE IS	8.38784	ON 90070503:	AT (703580.00, 4270240.00, 0.00, 0.00)	DC	
	HIGH 2ND HIGH VALUE IS	6.00033	ON 90072624:	AT (703580.00, 4270240.00, 0.00, 0.00)	DC	

*** RECEPTOR TYPES: GC = GRIDCART
GP = GRIDPOLR
DC = DISCCART
DP = DISCPOLR
BD = BOUNDARY

```
     JULY 1990 MESOPUFF II/ ISCST2 MERGING


VERSON=  5.1  LEVEL= 93181  NSYR=90  NSDAY=182  NSHR= 0  NADVTS=  744  IAVG=    3  NPUF=  1  NSAMAD=  1  IELMET=50  JELMET=35
DGRID=  20000.0  IASTAR=17  IASTOP=46  JASTAR= 4  JASTOP=33  ISASTR=28  ISASTP=35  JSASTR=15  JSASTP=22  MESHDN= 1  NPTS=  10
NAREAS=   0  NREC=  64  IPRINF=  36  LGAUSS=T  LCHEM=T  LDRY=T  LWET=T  LPRINT=T  L3VL=T  LVSAMP=T  WSAMP=   2.00  LSGRID=F
NSPEC= 5
LWETG=F  LWETNG=T  LDRYG=F  LDRYNG=T  LPRFLX=T


XREC=27.72 27.74 27.88 27.90 27.91 28.00 28.05 28.09 28.19 30.52 30.61 30.65 30.74 30.80 30.84 30.94 30.96 31.01 31.08 31.18
     31.24 31.27 31.28 31.37 31.42 31.51 31.57 31.65 31.67 31.70 31.83 31.85 31.91 31.99 32.02 32.11 32.17 32.23 32.25 32.31
     32.37 32.37 32.38 32.45 32.51 32.56 32.60 32.61 32.68 32.78 32.82 32.86 32.87 32.93 32.94 32.96 33.19 33.20 33.23 33.30
     33.33 33.50 33.52 33.56


YREC=14.05 13.88 13.99 13.83 14.19 13.97 13.85 14.10 14.01 16.93 17.40 17.97 17.62 16.88 18.05 17.71 17.19 18.26 17.45 19.51
     18.08 17.61 18.47 19.30 18.78 17.86 18.41 18.13 18.87 19.11 18.68 19.41 18.38 19.62 18.92 19.23 19.89 18.99 20.58 18.74
     20.09 21.12 19.41 20.86 21.31 20.22 19.22 20.49 19.88 19.59 20.31 21.26 19.84 20.70 20.06 21.02 20.82 21.83 21.48 22.02
     21.16 21.58 20.81 21.26
```

*** THE FIRST HIGHEST OF 3-HR AVERAGE CONCENTRATION VALUES AT EACH NON-GRID RECEPTOR FOR SO2 ***
CONCENTRATIONS IN MICROGRAMS/CUBIC-METER, RECEPTOR LOCATIONS IN METERS

REC NO	CONC	(YYMMDDHH)	AT	RECEPTOR (X,Y)		REC NO	CONC	(YYMMDDHH)	AT	RECEPTOR (X,Y)	
1	4.8388	(90072818)	AT	(554300.00,	280980.00)	2	4.3077	(90072818)	AT	(554880.00,	277560.00)
3	4.5770	(90072818)	AT	(557540.00,	279840.00)	4	4.0606	(90072818)	AT	(558020.00,	276620.00)
5	5.1683	(90072818)	AT	(558200.00,	283780.00)	6	4.4119	(90072818)	AT	(559900.00,	279380.00)
7	3.9992	(90072818)	AT	(560960.00,	277060.00)	8	4.7420	(90072818)	AT	(561720.00,	281980.00)
9	4.3328	(90072818)	AT	(563740.00,	280100.00)	10	5.5231	(90072815)	AT	(610340.00,	338580.03)
11	4.7055	(90072812)	AT	(612200.00,	348060.00)	12	6.5819	(90072206)	AT	(612940.00,	359360.00)
13	5.2547	(90072206)	AT	(614760.00,	352420.00)	14	6.5571	(90072815)	AT	(615920.00,	337520.00)
15	8.6506	(90072506)	AT	(616860.00,	360980.00)	16	4.6043	(90072506)	AT	(618880.00,	354199.97)
17	5.8416	(90072506)	AT	(619260.00,	343840.00)	18	8.3091	(90072706)	AT	(620140.00,	365260.00)
19	5.1203	(90072812)	AT	(621660.00,	349020.00)	20	11.4135	(90070503)	AT	(623580.00,	390239.97)
21	5.8279	(90072903)	AT	(624740.00,	361559.97)	22	4.9670	(90072809)	AT	(625500.00,	352240.00)
23	6.3105	(90072712)	AT	(625700.00,	369320.00)	24	6.1868	(90072712)	AT	(627380.00,	385940.03)
25	9.7763	(90072606)	AT	(628400.00,	375660.03)	26	6.0722	(90072709)	AT	(630180.00,	357260.03)
27	7.1578	(90072703)	AT	(631360.00,	368220.00)	28	11.0045	(90072703)	AT	(633000.00,	362640.00)
29	9.4161	(90072703)	AT	(633480.00,	377320.00)	30	7.8607	(90072700)	AT	(634020.00,	382180.00)
31	9.3962	(90072703)	AT	(636560.00,	373560.00)	32	6.8602	(90072712)	AT	(637020.00,	388200.00)
33	7.6521	(90072709)	AT	(638280.00,	367640.00)	34	6.6451	(90072712)	AT	(639740.00,	392380.00)
35	7.2901	(90072712)	AT	(640339.94,	378320.00)	36	7.4563	(90072712)	AT	(642260.00,	384640.00)
37	6.4944	(90072903)	AT	(643440.00,	397800.00)	38	7.4549	(90072706)	AT	(644600.00,	379780.00)
39	7.2647	(90072903)	AT	(645059.94,	411500.00)	40	8.1755	(90072709)	AT	(646200.00,	374740.00)
41	6.9826	(90072903)	AT	(647340.00,	401720.00)	42	9.1971	(90071412)	AT	(647480.00,	422440.00)
43	7.6686	(90072706)	AT	(647540.00,	388160.03)	44	8.2775	(90071412)	AT	(648960.06,	417120.03)
45	7.7897	(90071412)	AT	(650260.00,	426180.00)	46	7.2484	(90072903)	AT	(651300.00,	404400.00)
47	10.1468	(90072706)	AT	(651940.00,	384420.00)	48	8.0164	(90072903)	AT	(652260.00,	409880.00)
49	8.3982	(90072703)	AT	(653660.00,	397620.00)	50	9.5046	(90072706)	AT	(655560.00,	391760.00)
51	7.2208	(90072903)	AT	(656400.00,	406160.00)	52	8.5742	(90071412)	AT	(657220.00,	425140.00)
53	9.3857	(90072703)	AT	(657300.06,	396740.00)	54	8.7174	(90072903)	AT	(658600.00,	414100.00)
55	8.8118	(90072703)	AT	(658840.00,	401100.00)	56	10.3587	(90071412)	AT	(659240.06,	420500.00)
57	8.3657	(90071412)	AT	(663820.06,	416320.00)	58	6.0817	(90072900)	AT	(664080.00,	436660.00)
59	9.5684	(90072900)	AT	(664620.00,	429620.03)	60	4.8063	(90072715)	AT	(666039.94,	440379.97)
61	10.1119	(90072900)	AT	(666540.00,	423140.00)	62	10.3305	(90072900)	AT	(669980.00,	431640.00)
63	7.9922	(90071412)	AT	(670420.00,	416100.00)	64	10.5191	(90072900)	AT	(671160.00,	425180.00)

*** THE SECOND HIGHEST OF 3-HR AVERAGE CONCENTRATION VALUES AT EACH NON-GRID RECEPTOR FOR SO2 ***
CONCENTRATIONS IN MICROGRAMS/CUBIC-METER, RECEPTOR LOCATIONS IN METERS

REC NO	CONC	(YYMMDDHH)	AT	RECEPTOR (X,Y)	REC NO	CONC	(YYMMDDHH)	AT	RECEPTOR (X,Y)
1	3.2351	(90072815)	AT	(554300.00, 280980.00)	2	2.9588	(90072815)	AT	(554880.00, 277560.00)
3	3.2662	(90072815)	AT	(557540.00, 279840.00)	4	2.9756	(90072815)	AT	(558020.00, 276620.00)
5	3.6546	(90072815)	AT	(558200.00, 283780.00)	6	3.3077	(90072815)	AT	(559900.00, 279380.00)
7	3.1087	(90072815)	AT	(560960.00, 277060.00)	8	3.6305	(90072815)	AT	(561720.00, 281980.00)
9	3.5060	(90072815)	AT	(563740.00, 280100.00)	10	5.4423	(90072812)	AT	(610340.00, 338580.03)
11	4.3656	(90072615)	AT	(612200.00, 348060.00)	12	4.9327	(90072712)	AT	(612940.00, 359360.00)
13	4.4683	(90072615)	AT	(614760.00, 352420.00)	14	5.9293	(90072812)	AT	(615920.00, 337520.00)
15	5.2634	(90072712)	AT	(616860.00, 360980.00)	16	4.5566	(90072712)	AT	(618880.00, 354199.97)
17	5.6303	(90072812)	AT	(619260.00, 343840.00)	18	5.7724	(90072712)	AT	(620140.00, 365260.00)
19	4.5533	(90072818)	AT	(621660.00, 349020.00)	20	10.4414	(90072700)	AT	(623580.00, 390239.97)
21	5.5488	(90072712)	AT	(624740.00, 361559.97)	22	4.8869	(90072812)	AT	(625500.00, 352240.00)
23	5.4169	(90072809)	AT	(625700.00, 369320.00)	24	5.4463	(90072600)	AT	(627380.00, 385940.03)
25	6.7027	(90072712)	AT	(628400.00, 375660.03)	26	5.8470	(90072809)	AT	(630180.00, 357260.03)
27	6.3759	(90072712)	AT	(631360.00, 368220.00)	28	6.7959	(90072709)	AT	(633000.00, 362640.00)
29	7.0137	(90072712)	AT	(633480.00, 377320.00)	30	7.0098	(90072712)	AT	(634020.00, 382180.00)
31	6.9202	(90072712)	AT	(636560.00, 373560.00)	32	5.9444	(90072703)	AT	(637020.00, 388200.00)
33	7.5083	(90070203)	AT	(638280.00, 367640.00)	34	6.1067	(90072703)	AT	(639740.00, 392380.00)
35	6.2126	(90072709)	AT	(640339.94, 378320.00)	36	6.4216	(90072706)	AT	(642260.00, 384640.00)
37	6.2030	(90072712)	AT	(643440.00, 397800.00)	38	7.4279	(90072712)	AT	(644600.00, 379780.00)
39	5.8111	(90072900)	AT	(645059.94, 411500.00)	40	7.4911	(90072706)	AT	(646200.00, 374740.00)
41	6.0245	(90072703)	AT	(647340.00, 401720.00)	42	6.3134	(90072709)	AT	(647480.00, 422440.00)
43	7.6504	(90072712)	AT	(647540.00, 388160.03)	44	7.3222	(90072903)	AT	(648960.06, 417120.03)
45	5.7656	(90072709)	AT	(650260.00, 426180.00)	46	6.1225	(90072703)	AT	(651300.00, 404400.00)
47	7.7295	(90072712)	AT	(651940.00, 384420.00)	48	6.8271	(90072900)	AT	(652260.00, 409880.00)
49	7.3849	(90072712)	AT	(653660.00, 397620.00)	50	9.1159	(90072703)	AT	(655560.00, 391760.00)
51	6.6103	(90072703)	AT	(656400.00, 406160.00)	52	7.9734	(90072900)	AT	(657220.00, 425140.00)
53	7.8440	(90072712)	AT	(657300.06, 396740.00)	54	7.9002	(90072900)	AT	(658600.00, 414100.00)
55	7.4880	(90072712)	AT	(658840.00, 401100.00)	56	9.2875	(90072903)	AT	(659240.06, 420500.00)
57	8.3175	(90072903)	AT	(663820.06, 416320.00)	58	4.7874	(90072803)	AT	(664080.00, 436660.00)
59	5.4192	(90072903)	AT	(664620.00, 429620.03)	60	4.6170	(90072900)	AT	(666039.94, 440379.97)
61	9.5550	(90071412)	AT	(666540.00, 423140.00)	62	4.7610	(90072621)	AT	(669980.00, 431640.00)
63	7.3090	(90072900)	AT	(670420.00, 416100.00)	64	8.1059	(90071412)	AT	(671160.00, 425180.00)

*** THE 10 MAXIMUM OF 3-HR AVERAGE CONCENTRATION VALUES AT EACH NON-GRID RECEPTOR FOR SO2 ***
CONCENTRATIONS IN MICROGRAMS/CUBIC-METER, RECEPTOR LOCATIONS IN METERS

RANK	CONC	(YYMMDDHH) AT	(X,Y)	RECEPTOR NO.	RANK	CONC	(YYMMDDHH) AT	(X,Y)	RECEPTOR NO.
1	11.4135	(90070503) AT	(623580.00, 390239.97)	20	2	11.0045	(90072703) AT	(633000.00, 362640.00)	28
3	10.5191	(90072900) AT	(671160.00, 425180.00)	64	4	10.4414	(90072700) AT	(623580.00, 390239.97)	20
5	10.3587	(90071412) AT	(659240.06, 420500.00)	56	6	10.3305	(90072900) AT	(669980.00, 431640.00)	62
7	10.1468	(90072706) AT	(651940.00, 384420.00)	47	8	10.1119	(90072900) AT	(666540.00, 423140.00)	61
9	9.7763	(90072606) AT	(628400.00, 375660.03)	25	10	9.5684	(90072900) AT	(664620.00, 429620.03)	59

TECHNICAL REPORT DATA
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1. REPORT NO.	2.	3. RECIPIENT'S ACCESSION NO.
EPA-454/R-95-OO6		

4. TITLE AND SUBTITLE	5. REPORT DATE
Inter-agency Workgroup on Air Quality Modeling (IWAQM): Assessment of Phase 1 Recommendations Regarding the Use of MESOPUFF II	April 1995
	6. PERFORMING ORGANIZATION CODE
7. AUTHOR(S)	8. PERFORMING ORGANIZATION REPORT NO.
9. PERFORMING ORGANIZATION NAME AND ADDRESS Systems Application International San Rafael, CA 94903	10. PROGRAM ELEMENT NO.
	11. CONTRACT/GRANT NO. Contract 68-D-30019 Work Assignment 2-94
12. SPONSORING AGENCY NAME AND ADDRESS U.S. Environmental Protection Agency Office of Air Quality Planning and Standards Emissions, Monitoring and Analysis Division Research Triangle Park, NC 27711	13. TYPE OF REPORT AND PERIOD COVERED Final Report
	14. SPONSORING AGENCY CODE

15. SUPPLEMENTARY NOTES
EPA Work Assignment Manager: John S. Irwin

16. ABSTRACT

This report documents results from a case study to apply the MESOPUFF II air quality modeling system following the IWAQM interim recommendations (EPA, 1993). The study objectives were to identify and summarize the decisions made; record and summarize the resolution process for these decisions; and provide a written record of the resources used to complete the effort.

As will be seen in the discussion, limitations in funding resources necessitated only partial implementation of the interim recommendations. This was deemed acceptable because the purpose of the exercise was not to develop a meaningful assessment of actual air pollution impacts. The contractor was given a relatively free hand in suggesting and implementing strategies to automate processes and to accelerate the computations. Acceptance of these or similar strategies in an actual assessment can only be addressed on a case-by-case basis involving the relevant review authorities in the context of an actual situation. The IWAQM concludes that the findings confirm the need for active interaction between applicant and all the reviewing authorities (EPA, State, Federal Land Managers), and that this interaction should occur as soon as feasible.

17. KEY WORDS AND DOCUMENT ANALYSIS

a. DESCRIPTORS	b. IDENTIFIERS/OPEN ENDED TERMS	c. COSATI Field/Group
Air Pollution Long Range Transport Air Quality Dispersion Models	Dispersion Modeling Meteorology Air Pollution Control	

18. DISTRIBUTION STATEMENT	19. SECURITY CLASS *(Report)*	21. NO. OF PAGES
Release Unlimited	Unclassified	134
	20. SECURITY CLASS *(Page)*	22. PRICE
	Unclassified	

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