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INTERAGENCY WORKGROUP ON AIR QUALITY MODELING (IWAQM) PHASE 2 SUMMARY REPORT AND RECOMMENDATIONS FOR MODELING LONG RANGE TRANSPORT IMPACTS

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INTERAGENCY WORKGROUP ON AIR QUALITY MODELING (IWAQM) PHASE 2 SUMMARY REPORT AND RECOMMENDATIONS FOR MODELING LONG-RANGE TRANSPORT IMPACTS

U.S. Environmental Protection Agency
Air Quality Modeling Group (MD-14)
Research Triangle Park, North Carolina 27711

National Park Service
Air Resources Division
Denver, Colorado 80225

USDA Forest Service
Air Program
Fort Collins, Colorado 80526

U.S. Fish and Wildlife Service
Air Quality Branch Denver, Colorado 80225

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PREFACE

The Interagency Workgroup on Air Quality Modeling (IWAQM) was formed to provide a focus for development of technically sound recommendations regarding assessment of air pollutant source impacts on Federal Class I and Wilderness areas. Meetings were held with personnel from 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. The purpose of these meetings was to review respective modeling programs, to develop an organizational framework, and to formulate reasonable objectives and plans that could be presented to management for support and commitment. The members prepared a memorandum of understanding (MOU) that incorporated the goals and objectives of the workgroup and obtained signatures of management officials in each participating agency. Even though no States are signatories, they did participate in IWAQM functions.

This document is being released as a publication of the Environmental Protection Agency (EPA) in response to a request from the members of IWAQM. Members of the workgroup include representatives from the Environmental Protection Agency, the U.S. Forest Service, the National Park Service, and the U.S. Fish and Wildlife Service. The document includes IWAQM's recommendations for modeling methods that might be used to estimate Prevention of Significant Deterioration air quality impacts and National Ambient Air Quality Standards (NAAQS) air quality impacts associated with long-range transport of pollutant emissions to Class I and Wilderness areas . The IWAQM recommends that the CALPUFF Lagrangian puff dispersion modeling system be used for characterization of the transport and dispersion.

The recommendations of IWAQM contained in this document is considered technical guidance tailored for use in assessing air quality impacts associated with prevention of significant deterioration.

ACKNOWLEDGMENTS

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1.0 INTRODUCTION

Special protection from adverse air quality impacts is afforded certain national parks and wilderness areas, through the prevention of significant deterioration (PSD) program (U.S. EPA, 1980). These areas have been designated as Class I areas, and as such, increases of pollutant levels in these areas are strictly limited. Furthermore, the Federal Land Manager (FLM) of the Class I area is given an affirmative responsibility to ensure that Air Quality Related Values (AQRVs) are not adversely impacted. [The FLMs of the Class I areas are the U.S. Forest Service (USFS), the National Park Service (NPS), and the U.S. Fish and Wildlife Service (FWS).] Air quality models are one of the primary tools used to assess the impacts from sources of air pollution on both the established Prevention of Significant Deterioration (PSD) increments and the AQRVs. Steady-state models have been generally used for PSD analyses. As the PSD program has developed, the need for more sophisticated models to assess air quality impacts in Class I areas, from sources at relatively greater distances from the Class I areas, has arisen. In some areas, the FLMs have asserted that Class I areas have been adversely affected by air pollution and that new sources of pollution over a broad area are further harming the resource. The absence of any recommended long-range modeling techniques has left permitting authorities without the means to assess the assertions of the FLMs. The Environmental Protection Agency (EPA) and the FLMs have undertaken various model development efforts to address the air quality impacts of pollution transported over relatively long distances. The Interagency Workgroup for Air Quality Modeling (IWAQM) was formed to coordinate the independent modeling efforts of the EPA and the FLMs so that a consistent, technically credible approach can be recommended and used.

Models used to evaluate the impact of sources of air pollution on the PSD increments and National Ambient Air Quality Standards (NAAQS), are required to follow Appendix W to 40 CFR Part 51 (*Guideline on Air Quality Models),* U.S. EPA (1997). (Hereafter, referred to as the *Guideline*.) For many situations, preferred models, considered generally applicable under a variety of circumstances, are defined. Currently within the *Guideline* (Section 7.2.6), there is no preferred model listed for assessing impacts involving transport beyond 50 km. For those situations for which there are no preferred models, criteria are established in the *Guideline* to use appropriate methods on a case-by-case basis. These criteria are:

i. The model can be demonstrated to be applicable to the problem on a theoretical basis, and

ii. the data bases which are necessary to perform the analysis are available and adequate, and

iii. performance evaluations of the model in similar circumstances have shown that the model is not biased toward underestimates, or

iv. after consultation with the EPA Regional Office, a second model is selected as a baseline or reference point for performance and the interim procedures are then used to demonstrate that the proposed model performs better than the reference (preferred) model.

The processes which become important in the transport of pollution over long distances include the spatial and temporal variability of the winds which transport and disperse air pollutants in the presence of various terrain and water features, the chemical transformation of the pollutants as they travel, and the deposition of the pollutants along the way. Cummulative impact assessments likely will need to address multiple, geographically disperse sources. There are existing long-range transport models available which meet some, but not, all of these needs and some which meet these needs but either have not been sufficiently tested or are perceived to need further development for routine operational use in regulatory assessment analyses. One of the primary goals of IWAQM is to evaluate existing modeling codes and either recommend one as an accepted approach or combine the better elements of several of the existing codes, creating a new modeling construct.

The IWAQM work plan (U.S. EPA, 1992a) describes a phased approach to satisfy the modeling needs described above. Phase 1 consists of reviewing EPA guidance and recommending an interim modeling approach to meet the immediate need for a long-range transport model for ongoing permitting activity. In developing a Phase 2 recommendation, the workgroup was to review other available operational models and make a recommendation of the most appropriate modeling techniques. The Phase 2 recommendation was to be a compromise between the current modeling state-of-science and best available operational computer capabilities. If resources could be found to pursue a Phase 3 recommendation, the workgroup would add more advanced modeling techniques to its consideration, probably representing a greater level of scientific and computer hardware sophistication.

Given the practical limitations of resources and hardware, the Phase 1 interim recommendations (U.S. EPA, 1993) were designed to provide the best approach from existing "off-the-shelf" techniques. Two models were assessed, the MESOPUFF II model (U.S. EPA, 1994) and the Acid Rain Mountain Mesoscale Model (ARM3), Morris et al., (1988). Upon careful examination of both models, coding errors were discovered in the ARM3, which potentially invalidated its previous evaluations. With this in mind and other considerations as discussed in U.S. EPA (1993), the Phase 1 recommendation was to use on a case-by-case basis the Lagrangian puff model, MESOPUFF II, to evaluate the impacts of pollutants from sources located more than 50 kilometers from Class I areas, up to several hundred kilometers from Class I areas. The impacts are: 1) the allowable Class I increases (increments), 2) the National Ambient Air Quality Standards (NAAQS), and 3) Air Quality Related Values (AQRVs)

associated with emissions of sulfur, nitrogen and particulate matter. The PSD NAAQS pollutants were sulfur dioxide (SO_2) and particulate of size less than or equal to ten microns (PM_{10}). AQRV impacts include such effects as visibility degradation and acidic deposition. In order to focus this effort, increase the chance for success in at least certain scenarios, and to meet an articulated immediate need of permitting authorities and the EPA, IWAQM chose to address only sulfur and nitrogen derived pollutants. It was acknowledged that there are other pollutants such as photochemical oxidants that may injure components of the natural ecosystem, but assessment by IWAQM of the modeling needs and development of oxidant effects modules was postponed until a later date. The Phase I interim recommendations also provided a screening methodology, which (as is discussed later) proved to be too concervative to be of much use.

For the Phase 1 recommendation, MESOPUFF II was deemed suitable for conducting single source impact analyses, and in some circumstances cumulative impact analyses. As the dispersion characterizations in MESOPUFF II were not designed to handle local-scale dispersion effects, it was recognized that the MESOPUFF II results would frequently need to be combined with the results from other modeling techniques used to estimate concentrations from sources closer than 50 kilometers to a receptor area. The Phase 1 recommendation was structured to satisfy case-by-case *Guideline* criteria i, ii, and iii above. The iv criterion has meaning only when there is a preferred model, and such is not the case for modeling impacts involving transport beyond 50 kilometers.

By restricting the models considered for Phase 1 to "off-the-shelf" techniques, IWAQM recognized certain limitations. These include a lack of consideration of the effects of terrain on the long-range transport and dispersion, an underestimation of the conversion of sulfur dioxide, SO_2, to sulfate, $SO_4^=$, when polluted air interacts with clouds, and a possible overestimation of particulate nitrate when a limited number of sources are considered. Nonetheless, IWAQM considered the techniques, suggested to be a significant improvement to those previously used, in that previous techniques ignored many of the processes important to the assessment of air quality impacts in Class I areas. Thus, while under some circumstances the impacts on regional visibility may be underestimated, because the concentrations of sulfates in the atmosphere may be underestimated due to the inability of the model to treat in-cloud processes, IWAQM, including the representatives of the land management agencies, considered the suggested techniques to be technically superior to simply assuming that there are no impacts on regional visibility.

The IWAQM recognized that there were certain risks involved with recommending an interim modeling approach. From a regulatory perspective, it is generally desirable to use an interim model which will yield somewhat higher impact calculations than a more refined, preferred approach. In the case of steady-state air quality models, this can be relatively easily ensured because of the independence of the concentration calculations from one hour to the next. In the case of the Lagrangian

long-range transport models under consideration here, the concentration calculations for a given hour will be explicitly dependent on the spatially and temporally varying wind field from that hour and previous hours. Therefore, the exact behavior of a given modeling system relative to a similar but different modeling system can not be predicted with certainty.

Not long after the release of the Phase 1 recommendation, the EPA sponsored the Sixth Modeling Conference which was held August 9-10, 1995 in Washington, D.C. One of the main topics at this two-day event was a review of IWAQM Phase 1 recommendation, a summary of work in progress, with review comments provided by several groups. At the conference, IWAQM presented long-range trajectory comparison, that suggested that use of mesoscale meteorological analyses of wind fields provided a significant improvement in the accord of modeled and observed trajectories. The IWAQM endorsed specifically the use of mesoscale meteorological analyses that employ data assimilation. The IWAQM recommended that the Phase 1 recommendation to use the MESOPUFF II modeling system be replaced with a recommendation to use the CALMET/CALPUFF modeling system. This was a relatively new Lagrangian puff modeling system, which had additional algorithms to provide simulation of local-scale short-range dispersion using methods already endorsed by the EPA. Thus, use of this newer modeling system allowed one model to be used for all sources in an analysis, regardless of the transport distance involved. The IWAQM also endorsed the formation of public/private committees to manage the myriad of site specific technical decisions that are inherent in assessing mesoscale PSD and AQRV impacts on Class I areas. Appendix D provides a review of the information provided at the Sixth Modeling Conference, a summary of comments received, and IWAQM's response to these comments.

Section 2 presents the Phase 2 modeling recommendation, which represents a compromise between the current modeling state-of-science and best available operational computer capabilities. The IWAQM Phase 2 recommendations are for methods and procedures that might be used to estimate air quality Prevention of Significant Deterioration impacts to increments and AQRVs and National Ambient Air Quality Standards (NAAQS) impacts from pollutant emissions, that due to the transport distances and location are best treated using a long-range transport modeling system. The Phase 2 recommendations are not limited to recommendations on which modeling systems to use, as part of IWAQM's efforts are to assist in fostering best assessment of impacts. Briefly summarized, the Phase 2 recommendation consist of:

- a suggested screening technique for modeling worst-case estimates of long-range transport impacts,

- a recommendation that the CALPUFF modeling system be listed as the preferred model in Section 7.2.6 in the *Guideline*,

- recommendations for assessing PSD increment and NAAQS impacts of a new source's emissions (or change in an existent source's emissions) involving long-range transport of emissions,

- recommendations for assessing the AQRV impacts of a new source's emissions (or change in an existent source's emissions) of sulfur, nitrogen and particulate matter to regional visibility degradation and deposition, which requires a knowledge of the current state of the Class I area, and

- a recommendation that consideration be given to forming committees ('Regional Approach') to assist in the resolution of the myriad of decisions associated with mesoscale modeling of PSD and AQRV impacts for each Class I area (or groups of areas).

Section 3 discusses the chemistry limitations inherent in CALPUFF, and how results from CALPUFF can be used to estimate regional visibility impacts and deposition of sulfur and nitrogen.

From the comments received at the Sixth Modeling Conference, IWAQM concluded that in order to provide a firmer basis for a Phase 2 recommendation, more information was needed comparing mesoscale modeling dispersion results with tracer field data, and more comparisons were needed to stress test code modifications made to incorporate local-scale dispersion characterizations. Everyone was in agreement that the screening analysis, suggested by IWAQM in the Phase 1 recommendation, was inadequate. It was perceived as providing such large overestimates of SO_2 and sulfate impacts that it was of little use. Section 4 provides a review of the activities that IWAQM has sponsored in developing the Phase 2 recommendations, as well as, summaries of investigations that IWAQM is aware of that provide information regarding lessons learned in using and applying the CALPUFF modeling system.

2.0 MODELING RECOMMENDATIONS

For most of the modeling situations discussed in the *Guideline* where a refined modeling technique is recommended, a screening analysis is also provided. The screening analysis is meant to be easy to conduct and to provide a worst-case maximum impact estimate. If the results of the screening analysis show compliance with existing regulatory requirements, then no further modeling for compliance with standards and increments is required.

Basically, IWAQM's recommendations for a screening analysis is an approach of using a simplified set of meteorology with CALPUFF. To encourage the results to be higher than would be estimated using a fully developed CALMET and CALPUFF analysis, rings of receptors are used. The maximum concentration value found anywhere on the receptor rings are used (rather than restricting the analysis to receptors only located within the Class I area(s) of interest). More discussion of the steps to be taken and processing requirements for a screening analysis is provided in Section 2.1.

IWAQM's recommendations for a refined analysis involve the following differences from the screening analysis:

- use of a fully developed time and space varying characterization of the meteorology using CALMET, and
- the receptors are placed within the Class I area(s) of concern, and
- the background concentrations of ozone and ammonia are allowed to vary in time and space, and
- the concentration and AQRV impacts are computed to more directly correspond to the standards, increments, and thresholds of concern.

More discussion of the steps to be taken and processing requirements for a refined analysis is provided in Section 2.2.

Sections 2.1 and 2.2 focus on how to apply models, specific options and data sets to be employed, and the processing of the input and output data. Section 2.3 provides more general recommendations on practical issues and limitations of long-range transport modeling assessments.

2.1 Screening Analysis

Section 4.7 presents comparisons of puff and plume model simulation results to demonstrate what differences might arise in simulated concentration values when the plume and puff model employ essentially identical meteorology and dispersion characterizations. The results shown in Section 4.7 show striking evidence that treating the sequence of meteorological events of all hours (including calms), can result in puff simulated maxima that are considerably higher than plume simulated maxima for

almost any distance downwind or averaging time. This was most evident for the shorter averaging times that were 24-hours or less. The IWAQM concludes from these results that use of a plume model as a screen for a puff model's impacts is unlikely to be successful. In Section 4.8, a summary is presented of comparisons of results obtained by using a puff model with single station meteorology (a screening analysis) versus fully generated wind fields (a refined analysis) for each hour. These results suggest that the maximum concentration values simulated using the proposed screening approach for a receptor ring may occasionally underestimate results obtained from a refined model simulation. To address this tendency, IWAQM recommends use of the maximum concentration found anywhere on the receptor rings, rather than limiting the analysis to only receptors within the Class I area(s) of concern (as would be the case in a refined analysis). These conclusions are for maxima on receptor rings at fixed distances from isolated point sources where the terrain was relatively flat.

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With these thoughts in mind, the following CALPUFF screening procedure is suggested by IWAQM (as outlined in Table 1):

1) generate five years of ISCST3 input meteorology using PCRAMMET,

2) generate an ISCST3 control file (use standard ISC defaults and create receptor rings as appropriate for the application); use the ISC2PUF conversion program to create the CALPUFF control file,

3) edit the CALPUFF control file to select MESOPUFF II chemistry, and specify domain-wide background concentration values for ozone and ammonia (see Section 2.2.2),

4) run CALPUFF with the ISCMET.DAT data option, and pick the maximum concentration for each pollutant, for each receptor ring and averaging time modeled. Perform increment and AQRV comparisons as required. For haze impact assessment, use the FLM provided "clean" background extinction coefficient and assume a RH value of 90%.

In Step 1 above, it is anticipated that an update will be made to PCRAMMET and the Meteorological Processor for Regulatory Modeling (MPRM) so that they will list the relative humidity for each hour, along with the other parameters needed to compute deposition. With this update, the MESOPUFF II chemistry can be activated within CALPUFF. In Step 2 above, it is envisioned that receptor rings would be created that would pass through the Class I area(s) of interest. The IWAQM recommends that the placement of the receptor rings, and assumptions to be employed in the CALPUFF model runs be discussed with the applicable reviewing authorities, prior to actually

Table 1. Outline of recommendations for screening analysis. Given judgement required in receptor ring placement and background values to be assumed in CALPUFF and CALPOST analyses, applicants should gain agreement on how coordination with Federal Land Managers (FLM) and other reviewing authorities will be addressed, prior to conducting runs and analyses.	
Meteorology	Use five years of PCRAMMET (extended output for deposition).
Receptors	Receptors at least every two degrees on rings that encircle source and pass through the Class I area(s) of interest.
Dispersion	1. Use ISC2PUF to convert an ISC3 control input file for use by CALPUFF. 2. Edit control file to use MESOPUFF II chemistry; use wet and dry deposition (use default setups for these). 3. Use domain average background values for ozone and ammonia for area. 4. Run CALPUFF using ISC meteorology option (note, define 6 to 10 layers in vertical; top layer should extend above maximum mixing depth expected); horizontal domain extending 50 to 80 km beyond outer receptor ring.
Processing	**1. For PSD increments**: use maximum 3-hr, 24-hr and annual SO_2 and PM_{10} and maximum annual NO_2 for comparison with allowable limits. **2. For haze:** use maximum 24-hr $SO_4^{=}$, NO_3^{-}, and HNO_3 values; assume 90% RH for f(RH) for day, calculate extenction coefficients for each pollutant (see Section 3.2); and compute the precent change in extinction using the FLM supplied background extinction, as described in Section 3. **3. For total S or N deposition:** convert deposition flux to kg/(hectar•year) using maximum values of annual SO_2, $SO_4^{=}$, NO_3^{-}, HNO_3, and NOx as described in Section 3.

conducting any screening analyses. These up front discussions are essential for defining the AQRV's of interest, which dictate the averaging times and pollutants of interest for the AQRV assessments. The maximum 3-hr, 24-hr and annual SO_2 and PM_{10}, and the annual nitrogen dioxide concentrations would be compared with the current standards and PSD increments as required by the applicable reviewing authorities. If a haze impact assessment is required, then use the 24-hour maximum sulfate, nitrate and primary particulate concentrations in equation (8) of Section 3.2. If total nitrogen or total sulfur deposition impacts are required, then use the maximum annual concentration values and follow the procedures as described in Section 3.3.

2.2 Refined Analysis

Table 2 outlines the basic IWAQM recommendations for a refined analysis. It is understood that conducting a CALMET and CALPUFF analysis for any scale of application will necessarily involve case-specific judgements. It is IWAQM's conclusion that it is not possible to prescribe all the decisions needing to be made. We have attempted to provide suggestions where possible. We have recommended that all users of CALMET and CALPUFF start with a common set of default conditions and input data. Then, as the decisions are made to change default settings and discard or augment the input data, these can be discussed and reviewed with the applicable authorities, prior to actually committing expensive and time-consuming resources. Within this context use of technical review committees, as suggested in the Regional Approach (Section 4.5), would greatly assist applicants in these endeavors.

2.2.1 Meteorology

Expertise Needed

Currently, developing CALMET meteorological fields is considered a difficult task just managing the sheer volume of input and output data of CALMET, and excellent computer skills are needed to manage the operation of the various processors to CALMET. The software was not written to accept a variety of input data formats. The software was developed with the assumption that the user is capable of screening the data for anomalous values. It was assumed that if the data are not in the required format, the user has the programming skills to write special programs to translate the data format to the format required.

Renovating these programs was beyond the resources available to IWAQM. The IWAQM focused what resources it had to the issues of testing the technical aspects of the modeling system (comparisons with tracer experiments, enhancement of processing controls, etc.) to see if the CALMET/CALPUFF modeling system was technically sufficient for routine use. It has been assumed that support to renovate these processors can be found, if and when, the CALMET/CALPUFF modeling system becomes a recommended modeling approach.

Currently, adjusting and tailoring the CALMET options to see if the generated wind fields are reasonable requires strong computer graphics skills to visualize the results generated by CALMET. This component of the analysis can be simplified by using existing visualization software.

The control of the CALMET options requires expert understanding of mesoscale and microscale meteorological effects (such as terrain slope flows) on meteorological

Table 2. Outline of recommendations for refined analysis. Given judgement required in CALMET, CALPUFF and CALPOST processing, applicants must gain agreement on how coordination with Federak Land Managers (FLM) and other reviewing authorities will be addressed, prior to conducting runs and analyses.	
Meteorology	1. Use five years of representative hourly NWS surface and precipitation observations, and twice-daily upper air observations. On a case-by-case basis, one may use less than five years of *FDDA-MM* data with representative NWS data; or use less than five years of on-site meteorological data with available NWS data. 2. CALMET (minimum of 6 to 10 layers in vertical; top layer must extend above maximum mixing depth expected); horizontal domain extending 50 to 80 km beyond outer receptors and sources being modeled; terrain elevation and land-use data resolved for situation (tailor land-use parameters to situation).
Receptors	Within Class I area(s) of concern, provide coverage tailored to situation (insure FLMs concur).
Dispersion	1. CALPUFF with default dispersion settings. 2. Use MESOPUFF II chemistry; use wet and dry deposition (use default setups for these). 3. Define background values for ozone and ammonia for area (tailor spatial variability to situation needs and data availability).
Processing	**1. For PSD increments:** use highest second-highest 3-hr, 24-hr concentration values, and use the maximum annual concentration values of SO_2 and PM_{10} and maximum annual for NO_2 for comparisons with allowable limits. **2. For haze**: process the 24-hr $SO_4^{=}$, NO_3^{-}, and HNO_3 values adjusted using hourly RH as discussed in Section 3; calculate extinction coefficients for each pollutant (Section 3.2), compute the percent change in extinction using the FLM supplied background extinction, as described in Section 3; compare with thresholds as directed by applicable FLMs and reviewing authorities. **3. For total S or N deposition:** convert deposition flux to kg/(hectar•year) using maximum values of annual SO_2, $SO_4^{=}$, NO_3^{-}, HNO_3, and NOx as described in Section 3; compare with threshold as directed by applicable FLMs and reviewing authorities.

conditions, and finesse to adjust the available processing controls within CALMET to develop the desired effects (e.g., Section 4.9.2). The IWAQM does not anticipate a lessening in this required expertise in the future. Developing three-dimensional time-varying fields of meteorological conditions is a demanding task, which can not be left to unskilled or inexperienced staff. The IWAQM does not foresee a time when

development of time-varying mesoscale meteorological wind fields (by whatever means) will become as simplified as the running of the ISC3 modeling software has become in recent years.

Appendix A provides a listing of the default settings recommended by IWAQM at this time. Some of these settings require testing, and we have attempted note these. The information provided in Appendix A should not be interpreted as a cookbook approach to be applied, regardless of results obtained.

Length of Modeling Assessment

Significant year-to-year variations were seen in the Demonstration Assessment (Section 4.1) and also in the developmental work towards attempting to build a new screening methodology (Section 4.8). These results suggest that several years of refined analysis are needed to address the variation in pollution impacts likely to occur. For consistency with other *Guideline* requirements, a five-year period of analysis using representative NWS meteorological data is recommended. CALMET employs diagnostic algorithms to tailor the available meteorological data for slope flow effects, land-sea circulations, etc. If special meteorological observations are available within the modeling domain that would assist CALMET's diagnostic analysis, or if *FDDA-MM* data are to be employed in the CALMET analysis, then less than a five-year period of analysis can be accepted, on a case-by-case basis by the applicable reviewing authorities. This accommodates use of refined meteorological data for those locations where refined meteorological data have been suitably processed, or where mesoscale meteorological campaigns have been accomplished.

Geophysical Data

Terrain heights and land-use are needed for input to CALMET. The IWAQM has provided one set of these values for the contiguous United States. The grid resolution is approximately 900 m for the terrain data and 1/12 degree latitude (9.25 km) by 1/8 degree longitude (9.8 km at 45° latitude) for the land-use data (CALMET, CALPUFF, And CALPOST Modeling System (Version 1) CD-ROM; see Appendix C). Default values characterizing the surface parameters associated with each land-use class are also provided. The resolution of this data set is considered adequate for assessments involving transport distances of 50 km and greater, although the land-use categorization should be examined carefully. The resolution of this data set may also be adequate for many local-scale assessments.

The IWAQM recommends use of this data set, as a first choice. The IWAQM recognizes that there are instances when these terrain heights and land-use data must be considered inappropriate, such as the situation discussed in Section 4.9.2. It is anticipated that rejection of this data set will most often be for treatment of sources located in very rugged terrain, which is anticipated to significantly affect the transport trajectory of the plume. Using this data set, as a first choice with assignment of the

default surface parameters as listed on the distribution CD, should provide consistency in future analyses and helps to standardize the input requirements for software development.

Another source of terrain heights and land-use data is from the United States Geological Survey (USGS). Some of these data can be accessed through the World Wide Web. The general USGS site is at http://www.usgs.gov. At the time of this writing, the data was available at http://edcwww.cr.usgs.gov/doc/edchome/ndcdb/ndcdb.html.

Precipitation Data

Precipitation is notoriously spotty, with many localized maxima and minima. It is recommended by IWAQM that all precipitation reports reasonably available be used.

Precipitation data are available for the United States from the National Climatic Data Center (NCDC) in a format called TD-3240. No data filling is necessary for these data sets for use by CALMET. But as discussed in EPA (1995a), the formatting of these data for a large domain is not trivial. The software available is not robust and could stand to be improved.

Another source of precipitation data is from private firms that purchase the data from NCDC, repackage it, and provide software for extracting the repackaged data. This may be an attractive alternative to some users.

National Weather Service Data

The number of surface and upper air sites will be determined by the size of the modeling domain and the availability of meteorological data. It is recommeded that for refined analyses one would use all sites that are within and near the modeling domain, so as to provide as good a characterization as possible of the spatial variation of the meteorological conditions.

The CD-ROM data sets (Appendix C) are made available by the National Climatic Data Center. These hourly surface weather observations (*Solar and Meteorological Surface Observation Network* (SAMSON) and Hourly United State Weather Observations (HUSWO) 1990-1995), and twice-daily upper air observations (*Radiosonde Data for North America*) are recommended by IWAQM as first choice for acquiring access to these data. Using these data sets, as a first choice, should provide consistency in future analyses and helps to standardize the input requirements for software development.

The current CALMET software requires the user to closely inspect the upper-air data prior to use. Since the program does not fill in missing levels or time periods (which sometimes occur in the observations), the user should inspect the data to insure

that complete data is available at least for all levels below and just above the anticipated maximum mixing depth for the modeling domain. Furthermore, CALMET can not process if the time difference between successive upper-air soundings is greater than 12 hours. If this occurs, the user must use judgement to fill in the requisite data. When multiple NWS sites are used for characterizing the hourly surface weather conditions, missing observations from one station can be handled simply by filling in a missing data indictor for that site for that hour. But the user should review the hourly surface observations to insure that the data coverage in space and time is adequate. This requires judgement and finesse and given the complexities of long-range transport analysis, is not amenable to cookbook cures.

FDDA-MM Data

As mentioned in Section 4.4 there are various groups capable of developing *FDDA-MM* data suitable for use as input to the CALMET/CALPUFF modeling system. Alternatively, consideration could be given to using the 1990 MM4 data set (NCDC, 1995) or other data sets which might be completed for other years. The problem with these data sets is that the they are costly to construct and advances are currently being made at such a rapid pace, they are becoming dated almost as soon as they are constructed. Furthermore, there are situations defined in the *Guideline* when on-site meteorological data are to be collected and used in the modeling assessments (e.g., when using CTDMPLUS for a complex terrain impact assessment, where the transport distances are less than 50 km). Hence, there appears to be a never-ending need to construct additional years of data. The IWAQM recommends finding a link to some operational source of *FDDA-MM* data, as the optimal solution.

Towards this end, IWAQM recommends that links to the operational model outputs that are produced by the NOAA Mesoscale Modeling Branch (MMB) (see discussion by Schulze and Turner, 1998). This group is developing data suitable for use in the CALMET/CALPUFF modeling system. They have an active plan to refine and improve the modeling science and to reduce the grid size in future years. These model outputs are being developed to directly support operational needs of the National Weather Service, and should prove to be a stable source of such data in the future.

The major obstacle is access to these data. An operational means for gaining easy access to comprehensive mesoscale meteorological data sets has yet to be developed. Therefore, IWAQM recommends that a solution be developed that will provide the public routine, inexpensive access to such data. The data can be depended on being available in future years. Users who either are required to collect and use on-site data, or need such data for best characterization of their situations, can use CALMET to manage the blending of their on-site data, with routine NWS observations and available *FDDA-MM* data.

Once an operational link is established to an operational source of *FDDA-MM* data and a sufficiently long record of the data is available, IWAQM recommends the use of these data.

2.2.2 Chemistry

The MESOPUFF II chemistry option, currently available in CALPUFF, is adequate for representing gas phase oxidation of sulfur dioxide to sulfate and for the nitrate chemistry. The algorithms currently do not adequately account for the aqueous phase oxidation of sulfur dioxide to sulfate. The aqueous phase chemistry can dominate the formation of sulfate. Therefore, in many applications sulfate is likely to be underestimated.

The IWAQM recommends use of the MESOPUFF II chemistry option, although it is recognized that this module may grossly underestimate the conversion of sulfur dioxide to sulfate when the pollutants interact with clouds or fog.

Ozone Background

CALPUFF provides two options for providing the ozone background data: (1) a single, typical background value appropriate for the modeling region, or (2) hourly ozone data from one or more ozone monitoring stations. The second and preferred option requires the creation of the OZONE.DAT file containing the necessary data. For the Demonstration Assessment, the domain was large (700 km by 1000 km) such that the second option was necessary. The IWAQM does not anticipate such large domains as being the typical application. Rather, it is anticipated that the more typical application will involve domains of order 400 km by 400 km or smaller. But even for smaller domains, the ability to provide at least monthly background values of ozone is deemed desirable. The problem in developing time (and perhaps spatial) varying background ozone values is having access to representative background ozone data.

Ozone data are available from EPA's Aerometric Information Retrieval System (AIRS); however, AIRS data must be used with caution. Many ozone sites are located in urban and suburban centers and are not representative of oxidant levels experienced by plumes undergoing long range transport.

Ammonia Background

A further complication is that the formation of particulate nitrate is dependent on the ambient concentration of ammonia, which preferentially reacts with sulfate. The ambient ammonia concentration is an input to the model. Accurate specification of this parameter is critical to the accurate estimation of particulate nitrate concentrations. Based on a review of available data, Langford et al. (1992) suggest that typical (within a factor of 2) background values of ammonia are: 10 ppb for grasslands, 0.5 ppb for forest, and 1 ppb for arid lands at 20^{o}C. Langford et al. (1992) provide strong evidence

that background levels of ammonia show strong dependence with ambient temperature (variations of a factor of 3 or 4) and a strong dependence on the soil pH. However, given all the uncertainties in ammonia data, IWAQM recommends use of the background levels provided above, unless specific data are available for the modeling domain that would discredit the values cited. It should be noted, however, that in areas where there are high ambient levels of sulfate, values such as 10 ppb might overestimate the formation of particulate nitrate from a given source, for these polluted conditions. Furthermore, areas in the vicinity of strong point sources of ammonia, such as feed lots or other agricultural areas, may experience locally high levels of background ammonia.

2.2.3 Dispersion

Expertise Needed

The control of the CALPUFF options requires expert understanding of terrain affects on meteorological conditions and some finesse to adjust the available processing controls. Appendix B provides a listing of the default settings for CALPUFF recommended by IWAQM at this time. Some of these settings require testing, and IWAQM has attempted note these. The information provided in Appendix B should not be interpreted as a cookbook approach to be applied, regardless of results obtained.

Emissions

Developing an inventory with agreed upon emission rates is not trivial. The inventory could differ depending on whether the analysis is addressing NAAQS assessments (which typically address maximum allowable emission rates from only PSD sources) versus AQRV assessments (which typically address actual current emission rates from all existing sources). The IWAQM recommends that the manner in which the sources and emissions are to be characterized be agreed upon in the initial up-front discussions with the reviewing authorities.

Receptors

For some Class I areas the FLMs have developed receptor networks for use in the modeling analyses, which facilitates assessment of cumulative impacts from successive applicants. In such cases, the applicants should use these predefined receptor networks. In other situations, IWAQM suggests use of judgement. The more rugged the terrain and the presence of local sources being included in the analysis will necessitate use of more closely spaced receptor networks in order to adequately characterize the concentration patterns to be simulated for the Class I area(s). This is another area where judgement and review by others will be needed.

Local-scale

The IWAQM is recommending use of the CALPUFF modeling system for the characterization of all sources being explicitly modeled. This eliminates the need to simulate the long-range impacts (those involving transport greater than 50-km) separately, and then combine these results with those obtained using some other model for the local-scale impacts (those involving transport of less than 50-km). We have CALPUFF and ISC comparison results using both steady-state and non-steady-state hourly meteorology. It was the conclusion of IWAQM that CALPUFF could reproduce the steady-state results of the ISC plume dispersion model. A benefit of using one model for all sources is that CALPUFF has the MESOPUFF II chemistry, which provides characterization of pollutant species that are not treated by currently available local-scale models (such as ISC and CTDMPLUS).

Comprehensive tests results are not available comparing CALPUFF with CTDMPLUS for steady-state impacts on isolated hills and ridges. The IWAQM assumes that once these have been accomplished and the results have been shown to be similar, that long-range impact assessment with CALPUFF (using fully developed CALMET meteorology) can also include more explicit hill impaction assessments, as necessary, for all sources regardless of the transport distances involved.

2.3 Practicalities

The IWAQM recommendations for conducting a long-range transport screening analysis are presented in Section 2.1, and the IWAQM recommendations for conducting a long-range transport refined analysis are presented in Section 2.2. The focus of these discussions was how to run the simulations and the management of the input and output data. There are other practical concerns that applicants and reviewing authorities should be mindful of, namely: the uncertainties associated with the screening analysis, the uncertainties associated with the refined analysis, differences between plume and puff simulation results, and commensurate difficulties in providing technical oversight.

2.3.1 Screening procedures uncertainties

In Section 4.8 comparisons are presented of CALPUFF simulation results generated either through the use of ISC or CALMET meteorology. Anticipating that most analyses will involve a moderate to tall stack, of order 35-m to 200-m in height, it is seen that the screening estimates of sulfur-dioxide and sulfate concentration maxima obtained using ISC meteorology, typically range within ±70% of that simulated using CALMET meteorology. The sulfur dioxide and sulfate deposition fluxes obtained using ISC meteorology, typically range within ±60% of that simulated using CALMET meteorology. This suggest that the screening analysis as proposed is not providing a biased (overestimate) of these impacts. It was for this reason that IWAQM recommended that all receptors on the ring be included in the screening assessment. It

was hoped that this would provide a measure of conservatism to the screening analysis. Adding a measure of conservatism is deemed reasonable, as the proposed screening analysis completely disregards the terrain and land-use induced wind effects, that would arise if fully-developed three-dimensional wind fields were developed using available surface and upper-air observations. The IWAQM concludes that the impacts estimated by the screening procedure proposed are conservative and yet less onerous than results as would be obtained by the Phase 1 Level 1 screening, and addresses concerns raised at the Sixth Modeling Conference

2.3.2 Refined modeling uncertainties

In Section 4.6 comparison results of CALPUFF simulations with tracer field data are provided. The studies presented are considered representative of a few of the better tracer field studies that involve comprehensive sampling along arcs at downwind distances of order 50- to 100-km. As summarized in Section 4.6, in general the CALPUFF simulated concentration values were within a factor of two of that observed. Little differences in overall performance was seen, whether Pasquill or similarity dispersion curves were employed. This is understandable since as transport times and distances increase, the dispersing material is becoming well-mixed in the vertical, and the horizontal extent of the dispersing material is more related to the wind field variations than is the rate of relative dispersion about simulated puff centroids. This is dramatically made apparent by the results shown in Section 4.7, where direct comparisons were made of the ISC plume model and CALPUFF. In these comparisons it was shown that for steady-state assumptions, CALPUFF could suitably mimic results as would be obtained by ISC. And yet with identical specification of the dispersion and meteorology, once the puff model was allowed to simulate the 'causality' of hour-by-hour variations, the puff model's results no longer were similar to that obtained by ISC. In fact, as a result of explicitly treating calms and wind reversal effects by the puff model, the simulated maximum concentrations by CALPUFF were generally greater than that simulated by ISC for all transport distances and averaging times.

The quality and uncertainties associated with long-range transport simulations is driven more by the characterization of the mixing depth and by the characterization of the transport winds. Better characterization of the mixing depth may be possible in the future, but it should be understood that the mixing in the vertical reflects both local and mesoscale effects. The influence of local variations in land-use (forests, lakes, farmland, cities) can be significant. Hence uncertainties of order ±40% in mixing depth are likely (Irwin and Paumier, 1990) and will be difficult to avoid. Improvement in the characterization of the transport winds is possible through the use of *FDDA-MM* meteorological data, as discussed in Section 4.3. Both the comparisons of simulated trajectories and the comparisons of trajectories derived using the CAPTEX tracer field show improvement through the use of sophisticated mesoscale meteorological data employing FDDA.

Based on the tracer comparison results presented in Section 4.6, it appears that CALPUFF provides reasonable correspondence with observations for transport distances of order 100 km. Most of these comparisons involved concentration values averaged over 5 to 12 hours. The CAPTEX comparisons, which involved comparisons at receptors that were 300 km to 1000 km from the release, suggest that CALPUFF tends to overestimate surface concentrations by a factor of 3 to 4. Use of the puff splitting option in CALPUFF might have improved these comparisons, but there are serious conceptual concerns with the use of puff dispersion for very long-range transport (300 km and beyond). As the puffs enlarge due to dispersion, it becomes problematic to characterize the transport by a single wind vector, as significant wind direction shear may well exist over the puff dimensions.

With the above thoughts in mind, IWAQM recommends use of CALPUFF for transport distances of order 200 km and less. Use of CALPUFF for characterizing transport beyond 200 to 300 km should be done cautiously with an awareness of the likely problems involved. Since the long-range transport results appear to be relatively insensitive to the exact selection made for characterizing the puff dispersion parameters, IWAQM recommends use of dispersion parameters that provide results most similar to the local-scale model of choice (which currently is ISC). It would appear that CALMET is capable of treatment of highly complex wind fields that are strongly influenced by terrain slope flows (Section 4.9.2). However, as mentioned at the Sixth Modeling Conference, there are situations that one can imagine involving highly rugged terrain, that any model simulation's results must be viewed as uncertain.

2.3.3 Secondary pollutant uncertainties

The CALPUFF simulation for gas phase oxidation of sulfur dioxide to sulfate and for the nitrate chemistry is considered adequate. The algorithms currently do not adequately account for the aqueous phase oxidation of sulfur-dioxide to sulfate, which can become dominant in the presence of fog or clouds. Even if planned updates to CALPUFF include consideration of the aqueous phase chemistry, the input data may preclude routine use of this enhancement. Finally, it must be mentioned that evaluation studies have not been conducted regarding CALPUFF's simulations of secondary formed sulfate and nitrate. The IWAQM is not aware of comprehensive tracer-field-data studies that would lend themselves to such evaluation studies. Given that aqueous phase chemistry is not treated, it is likely that CALPUFF simulations of sulfate would be less than observed. Mention is made in Section 4.9.1 that the total nitrogen deposition estimates by CALPUFF were about a factor of 3 less than estimates provided by a more physically complete model (RADM). Notwithstanding these obvious deficiencies, IWAQM recommends use of CALPUFF's estimates of sulfate and nitrate for purposes of addressing the need to assess AQRV impacts in Class I areas (in lieu of assuming that there are no impacts at all).

2.3.4 Technical oversight and review

It would be convenient if objective criteria and cookbook procedures could be constructed that would preclude inappropriate application of air dispersion models. This has proved to be troublesome for local-scale modeling, and likely is impossible for mesoscale and long-range transport modeling. As in any air quality simulation, the usefulness of the results obtained depends mostly on the expertise brought to the analysis in characterizing the situation, and on the experience applied in interpreting the results obtained. In response to these considerations, IWAQM has attempted to warn the modeling community that conducting a long-range transport assessment requires esperts. We have also tried to warn the modeling community that application of the CALPUFF modeling system to any situation will require expert judgment, it will likely involve site-specific decisions, and it will require strong interaction and coordination with the applicable reviewing authorities.

In this regard, the use of technical review committees, as suggested in the Regional Approach (Section 4.5) would likely prove useful to both the applicants and to the reviewing authorities. These technical committees could assist in sorting through the site-specific decisions, and they could provide a forum for reaching consensus. Having a standing technical committee would provide applicants with some assurance of being treated equitably, and could provide data sets for use to facilitate comparability between individual analyses. Whether such a committee would prove useful is dependent on availability of experts and on the ability to obtain long-term commitments of service. Furthermore, not all Class I areas will require use of such committees. Hence, while IWAQM endorses the use of such committees, IWAQM does not recommend Federal agencies mandate or require their use.

3.0 TRANSFORMATIONS, VISIBILITY, AND DEPOSITION

In principle, estimating the impact of emissions from an individual source is best accomplished using a Lagrangian dispersion model, as a Lagrangian model 'follows' the emissions as they are transported downwind. This provides within the model the ability to directly assess how much each source's emissions are impacting each receptor in the analysis. However, there are some physical processes (like nonlinear chemical transformations) that can be more explicitly and completely characterized using Eulerian grid modeling techniques. To treat nonlinear chemical transformations within a Lagrangian modeling framework is presently so computationally demanding as to be impractical for routine use.

The IWAQM recognized these limitations and tradeoffs between Lagrangian and Eulerian grid modeling techniques. The purpose of the Phase 2 recommendations was to recommend techniques useful for permitting individual PSD sources. For individual source impacts involving complicated terrain and transport distances of order 50 to 250 km, a Lagrangian puff model like CALPUFF is an optimal choice. In this section we summarize the approximations made in the CALPUFF chemical transformations and associated inherent limitations. We then summarize the methodology recommended for computing haze and deposition impacts in Class I areas. Finally, we discuss conceptually how assessment of adverse impact of Air Quality Related Values is somewhat different than traditional NAAQS assessments.

While drafting this report, the National Park Service, the U.S. Fish and Wildlife Service and the U.S. Forest Service have been holding intensive meetings to promote a greater consistency in the procedures Federal Land Managers use in identifying and evaluating AQRV impacts. We have discussed in this report the assessment of regional visibility impacts using the deciview, which at the time of the drafting of this report was the preferred metric. As time progresses, it is looking more like the change of extinction may become the preferred metric. Hence, although the information provided here is useful, the details and implementation may be somewhat different as a consequence of the ongoing discussions. For the latest information on procedures and metrics, we suggest visiting the web site: **http://www.nature.nps.gov/ard/flagfree/index.html**.

3.1 Chemical Transformations

The MESOPUFF II chemistry option, currently available in CALPUFF(4.0), is adequate for representing gas phase oxidation of SO_2 to $SO_4^=$ and for the nitrate chemistry. The algorithms currently do not adequately account for the aqueous phase oxidation of SO_2 to $SO_4^=$. The aqueous phase chemistry can dominate the formation of sulfate. Therefore, in many applications sulfate is likely to be underestimated. A further complication is that the formation of particulate nitrate (NO_3^-) is dependent on the ambient concentration of ammonia, which preferentially reactswith $SO_4^=$. The ambient ammonia concentration is an input to the model. Appropriate specification of this

parameter is critical to the estimation of realistic values of particulate nitrate concentrations.

For instance, if we were simulating effects of emissions coming from an as yet to be built new single source, then the ammonia available to react with these new emissions could be estimated from monitored background levels of ammonia. If there are large major sources near the proposed new source included in the analysis, then the background ammonia should in principle be adjusted to a value somewhat above that monitored to reflect ammonia available that these existing sources typically scavenge from the atmosphere. By way of this example, we see that CALPUFF is most easily applied for isolated new emissions, and becomes more problematic as the number of sources increases. This supports limiting application of CALPUFF to a relatively few sources of emissions, so that the 'background' levels of ozone and ammonia can be derived using appropriate monitoring data.

The spatial and temporal scales, where CALPUFF might be used, are long enough so that the chemical conversion of SO_2 to $SO_4^=$ and NO_X to HNO_3 are of interest. The oxidation of SO_X and NO_X may occur by gas and aqueous phase reactions. The gas phase reactions for both SO_X and NO_X involve free radical photochemistry and, therefore, are coupled to the oxidation of reactive organic gases (ROG). Homogeneous gas phase reaction is the dominant SO_2 oxidation pathway during clear, dry conditions. Ozone and hydrogen peroxide are believed to be the principal oxidants for aqueous phase oxidation of SO_2. Homogeneous gas phase reactions may convert SO_2 at most a few percent per hour, whereas aqueous phase reactions can convert SO_2 up to 100% per hour.

The oxidation of NO_X is dependent on gas phase ROG/NO_X/O_3 photochemistry. It is generally more rapid than SO_2 gas phase oxidation. NO_X can be oxidized to nitric acid (HNO_3) and organic nitrates (RNO_3) such as peroxyacetylnitrate (PAN). HNO_3 combines with ammonia gas to form solid or aqueous ammonium nitrate (NH_4NO_3). Unlike sulfate formation, the nitrate process is reversible. Equilibrium is established between nitric acid, ammonia, and ammonium nitrate:

$$NH_4NO_3 \leftrightharpoons HNO_3 + NH_3$$

The equilibrium constant for this reaction is a nonlinear function of temperature and relative humidity. The equilibrium constant can vary several orders of magnitude over a typical diurnal cycle. Given fixed amounts of total nitrate, ammonia, and water vapor, higher NH_4NO_3 concentrations are expected at night due to lower nighttime temperatures and higher relative humidities. Thus, the nitrate aerosol can not be considered a stable product like sulfate.

The transformation rate expressions, used in the MESOPUFF II algorithm, were developed statistically analyzing hourly transformation rates produced by a

photochemical model. Plume SO_X/NO_X dispersing into background air containing ozone and reactive hydrocarbons was simulated over a wide range of conditions representing different solar radiation intensities, temperatures, dispersion conditions, background ozone concentration and surface-level relative humidity, RH, plume NO_X concentrations and emissions times. The following transformation rate expressions, representing curve fits to the daytime hourly conversion rates predicted by the photochemical model, were determined:

$$k_1 = 36R^{0.55}[O_3]^{0.71}S^{-1.29} + k_{1(aq)}$$
$$k_2 = 1206[O_3]^{1.5}S^{-1.41}[NO_x]^{-0.33}$$
$$k_3 = 1261[O_3]^{1.45}S^{-1.34}[NO_x]^{-0.12}$$

Where,
- k_1 is the SO_2 to $SO_4^=$ transformation rate (percent/hour),
- k_2 is the NO_X to HNO_3 + RNO_3 transformation rate (percent/hour),
- k_3 is the NO_X to HNO_3 (only) transformation rate (percent/hour),
- R is the total solar radiation intensity (kw/m^2),
- S is a stability index from 2 to 6 (PG stability A&B = 2, C=3, etc.,
- RH is the surface-level relative humidity (percent),
- $[O_3]$ is the background ozone concentration (ppm),
- $[NO_X]$ is the plume NO_X concentration (ppm), and,
- $k_{1(aq)}$ is the aqueous phase SO_2 oxidation term.

The term, $k_{1(aq)}$ peaks at a value of 3 percent/hour at 100% relative humidity. This is much less than might be expected if the plume interacted with clouds or fog. These transformation rate expressions only apply during the day. At night oxidation rates of 0.2% and 2.0% for SO_2 and NO_X, respectively, are suggested as default values in the model.

3.2 Visibility Analysis

In the context of the Phase 2 recommendation, the focus of the visibility analysis is on haze. These techniques are applicable in the range of thirty to fifty kilometers and beyond from a source. At source-receptor distances less than thirty to fifty kilometers, the techniques for analyzing visual plumes (sometimes referred to as 'plume blight') should be applied.

There are two approaches to determining visibility effects (NAPAP Report to Congress). One is a technically rigorous, complex, and situation-specific method, while the other is a more generalized approach. The more rigorous approach requires the calculation of aerosol growth dynamics and the application of Mie theory to determine the optical characteristics of the aerosol distribution. Sophisticated radiative transfer models are then applied, using the aerosol optical characteristics, the lighting and scene characteristics and the spatial distribution of the pollutants to calculate the path

and wavelength of image-forming and non-image-forming light that reaches a specific observer at a specific time and date from all points in the scene being viewed. While this detailed analysis may be useful for assessing specific cases, it is impractical for addressing haze issues where visibility is experienced in a nearly infinite variety of situations and where detailed characteristics of the pollution, lighting, and scene conditions are rarely known.

The generalized approach uses aerosol species extinction efficiencies, with water growth functions, to determine the light extinction coefficient of the aerosol, from its composition and from the relative humidity of the atmosphere. The extinction efficiencies and relative humidity dependence of the aerosol are based upon typical results from the more rigorous analyses mentioned above.

A generalized approach is recommended by IWAQM for Class I area analyses. Under this approach, the concentrations of pollutants (in this case calculated by an air quality model) are used to calculate the extinction coefficient due to these pollutants. This is then compared against the light extinction coefficient of the background air. A constant fractional change in the extinction coefficient produces a similar perceptual change for a scene regardless of baseline conditions. Therefore, under cleaner visibility conditions, relatively less pollution will cause a perceptible change than under more polluted background conditions.

Visibility is an instantaneous phenomenon. When an observer looks at a scene, the view is what is seen at that moment. Many of our measurements and modeling techniques deal with averaged values from one hour and longer. Therefore, some consideration is needed to accommodate this dichotomy.

Visibility Parameters

Visibility is usually characterized by either visual range (*VR*) (the greatest distance that a large dark object can be seen) or by the light-extinction coefficient (b_{ext}) (the attenuation of light per unit distance due to scattering and absorption by gases and particles in the atmosphere) (Sisler,1996). Under certain assumed conditions, these parameters are inversely related to each other by Equation 1.

$$VR(km) = \frac{3.912}{b_{ext}(km^{-1})} \qquad (1)$$

The dimensions of *VR* are length and the dimensions of b_{ext} are 1/length. Visual range is usually expressed in kilometers. The extinction coefficient is sometimes expressed as “inverse kilometers” (km^{-1}) or as “inverse megameters” (Mm^{-1}) (the reciprocal of 1 million meters). If b_{ext} is expressed in Mm^{-1}, the coefficient 3.912 in Equation 1 becomes 3912. The value 3.912 = -ln(0.02), which assumes a two percent contrast

threshold for the viewer. Other researcher have assumed a five percent threshold, which would change the value to 2.995.

A constant fractional change in the extinction coefficient produces a similar perceptual change for a scene regardless of baseline conditions. Using the relationship of a constant fractional change in the extinction coefficient resulting in a similar perceived visual change, an alternate visibility index, the deciview (*dv*) has been defined (Equation 2).

$$dv = 10 \ln \frac{b_{ext}(km^{-1})}{0.01(km^{-1})} \quad (2)$$

This index was specifically designed so that anywhere along its scale, haziness changes that are equally perceptible correspond to the same deciview difference. For example, a 3dv difference caused by a change in air quality should result in about the same perceived change in haziness, whether under clean or highly polluted conditions. This characteristic of the deciview scale requires that the scene being viewed has sufficient sensitive scenic features to detect changes in visibility from the baseline haze level. No one scene is likely to have such scenic features for all conceivable haze levels. However, the nearly infinite variety of scenes available, where hazes are concerned, ensures that many will have the desired characteristic for any haze level (NAPAP report to congress).

Calculating the Extinction Coefficient

Visibility is degraded by light scattered into and out of the line of sight and by light absorbed along the line of sight. Light extinction is the sum of light scattering and absorption, and is usually quantified using the light extinction coefficient (b_{ext}). Using the generalized approach to estimating visibility effects, outlined above, one can calculate the extinction coefficient as the sum of its parts, i.e., $b_{ext} = b_{scat} + b_{abs}$, where b_{scat} and b_{abs} are the light scattering and absorption coefficients. The light scattering and absorption coefficients can be further broken down by their respective components. The scattering coefficient is affected by Rayleigh scattering (b_{Ray}) from air molecules and from particle scattering (b_{sp}); the particles can be natural aerosol or result from air pollutants. The absorption coefficient is affected by gaseous absorption (b_{ag}) and particulate absorption (b_{ap}). Nitrogen dioxide is the only major light-absorbing gas in the lower atmosphere; it generally does not affect hazes, although it can be an important element in a coherent plume assessment. Therefore, only particle absorption is considered in the suggested haze analyses.

Particle scattering, b_{sp}, can be broken down by the contributions of different particulate species. It has been convenient to consider the scattering coefficients of

fine particles ($PM_{2.5}$) (particles with mass mean diameters less than or equal to 2.5 µm) and coarse particles (mass mean diameters greater than 2.5µm but less than or equal to 10µm). The fine particle scattering coefficient can be further defined by the sum of the scattering coefficient due to sulfates (b_{SO4}), nitrates(b_{NO3}), organic aerosols (b_{OC}), and soil (b_{Soil}); the coarse scattering coefficient (b_{Coarse}) is typically not refined any further. Thus the particle scattering coefficient (b_{sp}) can be expressed as in Equation 3.

$$b_{sp} = b_{SO4} + b_{NO3} + b_{OC} + b_{Soil} + b_{Coarse} \quad (3)$$

Each of the particle scattering coefficients can be related to the mass of the components using the relationships in Equation 4.

$$\begin{aligned} b_{SO4} &= 3\ [(NH_4)_2SO_4]\ f(RH) \\ b_{NO3} &= 3\ [NH_4NO_3]\ f(RH) \\ b_{OC} &= 4\ [OC] \\ b_{Soil} &= 1\ [Soil\ Mass] \\ b_{Coarse} &= 0.6\ [Coarse\ Mass] \end{aligned} \quad (4)$$

The quantities in brackets are the masses expressed in µg/m^3. (It is assumed that the forms of the $SO_4^=$ and NO_3^- are ammonium sulfate [$(NH_4)_2SO_4$] and ammonium nitrate [NH_4NO_3].) The numeric coefficients are the dry scattering efficiencies (m^2/g). The term *f(RH)* is the relative humidity adjustment factor. The extinction coefficients are in Mm^{-1}. If the dry scattering efficiencies are divided by 1000 (i.e., 0.003 instead of 3) the resultant extinction coefficients will be in km^{-1}.

Particle absorption (b_{ap}) is primarily due to elemental carbon (soot). For purposes of analyzing the effects of soot on visibility in a modeling analysis, the relationship in Equation 5 should be used. Again, the quantity in brackets is the mass of elemental

$$b_{ap} = 10\ [EC] \quad (5)$$

carbon in µg/m^3 and 10 is the extinction efficiency.

The total atmospheric extinction can be expressed as in Equation 6. To the extent that a source contributes to the formation of some of these constituents, those

$$b_{ext} = b_{SO4} + b_{NO3} + b_{OC} + b_{Soil} + b_{Coarse} + b_{ap} + b_{Ray} \quad (6)$$

contributions can be summed to yield the source's contribution to extinction. This will be discussed in more detail below.

Examination of Equation 4 reveals that the sulfate and nitrate components of the extinction coefficient are dependent upon relative humidity. These aerosols are hygroscopic and the presence of water enhances their scattering efficiency. It is sometimes convenient to consider the sulfate and nitrate components of extinction separately from the remaining components of Equation 6 and to keep the relative humidity adjustment factor (*f(RH)*) separate. Equation 6 can then be rewritten as in Equation 7,

$$b_{ext} = b_{SN}\, f(RH) + b_{dry} \qquad (7)$$

where

$$b_{SN} = 3\ [(NH_4)_2SO_4 + NH_4NO_3]$$
$$b_{dry} = b_{OC} + b_{Soil} + b_{Coarse} + b_{ap} + b_{Ray}$$

where b_{SN} is the combined extinction coefficient of sulfate and nitrate, excluding the relative humidity adjustment factor, and b_{dry} is the sum of b_{OC}, b_{Soil}, b_{Coarse}, b_{ap}, and b_{Ray}.

The relative humidity adjustment factor requires some further explanation. The variation of the effect of relative humidity on the extinction efficiency of sulfates and nitrates is shown in Figure 1. As can be seen, the effect of relative humidity on the extinction efficiency of these aerosols is non-linear, and is several times greater at higher relative humidities. These factors are applicable on a short-term basis. If the particulate concentrations are only available over a longer averaging time (i.e., a 24-hour sample or a seasonal average) then the average relative humidity adjustment factor for that time period must be applied, ***not*** the average relative humidity. (Alternately, short-term extinction coefficients (i.e., 1-hour) may be averaged to yield a longer-term average.)

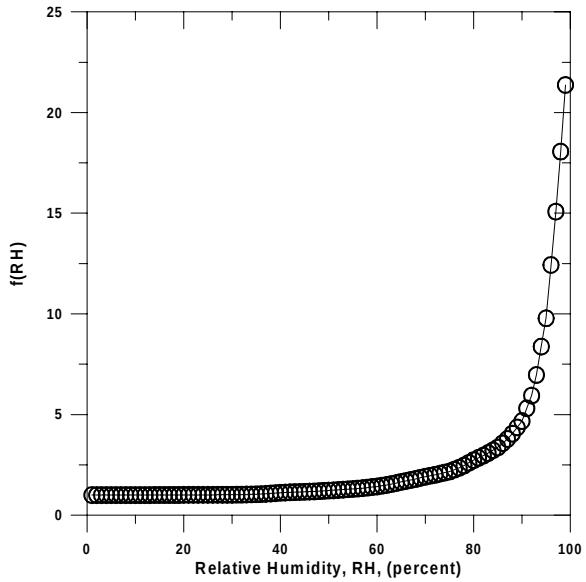


Figure 1. Variation of f(RH) (see Equation 7).

Background visibility conditions

As noted previously, visibility analyses are compared against a background condition. The estimates of background visibility conditions at Class I areas are derived from the IMPROVE (Interagency Monitoring of PRotected Visual Environments) network. There are several methods of obtaining estimates of the background visibility. These include reconstructed extinction from speciated measurements of particulate matter, direct measurement of extinction with a transmissometer, and estimates of extinction from photographs (Malm et al., 1996). Reconstructed extinction is usually used to estimate background conditions, since this can be directly related to pollutant loadings. It should be noted that reconstructed extinction values from the IMPROVE network are based on 24-hour average particulate concentrations. The temporal average at a point is used to represent a short-term spatial average.

The background conditions provided for a Class I visibility analysis will be representative of clean conditions. Changes in visibility are most sensitive under clean conditions. By using clean conditions for all comparisons in a Class I analysis, it ensures that already clean conditions will not be impaired. Additionally, the Clean Air Act states as a national goal that the visibility in Class I areas is to be unimpaired by man-made air pollutants and that any such impairment is to be remedied. To represent clean conditions, the average of the cleanest 20% of the data from IMPROVE, at that site, is generally used. Even the data from the cleanest days usually exhibit some made-made influence. This average of 24-hour values for the 20% cleanest conditions is used as representative of a clean background condition.

Background conditions may be provided using any of the visibility parameters, defined above, although the preferred method is to use the extinction coefficient, with the hygroscopic components and other components dissociated, as in Equation 7. Using the form of Equation 7 allows the effects of relative humidity to be applied consistently to both the background aerosol and the aerosol attributable to a new source. If only one of the other visibility parameters is available, without the dissociation of the hygroscopic components, then that value would be used. However, the relative humidity conditions that represent the average background will likely be different than the condition being analyzed. The usual effect of this is that the relative effect of sulfate and nitrate emissions is overstated under high relative humidity conditions.

Calculating a change in extinction

The modeling techniques outlined in this recommendation will provide ground level concentrations of visibility impairing pollutants. These concentrations are then used to calculate the extinction coefficient due to these pollutants, using the relationships outlined in Equations 4 and 5. The results of this are then compared against the background extinction from Equation 7. The metric used for this comparison is usually the change in deciview (Δdv) from a "clean" background condition. Thus, for a given background extinction, b_{back}, and a source or sources contribution to extinction of b_{source}, Δdv is given by Equation 8.

$$\Delta dv = 10 \ln \frac{b_{back} + b_{source}}{b_{back}} \quad (8)$$

These methods are embodied in the CALPOST program which post-processes the concentrations from the CALPUFF air quality model. However, if another model is used it is necessary to be able to perform these calculations separately. Even if the CALPUFF system is used, it is sometimes more convenient to calculate changes in visibility outside of the post-processor.

Example Problem

This example assumes that a dispersion model has been run and yielded concentrations of $SO_4^=$ and soot (elemental carbon). From these concentrations the analyst wishes to calculate a change in visibility.

First, we will consider the background visibility condition. If the background 24-hour average visibility at the Class I area of interest has a combined sulfate and nitrate extinction coefficient (b_{SN}) of 1.8 Mm^{-1} (neglecting the effects of relative humidity) and an extinction coefficient from the other components (b_{dry}) of 19.6 Mm^{-1}, then the background extinction (b_{back}), expressed in the form of Equation 7 would be:

$$b_{back} = 1.8\ f(RH) + 19.6$$

In a typical analysis, the model will be run for an extended period, such as a month, a season, annually, or for multiple years. This will produce a corresponding number of 24-hour averaging periods, which will each need to be analyzed against the background condition. In our example we are only considering one 24-hour averaging period. For this example we will assume that the sources in the analysis contributed 0.218 µg/m^3 of sulfate ($SO_4^=$) and 0.05 µg/m^3 of soot (elemental carbon). The first step is to convert the mass of $SO_4^=$ to ammonium sulfate ($(NH_4)_2SO_4$), which is accomplished by multiplying by the ratio of the molecular weights of $(NH_4)_2SO_4$ to $SO_4^=$, which is 1.375. This yields a concentration of $(NH_4)_2SO_4$ of 0.30 µg/m^3. This result is then multiplied by the dry scattering efficiency of $(NH_4)_2SO_4$ (which is 3, from Equation 4), yielding an extinction coefficient for the sulfate of 0.9 Mm^{-1}; the relative humidity adjustment has not yet been applied. In this example, our modeling does not require any conversion of the mass of soot, so we need only to multiply the soot concentration (0.05 µg/m^3) by the extinction efficiency of elemental carbon (which is 20, from Equation 5). This yields an extinction coefficient of 1.0 Mm^{-1}. Therefore, following the form of Equation 7, the source contribution would be:

$$b_{source} = 0.9\ f(RH) + 1.0$$

The relative humidity adjustment factor for this averaging period has not yet been applied. Our example is based on a 24-hour average. The representative hourly RH values for this day would need to be obtained. For each hour, the corresponding *f(RH)* must be obtained from Figure 28 (or a corresponding table). These values are then averaged together. Let us assume that for this day the average *f(RH)* is 3.4. With the day-average relative humidity adjustment factor (*f(RH)*) of 3.4, b_{back} would be 25.72 Mm^{-1} (corresponding to a visual range of 152 km from Equation 1) and b_{source} would be 4.06 Mm^{-1}. Using these values in Equation 8 would yield a Δdv of 1.46.

These calculations would be repeated for each 24-hour average concentration in the analysis, using the corresponding day-average *f(RH)*. Background visibility conditions may be given for seasons or months. The corresponding background values should be used. A spread sheet program is suggested if the results are not processed with the CALPOST processor.

Visibility Summary

The following list summarizes the steps necessary for conducting a visibility analysis under this recommendation.

- Consult with the appropriate regulatory agency and with the appropriate FLM
- Run an air quality model which yields ambient concentrations of visibility impairing pollutants
- Obtain data on the background visibility conditions for use in the form of Equation 7, $b_{ext} = b_{SN}f(RH) + b_{dry}$
- Calculate the extinction coefficient for the source or sources being analyzed using Equations 4 and 5.
- Apply appropriate and consistent relative humidity adjustment factors to both the source contribution to light-extinction and the background light-extinction.
- Calculate a change in deciview (Δdv) using equation 8.

3.3 Deposition Calculations

Estimates of atmospheric deposition are obtained by selecting the options in CALPUFF to calculate and output the wet and dry fluxes of the pollutants modeled. The units of the fluxes are in $g/m^2/s$ of the pollutant modeled (i.e., $g/m^2/s$ of HNO_3). Generally AQRV analyses require values of total deposition (background plus modeled impact) to be given in units of kg/ha/yr of an element, such as nitrogen (N) or sulfur (S). Therefore, the modeled deposition flux of each of the oxides of sulfur or nitrogen from CALPUFF must be adjusted for the difference of the molecular weight of their oxides and the element and the various forms must be summed to yield a total deposition of sulfur or nitrogen. This can be accomplished using a multiplier in CALPOST to do all of the conversions. The CALPOST program will produce an average flux (i.e., annual average), therefore, the average value must be multiplied by the number of seconds in an hour and the total number of hours used in the averaging period for the total deposition.

The wet and dry fluxes of SO_2, $SO_4^{=}$, NO_X, HNO_3, and NO_3^{-} need to be calculated and saved in a CALPUFF run. It is necessary to make a separate CALPOST run of the wet and dry fluxes for each species modeled, normalizing each species by the molecular weight of a common compound or element (usually S or N), converting the units, and adjusting for the total number of averaging periods used in the CALPOST run (i.e., 8760 for 1 year). Then the results of the sulfur CALPOST runs are summed and the results of the nitrogen CALPOST runs are summed to yield a total deposition value for sulfur and nitrogen, respectively. The following table indicates the multipliers to use to correct for molecular weight differences and unit changes, as well as the correction to go from a short-term flux to annual deposition.

Deposition of:	Ratio Mol wt. of Oxidant to S or N	g to kg	m2 to ha	sec to hours	Number of Hours in	Multiplier (a in CALPOST) x N
S from SO_2	0.50000	10^{-3}	10^4	3600	N	1.800000E+04
S from SO_4	0.33333	10^{-3}	10^4	3600	N	1.200000E+04
N from NOX	0.30435	10^{-3}	10^4	3600	N	1.095652E+04
N from HNO3	0.22222	10^{-3}	10^4	3600	N	8.000000E+03
N from NO3	0.22581	10^{-3}	10^4	3600	N	8.129032E+03

For example, if CALPUFF was run for SO_2 and $SO_4^=$, for one year, it would be necessary to run four different CALPOST runs for wet and dry deposition of SO_2 and $SO_4^=$. For the SO_2 runs, the multiplier in CALPOST would be set to $1.8x10^4x8760 = 1.576x10^8$, assuming a non-leap year with 8760 hours and to $1.2x10^4x8760 = 1.0512x10^8$ for the $SO_4^=$ runs. If one was interested in the deposition over the month of January, assuming a run length of 744 hours, one would use 744 in place of the 8760 to calculate the multiplier in CALPOST.

3.4 Assessing Air Quality Related Values - Background

It usually is not possible to assess Air Quality Related Values (AQRVs) in isolation of the existing background stress. To illustrate this point, we consider two examples. The first using a leaf injury model and the second discusses discerning differences in visibility.

Larsen et al., (1983) presented a model of leaf injury, in which leaf injury was seen to be a function of the hourly sulfur-dioxide concentration raised to the 1.845 power times the ozone concentration raised to the 1.271 power. The impact for a series of hours was to be computed as a summation over each hour's computed effect. What should be noted is the fact that the injury was not linear, but was proportional to a power, in this case, greater than 1. We can simplify this to an equation of the form:

$$D = a\ \chi^p$$
$$\chi = b + b'$$

where D = damage, a is some constant, p is a power (like those cited above), χ is the total concentration (or deposition, etc.), which is composed of a background concentration, b, and an additional concentration, b', associated with one or more sources. If p is not equal to 1, then it is not possible to assess the effects of the background concentration, b, separately from the effects associated with one or more sources, b'.

Example: Let p = 2, b = 10 and b' = 1, then D = 121a. If one separately computes the damage as a summation, as D = D(b) + D(b'), the result will underestimate the total damage, as D = 100a + a = 101a.

The deciview, dv change associated with adding some new source's effects onto an existing background haze effect can be computed as:

$$dv = 10 \ln[\frac{(b + b')}{b}]$$

where b is the extinction coefficient associated with the background and b' is the extinction coefficient associated with the additional source or sources. It is worth noting in the above equation that the human perception of a change in visibility is fundamentally a function of the existing background condition. A one dv change is computed whenever the ratio (b+b')/b = 1.11. Or stated in other terms, when b' is 11% of b, a one dV change in the visibility will be computed.

These two examples were provided to illustrate that assessing some Air Quality Related Vales (e.g., as might be related to crop injury, or visibility effects) is fundamentally tied to knowing the current stress (background) being exerted on the system. Assessing the response of a resource (plant health, visibility) is related to the cumulative effects of all the current existing stresses. Whether a model is used to estimate the existing condition, or whether existing monitoring measurements can be used to define the current stress (background), is decided for each case based on available information.

4.0 STUDIES AND FINDINGS

Sections 4.1 through 4.5 provide extended summaries of the investigations conducted prior to the Sixth Modeling Conference. Following the Sixth Modeling Conference, a series of investigations were conducted in response to the comments received, and these results are summarized in Sections 4.6 through 4.9. In Section 4.6, summaries are presented of several investigations in which surface concentration values estimated by the CALPUFF puff dispersion model were compared with tracer field data. These are presented to provide further information, as requested at the Sixth Modeling Conference, for deriving conclusions on the performance of the CALMET/CALPUFF modeling system in characterizing long-range transport. In Section 4.7, a summary is presented in which direct model-to-model comparisons are made between CALPUFF and ISC simulations of point source release dispersion. These are presented to provide evidence on the ability of CALPUFF to replicate the dispersion results of ISC for steady-state meteorological conditions. Some coding deficincies were detected in compariing the steady-state CALPUFF results with ISC, but the primary lessons learned were what differences could be expected due to the fact that puff models treat the sequence of meteorological events ('causality'). This information is valuable since CALPUFF was to be used to simulate all sources (even though for some, the transport may be less than 50 km) in a long-range transport assessment. Section 4.8 summarizes results available towards developing a new screening technique that might be used to see if it is worthwhile or needful to develop a full wind-field puff-dispersioin analysis using the CALMET/ CALPUFF modeling system. It was evident at the Sixth Modeling Conference that use of the ISC plume dispersion model to develop screening estimates of long-range transport impacts was not providing much help. Section 4.9 summarizes studies that have recently been completed of further enhancements and refinements, some of which are implemented in Version 5.0 of the CALMET/CALPUFF modeling system. Not all of these enhancements have been fully tested, but it was felt desirable to summarize that which was known.

4.1 MESOPUFF II Implementation Assessment

A case study was conducted to apply the MESOPUFF II air quality modeling system following IWAQM Phase 1 interim recommendations (U.S. 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. A complete description of the study results is presented in U.S. EPA (1995a). As part of this study 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 (SNP), including the James River Face (JRF) wilderness area. Demonstration model simulations were performed using three years of the developed five-year meteorological data set 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.

As discussed in the summary report for this project (U.S. EPA, 1995a), 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 area, and thus is incomplete. 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, 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.

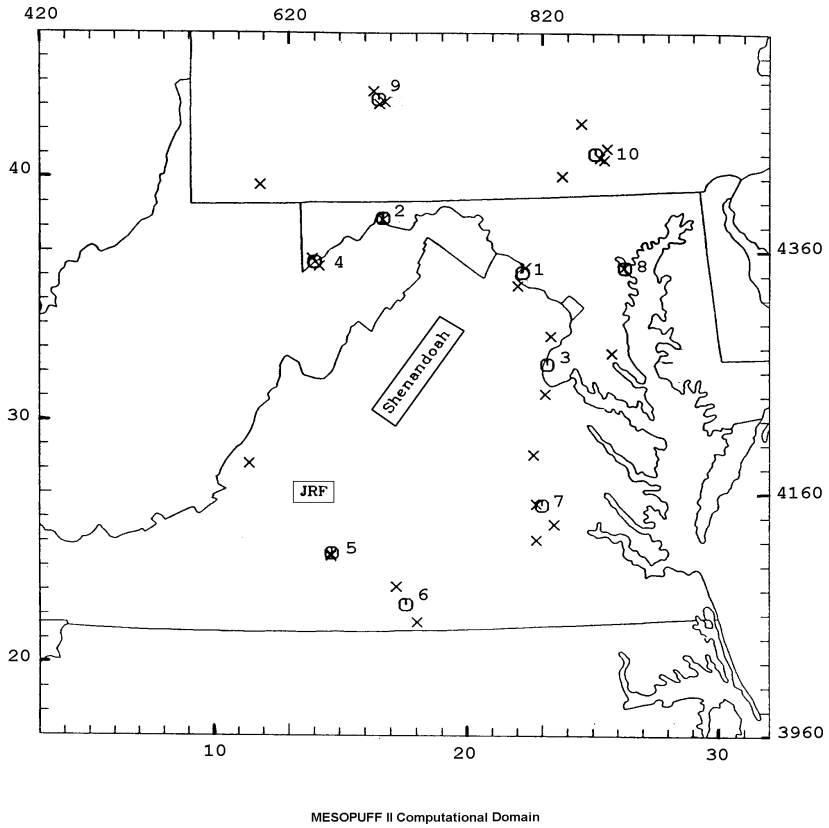


Figure 2. Display of the MESOPUFF II computational domain, showing positions of all PSD sources compiled for the demonstration assessment. Crosses represent all 27 original PSD sources, while circles denote the ten final aggregated sources used for the demonstration analyses. The source characteristics for the ten aggregate sources (numbered) are given in Table 2. One unit along left and bottom axes equals 20 km. Top and right axes are the UTM coordinates in km.

Demonstration Results

In the MESOPUFF II modeling for this project, 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 then added to ISCST2 results to demonstrate the integration process. For the demonstration study, sources were to be located as far as 200 km from SNP. All sources and receptors to be modeled must be contained within the computational domain. Puffs are not tracked after they leave this grid. To avoid underestimating concentrations by immediately losing puffs from near-boundary sources or missing short-term recirculation events at near-boundary receptors, all sources and receptors should be at least 20-50 km from the boundaries of

the computational grid. Provision for a 80 km buffer zone on all sides of this source region yielded a computational domain of 30 by 30 grid points (Figure 2), with a grid spacing of 20 km.

For the demonstration study, existing sources that began operation since the beginning of the PSD program would be modeled. For practical considerations and ease of communications between affected states, the sources were limited to those within EPA Region III, comprising the states of Delaware, Maryland, Pennsylvania, Virginia and West Virginia, and the District of Columbia. Small PSD sources, with emissions of both SO_2 and NO_x less than 5 g/s, were excluded. This resulted in a set of 27 sources (indicated by crosses in Figure 2). To reduce run times the set of 27 sources were consolidated into 10 sources. Table 3 shows the final set of 10 consolidated sources, the facilities that are included in each, and the location and emission parameters. Figure 2 also displays the locations of these ten sources (indicated by circles) in relationship to all 27 original PSD sources.

Table 3. Final condensed set of sources modeled with MESOPUFF II for the demonstration assessment. HS, DS, VS, and TS are the source's stack height, stack diameter, effluent exit velocity, and effluent exit temperature, respectively.

	Sources	UTM X (km)	UTM Y (km)	HS (m)	DS (m)	VSl (m/s)	TS (K)	SO_2 (g/s)	$SO_4^=$ (g/s)	NO_x (g/s)
1	PEPCO II, Patawmack	803.6	4341.0	48	8.77	36.6	557	348.2	15.7	230.4
2	Warrior Run	693.6	4385.0	82	3.75	23.6	398	54.8	2.5	26.0
3	Ogden-Martin, SEO Birch	823.6	4265.0	106	3.24	10.0	372	48.0	2.2	151.9
4	N. Branch, Mettike	639.6	4349.0	76	4.69	21.3	389	112.1	5.0	83.6
5	LG&E Altavista, Multitrade	653.6	4109.0	60	4.44	21.4	407	24.7	1.1	42.6
6	Mecklenburg, Old Dominion	711.6	4067.0	109	7.11	18.6	331	194.6	8.8	425.1
7	Doswell, Cogentrix-Richmond, Cogentrix-Dinwiddie, LG&E Hopewell	819.6	349.6	70	5.35	14.0	352	252.1	11.3	426.4
8	Brandon	885.2	4345.0	187	6.71	27.3	413.	1893.6	85.2	630.8
9	Cambria Cogen, Colver PP, Ebensburg	689.6	683.6	86	5.08	21.3	418	287.8	13.0	155.8
10	P.H. Glalter, Harrisburg, Lancaster, Solar Turbine, York Co.	861.6	4439.0	67	6.60	15.4	438	14.1	0.6	212.3

For this study, PM_{10} increments were calculated as described in the Phase 1 recommendations. Modeled concentrations of sulfate and aerosol nitrate were converted to ammonium sulfate and ammonium nitrate, and summed to estimate PM_{10} increments. The PSD increments were calculated for each receptor, and the highest values within SNP and JRF were identified. Since there are no standards or mandated increments for AQRVs, it was necessary to define AQRV criteria before postprocessing could begin. For visibility, incremental extinction coefficients were computed from 3-hour average modeled sulfate and nitrate concentrations using relative humidity data

and the equation provided in Appendix B of the Phase 1 recommendations. The maximum 3-hour extinction resulting from modeled emissions over all receptors was compared to measured total extinction from the SNP IMPROVE monitoring site. The number (and percentage) of 3-hour periods for which the maximum extinction represents 10 percent or more of the measured extinction for the 90th percentile cleanest day was reported. Deposition impacts were calculated for each 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 expressed as the cumulative annual sum of wet and dry deposition, in units of kg/hectare.

Table 4. PSD and AQRV parameters calculated from MESOPUFF II demonstration assessment.

		Shenandoah NP			James River Face			Allowable Class I Increment
Parameter	Averaging Period	1988	1989	1990	1988	1989	1990	
		PSD Increments						
SO_2	Annual (ug/m3)	0.23	0.32	0.21	0.08	0.10	0.06	2
	24-hour (ug/m3)	3.92	5.03	3.15	1.39	2.93	1.61	5
	3-hour (ug/m3)	16.56	19.62	9.55	5.38	7.35	3.65	25
NO_x	Annual (ug/m3)	0.12	0.15	0.13	0.05	0.07	0.04	2.5
PM_{10}	Annual (ug/m3)	0.08	0.12	0.07	0.05	0.07	0.04	4
	24-hour (ug/m3)	1.24	3.32	1.31	0.85	1.25	1.31	8
		Visibility						
Extinction	3-hour (% of year)	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 (km/Ha)	0.09	0.12	0.07	0.04	0.16	0.03	

Extinction = percent of 3-hour periods for which incremental extinction is greater than 10 percent of clear-day extinction levels.

Table 4 displays a summary of calculations from three years of MESOPUFF II output (1988-1990). Results are given for receptor groups in both SNP and JRF. There is considerable year-to-year variations in all of the simulated impacts, typically of order 20 to 25%. 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 second highest 3-hour and 24-hour average SO_2 concentrations approach or exceed the allowable Class I increments, while the second highest 24-hour average modeled PM_{10} is between an eighth and one-half the allowable limit. Also note, that

whereas the summer 1988 was characterized by widespread high pollution levels throughout the eastern U.S. (particularly for ozone), all modeled 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 4 corresponds to the percent of each year in which calculated sulfate plus nitrate concentrations lead to extinction levels more than 10 percent above the defined "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 JRF. 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 levels computed for SNP translate to minimum visual ranges of 59, 9, and 22 km, respectively, for each year modeled. The maximum extinction levels are quite high when one considers that these estimates were calculated solely as a result of particulate matter generated by these emission sources alone, and that other SO_2 and NO_x sources, and natural and anthropogenic sources of organics and dust, were not taken into account.

Source-Receptor Separation Distance Sensitivity Study

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 (U.S. EPA, 1995a). Four months of one year (representing each season of a year) 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 "spine" of the SNP. The source rings were established at 50, 100, 125, 150, 175, and 200 km from the spine (Figure 3).

The distribution of hypothetical point sources around each ring was determined such that the linear density of sources was held as constant as possible. The emission rates and source emission characteristics were set to be similar to those listed in Table 3. The emission rate and stack parameters used for the hypothetical sources are summarized in Table 5. The stack parameters are average values from the PSD source data in Table 3. 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 6, and the locations of the sources are shown in Figure 3.

Table 5. Emission rates and stack parameters for the idealized sources.	
Stack Parameters	Value for Idealized Sources
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 Im)	81.0
Stack Diameter (m)	3.97
Stack Gas Exit Velocity (m/s)	20.7
Stack Gas Exit Temperature (K)	425.0

A total of 24 MESOPUFF II runs were made, corresponding to six distances for each of the four months. MESOPUFF II output for the ring source analysis consisted of 3-hour average concentrations, and wet and dry fluxes of all species. 24-hour averages and monthly averages were produced for NO_x, nitric acid, sulfate ($SO_4^=$), nitrate (NO_3^-) and modeled PM_{10}, $SO_4^=$ 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 (these conversions are discussed further in Section 3). Following the Phase I 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. (For further discussion of the computations of total S and N deposition, see Section 3.3). An important AQRV associated with PM_{10} is visibility. MESOFILE was not capable of producing visibility estimates as outlined in the Phase I recommendations, where extinction is a function of relative humidity. Thus, visibility impacts were not assessed for the ring source analysis.

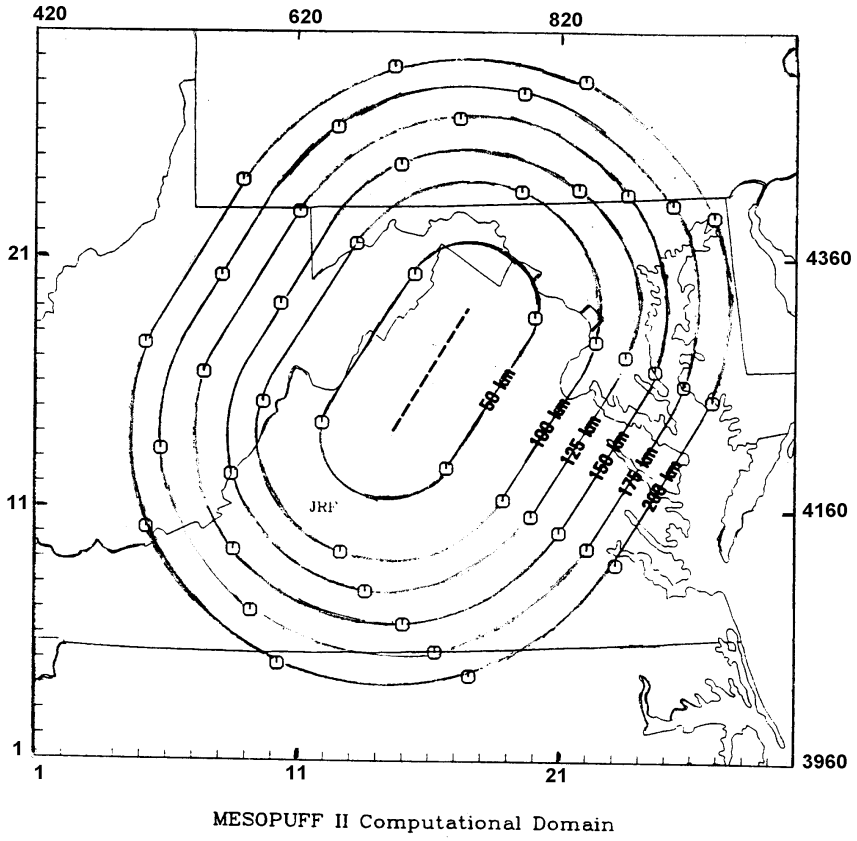


Figure 3. MESOPUFF II computation domain for ring source analyses, showing the location of the ring sources. One unit along left and bottom axes equals 20 km. Top and right axes are the UTM coordinates in km.

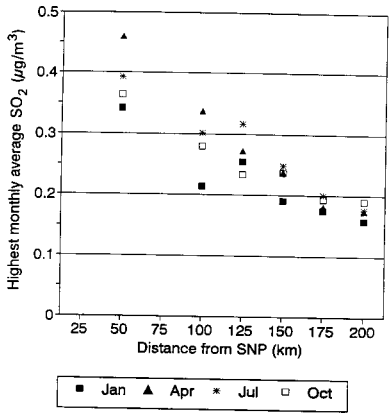
Figure 4a shows the results obtained for the monthly average SO_2 concentration for each of the four months as a function of source distance from SNP. The nearly linear decrease as a function of distance from SNP seen for these results is typical of that seen in the highest 24-hour average SO_2 results. As might be expected for a primary pollutant, the highest impacts occur for the 50-km source ring. The highest monthly average concentration is 0.45 µg/m^3, and decreases by a little over a factor of 2 for sources located on the 200 km ring. The maximum 3-hour and 24-hour SO_2 concentrations were also for the sources on the 50 km ring and were 20 µg/m^3 and 2.8 µg/m^3, respectively. The computed maximum 3-hour SO_2 concentration for sources on the 50 km ring is close to the allowable 3-hour increment of 25 µg/m^3. The computed maximum 24-hour SO_2 concentration for sources on the 50 km ring is slightly more than half the allowable Class I PSD increment of 5 µg/m^3.

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

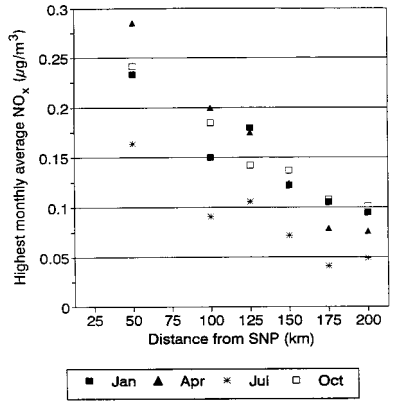
Figure 4b shows the highest monthly average concentrations for NO_x. (Plots of shorter-term NO_x concentrations were not prepared because there are no short-term PSD standards for NO_x.) Comparison of Figure 4a to Figure 4b for monthly average SO_2 illustrates the faster rate of chemical decay for NO_x. For sources on the 50 km ring, 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. For sources on the 200 km ring, 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.

Figure 4c presents the highest monthly 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, in that there is no clear decrease with source ring distance. This pattern is expected as, unlike SO_2 or NO_x, sulfate and nitrate are actively being formed during transport downwind. 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. Modeled sulfate and nitrate

(A)



(B)



(C)

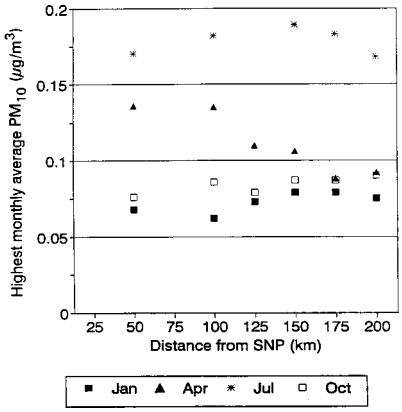


Figure 4. Highest monthly concentrations of (A) SO_2, (B) NO_x, and (C) PM_{10} (µg/m3) from ring sources for January, April, July and October, 1988.

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 the MESOPUFF II analysis 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.

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. For all sources, the highest S deposition occurred in July, and the lowest in January. Dry SO_2 deposition accounted for most of the modeled S deposition in all months. Deposition of $SO_4^=$ was small for all months except July. The main reason for this is that most of the total sulfur remained in the form SO_2 at all distances modeled. 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 random variability.

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. For all sources, 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. 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 solubility of HNO_3, the modeled wet deposition of HNO_3 appears surprisingly low.

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^-. Snow is assumed in MESOPUFF II to scavenge particles, but not gases. 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.

4.2 Revisions to CALMET and CALPUFF

In the course of completing the Phase 1 recommendations, IWAQM had become aware of the CALMET/CALPUFF modeling system (Scire et al., 1990ab), which was actively under development. Building from lessons learned from the MESOPAC/MESOPUFF II modeling system, the CALMET/CALPUFF modeling system was a Lagrangian puff model designed to include: 1) the capability to treat time-varying point and area sources, 2) suitability for modeling domains from tens of meters to hundreds of kilometers from a source, 3) predictions for averaging times ranging from one-hour to one year, 4) applicability to inert pollutants and those subject to linear removal and chemical conversion mechanisms, and 5) applicability for rough or complex terrain situations. The CALMET meteorological processor was designed to be compatible with both CALPUFF and a photochemical grid model, called CALGRID (Scire et al., 1989). Even though the current focus of IWAQM was on puff model simulations, the Phase 3 work was anticipated to include grid modeling. Hence the compatibility of CALMET to a grid model was considered advantageous.

There were two areas where IWAQM felt further enhancements were needed. With a view towards allowing one model to be used for all sources (which might include sources-receptor distances of less than 50 km), the first area for enhancement was to include within CALPUFF dispersion additional algorithms, so that CALPUFF simulation results would be consistent with ISC and CTDMPLUS (Perry et al., 1989) modeling results for steady-state meteorological conditions. The ISC plume dispersion model is recommended in the *Guideline* for use in gently-rolling terrain, and the CTDMPLUS plume dispersion model is recommend in the *Guideline* for use in complex terrain where plume impaction on elevated isolated terrain features is likely. Both ISC and CTDMPLUS are limited to source-receptor distances of less than 50 km. The IWAQM has concluded that one of the most challenging issues for long-range transport is the characterization of the time-varying three-dimensional wind field. Therefore, the second area for enhancement to the CALMET/CALPUFF modeling system was to include provisions within CALMET to allow use of mesoscale meteorological modeling results created using data assimilation techniques, for example Stauffer and Seaman (1989) and Stauffer et al., (1990).

At the time of the Sixth Modeling Conference, there were only preliminary sensitivity testing results to show that the modifications to CALPUFF would be successful in replicating ISC. There were no comparison results available showing consistency between CALPUFF and CTDMPLUS. Comparisons of CALPUFF with ISC are presented in Section 4.7. In following discussion, we summarize the modifications that were made to CALMET to expand its use to long-range transport applications.

The wind field module in CALMET is based on the Diagnostic Wind Model (DWM). In anticipation of using CALMET and CALPUFF for long-range transport distances, a series of modifications were made (U.S. EPA, 1995b). These included options to use a spatially variable initial guess field based on observations or results

from coarse-grid mesoscale meteorological modeling analyses, optional use of Lambert conformal coordinates for sources and receptors versus Universal Transverse Mercator (UTM) Cartesian coordinates, and (as mentioned before) provisions to allow processing of mesoscale meteorological modeling results created using data assimilation techniques.

The DWM in CALMET uses a two step procedure in developing the final wind fields. An initial guess field is developed based on a domain-average wind profile, and this domain-average profile of winds is adjusted for terrain effects and divergence minimization to produce a “Step 1" wind field. The second step in the processing of the wind field is the introduction of the observational data into the terrain-adjusted Step 1 wind field. As originally configured, the initial guess domain-average profile was constant over the domain. For long-range transport analyses, it is easily conceivable that terrain features (such as a ridge, or a deeply cut river gorge that turns sharply within the computational domain) would invalidate the appropriateness of using an initial guess wind profile that is everywhere the same over the domain (i.e., homogeneous). To address this, options were added to CALMET that allow spatially variable winds as an initial guess field. The spatially variable winds are computed using an inverse-distance interpolation from the available wind profile observations. The provision to allow use of a Lambert conformal projection versus a flat Cartesian mapping of receptors and sources was perfunctory, but necessary, in anticipation of analyses that might include transport distances where the curvature of the earth might become a significant factor in the analyses (say computational domains larger than 200 km by 200 km).

The adaptations needed to allow use of meteorological wind fields as analyzed by sophisticated mesoscale meteorological models (hereafter referred to as *FDDA-MM data*) involved more than simply providing a new data input option. Four Dimensional Data Assimilation (FDDA) and the development of *FDDA-MM* data are discussed further in Section 4.4. The representativeness of the fine-scale observations (which can be viewed as point-value observations) as compared with winds derived from *FDDA-MM* analyses (which can be viewed as grid-average observations) was expected to depend on such factors as the height above the surface, subgrid-scale terrain variations, and the ratio of the input *FDDA-MM* data grid size to the output grid size of the CALMET analyses. For example, the *FDDA-MM* results having a grid spacing of 80-km will not reflect potentially important local features of the surface flow field induced by terrain variations (e.g., in vicinity of the Shenandoah National Park or the Columbia river gorge) which can not be resolved by a grid resolution of 80 km. On the other hand, the point-value observations in such areas do not necessarily represent larger-scale flow fields as well as the *FDDA-MM* data fields. Therefore, IWAQM investigated development of a weighting factor based on the subgrid-scale terrain variations, that could be employed to blend the *FDDA-MM* data fields into the network of available surface and upper air observations. The developmental work to define the blending weights is described in the summary project report U.S. EPA (1995b). The

detailed description of how to compute the weights is provided in the current CALMET user's guide.

The decision as to where to introduce the *FDDA-MM* winds in the CALMET processing involves judgment. Basically, the finer the grid resolution used in developing the *FDDA-MM* winds the more reasonable it is to bring these data directly in as observations in developing the Step 2 winds. The coarser the grid resolution used in developing the *FDDA-MM* winds, the more reasonable it is to bring in these data to initialize the Step 1 analyses, and allow the diagnostic wind model of CALMET to develop the local terrain effects.

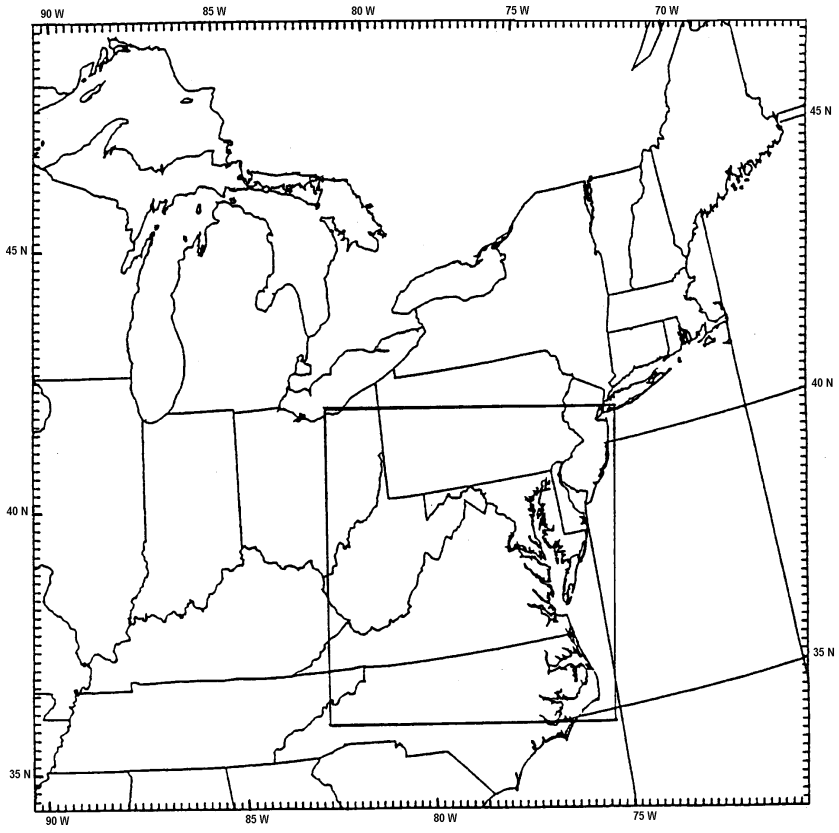


Figure 5. The MM4 domains for the 54-km grid (outer box) and the 18-km grid (inner box).

Table 7. Summary of statistical comparisons of wind fields.

	54-km Results		18-km Results	
	R^2	RMSE	R^2	RMSE
80-km MM4 Interpolated	0.961	0.992	0.958	0.949
CALMET-L Observations only	0.789	2.211	0.858	1.774
CALMET-S Observations only	0.542	3.220	0.814	2.039
CALMET-L MM4 as initial guess field	0.926	1.378	0.920	1.328
CALMET-S MM4 as initial guess field	0.932	1.316	0.922	1.300
CALMET-L MM4 as Step 1 field	0.962	0.992	0.959	0.932
CALMET-S MM4 as Step 1 field	0.962	0.993	0.959	0.938
CALMET-L MM4 as observations	0.960	1.020	0.952	1.011
CALMET-S MM4 as observations	0.959	1.021	0.952	1.011

R^2 = correlation coefficient, and RMSE = root mean squared error.
L = large radius of influence settings, and S = small radius of influence settings.
R^2 and RMSE are computed on a concatenation of the time series of the east-west (u) and north-south (v) components of the wind (each of length N) into one time series (of length 2N).

The radii used were defined as:

	Small	Large
R1	50 km	500 km
R2	100 km	1000 km
Rmax1	100 km	500 km
Rmax2	200 km	1000 km
Rmax3	1000 km	1000 km

where R1, R2 = the distances at which the Step 1 wind and observations have equal weight in the surface layer (R1) and the upper layers (R2), Rmax1, Rmax2 = the maximum radius of influence of observations in the surface (Rmax1) and upper layers (Rmax2), and Rmax3 = the over-water radius of influence.

To investigate the effectiveness of the terrain weights developed, the CALMET diagnostic wind field model was used to analyze two episodes, one summer episode (August 1-6, 1988) and one winter episode (December 3-10, 1988). The summer episode was characterized by light wind, stagnating conditions. The winter episode was characterized as an active period that included the passage of a front and low-pressure system through the domain. Penn State Mesoscale Meteorological (MM4) results were available employing four dimensional data assimilation (Stauffer and Seaman, 1989) for both episodes, for three different grid resolutions, 18-, 54- and 80-km. Figure 5 depicts the domains over which comparisons were made of CALMET simulated wind fields, developed for comparison with the MM4 54-km winds (outer box in Figure 5) and with the MM4 18-km winds (inner box in Figure 5). The CALMET winds were developed using the MM4 80-km winds as input (at various stages in the CALMET processing),

and CALMET winds were developed using only the hourly surface weather observations and twice-daily upper air observations from the National Weather Service.

Table 7 summarizes the comparison results obtained by using the available 80-km MM4 winds in various ways with CALMET to develop either 54- or 18-km gridded wind fields. As a further comparison, the hourly 80-km MM4 winds were linearly interpolated directly to the 54- or 18-km grid resolution. In general, the introduction of the 80-km MM4 winds improves the ability of CALMET to reproduce the reference 54- and 18-km MM4 wind fields. Slightly better agreement was achieved when the 80-km MM4 winds were brought in after the diagnostic terrain adjustment procedures (i.e., as the Step 1 wind fields or as "observations"). This is conjectured to occur due to the fact that 1) the 80-km MM4 are already close to the 54- and 18-km MM4 results, and 2) the CALMET diagnostic adjustments may duplicate terrain effects that were already accounted for in the development of the 80-km MM4 winds. The similarity of the interpolated 80-km MM4 winds to the 54- and 18-km MM4 winds (as evidenced by the close agreement achieved by simple linear interpolation) suggest that there might not be significant new terrain effects between the 80-, 54-, and 18-km scales for this region of the United States.

4.3 Trajectory Comparisons

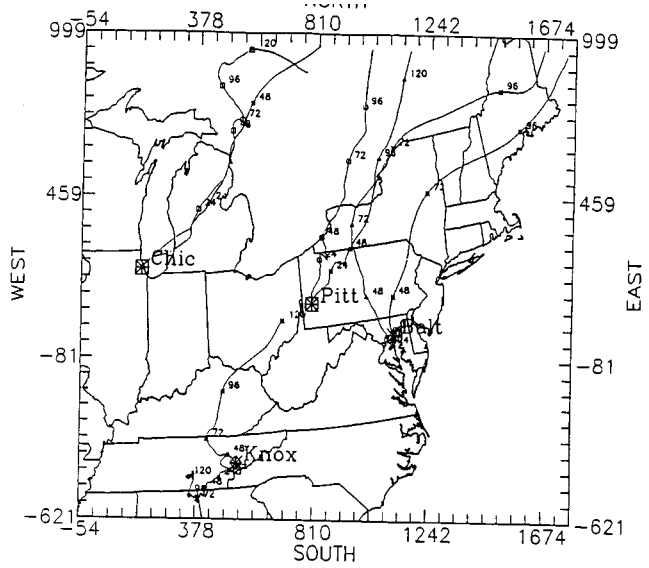
As discussed in the previous section, modifications were made to CALMET in anticipation of using CALMET and CALPUFF for long-range transport distances (U.S. EPA, 1995b). It was anticipated that use of *FDDA-MM* winds would improve CALPUFF's characterization of trajectories of dispersing pollutants. To investigate this, two trajectory studies were conducted: 1) a numerical simulation study, and 2) a comparison with regional-scale observations of trajectories.

Numerical simulation study

Trajectories were computed from four release locations at three levels (10 m, 200 m, and 400 m) for each of the wind fields discussed in Section 4.2 for the summer episode (U.S. EPA, 1995b). Trajectories were generated at each location every 4, 6 and 12 hours from the beginning of the simulation, for up to 24 hours before the end of the simulation. A statistical analysis was conducted on the trajectories to assess the effect of the different wind fields.

Figures 6a and 6b show the trajectories at an elevation of 10 m on the 54 km grid for each of the four locations. The trajectories developed using the MM4 54 km gridded meteorology directly are shown in both figures with small "x's." The trajectories developed using the CALMET generated 54 km winds are shown in both figures with

(A)



(B)

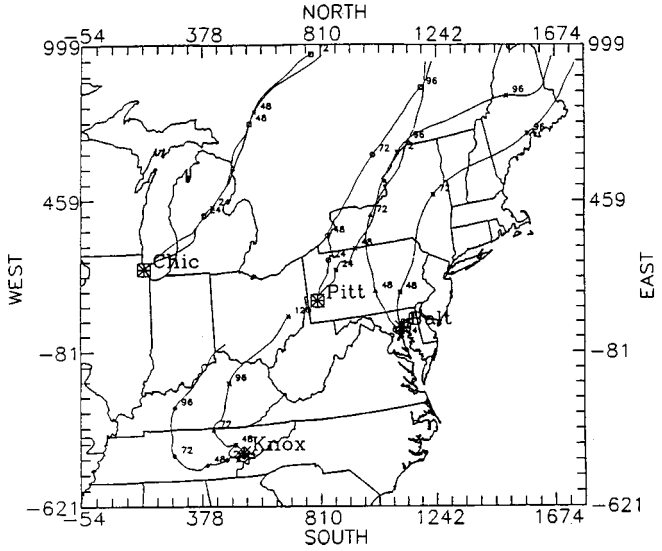


Figure 6. Trajectories at 10 m on the 54 km grid produced by CALMET (A) using the large radius of influence and observations only, and (B) using the large radius of influence and introducing the MM4 80 km winds in the Step 1 initial guess. CALMET results are shown with "o" and trajectories developed directly from MM4 54 km winds are shown with "x". The starting date was August 1, 1988 at 7 AM. The small numbers indicate hours after release.

small "o's." Figure 6a illustrates the results obtained by CALMET with observations only, and Figure 6b illustrates the results obtained by CALMET by introducing the MM4

80 km winds in the development of the Step 1 initial guess wind fields. The most striking differences between the two figures is for the trajectory developed from the Knoxville release location. The CALMET winds (based on observation only) show a light southwest flow, whereas the winds resulting from introducing 80 km MM4 winds to CALMET show the corrent movement towards the north and northeast.

Trajectory statistics were computed from each release time for each site and three levels. In general, the introduction of the 80 km MM4 winds into CALMET to develop either 54 km or 18 km gridded wind fields significantly improved the comparisons with the trajectories developed from the 54 km and 18 km MM4 wind fields directly, versus using only the routine hourly weather observations and twice-daily upper air observations as input to CALMET. There was a slight difference to be seen in using a large or small radius of influence in developing the trajectories with CALMET when only observations were input to CALMET. When the MM4 data are used as input to CALMET, the choice of the radius of influence appears statistically to have no effect on the trajectory comparisons.

CAPTEX comparisons

One of the objectives of the CAPTEX comparisons (Irwin et al., 1996) was to assess whether use of mesoscale dynamic wind fields developed using Four-Dimensional Data Assimilation (FDDA), exhibiting improved spatial and temporal resolution versus typical mesoscale wind fields determined diagnostically from the available hourly surface and twice-daily upper air observations, would improve the quality of the characterization of the transport and dispersion. Results were generated for CAPTEX releases 3, 5 and 7.

The Cross-APpalachian Tracer EXperiment (CAPTEX) is a unique series of tracer releases, which besides testing a particular tracer technology, was conducted for the purpose of providing data to evaluate and improve computer models of pollutant dispersion and to provide insight into the mechanisms involved in long-range transport and dispersion (Ferber et al., 1986). A three-hour ground-level release of perfluoromonomethylcyclohexan (C_7H_{14}, PMCH) was made five times near Dayton, Ohio and twice from near Sudbury, Ontario when winds were expected to transport the tracer over the ground-level sampling network. Samplers were operated at 86 sites in Ohio, Pennsylvania, New Jersey, New York, New England and southern Canada at distances from 300 to 1100 km from the release site. Air concentrations were collected for 3- and 6-hour durations for several days following each release.

Meteorological data available for use in developing the CAPTEX wind fields consisted of 122 National Weather Service (NWS) surface locations reporting hourly and 13 upper-air locations reporting twice-daily (0000 GMT and 1200 GMT) throughout the region. Furthermore, mesoscale wind fields developed using FDDA were available on an 80-km grid. Three wind field models were used to obtain a gridded field of meteorological data with a horizontal resolution of 18-km: MESOPAC II, CALMET, and

CALMET using the mesoscale wind fields as STEP-1 inputs. In the discussion to follow, the latter modeled wind field is referred to as CALMET/MM4.

Version 8 of the Penn State/NCAR Mesoscale Model - Generation 4 (MM4) was used to develop profiles of atmospheric wind, temperature, and moisture. The MM4 is a primitive equation, mesoscale, hydrostatic Eulerian modeling system of the atmosphere (Anthes et al., 1987). The vertical layers are terrain following. FDDA is incorporated as Newtonian nudging by adding to the general momentum and thermodynamic equation a "Force-Restore" term, to effectively nudge the numerical solution towards the observed data (Stauffer and Seaman, 1989; Stauffer et al., 1990). Nudging was applied for the east-west and north-south wind components, temperature and mixing ratio at all levels, except for temperature at the surface and at levels aloft within the lowest 6 layers of the analyses (top of sixth layer is typically 1500m). The horizontal grid spacing of the MM4 simulation was 80 km in both dimensions, with a grid array size of 84 by 55 centered on 90°W longitude and 40°N latitude to cover the domain of the CAPTEX releases.

MESOPUFF II was driven by each of the modeled wind fields to produce a set of three simulations of ground-level concentrations for each of the three CAPTEX releases (9 simulations in all). CALPUFF was driven by two of the modeled wind fields, CALMET and CALMET/MM4, to produce a set of two simulations of ground-level concentrations for each of the three CAPTEX releases (6 simulations in all).

In both the MESOPUFF II and CALPUFF simulations, chemical transformations, dry deposition and wet removal were not modeled because PMCH was assumed to be inert and non-depositing. No attempts were made to optimize the choice of model options within CALPUFF, such as the dispersion coefficients, mode of incorporation of MM4 data, and meteorological vertical layer structure. In effect, CALPUFF was run in a mode designed to make it most like MESOPUFF II, in order that the effects of different wind fields and transport characterization could be identified. MESOPUFF II and CALPUFF differ in the way transport winds are computed for each puff. MESOPUFF II uses a two-layer wind field, the lower layer for the transport of puffs within the mixed layer, and an upper layer field for puffs above the mixing height. For a surface release, as in CAPTEX, MESOPUFF II will always use the lower layer (mixed-layer averaged) wind field. CALPUFF internally computes for each sampling step, a transport wind averaged over the depth of the puff from the multi-layer winds provided to it from CALMET. As the puff grows in the vertical, the depth through which the wind is averaged is increased.

The distance from the nearest to furthest receptor was approximately 800 km and there where 86 receptor locations. The average distance between the receptors was roughly 86 km = $[(800)^2/86]^{1/2}$, which meant that typically there were 4 to 6 receptors with nonzero concentration values for analysis for the shorter travel times (300 to 600 km transport) and from 8 to 16 receptors with nonzero concentration values for analysis for the larger travel times (600 to 900 km transport). This suggests that the

maximum concentration was likely not well characterized and is uncertain both in the observations and in the simulations.

For each 6-hour period, the centroid position was computed for the observed and simulated tracer puff as it was transported downwind over time. The results for each release are shown in Figure 7. It was concluded that the simulated trajectories are sensitive to the manner in which the wind field is characterized, but are insensitive to the model employed. This can be seen by the fact that the simulated trajectories are nearly identical for MESOPUFF and CALPUFF when the models have the same input wind fields.

Ratios were formed by dividing the simulated and observed maximum concentration values for each six-hour period. There was no noticeable trend seen as a function of travel time (hours after release), but clearly there was a tendency to overestimate the maximum concentration value by roughly a factor of 3.7. To further investigate the tendency to overestimate the surface concentration maxima, ratios were formed by dividing the simulated and observed lateral dispersion (as determined from the second moment of the concentration values about the centroid positions) for each six-hour period. There was no apparent trend in the ratio values with travel time following release, however there was a clear trend to underestimate the horizontal extent of the tracer puff for each six-hour period. There were only slight differences seen for the different wind fields employed. The overall geometric average was 0.54 and the geometric standard deviation was 1.81. If the only difficulty or "bias" in the simulation was to underestimate the horizontal extent of the puffs, the effect on the simulated maximum concentration values would be proportional to the inverse square of the bias in the horizontal dispersion, which would be $3.43 = (1/0.54)^2$. It is concluded that the underestimation seen in the simulated horizontal dispersion is able to explain the overestimates seen in the simulated maximum concentration values. The large scatter seen in concentration and lateral dispersion ratio values in part may relate to the stochastic nature of atmospheric dispersion, but also is traceable to poor definition of the maximum concentration values and lateral dispersion.

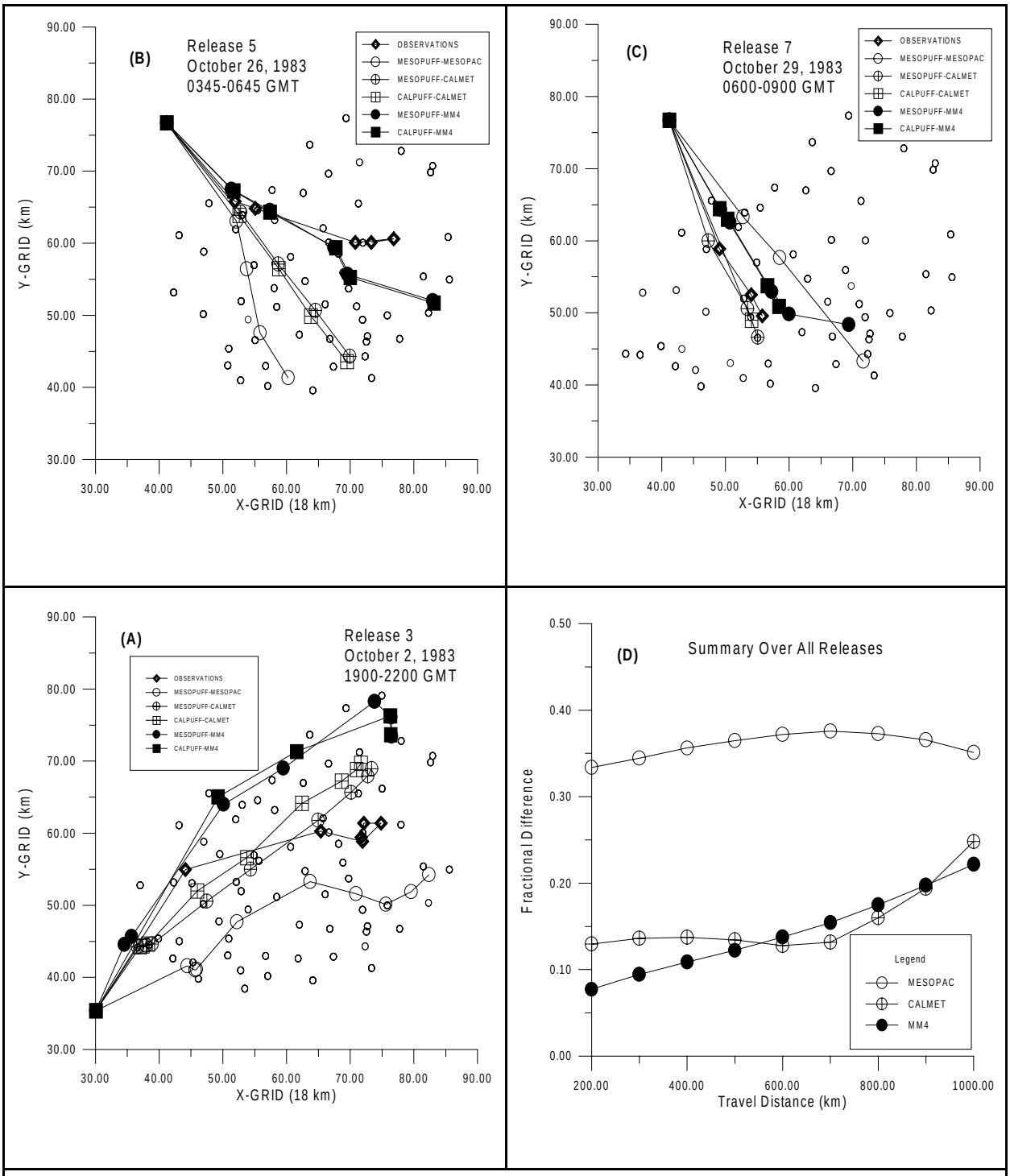


Figure 7. Summary of trajectory results for each of the releases are shown in parts (a), (b) and (c). In part (d) is shown the fractional difference computed between the observed and simulated trajectories, summarized over all releases for each of the three wind fields. The open smaller circles indicate sampling locations. The X and Y coordinates have been specified in terms of the meteorological grid, which had an 18-km size.

The purpose of this investigation was to assess whether different methods of characterizing the wind fields affect the performance of the simulated trajectory. The comparison results presented were conducted with simplified puff dispersion model assumptions, hence the model-to-model differences were minimized. The results shown in Figure 7 suggest a noticeable improvement in the puff simulation results of the centroid trajectory when mesoscale dynamic wind fields developed using FDDA were used to characterize the time and space varying wind field, versus using mesoscale wind fields determined diagnostically from the available hourly surface and twice-daily upper air observations. The favorable comparison of the CALMET wind field results with the MM4 results is influenced by Release 3 results, where CALMET happened to well characterize the average transport direction. The trajectory simulations for Releases 5 and 7 derived using MM4 winds are as good or better than the results obtained with CALMET wind fields derived solely from routine National Weather Service observations. It was concluded that use of MM4 is preferred and that both CALMET and MM4 wind fields provide better simulations of the trajectories than MESOPAC wind fields.

The analysis of the concentration maxima and lateral dispersion values suggest that the simulation assumptions employed in these results consistently underestimate the horizontal extent of the tracer puff as it is transported downwind. The centroid maximum surface concentration was found to be correspondingly overestimated and relatively insensitive to the mesoscale wind characterization. In these simulations, no provisions were made to address delayed shear enhancement of the dispersion as described by Moran and Pielke (1994) and Shi et al. (1990). Inclusion of some sort of puff splitting is obviously warranted, but the computational demands are not trivial if one is attempting to develop an operational model for routine use. Furthermore, in those cases where the puff model dynamics have been enhanced, for example Draxler (1987) and Davis et al. (1986), there was a tendency to underestimate the surface maximum concentrations.

4.4 Constructing *FDDA-MM* Data Sets Assessment

To foster interest in the use of mesoscale meteorological (MM) data processed using Four Dimensional Data Assimilation (FDDA) in routine air pollution modeling assessments and to learn what problems might be associated with such a project, IWAQM sponsored the development of a one-year meteorological data set for 1990 that spans the contiguous United States, southern Canada and northern Mexico. Hourly profiles of wind, temperature and moisture were provided at 23 levels in the atmosphere on an 80-km gird. The Penn State mesoscale meteorological model (MM4) with FDDA was used in developing these data. The horizontal grid spacing of the MM4 simulation was 80 km in both dimensions, with a grid array size of 85 by 56 centered on 90 W longitude and 40 N latitude to cover most of the North American continent and adjacent oceanic areas (Bullock, 1993). The model simulation variables from the outer 2 columns and rows of grid points were not included in the published data set to avoid the boundary effects typical of fixed-grid numerical models. The

domain of the model's vertical coordinate system extended from the earth's surface to the 100 millibar pressure level (approximately 15 km above sea level). The 15-level structure provides height-resolved information similar to that routinely obtained by the National Weather Service at 12-hour intervals from approximately 80 rawinsonde balloon sounding locations across North America. However, the data set obtained from the MM4 simulation provides synthetic soundings at 1-hour intervals for 4080 model grid-point locations, or about 600 times more information than is available from routine observational networks. The 1990 data set contains over 20 billion bytes of information.

The annual data set was developed from the MM4 output of 80 separate simulations. Each simulation was 5 days in length with a 12-hour overlap with chronologically adjacent simulations. This 12-hour overlap was used to allow a model "spin-up" so each simulation's hour 12 conditions would match the previous simulation's ending conditions without the detrimental effects of model initialization. The first 6 hours of each simulation were not used in the definition of the final data set. Hour 7 thru 11 results were blended with the previous simulation results with a time-linear weighting function to produce temporally continuous fields in the final data set. Beginning at hour 12, the simulation results were copied directly in the production of the annual data set. Differences between adjacent simulations for these overlap periods were monitored and no significant discontinuities were detected. At hour 12, the differences were often zero at the floating-point numerical precision of the CRAY Y/MP at EPA's National Environmental Supercomputing Center where the 80 MM4 simulations were performed. Each of these simulations required about 2.5 hours of CPU time to compute on the Cray Y/MP. The MM4 output files were then transferred to a DEC 3500 AXP workstation where the data were chronologically blended and chained and various QA checks were performed. The final product was then re-partitioned into 36 sequential files of about 600 Mbytes each. Three files were produced for each month, the first containing days 1 thru 10, the second containing days 11-20, and the third containing day 21 through the end of each month. These files were then processed by the National Climagic Data Center to produce a 12 Compact Diskette data set (NCDC, 1995).

The science of mesoscale analysis using data assimilation is rapidly developing. Major advancements have been occurring every several months during the period from 1995 through 1997. There are various research groups who have active development programs investigating mesoscale meteorological modeling employing data assimilation, e.g., Pielke et al., (1997), Turner and DeToro, (1998).

A major obstacle is access to these data. The 1990 MM4 data set in a compressed format, and providing only profiles of wind, temperature and moisture, requires 12 Compact Diskettes. An operational means for gaining easy access to comprehensive mesoscale meteorological data sets, as alluded to here, has yet to be developed.

4.5 Regional Approach

Federal and State modelers have struggled with the issues related to Class I area analyses and have found their resolutions to be elusive. Currently the consensus opinion within IWAQM is that air quality impact assessements for Class I areas are fundamentally different from local-scale assessements, typically associated with Class II assessments and State Implementation Plans (SIP's). Unfortunately, the Federal Agencies have attempted to implement the assessment of Class I impacts as if the assessment is similar to that associated with Class II and SIP impacts. This has lead to a significant mis-match between the analysis process and the inherent needs of a Class I impact assessment.

Local-scale assessments require that analyses be performed within a domain on the order of 50 km or less and centered on the source (the domain changes from permit to permit). Given the small domain, Class II analyses lend themselves to individual state implementation. Class I analyses, on the other hand, are centered on specific land areas. Therefore, the modeling domain does not change from permit to permit. Furthermore, these analyses involve a modeling domain on the order of hundreds of km, thus requiring multi-state coordination. Additionally, Class I area analyses for AQRV's may require estimating the deposition of secondary pollutants and their impact on visibility. Finally, the affirmative responsibilities of the FLM's inherantly adds to the coordination difficulties.

As an alternative to the current permit-by-permit practice, Class I air quality modeling assessments could be designed for each Class I area (or cluster of Class I areas). The cornerstone of this approach is an up-front comprehensive increment and AQRV analysis of the area. We envision an "initialization" study being accomplished outside the context of a permit application. An up-front study is preferred since many of the decisions which need to be made (e.g., inventory, AQRV's criteria, etc.) are specific to the Class I area, not the applicant's source. Further, it avoids having these decisions colored by the negotiations which occur for a single source. If desired, the "initialization" can involve technical experts from private and public groups. Finally (and perhaps most importantly), it provides future applicants with up-front information needed for planning and assurance of what is expected for the given situation.

In large part, the emissions inventory and meteorological data which are developed during the initializing process remain fixed in subsequent analyses. Therefore, once "initialization" is complete, each additional new source need only determine its additive contribution; as such, increment and AQRV's are directly tracked. This approach has the benefit of removing the burden, from each applicant, of developing an emissions inventory specific for their application. Updates may be necessary to account for changes in actual emissions from other sources. Within this approach, provisions can be made for updating the initial analysis under certain circumstances. For instance, a re-initialization analyses could result from any one of

the following: 1) periodic State audit as contemplated by the PSD regulations, 2) by choice of the permit applicant, or 3) as the scientific understanding changes. Once the system is "re-initialized", new meteorological data and grids may result.

4.5.1 A Regional Approach to Implementing a Class I Area Assessments

The following outline presents a conceptual approach how the air quality modeling could be accomplished for Class I areas. This approach was designed to provide a framework in which many of the issues could be resolved.

I. **INITIALIZING ANALYSIS**: Use the recommendations of the Interagency Workgroup on Air Quality Modeling (IWAQM) to initialize each Class I area outside the context of a permit application.
   A. Preprocess a fixed 5 year data base. All subsequent analyses will use this data set. That is, the meteorological grid will be fixed for all future analyses.
   B. Define both the computational and receptor grids. These grids are also fixed for all future analyses (unless a reanalysis warrants changes).
   C. Decide on the measures to be used in the Air Quality Related Values (AQRV's) analyses, and determine the significance (*de minimis*) criteria for the AQRV's (this should be done specific to the Class I area)
   D. Develop an Inventory:
      1. Source inventory for PSD increment analyses.
      2. Source inventory for AQRV analyses.
   E. Run IWAQM recommended approach to produce appropriate concentration/impact fields.
   F. Archive these fields for use by future Prevention of Significant Deterioration (PSD) applicants.

II. **INITIALIZATION STUDY PARTICIPANTS**: The initialization work should be a cooperative effort among the FLM for the area and the EPA regions and states who have or could have sources which affect the Class I area. The initialization study participants could include technical experts from industry and academia.

III. **PERMITTING**:
   A. The State within which the Class I area resides could be the ultimate caretaker of all data bases[1]. The data bases would include the meteorological data, the computation and receptor grid definitions, the Class I area specific emissions inventories, the various topographical and other data and the concentration/impact fields.

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[1] An issue yet to be resolved is developing an effective means to assist those States faced with assessing impacts on Class I areas not within their respective borders. Will coordination problems arise between States on roles and responsibilities?

B. Using the data provided, an applicant need only determine its own incremental impacts. These impacts will then be added to the archived concentration/impact fields for comparison against appropriate increments and AQRV's.

IV. **DATABASE UPDATES**: It is envisioned that re-initialization analyses could result from the following:

A. Periodic state audit as contemplated by the PSD regulations.
B. By choice of the permit applicant. An applicant will be permitted to use a more recent 5 year set of meteorological data with the requirement that they perform a complete re-initialization analysis. Such an analysis would update the comprehensive data base for future analyses.
C. As scientific understanding changes.

4.6 Comparisons of CALPUFF with Tracer Field Data

There are very few intensive tracer field experiments available for investigating model simulations of mesoscale transport and dispersion. The IWAQM is aware that there are several other expriments for which the CALMET/CALPUFF modeling system has not been exercised (mostly in Europe). The results that are summarized here represent those that IWAQM was aware of and for which the data could be obtained.

4.6.1 1975 Savannah River Laboratory Tracer Study

In this study (U.S. EPA, 1998a), concentration estimates from the CALPUFF dispersion model were compared to observed tracer concentrations from a short-term field experiment conducted at the Savannah River Laboratory (SRL) in South Carolina on December 10, 1975 (U.S. DOE, 1978). This experiment was designed to examine long-range transport of inert tracer materials to demonstrate the feasibility of using other tracers as alternatives to the more commonly used SF_6. Several tracers were released for a short duration (3-4 hours) and the resulting plume concentrations were recorded at an array of monitors downwind from the source.

For the CALMET/CALPUFF simulations, a meteorological grid extending from 32° N to 34° N latitude and from 80° W to 82° W longitude was used. Figure 8 shows the region of the SRL field experiment. The SRL facility is near the west edge of the domain and the sampling monitors are located along Interstate 95. A 24-by-24 horizontal grid with a 10-kilometer resolution was used for the SRL modeling. To adequately characterize the vertical structure of the atmosphere, six layers were defined: surface-20, 20-50, 50-100, 100-500, 500-2000, and 2000-3300 meters.

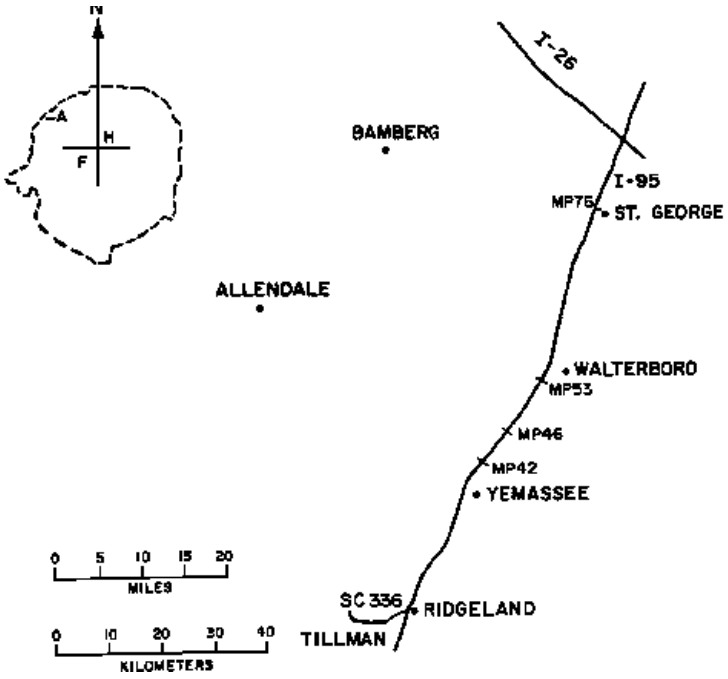


Figure 8. Savannah River Laboratory field experiment site.

The CALMET preprocessor utilizes National Weather Service (NWS) meteorological data and on-site data to produce temporally and spatially varying three dimensional wind fields for CALPUFF. Only NWS data were used for this effort and were extracted from two compact disc (CD) data sets (see Appendix C). The first was the *Solar and Meteorological Surface Observation Network* (SAMSON) compact discs, which were used to obtain the hourly surface observations. The following surface stations were used:

Georgia:	Athens, Atlanta, Augusta, Macon, Savannah
North Carolina:	Asheville, Charlotte, Greensboro, Raleigh-Durham, Wilmington
South Carolina:	Charleston, Columbia, Greer-Spartanburg

Twice daily soundings came from the second set of compact discs, the *Radiosonde Data for North America*. The following stations were used:

Georgia:	Athens, Waycross
South Carolina:	Charleston
North Carolina:	Greensboro, Cape Hatteras

The geophysical parameters were derived from geographical information system (GIS) land-use categories. Terrain and land-use data were available on the CALMET, CALPUFF, and CALPOST Modeling System (version 1.0) CD (hereafter referred to as the CALPUFF CD, see Appendix C). The terrain and GIS land-use data on the CALPUFF CD were used to define gridded land-use data for each field experiment. These data are defined with a resolution of 1/6° latitude and 1/4° longitude.

SF_6 and two heavy methanes were released. For this analysis, the SF_6 tracer emission rates were used. The source parameters for this analysis were, a release height of 62 m, with 154 kg of SF_6 tracer released over a 4 hour period (10.69 g/s) with no buoyant plume rise.

The distance to the monitoring arc was approximately 100 kilometers. The monitors were located along I-95 (Figure 8) from MP76 on I-95 near St. George south to Hwy 336 west of Tillman, SC and along SC 336. The monitors subtended an arc of about 70°. Receptors for modeling were placed along an arc every 1/4° degree from MP76 to MP22 near Ridgeland, resulting in 261 receptor locations. The distance between receptors was about 450 meters.

Two separate CALPUFF model runs were made: 1) using Pasquill-Gifford (PG) dispersion parameters, and 2) using dispersion coefficients from internally-calculated σ_v and σ_w from the micrometeorological variables calculated in CALMET (hereafter referred to as similarity dispersion). The central maximum concentration is estimated from a Gaussian fit to the modeled and observed data (Cmax) and computed from the crosswind integrated concentration (CWIC) and the lateral dispersion, σ_y, as Cmax = CWIC/($\sqrt{2\pi}$ σ_y). The CWIC was computed by trapezoidal integration. The program that computed these measures utilized only those values that were 1% or greater of the maximum.

The observed concentrations are the cumulative concentration from bag samples located along Interstate 95 from about St. George south to Ridgeland (Figure 9). Background concentration was estimated to be 0.5 ppt (DOE, 1978). The tracer release started at 10:25 Local Standard Time (LST) and continued until 14:25 LST. The bag samplers were started at different times, ranging from about 10:40 to 12:30 LST, and the duration of the sampling ranged from 7.0 to 7.5 hours. Since the release started at 10:25 LST, it seems likely that sampling at the monitors would have begun prior to the arrival of the plume. The arrival time of the modeled plume was the hour ending at 13:00 LST for both PG and similarity dispersion. The simulated plume required seven hours to pass the arc with the PG dispersion coefficients, but only six hours with similarity dispersion coefficients. Therefore, seven-hour-average modeled and observed concentrations were computed for comparison with the measurements. Since the first monitors were turned on prior to 11:00 LST and only cumulative concentration is reported for the observed data, the simulated concentrations were summed over the seven-hour period from 11:00 LST through 1800 LST.

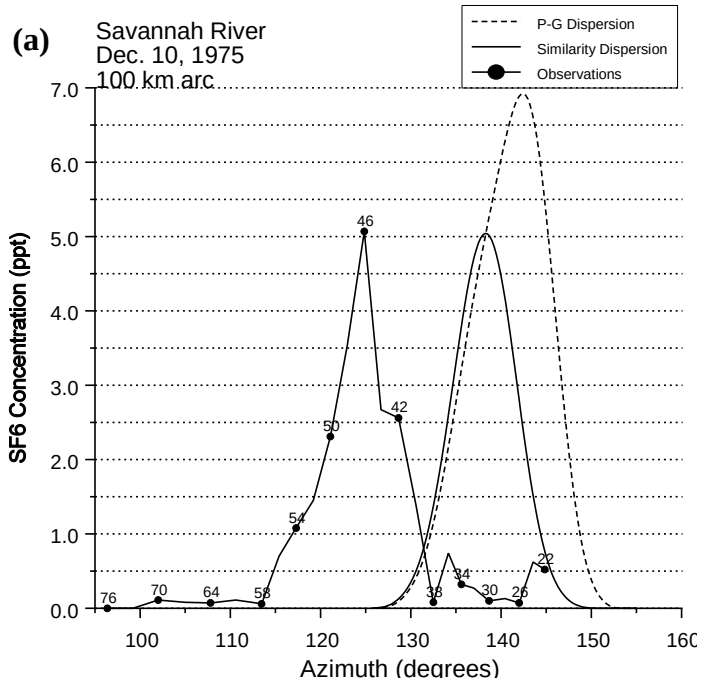


Figure 9. Simulated and observed seven-hour average concentration values along sampling arc for the Savannah River Laboratory December 10, 1975 tracer field experiment.

Figure 9 shows the plots of the concentration estimates at the receptors (continuous curves) and the observed concentrations at the receptors (labeled points). The modeled peaks are 10° to 20° further to the south than the observed peak. It appears that the CALMET meteorology derived using routine NWS was not able to characterize this initial difference in wind direction sufficiently to transport the plume more toward the north.

Clearly, there is general agreement in the shape and magnitude of the distributions. Note that there are two local maxima in the observations near 135° and 145°. The winds were more northerly shortly after the release and may have resulted in the observed local peaks (DOE, 1978) that were not captured in the modeled meteorology. The observed lateral dispersion is 50-100% larger than the modeled dispersion due to these local peaks. If these two secondary peaks are omitted from the analysis, then the statistical measures of the simulated plumes are in better agreement with the measures of the observed plume. Without these secondary peaks, the fitted central maximum to the observations increases by 37% to 3.8 ppt (modeled: PG 7.2 ppt and Similarity 5.1 ppt), The observed computed lateral dispersion is reduced by 33% to 7.77 kilometers (modeled: PG 6.9 km and Similarity 5.0 km). The observed CWIC is reduced only slightly to 0.732 ppt-m (modeled: PG 1.29 ppt-m and Similarity 0.8 ppt-m).

With only one realization for comparison, general conclusions regarding model performance are not possible. But the simulation results are in reasonable accord and do not suggest there are severe problems in the modeling system. It is encouraging that the correspondence is as close as it is given that only routine NWS observations were employed in developing the meteorological fields.

4.6.2 1977 Idaho FallsTracer Study

CALPUFF dispersion modeling results (Irwin, 1997) were compared with data obtained following a single 3-hour late afternoon tracer release, lasting from 1240 to 1540 Mountain Standard Time (MST), conducted on April 19, 1977 near Idaho Falls, Idaho. The tracer release results (Clements, 1979) were obtained as a consequence of an investigation into the feasibility of using certain perfluorocarbons and heavy methanes as alternative tracers in place of sulfur hexafluoride (SF_6). Hence, although the results have found use for testing alternative characterizations of dispersion and transport, this was not a primary purpose in the original design of the investigation. Draxler (1979) included this experiment in an assessment of the effects of alternative methods of processing wind data for characterization of the mesoscale trajectory and dispersion. He concluded that a network of wind observations having a spacing on the order of 25 kilometers might be needed to simulate mesoscale transport associated with variable-flow situations, and that spacing of order 100 kilometers might prove adequate for stationary and homogeneous flow situations.

The design for meteorological data collection and sampling locations relative to the release location is shown in Figure 10. Since locations of towers and sites were extracted from data volume figures, the relative positions are likely accurate but the absolute positions are no better than 0.5 km. The receptor arcs at 48 and 90 km downwind from the release are shown in Figure 10. Meteorological data were available from eleven sites providing hourly-averaged winds; four sites providing hourly-averaged winds and temperatures, three sites providing hourly pibal observations of winds aloft (CFA, MTV, DBS). Two of the pibal sites (CFA and DBS) also provided hourly-averaged winds and temperatures. Hourly rawindsonde observations were taken at about 600 m northwest of the release location. The meteorological masts ranged in height above ground with two at 6.1 m, eleven at 15.2 m, three at 22.8 m, and two at 30 m. The pibal observations taken at Billings, Montana (well past the farthest sampling arc downwind) were not used in this investigation. The skies were clear of clouds and no precipitation occurred during the experiment. The National Weather Service observations taken at Pocatello, Idaho (approximately 75 km southeast of the release location) were included to provide station pressure (required input for CALMET).

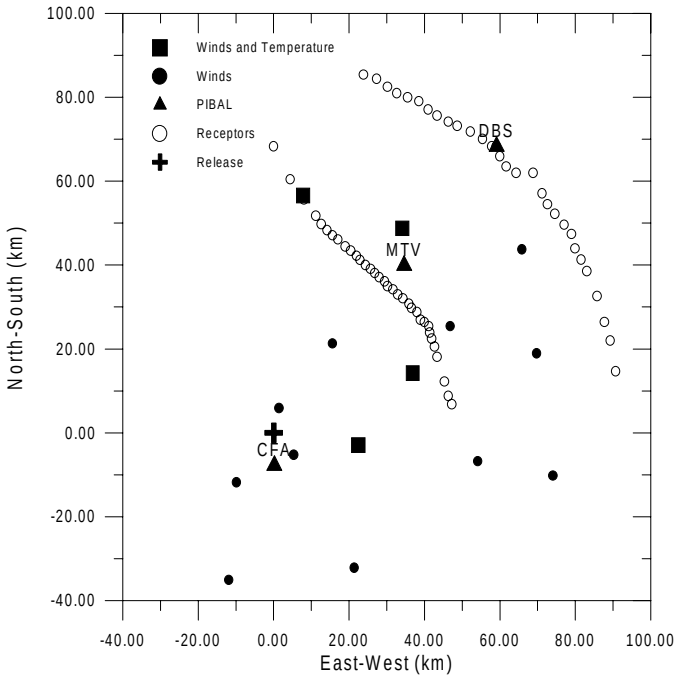


Figure 10. The Idaho tracer experiment sampling arcs and meteorological data collection network. The sampling arcs at 48 km and 90 km are shown. The receptor arc at 3.2 km downwind of the release is omitted for clarity.

To estimate the effects of drainage flow on the near-surface wind field, gridded values of land-use and terrain heights are needed. The land-use data are used as surrogates for typical values of surface roughness, albedo, soil heat flux, anthropogenic heat flux and leaf area index. These surface parameters are used in estimating the surface energy balance. For this analysis, U.S. Geological Service land-use and terrain height data were extracted from data bases included in U.S. EPA (1996). The basic grid size for these data is approximately 900 m. They were processed into a 20 by 20 grid with a grid resolution of 10 km. Default values, as defined in U.S. EPA (1996), for the surface parameters to be associated with the land-use data were used. The southwest corner of this grid was approximately 50 km southwest of the release. The area depicted in Figure 10 is fairly flat, but the terrain sharply increases in height to the west and north of the area depicted. The dominant land-use was rangeland; and the surface roughness was estimated based on land-use to be on the order of 10 centimeters.

Hourly-averaged winds and temperature were available from midnight April 18 through midnight April 19. To mitigate the effects of not having surface data beyond midnight of April 19, the surface meteorological tower data were duplicated to form two

24-hour periods, having identical meteorology. The assumption being made is that conditions were steady-state. The pibal and rawindsonde data, which were available from 0700 MST to 1900 MST, were treated in a similar manner. CALMET assumes all upper-air observations are from rawindsondes, and thus expects upper-air observations to provide winds, dry-bulb temperature and pressure with height. CALMET interpolates in height for missing data values at intermediate heights in an observation, but CALMET will not extrapolate upper air data. Thus observations are rejected that fail to reach the user-prescribed top of the modeling domain (3300 m for this analysis), or have missing data values at the surface. To make use of the hourly pibal observed winds, temperature and pressure values were added by linearly interpolating in time and height between available rawindsonde observations, which were available every 1 to 3 hours. The pibal wind directions were consistent with those from the one rawindsonde, but the wind speeds were generally less in magnitude.

A purpose of this investigation was to assess the effects of having different amounts of meteorological data for use in the development of the time varying field of meteorological data. For this purpose four separate runs were made: Case 1 using all available upper-air and surface mast observations, Case 2 using all surface mast observations but only the one on-site rawindsonde upper-air observation, Case 3 using only the CFA wind and temperature observations with the one on-site rawindsonde upper-air observations, and Case 4 using only the CFA wind and temperature observations with all upper-air observations. In Cases 1 and 2, all the on-site hourly wind and temperature data are employed but different amounts of upper-air observations are used. In Cases 3 and 4, hourly winds and temperatures taken close to the release are used with different amounts of upper-air observations. For all the CALMET simulations, winds and temperatures were computed for six layers in the vertical, the midpoints of which were: 10 m, 35 m, 75 m, 300 m, 1250 m, and 2650 m.

The winds at CFA were higher than those generally seen throughout the network. Hence in Cases 1 and 2 when all the on-site winds were employed the low-level winds were lower than when only CFA data were used. In Cases 1 and 2, the afternoon stability was Pasquill category B/C (Monin Obukhov lengths of order -30 m). As a consequence of higher winds in Cases 3 and 4, the surface friction velocities were higher, and the Monin Obukhov lengths were larger (in magnitude), thus closer to neutral stability. The afternoon mixing heights are similar regardless of data used. This results because the “upper-air” temperatures all have a common source, namely the rawindsonde observations taken 600 m northwest of the release. The nighttime mixing heights are mostly a function of the magnitude of the friction velocity. Hence, where estimated friction velocities were largest and differ most among the various processing methods, differences were seen in the nighttime mixing height values.

Each of the four analyses of meteorology was used to produce two CALPUFF simulations of ground-level concentrations for each of the three sampling arcs. In the first simulation, the dispersion was described using Pasquill-Gifford dispersion parameters. In the second simulation, the dispersion was described using dispersion

parameters suggested by Draxler (1976), which require values of the standard deviation of the vertical and lateral wind fluctuations (referred to hereafter as “similarity dispersion”). The wind fluctuation standard deviations estimated within CALMET are primarily dependent on the surface friction velocity. The surface friction velocity is a strong function of stability (largest during unstable conditions), roughness length and wind speed (increases as roughness length or wind speed increase).

For each sampling step, CALPUFF internally computes a transport wind averaged over the depth of the puff from the multi-layer winds provided to it from CALMET. As a surface release puff grows in the vertical, the depth through which the wind is averaged increases. The SF_6 tracer emission was reported to be steady at 25.37 g/s over the three hour period, and was simulated within CALPUFF as a 3-hour point-source release at 10-m starting at 1300 MST. The release height was set at the midpoint of the lowest CALMET layer, to insure that the internally computed standard deviations of lateral and vertical velocity fluctuations (for use in the similarity dispersion parameter characterizations) at the specified release height, were in accord with the wind speed used by CALPUFF for the lowest layer.

For each 6-hour period, the second moment (lateral dispersion, σ_y) of SF_6 concentration values about its centroid position along the arc was computed. The crosswind integrated concentration, CWIC, was computed by trapezoidal integration. By assuming the concentration profile along the arc is Gaussian, the central maximum, Cmax, was computed as, $Cmax = CWIC/(\sqrt{2\pi}\ \sigma_y)$.

A goal of this investigation was to assess the sensitivity of the modeling results to different treatments of processing the meteorology, as well as to assess the performance of CALPUFF in characterizing dispersion for transport distances beyond 50 km. Figure 11 depicts the observed SF_6 concentrations with the simulation results where all the surface and upper-air observations were used to generate the hourly wind fields. For the observed values, there were from 14 to 17 receptors along each arc with valid data for analysis. For analysis of the simulation results, receptors were spaced at each arc distance at 2 degree intervals, over the 90 degree sector northeast of the

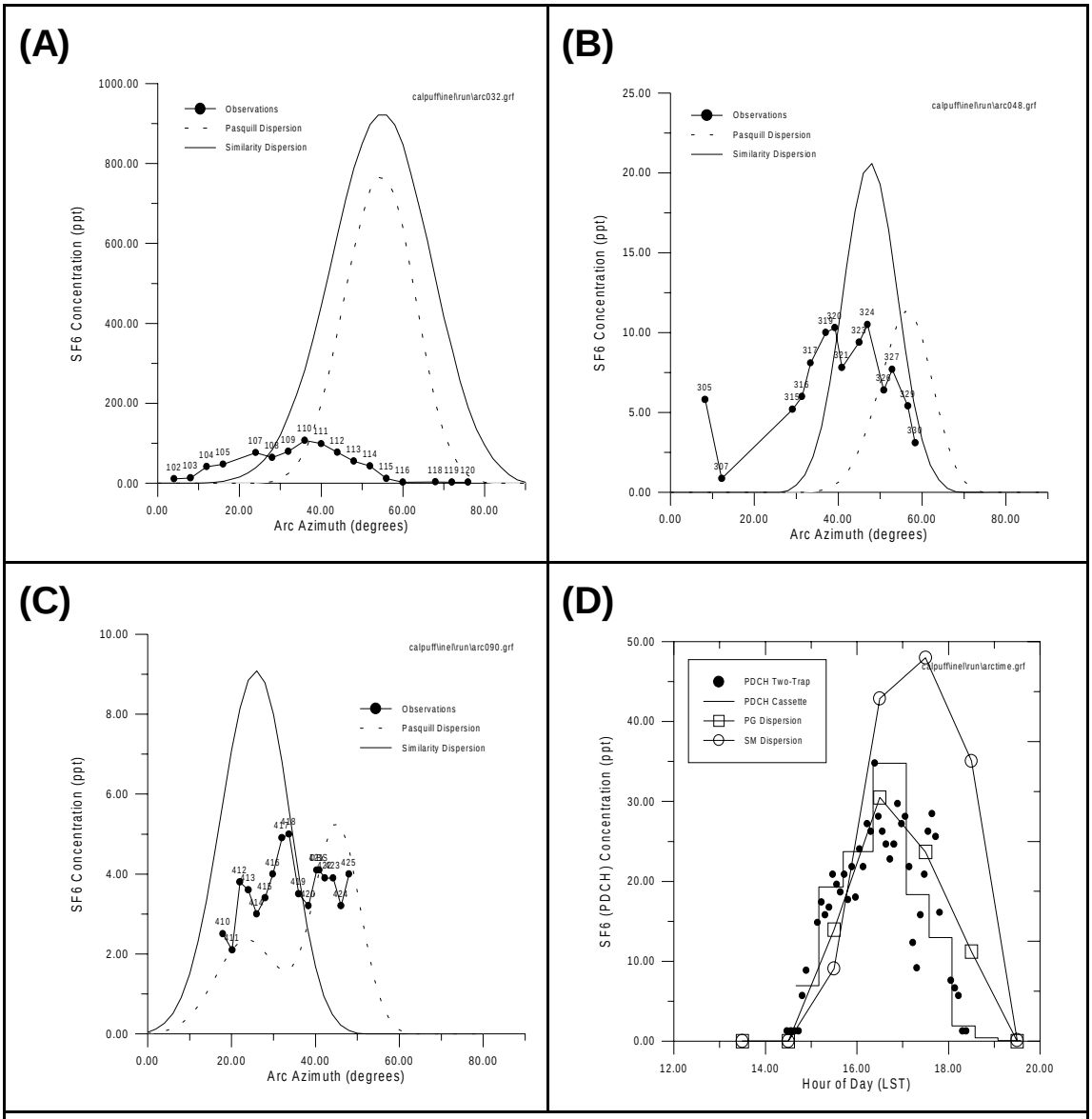


Figure 11. Six-hour average SF_6 concentration values observed and estimated for April 19, 1977, (A) 3.2-km arc, 1300-1900 MST; (B) 48-km arc, 1400-2000 MST; (C) 90-km arc, 1600-2200 MST. Azimuth is defined as viewed from the release position with 0 due North and 90 due East (see Figure 9). Receptor numbers are shown just above each observed concentration value. (D) Time history of observed PDCH and estimated SF_6 concentrations along the 48-km arc for April 19, 1977. Observed PDCH values were multiplied by 3.16 for comparison with estimated SF_6 values (volume of SF_6 divided by volume of PDCH released equals 3.16).

release location. The second moment, σ_y , represents a measure of the puff horizontal dispersion. For these 6-hour periods, the observed lateral dispersion ranged from roughly 22% to 15% of the travel distance downwind. The crosswind integrated concentration (CWIC) value characterizes the amount of pollutant mass seen at the surface. The observed CWIC values at all of the arcs is close to what one would expect if the tracer had become well mixed in the vertical. As shown in Figure 11 (which is typical for all of the simulations), the simulated transport was somewhat south of the observed position along the first two arcs. It is also apparent that the concentrations simulated for the first arc are at least a factor of 5 higher than observed.

Figure 11d provides a comparison of the time history of the puff, as it passed by the 48-km arc. Sampling results are shown for the two-trap sampler which provided 5-minute samples, and a cassette sampler which provided approximately 15-minute samples. These samplers were quite close to the observed position of the 6-hour SF_6. maximum along this arc. The dispersion results are for the simulated position of the maximum, which was somewhat displaced from that observed. The Pasquill dispersion results are in remarkable accord with the tracer results. The similarity results arrive and depart slightly later than observed. The slower transport for the similarity dispersion occurs because the vertical dispersion was less than that simulated by Pasquill dispersion, hence the transport speed was computed over a more shallow layer for the similarity results. These results and those discussed above suggest that the similarity dispersion was underestimating the vertical dispersion for this case.

The primary purpose of this investigation was to assess whether the CALPUFF simulations were in reasonable accord with the observed concentrations. The comparison results presented reveal as yet unexplained differences for the nearest arc, 3.2 km downwind from the release. The simulated pattern of dispersion was displaced as much as 40 degrees from that observed, regardless of how the wind fields were characterized. For all arcs, the lateral dispersion along the sampling arcs was best characterized by both dispersion characterizations when all the surface tower winds were used. Except for the first sampling arc, the simulated maxima along the arcs were typically within a factor of 2 of that observed. The Pasquill simulations were most sensitive to how the wind fields were characterized, showing the most variability between the various wind field results. Having but one puff release limits conclusions to be reached. For this one realization, it would appear that simulations by both dispersion characterizations were in best accord overall with observations when all the low-level winds and upper-air observations were used. And for this case, the similarity dispersion simulations may have underestimated the vertical dispersion.

4.6.3 1980 Great Plains Tracer Study

In this study (U.S. EPA, 1998a), concentration estimates from the CALPUFF dispersion model were compared to observed tracer concentrations from a short-term field experiment (the Great Plains experiment) near Norman, Oklahoma (Ferber et al., 1981) in July 1980. This experiment examined long-range transport of inert tracer

materials to demonstrate the feasibility of using other tracers as alternatives to the more commonly used SF_6. Several tracers were released for a short duration (3-4 hours) and the resulting plume concentrations were recorded at an array of monitors downwind from the source. For the Great Plains experiment, arcs of monitors were located 100 and 600 kilometers from the source.

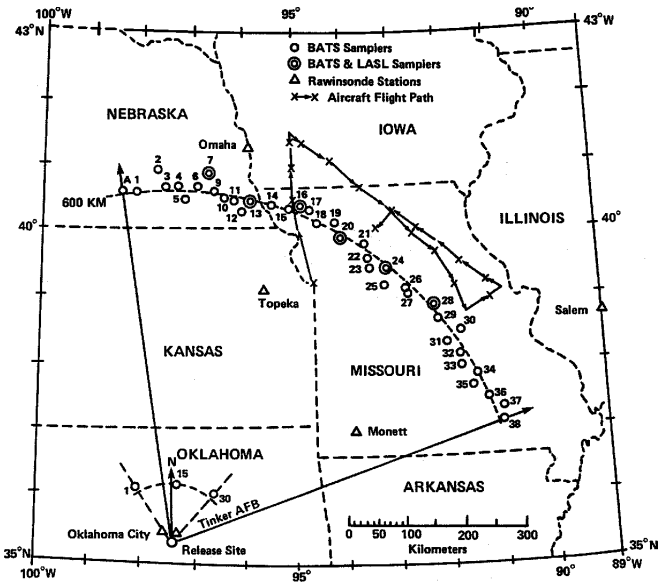


Figure 12. Great Plains field experiment site.

Previous studies have compared the results from the Great Plains experiment to dispersion model results. Carhart et al. (1989) intercompared the results from eight short-term, long-range dispersion models to the Great Plains results and to a longer-term study at the Savannah River Laboratory (not the study discussed in Section 4.6.1). The primary method for evaluating model performance was the use of the American Meteorological Society (AMS) statistical measures (Fox, 1981) and graphical techniques. They concluded that model results compared in space and in time to observations were generally poor and that predictions for a specific location and time for averaging periods less than one day were not reliable. They also noted that unpairing decreases the scatter. They concluded that "model improvement can be made by better representing the wind field. The use of multiple layers seems to improve results substantially."

The transport and diffusion of a tracer gas was simulated by Moran and Pielke (1995a,b) using the Colorado State University mesoscale atmospheric dispersion modeling (CSU MAD) system, which consists of a prognostic meteorological model coupled to a mesoscale Lagrangian particle dispersion model. Results from several simulations with the model were compared to observations from the Great Plains experiment. Their baseline simulation generally compared favorably to observations for

both arcs although directional errors of up to 20° were apparent. The results also suggest that the nocturnal low-level jet plays an important role in transport and deformation of the tracer plume and that some flow regimes require better temporal resolution of boundary layer winds than is available from the National Weather Service (NWS) twice-daily rawinsondes.

The Great Plains site is shown in Figure 12. Two arcs of monitors were deployed during the field experiment -- 100 and 600 kilometers. For this analysis, two separate grids were defined. For the 100-kilometer arc, a grid extending approximately from 35° N to 36.5°N latitude and from 96° W to 98.5° W longitude was defined. A 42-by-40 horizontal grid with a 10-kilometer resolution was used for this arc. For the 600-kilometer arc, the grid extended from approximately 35° N to 42°N latitude and from 89° W to 100° W longitude. A 44-by-40 horizontal grid with a 20-kilometer resolution was used for this arc.

To adequately characterize the vertical structure of the atmosphere, six layers were defined: surface-20, 20-50, 50-100, 100-500, 500-2000, and 2000-3300 meters. The CALMET preprocessor utilizes NWS meteorological data and on-site data to produce temporally and spatially varying three dimensional wind fields for CALPUFF. Only NWS data were used for this effort and came from two compact disc (CD) data sets (see Appendix C). The first was the *Solar and Meteorological Surface Observation Network* (SAMSON) compact discs, which were used to obtain the hourly surface observations. The following surface stations were used:

Arkansas:	Fort Smith
Iowa:	Des Moines
Illinois:	Springfield
Kansas:	Dodge City, Topeka, Wichita
Missouri:	Columbia, Kansas City, Springfield, St. Louis
Nebraska:	Grand Island, Omaha, North Platte
Oklahoma:	Oklahoma City, Tulsa
Texas:	Amarillo, Dallas-Fort Worth, Lubbock, Wichita Falls

Twice daily soundings came from the second set of compact discs, the *Radiosonde Data for North America*. The following stations were used:

Arkansas:	Little Rock	Nebraska:	North Platte, Omaha
Illinois:	Peoria	Oklahoma:	Oklahoma City
Kansas:	Dodge City, Topeka	Texas:	Amarillo
Missouri:	Monett		

CALMET requires a file of terrain elevations and geophysical parameters in order to prepare the wind fields and other meteorological parameters. The geophysical parameters were derived from geographical information system (GIS) land-use categories. Terrain and land-use data were available on the CALMET, CALPUFF, and

CALPOST Modeling System (version 1.0) CD (see Appendix C). These data are defined with a resolution of 1/6° latitude and 1/4° longitude.

The primary purpose of the Great Plains field study was to demonstrate the efficacy of perfluorocarbons as tracers in atmospheric dispersion field studies. Perfluoromonomethylcyclohexane (PMCH), perfluorodimethylcyclohexane (PDCH), SF_6, and two heavy methanes were released during this experiment. For this analysis, the PDCH emission rates were used since the monitoring data appeared to have a more complete record of PDCH concentrations. The following source parameters were used for this analysis:

Source	Release height (m)	Stack diameter (m)	Exit velocity ($m\ s^{-1}$)	Exit temp. (K)	Total tracer released (kg)	Length of release (hr)	Emission rate ($g\ s^{-1}$) and tracer
Oklahoma (July 8)	10.0	1.0*	0.001	ambient	186	3.0	17.22 PDCH
Oklahoma (July 11)	10.0	1.0*	0.001	ambient	26	3.0	2.41 PDCH

* The stack diameter for each study is the same as was used for the study with the INEL data

For both experiments, the emission rate was assumed to be constant over the entire period of the release, and the release was assumed to be nonbuoyant.

For the July 8 Great Plains experiment, sampling was conducted using two arcs of monitors: 100 kilometers and 600 kilometers as shown in Figure 12. Two separate CALPUFF model runs were made: 1) using Pasquill-Gifford (PG) dispersion parameters, and 2) using dispersion coefficients from internally-calculated σ_v and σ_w from the micrometeorological variables calculated in CALMET (hereafter referred to as similarity dispersion).

Beginning at 1300 LST on July 8, the PDCH and PMCH tracer gases were released at a constant rate for a three-hour period from an open field at the National Severe Storms Laboratory in Norman, Oklahoma. A background concentration for PDCH of 26 ppt (Ferber et al., 1981) was removed from the observed concentrations. The five-hour average modeled and observed concentrations for the 100-kilometer arc on July 8 of the Great Plains field experiment are shown in Figure 13a along with Moran and Pielke's baseline simulation (experiment 4b). Two things are immediately apparent: the monitoring did not capture the entire plume and the observed maximum concentration is very likely less than the simulated maxima. Given the incomplete sampling of the observed plume at 100 kilometers for this release, the statistical measures of the observed plume likely are suspect and are not sufficient to draw conclusions regarding model performance. In comparing the CALPUFF results to Moran and Pielke's simulation, the CSU MAD model placed the maximum about 25°

west of the actual plume. Moran and Pielke's result for the 100 kilometer arc are very similar to the CALPUFF simulations.

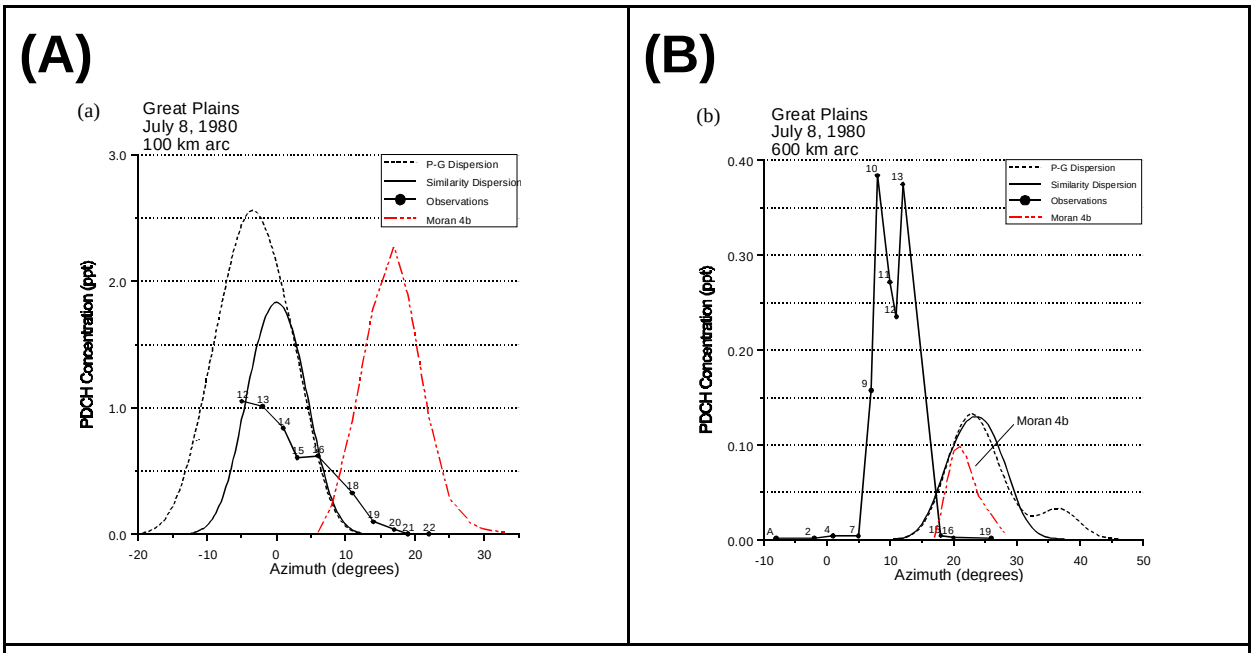


Figure 13. Simulated and observed concentrations for the Great Plains tracer field study for July 8, 1980 for A) 5-hour average concentrations along the 100-km arc, and B) 12-hour average concentrations along the 600-km arc.

The 12-hour average modeled and observed concentrations for the 600-kilometer arc on July 8 are shown in Figure 13b. Two things are apparent: 1) the observed maximum concentration is about three times higher than the simulated concentrations and 2) the maxima of the simulations are in relatively good agreement with each other. As noted above, the tracer arrived at the sampling arc earlier than anticipated and the sampling likely missed some of the tracer material. Ferber et al. (1981) speculate that the plume probably arrived just before the samplers were activated and a small amount of plume material was not collected. As described by Moran and Pielke (1995a), the most likely reason for the earlier-than-expected arrival was the formation of a low-level nocturnal jet. Hoecker (1963), in detailed studies of the low-level jet over the Midwestern plains (from Amarillo, TX to Little Rock, AR) using a series of pibal stations, found that jet speed maxima occur between 300 and 800 meters above local ground. In examining available data for the 1980 Great Plains field experiment, Moran and Pielke (1994) note an approximate doubling of the average nocturnal wind speeds from their daytime values. Examination of the upper air wind profiles for Oklahoma City through the period indicate the presence of a jet between 500 and 1000 meters for the 1200 Greenwich Mean Time (GMT) soundings.

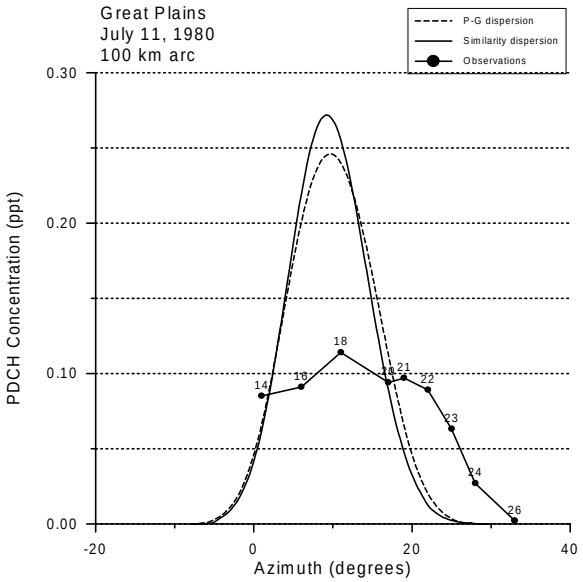


Figure 14. Simulated and observed 6-hour average concentration for the Great Plains tracer field study on July 11, 1980 along the 100-km arc.

Beginning at 1300 LST on July 11, tracer gases were released for a three-hour period using the same system as on July 8. The PDCH was released as an aerosol spray at an average rate of 2.41 g/s, about 1/7 the release rate on July 8. A background concentration for PDCH of 26 ppt was removed from the observed concentrations. The transit time for the observed plume was six hours. The transit time of the simulated plume in CALPUFF using both P-G and similarity dispersion coefficients also was six hours. Therefore, six-hour average concentrations were used in this part of the analysis.

The six-hour average modeled and observed concentrations for the 100-kilometer arc are shown in Figure 14. As with the July 8 study, the monitoring did not capture the entire plume at 100 kilometers, although the peak appears to be a little better defined, with an observed maximum at receptor 18. There were no aircraft flights to assist in determining the western extent of the plume. The simulated plumes using PG and similarity dispersion agree with each other very well, but, as with the July 8 results for the 100-kilometer arc, the peaks are more than twice the magnitude of the observed plume and the simulated lateral dispersion is less than the observed plume. .

As with the 100 kilometer arc for the July 8 study, the question remains - why do the simulated plumes have higher central maxima and narrower dispersion. With a more sophisticated modeling system, Moran and Pielke (1995a,b) encountered similar differences in their examination of the July 8 simulation at 100 kilometers, and they could not explain to their satisfaction why their dispersion model was not able to more closely represent the observed dispersion patterns at the receptor arcs.

4.6.4 1992 Project MOHAVE Tracer Study

In this investigation (Vimont, 1998), the CALMET/CALPUFF modeling system's simulation of tracer gas dispersion was compared with field measurements collected during the 1992 summer intensive monitoring period of Project MOHAVE. The Project MOHAVE tracer monitoring sites used in this analysis were at Dolan Springs (DOSP), Las Vegas Wash (LVWA), Meadview (MEAD), and Overton Beach (OVBE), (Figure 15). The tracer was released from the stack of the Mohave Power Plant (MOPP) in direct proportion to the time-varying sulfur dioxide emissions. The tracer was collected in 24-hour samples starting at 7 AM Mountain Standard Time (MST) at each of the sites, except at MEAD which had two 12-hour samples with start times of 7 AM and 7 PM MST. The monitoring network is not well suited for rigorous model evaluation as it is too sparse. Ideally, a network designed for model evaluation would have arcs of monitors placed at distances of interest (as in the studies mentioned in previous sections of this report). Also, it would be of interest to have sufficiently short sampling intervals so that passage of tracer past and along an arc could be analyzed.

The meteorology is strongly influenced by the east-west river canyon that runs from Las Vegas Wash and past Meadview. The Colorado River sharply turns south at Las Vegas Wash along a north-south transect that connects Las Vegas Wash with the location of the Mohave Power station. Upper air wind measurements were available from three radar profiles located at the Mohave Power Plant (MOPP), Meadview (MEAD), and Truxton (TRUX); RASS temperature profiles were available at MOPP, (Figure 14). Twice-daily balloon soundings (winds and temperature) were available from Dolan Springs (DOSP). Since CALMET requires both winds and temperatures at each upper air station, it was necessary to generate temperature profiles for the radar wind profiles collected at MEAD and TRUX. These were constructed by linear interpolation in time using the temperature profiles at DOSP (DOSP is closer in elevation to MEAD and TRUX, whereas MOPP is 600 to 800 m lower in elevation). The radar winds were reported in both a high resolution mode, and a low resolution mode. The high-resolution data does not extend as high, but provides more details. Thus the high-resolution data were combined with the low resolution data before processing by CALMET.

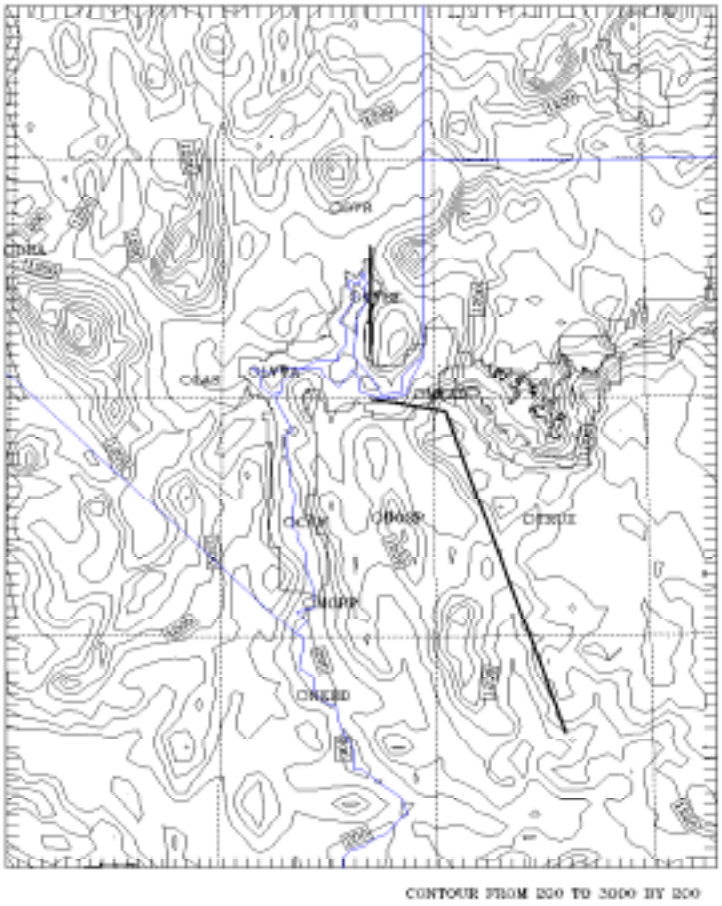
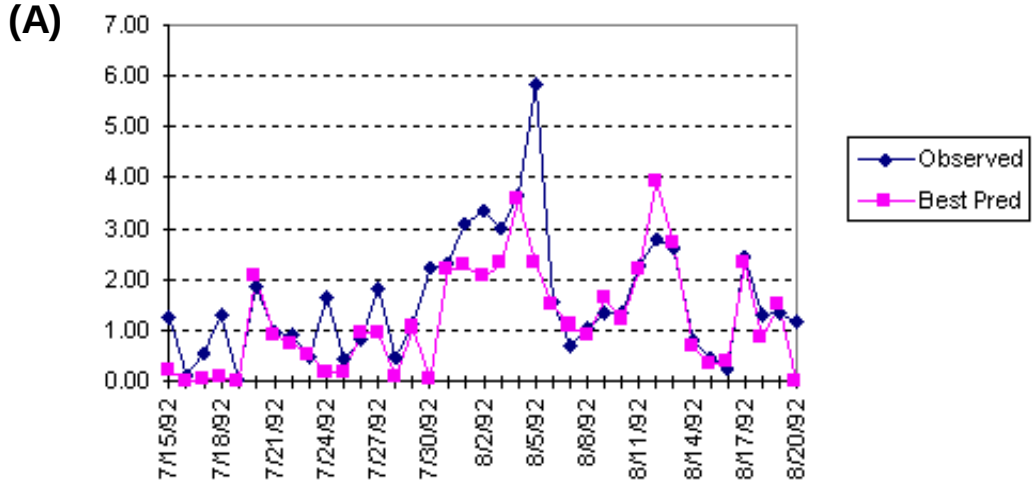


Figure 15. The Project MOHAVE tracer field study collected tracer samples at Dolan Springs (DOSP), Las Vegas Wash (LVWA), Meadview (MEAD), and Overton Beach (OVBE). The tracer was released from the stack of the Mohave Power Plant (MOPP). The bold solid lines are the CALMET "barriers" that were employed in developing the CALMET analyses.

A number of diagnostic model runs were made, and some general conclusions were reached. The initial CALPUFF runs with no complex terrain treatment grossly underestimated concentrations, especially at the nearest monitoring site at DOSP. The inclusion of the partial plume path adjustment terrain treatment option in CALPUFF improved the correspondence of the calculated concentration with the measurements, which is not surprising since several of the monitoring sites are more than 600 m higher than the base of the Mohave Power Plant stack. It was also concluded that the monitoring sites were too sparse to be used in a conventional manner. The narrowness of the dispersing plume meant that even a very small shift of a few kilometers in the plume position would result in major (in some cases orders of



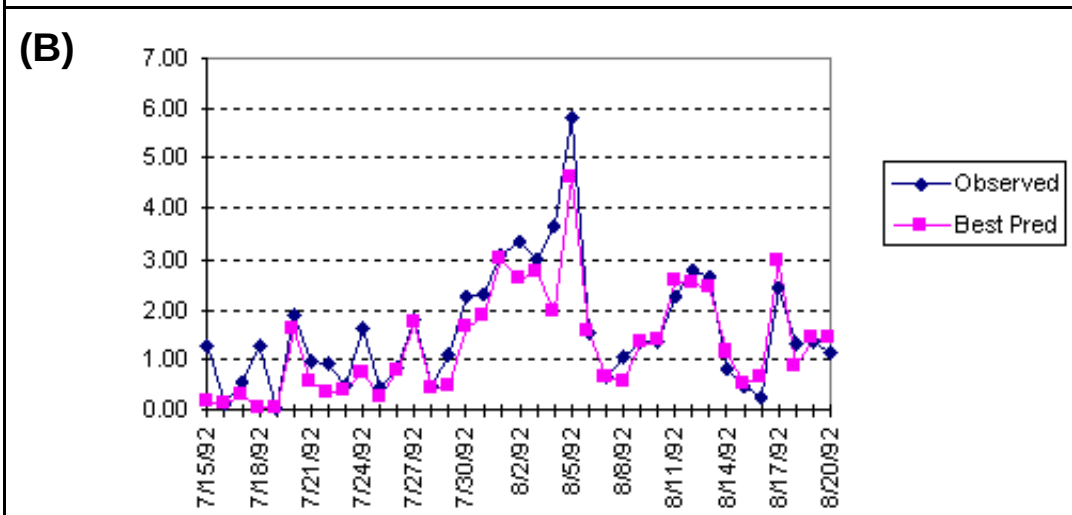


Figure 16 Tracer concentrations (femtoliters/liter) predicted and observed for the Las Vegas Wash (LVW) monitoring site, (A) are results obtained without use of barriers, and (B) are results obtained using barriers in the CALMET processing.

magnitude) changes in the simulated concentration values. To counter this deficiency, eight receptors were placed 15 km around each monitor's location. The estimated concentration in closest correspondence to that measured was selected for use in assessing model performance.

When CALMET was initialized using the wind and temperature profiles from all three sites, the CALPUFF tracer simulation results were in poor agreement with the observations. It was determined that the $1/(\text{distance})^2$ initialization used in CALMET was not capturing the fact that each of these sites were located in very unique settings. The TRUX profiler is located at a high elevation in a valley with a southwest to

northeast orientation. The MOPP profiler is located in the Colorado River Valley, which encompasses the DOSP location and continues up to the MEAD monitoring site. The MEAD site is located near the west entrance of the Grand Canyon, which runs east-west. CALMET was modified to allow 'barriers' to be placed in the Step 1 initialization process, so that the influence of observations could be limited to better reflect the unique settings of the profiler locations. The bold solid lines in Figure 15 show the placement of the barriers. Figures 16a and 16b illustrate the differences seen in the simulated concentrations without and with the barriers in the CALMET processing. The correspondence of the simulated tracer concentrations with those monitored seems to have been improved by allowing the barriers to influence the development of the CALMET Step 1 wind fields.

4.7 Comparisons of CALPUFF With ISC3

A sensitivity study comparing the ground level concentration values of CALPUFF (Scire et al, 1995b) with those of the Industrial Source Complex Short Term (ISC3) model (U.S. EPA, 1995c) for steady state and nonsteady state conditions was performed. The study (U.S. EPA, 1998; Eckhoff and Coulter, 1998) was divided into two parts. First, specific CALPUFF model input settings were tested for the best setting for emulating ISC3 under steady-state conditions. In the second part, the same input settings were then used to compare CALPUFF to ISC3 results under nonsteady state conditions.

For the first part of the study, CALPUFF (4.0) was compared with the latest version of ISC3 (Version *96113*). ISC3 was implemented in the 'Regulatory Default' mode and the input file for CALPUFF was configured so as to emulate ISC3 as closely as possible. Point sources were simulated for rural environments free of obstacles and with stack heights of 2 m, 35 m, 100 m and 200 m above ground level. Meteorological data sets were synthesized with fixed meteorological conditions (Pasquill-Gifford stability category, wind speed, and mixing height) and were of duration estimated to be sufficient to advect CALPUFF's puffs to the edge of the domain. A line of 62 receptors out to 100 km was placed along the 360° radial, aligned with the transport wind flow, and spaced at increasing intervals from the source.

For each pair of model runs (CALPUFF and ISC3), a residual concentration was computed at each of the 62 receptors. From the 62 residuals (one for each receptor), a mean, standard deviation (σ_R), and sum of residuals squared were computed. The mean provides an indication (sign) of bias along the receptor radial. The variance of the residuals provides general indication of the variance along the receptor radial. Because many of the absolute residuals were quite small, the sum of the residuals squared was also computed to provide a relatively robust indicator of accord along the receptor radial. A Fractional Bias equation, FB = 2*(CALPUFF-ISC)/(CALPUFF+ISC) was also computed. The steady state agreement between CALPUFF and ISC3 was very good. Minimum and maximum fractional bias values of -0.18 and 0.06 are an

indication of how well CALPUFF, with the slug model invoked, can emulate ISC3 in a steady-state environment using point source input data.

Having confirmed that the dispersion algorithms within CALPUFF do emulate quite well those within ISC3, the second part of the study was to compare modeling results when the meteorological conditions were allowed to varying each hour. Hourly meteorological data processed for input into ISC3 were selected from three stations to simulate three climatically different regions of the United States: 1991 Boise, Idaho; 1990 Medford, Oregon; and 1964 Pittsburgh, Pennsylvania. Each set contains a year of hourly averaged values of wind speed, wind direction, ambient temperature, stability class, and mixing heights. In these simulations, wind fields were not generated for the CALPUFF simulations. Instead, the ISC option was used, which allows CALPUFF to operate using meteorological data processed for input to ISC3. This means that the meteorology for these simulations is assumed to be everywhere the same, over the entire CALPUFF computational domain. This admittedly artificial assumption for the CALPUFF meteorology at least insured that the only reason for differences in the modeling results, resulted from the fundamental differences in the treatment of transport between a plume and a puff model.

The Boise data were selected because they were obtained in a river valley which has highly directional wind flows. More than 33% of the recorded winds have a northwesterly component and more than 33% of the winds have a southeasterly component with the majority of those winds having speeds greater than two m/s. Some of the modeled puffs were expected to be transported directly to the most distant receptors. The Medford data were selected because they were obtained in an area surrounded by mountains with a high number of calm wind hours. In 1990, 22% of the Medford Oregon winds were calm winds (<1 m/s). This compares to the average of 6.5% occurrence of calm winds for the other two sites. During calm wind events, CALPUFF calculates concentrations while ISC3 does not calculate concentrations. ISC3 treats the hour as missing when determining concentration averages. There was an expectation that there would be large differences in concentration averages because of the high number of calm winds. The Pittsburgh data were selected because the recording site is located on an open plain above a river valley and that the data have been used as a standard test set for a number of years. The wind directions and wind speeds are fairly well distributed, although there is a tendency for southwesterly winds.

The main receptor placement consisted of 15 rings of 36 receptors each, with receptors spaced every 10 degrees starting at 360 degrees. The rings were spaced at distances of 0.5, 1, 2, 3, 5, 10, 15, 20, 30, 50, 100, 150, 200, 250, and 300 km from the

Table 8. Characteristics for point sources used in the CALPUFF/ISC3 comparisons.

Stack Height (m)	Emission Rate (g/s)	Exit Velocity (m/s)	Stack Diameter (m)	Exit Temperature (K)
2	100	10.0	0.5	300
35	100	11.7	2.4	432
100	100	18.8	4.6	416
200	100	26.5	5.6	425

source. Four point sources (Table 8) were used in these ISC3/CALPUFF comparisons with hourly varying meteorology. For each year of hourly meteorology, and for each of the 15 rings of receptors, the highest and second-highest concentration was determined for four averaging times (1-hour, 3-hour, 24-hour, and annual) for each model. It was anticipated that some differences would be seen in the simulated maxima, since ISC3 ignores hours with wind speed less than or equal to 1 m/s (calms), for which CALPUFF continues to process, and because ISC3 can not treat the consequences of a flow reversal between hours, a situation easily interpreted by a puff model. Even though such differences were anticipated, the magnitude of these differences, and sensitivity to release height was not known.

As a case study, a ten-hour period was examined to determine the cause of large differences detected in the concentrations simulated by the two models using the Boise meteorological data. The large differences were detected 5 to 15 km downwind from the 2 -m point source for Hour 62 of the simulation, following a 4 hour period of calm winds and then a wind reversal. Figure 17a illustrates the distribution of the pollutant mass, in which emissions from particular hours, preceding Hour 62 have been depicted so that it is possible to see how the sequence of events preceding Hour 62 has affected the results seen. Starting with Hour 52 there was a 5-hour period for which the winds were from the east-southeast. Then there was a period of 4 hours of calm winds, which was followed by a 180-degree wind shift for 2 hours. Thus the pollutant mass which had started out moving towards the west-northwest, for the last two hours is seen moving back towards the southwest. As illustrated in the figure, the result is that a broad area upwind (in terms of Hour 62) is being affected by emissions that were released during Hours 52-60. The subsequent superposition of all of the puffs is shown in Figure 17b. For receptors 5 to 12 km southwest of the stack, the superposition of all the puffs results in concentration values that are more than a factor of two greater than that simulated by ISC3 for Hour 62. During one of the calm hours, Hour 57, the emissions were simulated to penetrate a low-level inversion. CALPUFF

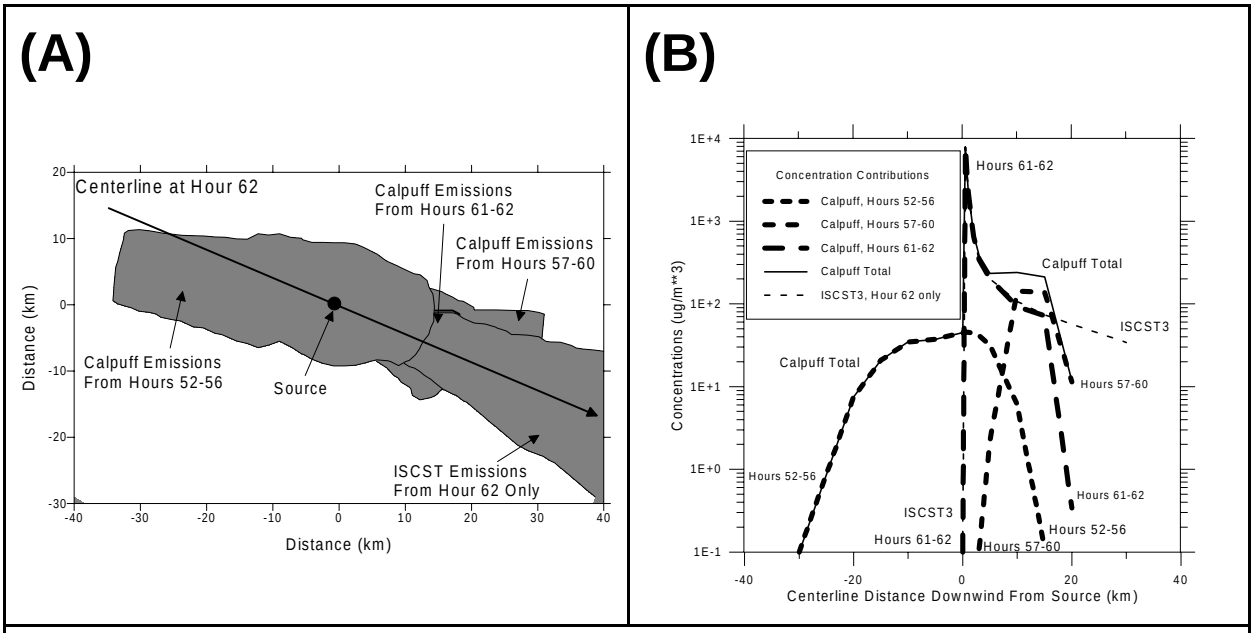


Figure 17. Case study of a ten-hour period of simulated dispersion by CALPUFF. (A) depicts impacts for Hour 62, showing contributions from emissions released prior to Hour 62, (B) depicts centerline concentrations from CALPUFF and ISC.

tracked the puffs and the subsequent fumigation to the ground once the inversion grew to encompass the puffs which were aloft.

The ten-hour example just described is illustrative of how differences can arise. It also serves notice that large differences can arise, and that these differences may arise from a rather complicated history of events. Both the sequence of events, as well as the dispersiveness of the atmosphere are important in understanding the puff simulation results. Unlike in plume simulations, the concentration results obtained for a given hour are unlikely to be understood simply by knowing the meteorology for the given hour. The sequence of the meteorological conditions leading up to the hour in question may be all important.

For each of the three sites, the results for each averaging time were summarized by plotting on a common graph the percent difference, PD = 100(C-I)/I, where C equals the highest (or second-highest) CALPUFF concentration along a receptor ring, and I equals the highest (or second-highest) ISC3 concentration along the same receptor ring for the given averaging time. Figure 18 is an example of some of the CALPUFF/ISC3 comparison results obtained by this sensitivity study. Illustrated in the figure are results for the Medford meteorology, and the results shown are for the 1-, 3-, 24-hour and annual average comparisons of the second-highest concentration values for each of the 15 receptor rings. As each receptor ring is at a prescribed distance, the results illustrate as a function of downwind distance and source-type whether CALPUFF is providing higher (PD>0) or lower (PD<0) concentrations than ISC3. The Medford

meteorological data had the highest occurrence of calm wind conditions, and some of the largest differences. CALPUFF was seen to provide concentration values greater than ISC3, for this site for all averaging times. It is instructive to note that CALPUFF can produce nonzero concentration values at the base of an elevated point source release (when flow reverses and pollutants previously released are transported back towards the source). ISC3 can never produce such an effect. It is also instructive to note that CALPUFF can yield much greater concentrations than ISC3 at most any distance downwind and for most any averaging time. The exact timing and distance downwind of such occurrences is dependent on the sequence of meteorological events, but typically can occur whenever there is a period of calm winds of extended length (say more than three hours in duration).

Figure 19 provides a sense of the differences to be seen between sites. Here annual averages are compared for each site. Typically, the greatest differences seen between the two models are seen in the shorter averaging times. The comparisons of the annual averages most clearly illustrate that as release height increases, CALPUFF tends to increasingly provided higher concentration impacts in comparison to ISC3. Also the comparisons of the annual averages best illustrate the occurrences of nonzero concentration values being simulated by CALPUFF and the lack thereof by ISC3. The effect on the model simulations and resulting comparison of concentration values of the high incidence of calm wind conditions (~23%) at Medford is apparent. The Pittsburgh and Boise meteorological data had similar incidences of calm wind conditions (7% and 6% respectively), but the Boise data was highly directional, with 33% of the wind towards the southeast and 33% of the winds towards the northwest (suggestive of high incidences of flow reversals). Thus it is that the Boise comparisons show CALPUFF yielding higher percentage difference in the annual averages than those seen using the Pittsburgh meteorological data.

In the above comparisons discussed, it is important to remember that no terrain effects on the meteorology were modeled (other than that which is inherent in the climatology of the surface weather observations). Hence, the percentage differences seen could have occurred at any of the sites, given the correct sequence of meteorological events. In this sensitivity analysis, one year of data was used from each site. The site-to-site differences is seen to be large. In the comparisons to be discussed in the next section, several years of data are used from one site.

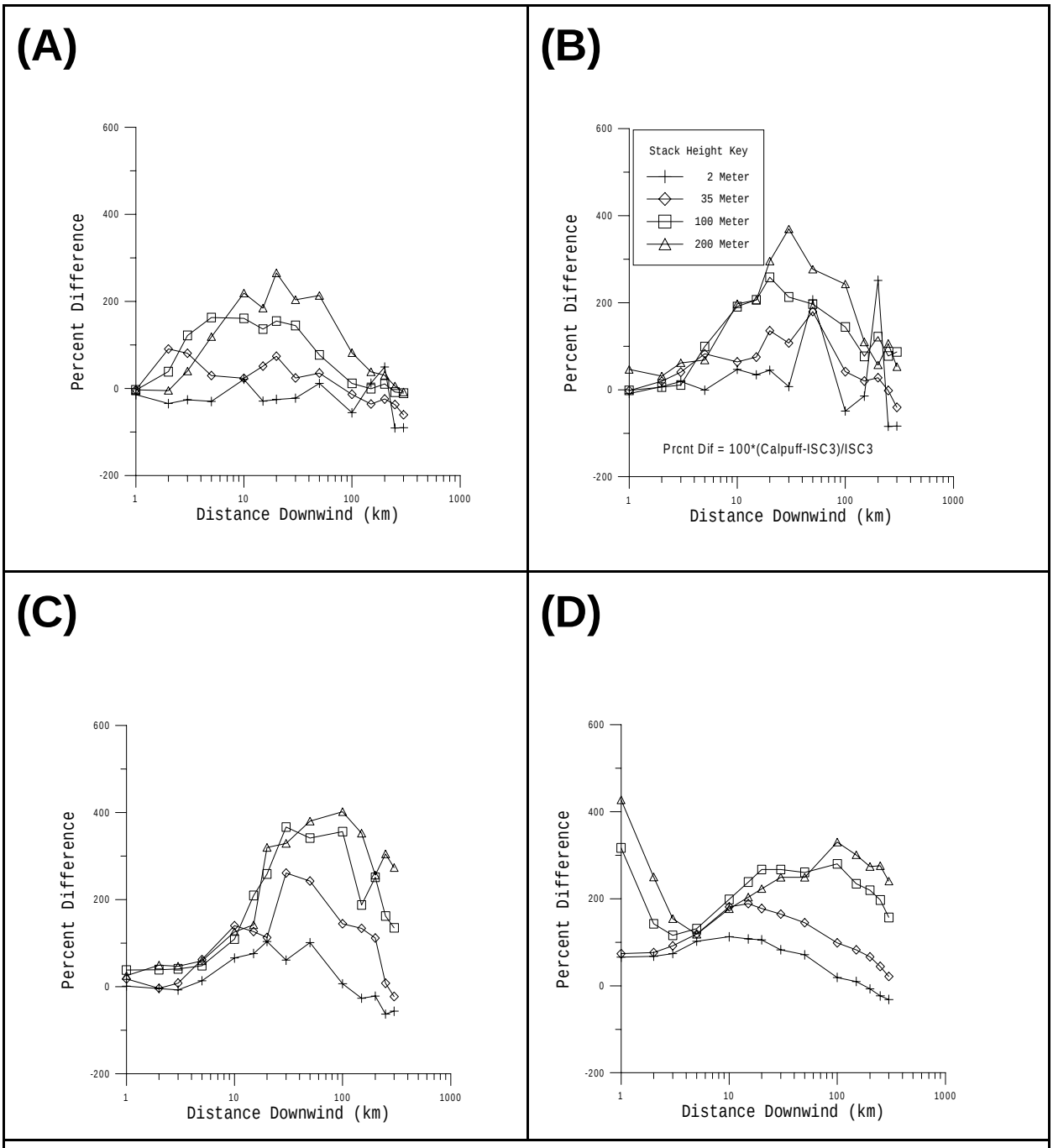


Figure 18. Percent differences (CALPUFF versus ISC3) as a function of downwind distance for the second-highest concentrations; (A) 1-hr, (B) 3-hr, (C) 24-hr, and (D) annual averages. Data are for Medford, Oregon.

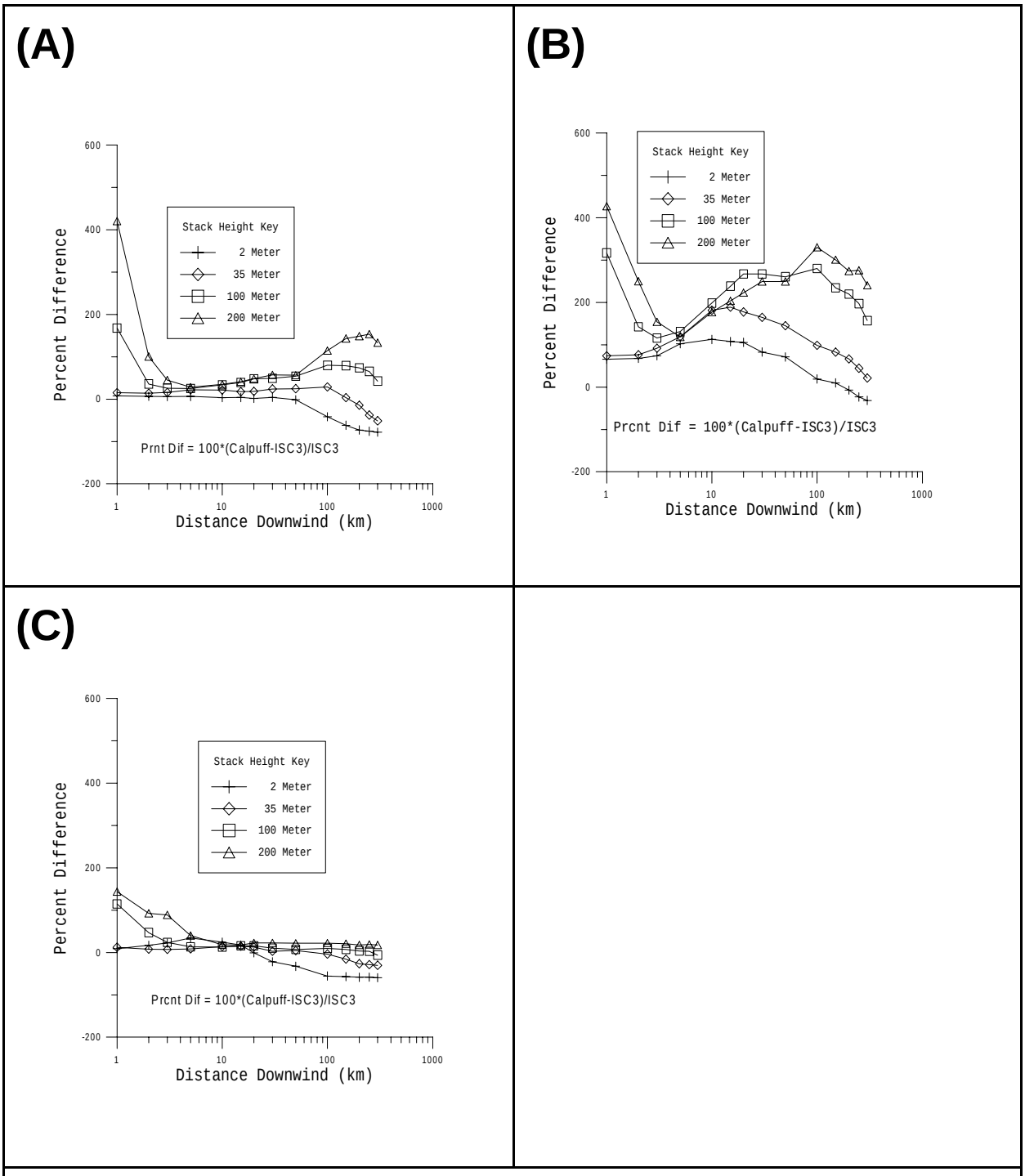


Figure 19. Percent differences (CALPUFF versus ISC3) as a function of downwind distance for the annual average: (A) Boise, (B) Medford, and (C) Pittsburgh.

4.8 CALPUFF SCREEN

By far, one of the most demanding tasks in performing refined puff model simulations is to successfully develop a valid time and space varying characterization of the meteorological conditions for use by the CALPUFF puff dispersion model. The processors that format and organize the input data to CALMET are not presently user-friendly and demand strong computer skills. Often special custom routines are needed to format available data into the acceptable formats for use by CALMET. Even if the logistics of manipulating the data were simplified, developing realistic characterizations of the time-varying three-dimensional wind fields will always require specialized skills. Developing mesoscale and microscale meteorological characterizations requires having not only the specialized understanding of micrometeorological wind effects, but also the experience and expert judgement to know when a characterization developed by the meteorological processor is unreasonable. Furthermore, to review and critique the CALMET results requires strong computer skills for visualization of the CALMET results, or for listing out for special inspection portions of the CALMET results.

In this section, we summarize the results from a study in which a methodology was tested whereby CALPUFF could be used with a simplified set of meteorological data, for the purpose of providing screening estimates of concentration and deposition impacts (U.S. EPA, 1998b). The methodology was tested in two ways: 1) five years of hourly meteorology were used to develop data for assessing the year-to-year variability, and 2) one year of hourly meteorology was fully processed through CALMET to assess whether the screening methodology devised did indeed provide concentration impacts greater than would be developed using a fully developed set of meteorology.

4.8.1 Screening methodology

As a design goal, it was our intention to minimize the effort needed to create the meteorological input for use by CALPUFF. CALPUFF has a built-in mode whereby it can use the meteorological data file generated by PCRAMMET for the Industrial Source Complex Short Term (ISCST3) model, thus bypassing the need to run CALMET.

The following approach was devised for running CALPUFF in a screening mode to estimate ground-level concentrations over a large area:

1) generate five years of ISCST3 input meteorology using PCRAMMET,

2) generate an ISCST3 control file and use the ISC2PUF conversion program to create the CALPUFF control file,

3) use the CALPUFF Graphical User Interface (GUI) to finalize the CALPUFF control file before running the CALPUFF model,

4) run CALPUFF with the ISCMET.DAT data option, and

5) pick the maximum concentration for each pollutant, for each distance and averaging time modeled (see discussion below on receptor placement).

Generating ISC3 input meteorology

PCRAMMET can be used to generate the meteorological data files for CALPUFF. Using hourly surface observations and twice-daily mixing heights, PCRAMMET computes atmospheric stability in the form of Pasquill-Gifford (PG) categories and rural and urban mixing heights. These data, along with the wind direction, wind speed, and temperature, are read directly by CALPUFF without any modification to the data file. It is recognized that this characterization of the meteorology will not vary spatially as in a refined modeling effort, and the consequent differences will be significant as the terrain becomes more rugged and complicated. As is known by those experienced in puff dispersion modeling, one can make conservative choices and assumptions, but it is difficult to guarantee that the results obtained will always be more conservative (but not onerously so) than that derived using fully developed time and space varying meteorological input data. In order to encourage the resulting concentration estimates to be higher than would be obtained using a refined set of meteorology, we have made conservative assumptions as to how the receptors will be placed, and which concentration values will be selected for use.

To perform dry deposition calculations, the surface roughness, friction velocity, and Monin-Obukhov length are required. These parameters can be computed by PCRAMMET and written to an output file for use. In order to estimate these additional parameters, several additional input values are required by PCRAMMET, including: surface roughness at the site where the wind measurements are taken (usually an airport), surface roughness at the site where the model is to be applied, noon-time albedo, Bowen ratio, and fraction of the net radiation absorbed by the ground.

For the test results to be discussed, we applied the screening methodology to the region about Oklahoma City depicted in Figure 12. We had previously developed the CALMET terrain and land-use files as discussed in Section 4.6.3. A surface roughness length at the measurement site (Oklahoma City airport) of 0.10 meters was assumed. An average roughness length of 0.34 meters was computed from the GEO.DAT file created for the entire modeling domain, as well as, an average noon-time albedo of 0.15 and Bowen ratio of 1.00. A value of 0.15 was assumed for the fraction of net radiation absorbed by the ground.

ISC3 control file settings

Using this proposed methodology, the control file and meteorology input can be created as if preparing for an application of the ISCST3 dispersion model. This approach has the advantage that many dispersion modelers are familiar with both the meteorological data and control file structures. The rural dispersion coefficients with the regulatory default settings were selected, which include use of stack-tip downwash, buoyancy induced dispersion, final plume rise, default wind speed profile exponents, and default vertical potential temperature gradient. Averaging times for the model runs were 1-hr, 3-hr, 24-hr, and annual averages.

A polar grid was used to define the receptor locations. CALPUFF does not accept a polar grid directly. Receptors must be a subset of the CALPUFF computational domain (which is a subset of the meteorological domain), i.e., a Cartesian grid, or they must be discrete receptors. The ISC2PUF program can convert a polar grid and associated terrain to discrete receptors with terrain. The ISC2PUF limits the number of receptors that can be processed to 1200. Hence very large applications, may require two or more runs of this program followed by merging the results into a single CALPUFF control file.

For the test results to be discussed, the following polar receptor networks were used:

Distance (km)	Receptor Spacing Along Each Ring	Number of Receptors	Distance Along Ring Between Receptors
1, 2, 3, 5, 10, 15, 20, 30, 50	every 10°	324	0.2 - 8.7 km
75, 100, 150, 200, 250, 300	every 5°	432	6.5 - 26.2 km

These two polar networks result in 756 receptors, well below the limit of about 1200.

CALPUFF control file settings

The CALPUFF system includes a program (ISC2PUF) that translates an ISCST3 control file to a CALPUFF control file. The converted control file must be edited prior to running CALPUFF. This can be accomplished in one of two ways: using a text editor to modify the control file directly, or using the CALPUFF graphical user interface (GUI) to guide the user through the options.

The CALPUFF control parameters that must be set by editing the ISC2PUF generated CALPUFF control file include: the use of puffs or slugs, and the type of dispersion - Pasquill-Gifford or internally-computed σ's. Also to be considered are the pollutants of interest, modeling of chemical transformations, and modeling dry deposition processes.

Pollutants: The transformation pathways for five active pollutants are treated by the MESOPUFF II scheme in CALPUFF: SO_2, $SO_4^{=}$, NO_x, HNO_3, and NO_3^{-}. Since haze and visibility are of concern in areas such as national parks, CALPUFF is most likely to be applied to model sulfates and nitrates. For the testing results to be presented, the focus was on SO_2 and $SO_4^{=}$.

Slug model versus puff model: The slug model was used, with the set of default options for slugs.

Dispersion coefficients: Pasquill-Gifford dispersion coefficients for both the screening and refined CALPUFF modeling were used.

Concentration estimates: CALPUFF was run initially for both the refined (one year) and screening modes (five years) without any chemistry or deposition. This provided 'baseline' concentration estimates without the effects of chemistry and deposition. CALPUFF was then run for one year with chemistry and deposition activated.

Chemical transformations: There are two transformation options in CALPUFF: 1) MESOPUFF II mechanisms and 2) a file with a diurnal cycle of transformation rates. The MESOPUFF II option requires relative humidity as one of the input variables for chemical transformations. However, this variable was not present in the current ISCST3 meteorological data file. The second mode requires a file of diurnal transformation rates specified by the user. In this mode, transformation rates are spatially uniform but provides for some temporal variability. The second method, with the file of transformation rates, was used in this modeling effort.

For the test results to be discussed, we used a 3.0 %/hr transformation rate for daylight hours and 0.2 %/hr at night for the SO_2 to $SO_4^{=}$ transformation. These rates were used for both CALPUFF refined and screening modes. The daytime period was defined as 0700 to 2000 LST, which biases the daylight period towards a summer day and should result in production of more sulfates.

Dry deposition: In CALPUFF, deposition can be modeled as either particle or gas, depending on the pollutant. To estimate deposition, the surface roughness length, surface friction velocity, and Monin-Obukhov length are estimated by CALMET and vary temporally and spatially when CALPUFF is run in a refined mode. In the screening mode, though, these variables are specified for each hour on the 'extended' data record in the meteorological file. PCRAMMET was run to generate these extended data records for the CALPUFF screening mode.

To compute dry deposition of particles or gases, CALPUFF requires one of the following: 1) a file of the diurnal variation of deposition velocities for each pollutant modeled, or 2) specification of the mass mean diameter, geometric standard deviation,

and number of particle size intervals to evaluate the effective particle deposition velocity. For the latter option, CALPUFF has default parameters for several pollutants, including SO_2 and $SO_4^=$. For this modeling effort, we used the second option with the gaseous SO_2 default parameters and the particulate $SO_4^=$ default parameters.

4.8.2 Year to year variability

Five years of meteorological data were processed through PCRAMMET to create the necessary input meteorology for the CALPUFF screening model runs. Oklahoma City was used for the hourly surface observations and Oklahoma City/Norman for the upper air data. Data from the Solar and Meteorological Surface Observation Network (SAMSON) compact disc (see Appendix C) were used to obtain the hourly surface data. The twice-daily mixing heights were retrieved from EPA's Support Center for Regulatory Air Models (SCRAM) system. The mixing height data on SCRAM restricted the period of choice from 1984 through 1991. Oklahoma City for 1985-1988 were used for this modeling effort. There were no mixing height data for 1989 on SCRAM. The upper air station changed from Oklahoma City to Norman in 1989. Since Norman is only 25-30 kilometers from Oklahoma City, data from Norman for 1990-1991 was used. There were no periods of missing data for Oklahoma City that required filling. There were five 2-hour periods of unfilled mixing heights for the two years of data at Norman. Following EPA guidance, the mixing heights were filled by linearly interpolating between the hours before and after the missing periods to fill in the mixing heights.

The 2-m, 35-m and 200-m point sources listed in Table 8 were used in this assessment. The rings of receptors (as listed earlier) were placed around each source, and the five years of ISC-type meteorology were processed by CALPUFF. For this assessment of year to year variations, inspection was made of the variations seen in the highest 1-hr, 3-hr, 24-hr and annual simulated SO_2 concentration, along each receptor ring. Table 9 summarizes the maximum and minimum value seen for C/Cavg, where C is the maximum concentration seen in any one year along a receptor ring for a particular source and averaging time, and Cavg is the average of the five values seen for this source along this ring for the five years simulated. Rather than list the results separately for each of the 15 receptor rings, we have compiled the results for three groups, with group 1 having four receptor rings at distances 1-, 2-, 3-, and 5-km; group 2 having five receptor rings at distances 10-, 15-, 20-, 30-, and 50-km; and group 3 having six receptor rings at distances 75-, 100-, 150-, 200-, 250-, and 300-km. These three groups subjectively relate to near-field impacts (group 1), mesoscale impacts (group 2), and longer-range impacts (group 3).

Table 9. Summary for three hypothetical sources and for four averaging times in the variation seen in the ratio C/Cavg, where Cavg is the average of the 5 maximum SO_2 concentrations for a receptor ring and averaging time, and C is the maximum SO_2 concentration simulate during one of the five years. The variations listed in C/Cavg reflect both variations seen with the distance range and variations over the five year period of the analysis.

		2-m Source		35-m Source		200-m Source	
1-Hour	Range	Min	Max	Min	Max	Min	Max
	1-5 km	0.79	1.52	0.89	1.14	0.68	2.05
	10-50 km	0.65	1.86	0.76	1.47	0.47	2.32
	75-300 km	0.56	1.66	0.72	1.23	0.44	1.74
3-Hour	1-5 km	0.83	1.26	0.89	1.21	0.80	1.49
	10-50 km	0.58	1.43	0.80	1.48	0.58	2.19
	75-300 km	0.59	1.87	0.60	1.52	0.71	1.51
24-Hour	1-5 km	0.85	1.16	0.80	1.26	0.75	1.29
	10-50 km	0.64	1.55	0.79	1.45	0.77	1.60
	75-300 km	0.61	2.13	0.59	1.52	0.68	1.41
Annual	1-5 km	0.90	1.11	0.88	1.13	0.83	1.26
	10-50 km	0.88	1.13	0.90	1.12	0.88	1.17
	75-300 km	0.81	1.29	0.89	1.25	0.86	1.17

As averaging time increased, there was less variation between years. For instance, for the 75 to 300 km receptor rings, the ratio of the one-hour maxima to the five-year average one-hour maxima varied from 0.45 to 2.30. Whereas the ratios for the annual-averages ranged from 0.80 to 1.30. For these results it is concluded that we might expect variation in the maximum concentrations of at least 20 to 30 percent.

4.8.3 SO_2 concentrations

One of the comments received at the Sixth Modeling Conference was the perception that the Phase 1 (Level I) screening procedure (U.S. EPA, 1993) was too conservative to be of practical use. Thus a second part of developing a new screening methodology was to test the results obtained with the new methodology with those that would be obtained in a refined modeling analysis. Table 10 summarizes the maximum

Table 10. Summary for three hypothetical sources and for four averaging times in the variation seen in the ratio Cs/Cr, where Cs is the SO_2 maximum concentration for a receptor ring and averaging time using CALPUFF with ISC meteorology, and Cr is the second highest SO_2 concentration simulated for the same ring using CALPUFF with CALMET meteorology. Results were generated for only 1990, so the minimum and maximum values for Cs/Cr, reflect variations seen over the receptor rings included in the range.

		2-m Source		35-m Source		200-m Source	
1-Hour	Range	Min	Max	Min	Max	Min	Max
	1-5 km	0.59	1.31	1.03	1.51	0.86	3.07
	10-50 km	0.74	1.30	0.87	1.86	1.27	3.29
	75-300 km	0.99	3.20	1.55	2.09	0.68	1.09
3-Hour	1-5 km	0.82	1.42	1.02	1.08	0.77	1.56
	10-50 km	0.88	1.43	0.80	1.53	0.72	2.71
	75-300 km	0.96	3.89	1.17	3.35	0.73	1.04
24-Hour	1-5 km	0.95	1.00	0.86	0.98	0.73	0.99
	10-50 km	0.88	1.21	0.86	1.28	0.92	1.54
	75-300 km	1.57	4.48	1.11	2.55	0.96	1.50
Annual	1-5 km	1.28	1.37	1.41	1.47	0.58	1.13
	10-50 km	1.49	2.28	1.59	2.29	1.16	1.30
	75-300 km	1.82	3.47	1.85	2.89	1.07	1.27

and minimum value seen for Cs/Cr, where Cs is the maximum SO_2 concentration seen for 1990 along a receptor ring for a particular source and averaging time using the CALPUFF with ISC meteorology (a screening estimate), and Cr is the second-highest SO_2 concentration seen along the same receptor ring resulting from using the CALPUFF with fully developed CALMET meteorology (a refined estimate). Comparing the CALPUFF screening estimate of the maximum concentration along a ring versus the second-highest concentration from a refined model run, provides an assessment of whether the new screening methodology is a conservative screening estimate.

In each of the three ranges, instances can be found where the maximum SO_2 concentration obtained using ISC meteorology as input to CALPUFF (screening estimate), Cs, was not as high as the second-highest concentration obtained from using CALMET meteorology as input to CALPUFF (refined analysis), Cr. It is important to

remember that these comparisons are between the maximum screening estimate found anywhere along the receptor ring and the refined modeling results for the maximum of the second-highest concentrations found anywhere along the ring. If an actual source were being modeled for a particular Class I area, we would anticipate that it is quite likely that the refined model's estimate of the highest of the second-high concentrations for the segment of a receptor ring passing through the Class I area would be lower than what would be found anywhere around the receptor ring.

For the receptor rings at 75-km to 300-km, the Cs/Cr ratios for the 1-hour comparisons range from 1.00 to 3.0 for the 2-m source, and from 0.70 to 1.10 for the 200-m source. As averaging time increases, the screening estimate of the maximum concentration tends to be greater than the second-highest concentration obtained in the refined analysis. The IWAQM concludes the new screening method (ISC meteorology as input to the CALPUFF model) provided conservative estimates of maximum SO_2 concentration values, that were not overly conservative for practical use. Although there is a finite possibility for the refined analyses to develop higher concentration impacts, the likelihood of this result is low for specific source-receptor pairings.

4.8.4 $SO_4^=$ concentrations

Table 11 summarizes the maximum and minimum value seen for Cs/Cr, where Cs is the maximum sulfate concentration seen for 1990 along a receptor ring for a particular source and averaging time using the CALPUFF with ISC meteorology, and Cr is the maximum sulfate concentration seen along the same receptor ring resulting from using the CALPUFF with fully developed CALMET meteorology. In each of the three ranges in Table 11, instances can be found where the screening estimate for sulfate concentration, Cs, is not as high as that obtained from the refined analysis, Cr. The 24-hour ambient sulfate concentrations are typically used in long-range haze impact assessments. For the 24-hour averaging time, the 2-m source maximum sulfate concentrations obtained with CALPUFF using ISC meteorology are typically greater than were obtained for this site in 1990 using CALPUFF with CALMET meteorological data. For the 200-m release, the CALPUFF screening estimates are less than that obtained using CALPUFF with CALMET meteorology.

Table 11. Summary for three hypothetical sources and for four averaging times in the variation seen in the ratio Cs/Cr, where Cs is the maximum sulfate concentration for a receptor ring and averaging time using CALPUFF with ISC meteorology, and Cr is the maximum sulfate concentration simulated for the same ring using CALPUFF with CALMET meteorology. Results were generated for only 1990, so the minimum and maximum values for Cs/Cr, reflect variations seen over the receptor rings included in the range.

		2-m Source		35-m Source		200-m Source	
1-Hour	Range	Min	Max	Min	Max	Min	Max
	1-5 km	0.52	0.89	0.80	2.12	0.56	1.72
	10-50 km	0.44	0.73	0.65	1.74	0.72	1.16
	75-300 km	0.76	2.57	0.58	2.11	0.33	0.51
3-Hour	1-5 km	0.42	0.76	0.91	1.02	0.42	1.27
	10-50 km	0.50	0.72	0.38	1.15	0.65	1.55
	75-300 km	0.56	3.25	0.54	2.16	0.25	0.50
24-Hour	1-5 km	0.62	1.04	0.55	0.83	0.30	0.70
	10-50 km	0.61	0.91	0.36	0.50	0.32	1.39
	75-300 km	0.58	3.07	0.38	1.51	0.16	0.33
Annual	1-5 km	1.10	1.17	1.23	1.43	0.47	0.89
	10-50 km	1.20	2.02	1.16	1.52	0.82	0.93
	75-300 km	2.00	3.20	1.50	1.88	0.68	0.80

4.8.5 SO_2 deposition

Table 12 summarizes the maximum and minimum value seen for Cs/Cr, where Cs is the maximum SO_2 deposition seen for 1990 along a receptor ring for a particular source and averaging time using the CALPUFF with ISC meteorology, and Cr is the maximum SO_2 deposition seen along the same arc resulting from using the CALPUFF

Table 12. Summary for three hypothetical sources and for four averaging times in the variation seen in the ratio Cs/Cr, where Cs is the maximum SO_2 deposition for a receptor ring and averaging time using CALPUFF with ISC meteorology, and Cr is the maximum SO_2 deposition simulated for the same ring using CALPUFF with CALMET meteorology. Results were generated for only 1990, so the minimum and maximum values for Cs/Cr, reflect variations seen over the receptor rings included in the range.

		2-m Source		35-m Source		200-m Source	
1-Hour	Range	Min	Max	Min	Max	Min	Max
	1-5 km	0.95	1.29	0.81	0.96	0.33	0.99
	10-50 km	0.69	1.47	0.48	1.16	0.28	1.03
	75-300 km	0.70	1.18	0.85	1.27	0.23	0.62
3-Hour	1-5 km	0.73	0.81	0.73	0.78	0.26	0.60
	10-50 km	0.52	1.06	0.59	0.91	0.27	0.87
	75-300 km	0.70	1.05	0.71	1.47	0.27	0.47
24-Hour	1-5 km	0.65	0.70	0.50	0.55	0.16	0.55
	10-50 km	0.80	1.14	0.55	0.63	0.44	0.62
	75-300 km	1.04	1.25	0.58	1.11	0.41	0.77
Annual	1-5 km	1.16	1.00	0.90	0.99	0.30	0.64
	10-50 km	1.32	1.76	1.14	1.71	0.70	0.91
	75-300 km	1.50	2.54	1.48	2.13	0.89	1.02

with fully developed CALMET meteorology. In each of the three ranges in Table 12, instances can be found where the screening estimate of SO_2 deposition, Cs, is not as high as that obtained from the refined analysis, Cr. For SO_2 deposition, the annual or seasonal average deposition is of most interest. For the lower release heights of 2-m and 35-m, the maximum annual SO_2 deposition obtained with CALPUFF using ISC meteorology are consistently greater than were obtained for this site in 1990 using CALPUFF with CALMET meteorological data. For the 200-m release, the CALPUFF screening estimates of SO_2 deposition are similar to those obtained using CALPUFF with CALMET meteorology.

Table 13. Summary for three hypothetical sources and for four averaging times in the variation seen in the ratio Cs/Cr, where Cs is the maximum sulfate deposition for a receptor ring and averaging time using CALPUFF with ISC meteorology, and Cr is the maximum sulfate deposition simulated for the same ring using CALPUFF with CALMET meteorology. Results were generated for only 1990, so the minimum and maximum values for Cs/Cr, reflect variations seen over the receptor rings included in the range.

		2-m Source		35-m Source		200-m Source	
1-Hour	Range	Min	Max	Min	Max	Min	Max
	1-5 km	3.60	6.79	2.66	4.09	1.20	2.20
	10-50 km	1.39	3.90	1.21	3.43	1.01	1.67
	75-300 km	1.32	2.76	0.94	2.63	0.45	1.04
3-Hour	1-5 km	2.05	3.68	1.54	1.97	0.59	1.31
	10-50 km	1.63	3.77	0.96	1.72	0.96	2.06
	75-300 km	1.21	3.47	0.83	2.26	0.34	0.62
24-Hour	1-5 km	0.93	2.38	0.98	1.06	0.30	0.74
	10-50 km	2.32	2.79	0.78	1.35	0.72	1.38
	75-300 km	1.50	4.50	0.90	1.58	0.31	0.68
Annual	1-5 km	1.41	1.51	1.54	1.90	0.80	1.39
	10-50 km	1.61	2.05	1.54	1.87	1.11	1.37
	75-300 km	1.98	4.07	1.38	2.63	0.81	1.27

4.8.6 $SO_4^=$ deposition

Table 13 summarizes the maximum and minimum value seen for Cs/Cr, where Cs is the maximum sulfate deposition seen for 1990 along a receptor ring for a particular source and averaging time using the CALPUFF with ISC meteorology, and Cr is the maximum sulfate deposition seen along the same arc resulting from using the CALPUFF with fully developed CALMET meteorology. In each of the three ranges in Table 13, instances can be found where the screening estimate of sulfate deposition, Cs, is not as high as that obtained from the refined analysis, Cr. For sulfate deposition, the annual or seasonal average deposition is of most interest. For the lower release heights of 2-m and 35-m, the maximum annual sulfate deposition obtained with CALPUFF using ISC meteorology are consistently greater than were obtained for this site in 1990 using CALPUFF with CALMET meteorological data. For the 200-m

release, the CALPUFF screening estimates of sulfate deposition are generally higher than those obtained using CALPUFF with CALMET meteorology.

4.8.7 Old screen versus new screen estimates

Ambient SO_2 concentrations

In Section 4.7, it was shown that when both CALPUFF and ISC use the ISC meteorology with assumed flat terrain, there was for these comparisons a clear tendency for CALPUFF to develop higher maximum concentration estimates the ISC for all averaging times and for all distances downwind. Whether this will happen for a particular source-receptor pairing, is dependent on whether calms and wind reversal are existent in the proper sequence. The more frequently calm conditions occur for a site, the more likely CALPUFF can develop higher concentration impacts. It is concluded from comparisons results as summarized in Section 4.7 that it would be a misconception to consider the Level I screening estimates for ambient SO_2 concentration values as being overly conservative (i.e., too high). CALPUFF is capable of providing higher SO_2 concentration values than ISC simply due to the fact that calms and wind reversals are not ignored.

Ambient sulfate concentrations

In the IWAQM Phase 1 and Phase 2 recommendations, ambient sulfate concentrations are used in assessing long-range transport haze impacts. And in this context, the 24-hour averages are used (as explained in Section 3) to address the 'regional' nature of the haze assessment. In the Phase 1 recommendations, the screening estimate (Level 1) of sulfate concentration was obtained by multiplying the SO_2 concentration by 1.5 (to account for the difference in molecular weight between $SO_4^=$ and SO_2).

Shown in Figure 20 is a comparison of the 24-hr maximum sulfate concentrations derived using the Phase 1 screening procedure and using CALMET meteorology as input to CALPUFF. The Phase 1 screening procedure is seen to be considerably higher (on the order of 30 times higher) than that derived using CALPUFF. For the 200-m source, The Level 1 screening estimates are seen to be higher than that derived using CALPUFF for receptor rings of 50-km or less. Beyond 50-km, the Level 1 24-hr sulfate concentration estimates are similar to that derived using CALPUFF.

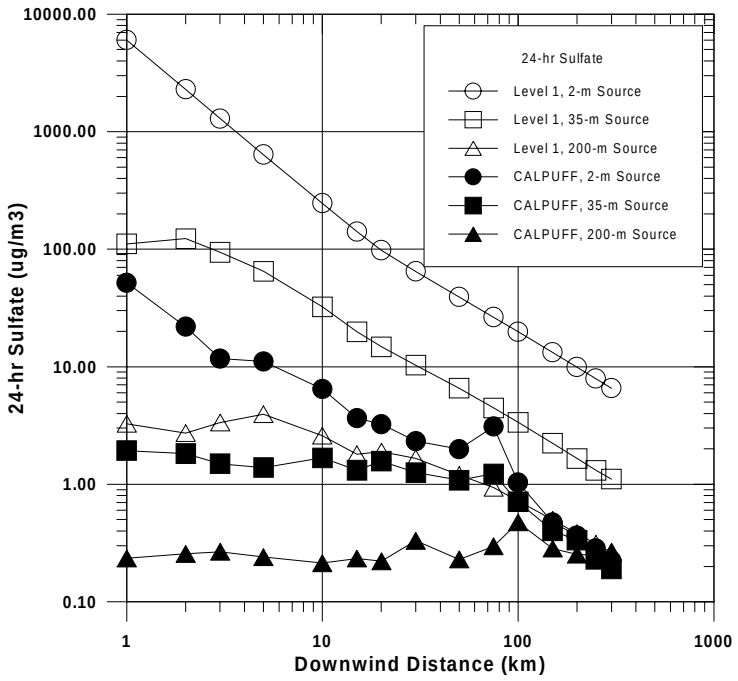


Figure 20. Comparison of Phase 1 Level 1 screening estimates of maximum 24-hour ambient sulfate concentrations versus maximum 24-hour ambient sulfate concentration derived using CALMET meteorology as input to CALPUFF.

Total sulfur deposition

In the IWAQM Phase 1 and Phase 2 recommendations, sulfur deposition is used in assessing air quality related values associated with forest health. In this context, the seasonal or annual averages are used (as explained in Section 3). In the Phase 1 recommendations, the screening estimate (Level 1) of total sulfur deposition flux was obtained by multiplying the SO_2 concentration by an assumed deposition velocity of 0.005 m/s, which was then multiplied by 0.5, since each gram of SO_2 deposited contributes 0.5 grams of sulfur. In the Phase 1 screening estimates, the sulfur deposition was assumed to be mostly from SO_2 gaseous deposition. In CALPUFF we can simulate the dry deposition of both SO_2 and sulfate. The total sulfur flux is then computed as 0.5 times the SO_2 deposition flux plus 0.33 times the $SO_4^=$ deposition flux (to account for amount of sulfur provided by $SO_4^=$ and SO_2).

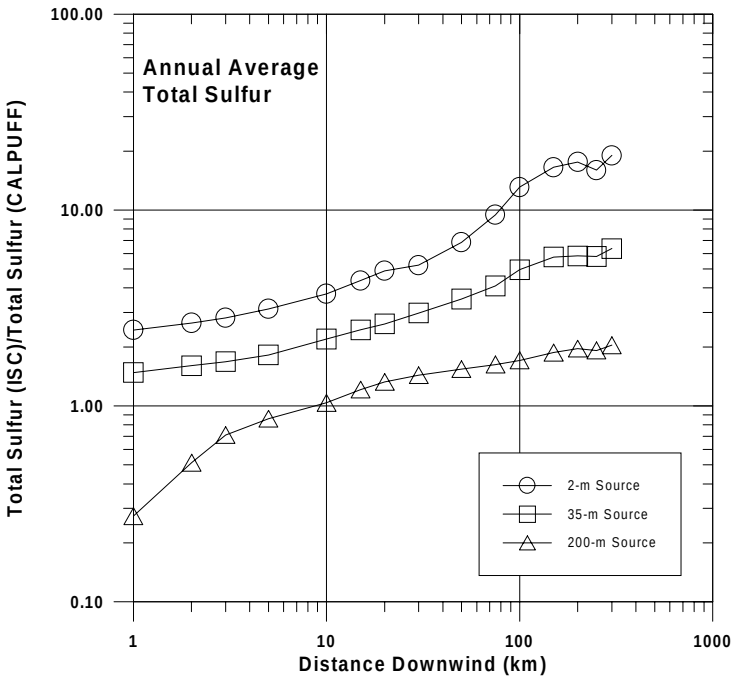


Figure 21. Comparison of annual average total sulfur flux as derived using the Phase 1 Level screening procedure and using CALMET as input to CALPUFF. Shown in the figure is the ratio formed by dividing the Level 1 result by the CALPUFF result.

Shown in Figure 21 is a comparison of the annual average total sulfur flux, derived using the Phase 1 Level 1 screening procedure and using CALMET as input to CALPUFF. In Figure 21, the comparison is shown by dividing the Phase 1 screening estimate by the CALPUFF result. For the more distant receptor rings, the Phase 1 screening procedure is seen to provide higher (by a factor of 2 to more than a factor of 10 times higher) than that derived using CALPUFF.

4.8.8 Findings and conclusions

In this section, we have summarized the results from a study in which a methodology was tested whereby CALPUFF was used with a simplified set of meteorological data, for the purpose of providing screening estimates of concentration and deposition impacts. It was seen that there were reasonably large variations in the SO_2 concentration maxima from one year to the next. There are limitations to the conclusions that can be reached, due to the limited nature of the testing that has been thus far accomplished. Comparisons of results obtained using the new screening methodology versus results obtained using fully developed CALMET meteorology has only been conducted for one location and for one year. In all cases examined, cases could be found where the CALPUFF screening results underestimated the maximum impacts simulated using more fully developed (CALMET) meteorology as input to CALPUFF. Thus IWAQM concludes that the screening method that has been tested

does not guarantee that the pollutant impacts will always be greater than that obtained using refined meteorology. Whether this precludes its use is a judgement decision. There is a certain degree of conservatism inherent in the screening procedure tested. This arises because the screening procedure requires use of receptor rings that completely surround the source being assessed, and it requires use of the maximum impact found anywhere along the receptor ring. In an actual situation, it is unlikely that the Class I area will completely surround the source being analyzed. It is more likely that the actual Class I area is limited to a small segment of a receptor ring. Thus if actual refined (fully developed) meteorology were developed and used, with actual source locations and receptors limited to the Class I area, one is likely to find the impacts simulated within the Class I may be considerably lower than that derived from the screening procedure for receptors that encircle the source.

4.9 CALMET/CALPUFF Enhancements

4.9.1 Use of *FDDA-MM* data with CALMET

Results of an ongoing investigation were reported by Sherwell and Garrison (1997). The study was being conducted by the Maryland Department of Natural Resources Power Plant Research Program (PPRP), in cooperation with EPA, to investigate the results that might be obtained using the CALMET/CALPUFF modeling system to simulate the magnitudes, sources, and possible reductions of NOx deposition to the Chesapeake Bay. In this study, the Penn State MM4 gridded 1990 meteorology data (discussed in Section 4.4) were employed. The EPA 1990 National Emissions Inventory for NOx has been used to derive source inputs. In the presentation by Sherwell and Garrison (1997), an overview was presented of the experiences gained in preparing and running the CALMET/CALPUFF system, and on the preliminary results of the analysis of NOx deposition to the Chesapeake Bay. A large part of their effort was developing the NOx inventory, due to its sheer size, as the raw inventory contained almost 90,000 entries for point sources and over 1100 counties in the defined domain.

The selection of their modeling domain was guided in part by a desire to compare results obtained using the CALMET/CALPUFF modeling system with those available from modeling runs from the Regional Acid Deposition Model (RADM). The RADM contains a more detailed treatment of the atmospheric chemical transformations and removal processes, and thus provides an interesting ‘check’ of the CALMET/CALPUFF modeling results. The final domain selected extended west through Illinois, north almost to the northern border of New York, south through most of

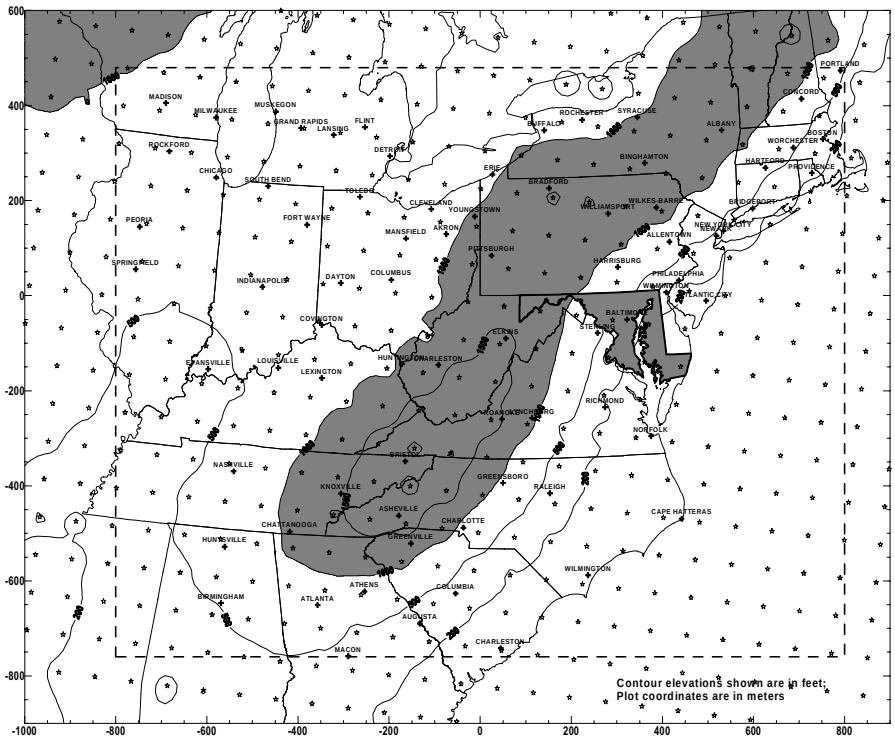


Figure 22. CALMET computational domain.

South Carolina, and covers most of southern New England (Figure 22). The MM4 data has a grid interval of 80 km. CALMET was used to produce 40 km gridded wind and meteorological fields. The fields had seven layers in the vertical: 10, 50, 150, 300, 750, 1500 and 3000 meters. Precipitation data were derived from the stations available on the Samson CD-ROM obtained from the National Climatic Data Center. Given the large computational domain, a lambert conformal projection scheme was selected. Figure 22 shows the location of the MM4 profile points throughout the domain, contours of terrain elevations based on the MM4 grid points, and the locations of the surface stations from which precipitation measurements were obtained and used.

To reduce the CALPUFF simulation times, a series of overlapping receptor grids were constructed, with the density of receptor increasing in the Chesapeake Bay area. The meteorological grid is displayed in Figure 22. The computation domain was sized to be somewhat larger than the domain of the sources being modeled. They had divided the source inventory into four 'zones', with zone 1 including sources within 50 km of the Chesapeake Bay, zone 2 including all sources out to 210 km, zone 3 including all sources out to 500, and zone 4 including all sources from 500 out to the edge of the domain shown in Figure 22. The CALPUFF simulations where configured to use the MESOPUFF II fine species chemical transformation scheme, and wet and

dry fluxes for HNO_3 and NO_3^- were calculated and stored. Constant background concentrations of ozone (80 ppb) and ammonia (10 ppb) were specified.

CALPUFF was run in one-month segments on a 200 MHZ Pentium Pro computer. Storage requirement per month were approximately 220 MB for the raw MM4 data for the selected domain, 75 MB for the CALMET output file used to drive CALPUFF, and 40 MB for the output files of wet and dry fluxes for two species (HNO_3 and NO_3^-). Each month took approximately 10 hours to run.

Total deposition due to dry and wet processes were roughly equal, with predicted wet deposition dominated by deposition of HNO_3 and dry deposition dominated by NO_3^-. On a domain-wide basis , the average total Nitrogen deposition rate was calculated to be about 3.64 kg/(hectare•year). This can be compared to the RADM results for 1990 (Dennis, 1997), which estimated the total Nitrogen deposition rate to be approximately 10 kg/hectare/year in the Chesapeake Bay area. In the most recent RADM simulations (R. Dennis, personal communication), the observations in the vicinity of the Chesapeake Bay and the current RADM seem to be in accord, with most of the wet and dry deposition resulting from HNO_3. In the Demonstration Assessment (Section 4.1), the low amount of wet deposition of HNO_3 estimated by CALPUFF was considered a surprise, given the high aqueous phase solubility of HNO_3. Given these more recent results and comparisons of RADM with observations, there is further cause to suspect the wet deposition results for HNO_3 to be underestimated by CALPUFF.

Of interest is that this analysis has in fact used the *FDDA-MM* meteorological data with the CALMET/CALPUFF modeling system successfully. They provide an independent check of the resources needed. The results are consistent with those found in performing the demonstration analyses, discussed in Section 4.1.

4.9.2 Use of CALMET to Develop Wind Fields

Scire and Robe (1997) reported on a series of enhancements to CALMET for improving the characterization of wind fields in the presence of topographical features that might be anticipated to induce strong upslope and downslope winds. Many industrial facilities are located in river valleys where the terrain effects can have a dominant influence on pollutant transport and dispersion. Furthermore, it is quite likely that the surface wind observations available may not be representative of the flow in the near vicinity of the facility (or conversely may only be representative in the near vicinity and not representative of flow conditions downwind). Attempting to resolve the fine-scale wind effects prognostic meteorological modeling is not only computationally demanding, but often beyond the state-of-the-art. CALMET uses diagnostic (empirical) models of these local-scale effects (upslope and downslope winds), which is computationally more cost-effective and provides a pragmatic solution to a complex problem.

The original wind field module in CALMET, was based on the parameterizations in the Diagnostic Wind Model (DWM) of Douglas and Kessler (1988). This module computed a slope flow (a vector oriented in the drainage direction) which was added to the initialized wind field components (Step 1 initialization). Time of day was used to deduce whether the slope flow was upwind or downwind. The magnitude of the slope flow was based on the local steepness of the terrain, the terrain elevation, the vertical temperature lapse rate, and the maximum terrain height within a radius of influence about the local point under consideration. An undesirable trait of this algorithm was that it would yield larger slope flows for higher terrain elevations, all other factors being equal. The original module used the ambient temperature lapse rate, whereas the potential temperature lapse rate provides the proper characterization of the static stability of the atmosphere. To address these concerns, a new downslope flow module was developed based on the shooting flow parameterization of Mahrt (1982) and a new upslope module was develop based on surface drag concepts. These new modules are no longer restricted to the first layer within CALMET, but instead can affect flow in upper layers.

The local sensible heat flux is an important parameter in deducing the magnitude and direction of the slope flows. This module in CALMET was upgraded to account for the angle of the terrain relative to the sun. For the sensible heat flux computations, the original algorithms assumed the terrain was horizontal to the earth. An east facing terrain slope will “feel” the effects of the sun’s heating in the morning and cooling in the afternoon sooner than a west facing terrain slope. To address this concern, algorithms by Whiteman and Allwine (1986) were added to CALMET that compute the solar radiation for a surface of arbitrary inclination and azimuth.

No matter how much skill is added in the computation of the slope flows, if the initial guess field in the Step 1 initialization is too far off, CALMET will poorly characterize the local wind flows. To address this concern, two enhancements were added to CALMET. First, instead of relying on only the upper-air observations to characterize the local vertical temperature profiles, an option was added to CALMET that allows the vertical temperature profiles using similarity theory (van Ulden and Holtslag, 1985). Second, a modification was added to CALMET that allows the user to control the influence of the upper-air observations and local surface observations in the construction of the Step 1 initialization wind fields. The user is allowed to specify height dependent factors, B, ranging from -1 (no influence by upper air observations) to +1 (no influence by surface observations). If the local surface observations are within the valley, they might be restricted to influencing the Step 1 initialization only for heights below the top of the valley, above which the upper-air observations could be given dominance.

Scire and Robe (1997) illustrated the enhancements discussed above by calculating wind fields in the Columbia River Valley. The region of interest included the City of Wenatchee, WA and the region to the southeast of the city. Wenatchee is located on both sides of the river and includes a relatively flat elevated plain. Figure 23

shows the CALMET modeling domain. The terrain variation is substantial, extending from under 200 meters elevations above mean sea level (MSL) to over 1700 meters MSL at the higher peaks in the southwest part of the domain. The Columbia River runs to the southeast, turns roughly east, and then turns again to the south over a distance of 20 kilometers. The high terrain features change orientation from east-west to north-south in the southern part of the domain.

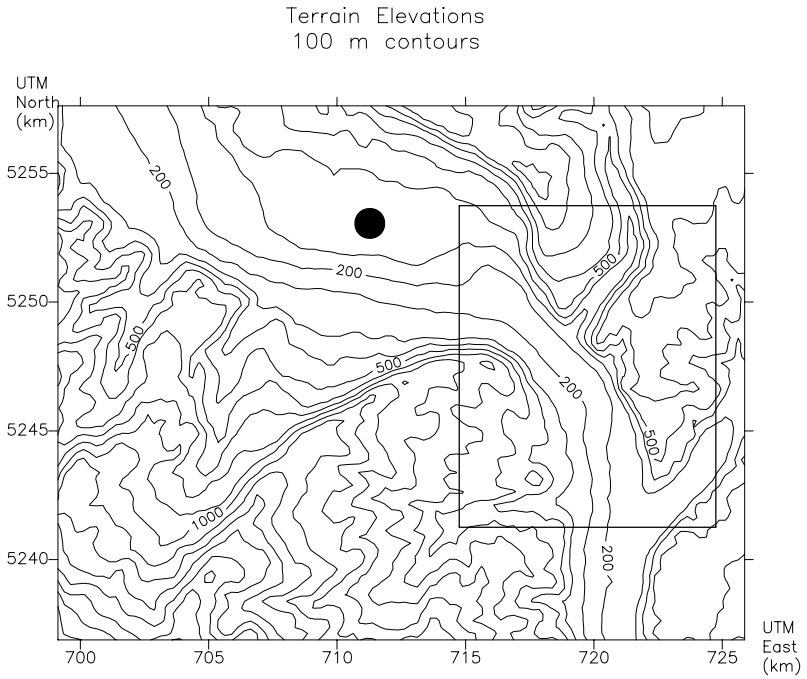


Figure 23. Terrain contours for the Wenachee, WA domain. Contour internal is 100 m, and the location of the Wenatchee (Pangborn) Airport is indicated by the filled circle. The box inset shows the subdomain for which slope flows are presented.

To characterize the terrain, a grid resolution of 250 meters was used in CALMET. The modeling domain consisted of 108 by 84 horizontal grid cells. Nine levels were used in the vertical: 10, 50, 120, 230, 450, 800, 1250 and 2600 meters above ground. The lower four levels are within the valley, the upper three levels are above most of the terrain features. The local wind observations were available at the location shown with a filled circle in Figure 23. This location is within the valley, and the wind rose for the location shows the influence for the local winds to channel and align with the local orientation of the valley. The height dependent factors, B, were set at -1, -1, -1, -1, +0.5, +0.8, +1, +1, +1. The nearest upper air observation station is Spokane, WA, which is over 200 km to the east of the CALMET domain.

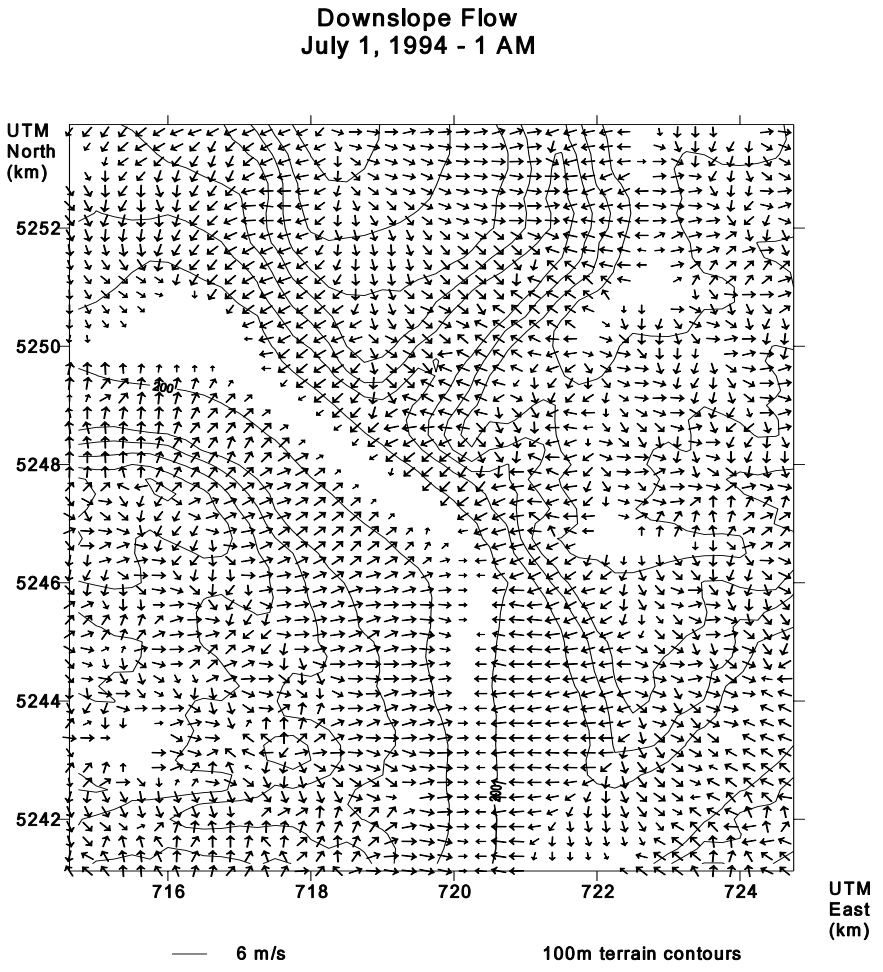


Figure 24. Down slope flow components for 1:00 AM July 1, 1994 for Wenatchee, WA . Wind vectors are plotted every 500 meters (at every second grid point).

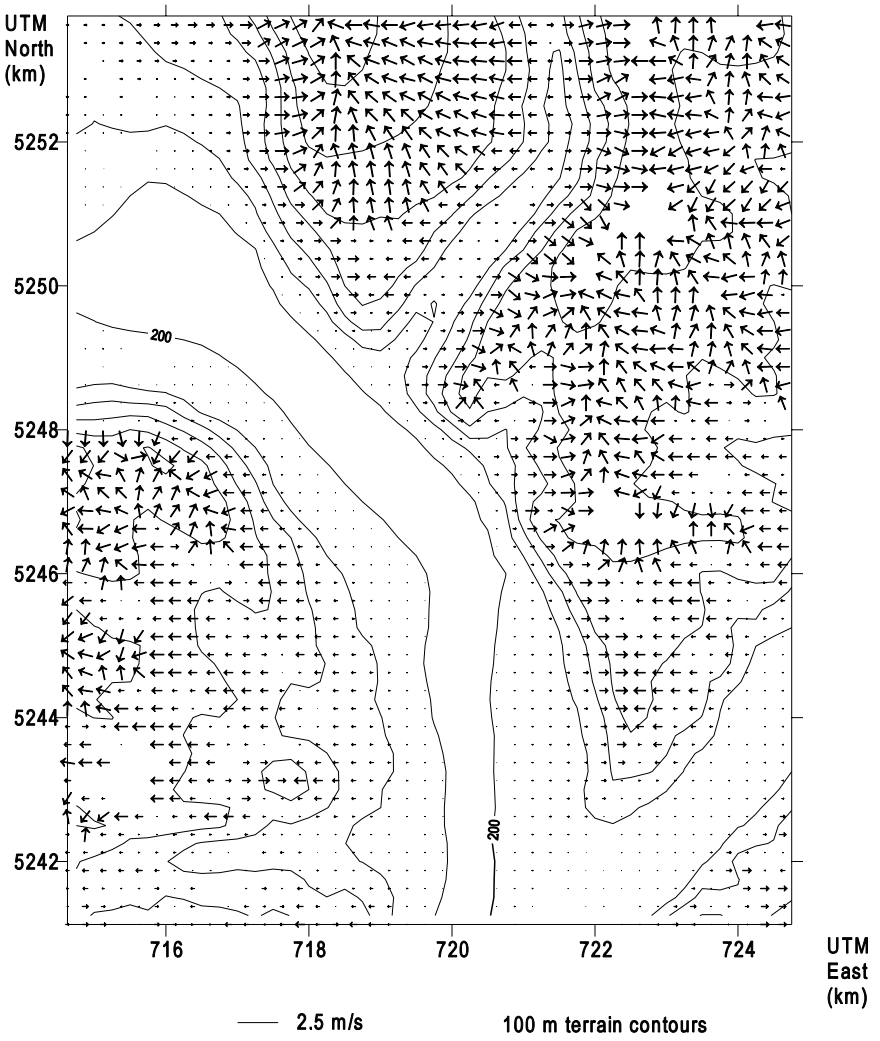


Figure 25. Upslope flow components for 3:00 PM July 1, 1994 for Wenatchee, WA . Wind vectors are plotted every 500 meters (at every second grid point).

Figure 24 shows the computed CALMET layer 1 downslope flows and Figure 25 shows the computed CALMET layer 1 upslope flows. The region shown in these figures is the box inset of Figure 23. The moderately strong nighttime drainage flows (1:00 AM, July 1, 1994) are shown in Figure 24. Figure 25 shows the computed upslope flows, which are (as expected) weaker than the downslope flows. Upslope flows are not expected to accelerate as rapidly as downslope flows.

The pattern and magnitude of the CALMET winds were considered consistent with expectations. These winds were developed using a single surface station in the valley and an upper air station located well outside of the valley. The computed wind fields show the expected diurnal cycle of nighttime drainage followed by daytime upslope flows. The patterns are consistent with the strong terrain channeling of the main valley and within the smaller side canyons. These wind fields would be expected to better characterize the transport of the pollutants. It was anticipated that the proper characterization of the local terrain influences on the wind field would provide a more realistic characterization of the transport around major terrain features rather than directly impacting apon such features.

These results are relevant to the Phase 2 recommendations. They demonstrate that realistic wind fields can be produced using diagnostic techniques. They illustrate that in some situations, the proper characterization of the terrain's influence on the wind fields will require gridded terrain heights, with a grid resolution of order 250 m. This would not be expected for resolving transport and dispersion of plumes that have already traveled large distances and are already quite broad relative to the local terrain features. But it is reasonable to expect that sources within such terrain would require more care to be taken in the characterization of the wind fields, otherwise the transport and resulting dispersion would be poorly characterized. These results also illustrate the feasibility of performing local-scale impacts assessments of the transport and dispersion of emissions from sources located in severe terrain, even when available meteorological observations are sparse.

4.9.3 Kincaid SF_6 and Lovett SO_2 Comparisons

The goal of this study (Strimaitis et al., 1997) was to conduct an evaluation of CALPUFF in comparison with ISCST3 (U.S. EPA, 1995c) for the Kincaid data set, and CTDMPLUS (Perry et al., 1989) for the Lovett data set. Also, enhancements were tested in a special version of CALPUFF (4.07), in which convective scaling parameterizations and concepts were implemented to better characterize dispersion from tall stacks during unstable conditions. Earlier versions of CALPUFF use a simple Gaussian distribution to characterize the vertical distribution of puff material within the convective boundary layer (CBL). As the puff grew, it soon filled the layer between the ground and the mixing height, resulting in a uniform vertical distribution. Within this framework, the primary effect of the convective motions in the mixed layer was to cause a rapid growth in the vertical size of a puff. Depending on the CALPUFF dispersion option selected, this growth rate is either parameterized by the stability class, scaled by measured turbulence intensity, or scaled by a turbulence intensity computed from the surface layer parameters.

In the last decade, modeling techniques that recognize the asymmetry of the vertical dispersion process in the CBL have matured. These techniques explicitly account for the differences between the distribution and strength of updrafts and downdrafts in the layer as they relate to the ensemble-mean concentration distribution.

One such technique that is simple yet effective is the “p.d.f.” approach that relates the probability density function of the vertical position of puff mass in the layer to the skewed probability density function of vertical velocity. Using the superposition of two Gaussian distributions to characterize the skewed p.d.f of the vertical velocity, the p.d.f. model produces a “dual plume” formulation that maps the evolution of one plume that is initially carried toward the ground in a (mean) downdraft, and a second plume that initially rises toward the top of the mixed layer in a (mean) updraft. Subsequent “reflections” from both the ground and the lid are simulated using image sources. Because each of these plumes has its own mean vertical velocity and rate of spread, the resulting vertical distribution of mass is skewed in much the same way as the observed distributions. The initial downdraft plume is called the direct source because it travels directly from an elevated source (accounting for the plume rise velocity) to the ground, while the initial updraft plume is called the indirect source because it reaches the ground only after traversing the full depth of the mixed layer.

U.S. EPA (1995d) extended the p.d.f. CBL formulation to include a simple way of simulating the tendency of highly buoyant plumes to “loft” at the top of the mixed layer, remaining there for some time before the convective eddies are able to overcome the buoyancy and mix their mass to the surface. This formulation forms the basis of the CBL component of AERMOD, U.S. EPA (1995d), and has been adapted for use in CALPUFF (4.07). Strimaitis et al. (1997) adopted AERMOD’s CBL parameterizations for obtaining the mean updraft and downdraft properties, and also their novel simulation of the lofting plume by means of the effective rise of the indirect source. However, the CALPUFF algorithms for treating partial penetration and subsequent entrainment into the mixed layer as the layer grows remain unchanged.

The Kincaid Generating Station is a coal-fired electric generating station with two 606 megawatt (MW) units vented through a single 187 meter stack. It is located in Kincaid, Illinois, approximately 25 kilometers southeast of Springfield. The power plant is in an area of relatively flat terrain surrounded by farmland. As part of an intensive monitoring program sponsored by the Electric Power Research Institute (EPRI), SF_6 tracer was released as a gas continuously through the stack for approximately 30 experiments of 6-9 hours in length during 1980 and 1981. A network of 200 samplers located from 0.5 to 50 km from the stack measured hourly SF_6 concentrations at the ground level. The SF_6 samplers were located approximately in arcs at distances of 0.5, 1, 2, 3, 5, 7, 10, 15, 20, 30, 40, and 50 km from the stack. In addition to measurements of winds and turbulence made at four levels on a 100-m tower, other meteorological data collected include vertical profile data from balloons, solar and net radiation, and cloud cover.

In this study the meteorological data files were developed by emphasizing the tower winds and temperatures, the “observed” mixing heights, and by computing the surface layer parameters using the RAMMET (U.S. EPA, 1995e) preprocessor. One major element in preparing the data files for CALPUFF relates to the transport time from the stack to the outermost receptor arc, which is frequently greater than 1 hour.

While plume models neglect this feature of the study, puff models do not. The tracer gas was typically started 1 to 4 hours before the sampling network, so emissions during the initial transport period are known. Therefore, the full meteorological data set was used (not just the meteorological hours for when tracer data were available) to extract data for complete days (24 hours) for each of the tracer experiments. This allowed development of all of the data needed to properly simulate each period.

The Lovett Power Plant is located in the Hudson River Valley approximately 70 km north of New York City. The terrain in the area rises to approximately 330 meters above the stack base elevation along a ridge 2.5 km north of the stack. The highest point in the area is 340 meters above stack base at about 3 km north of the facility. SO_2 emissions were released from a 145 meter stack containing two flues. Hourly stack parameters (temperatures and flows) were derived from continuously reported load data. The monitoring period is one full year. Twelve continuous SO_2 monitors were located to the west, south, and north of the facility. Ten of the twelve monitors were located in complex terrain from 2 km to 3.5 km from the stack. These ten monitors were all located at or above the elevation of the stack top. Two monitors were located south of the facility at distances of 2 km and 8.5 km for purposes of estimating background concentrations.

Meteorological data were collected on a 100 meter tower located in the valley south-southwest of the stack. The tower was instrumented at three levels (10 m, 50 m, and 100 m). Wind speed, wind direction, and horizontal turbulence (σ_θ) were measured at all three levels. In addition, four 10 meter meteorological towers collecting wind speed, wind direction and σ_θ were located in an arc on the high terrain to the west, west-northwest, north-northwest, and north of the stack. Much of the data needed to apply CALPUFF to this site was prepared by Paumier et al. (1992) for their evaluation of CTDMPLUS. These data files were used in this evaluation, and all but the hourly emissions data could be applied directly to CALPUFF.

For the Kincaid data, quality indicators of 1, 2, and 3 had been assigned to the data. A quality indicator of 1 meant that sampling was very incomplete and no maximum concentration could reliably be determined for the arc. A quality indicator of 3 meant that a distinct pattern could be seen in the data for the arc, and a maximum concentration could be determined reliably. Model performance results for the Kincaid data set were presented for two subsets of the data. The first were comprised of all arc-hours for which the peak concentration on the arc was given a quality indicator (QI) of 2 or 3; the second was the subset of these arc-hours with a QI of 3.

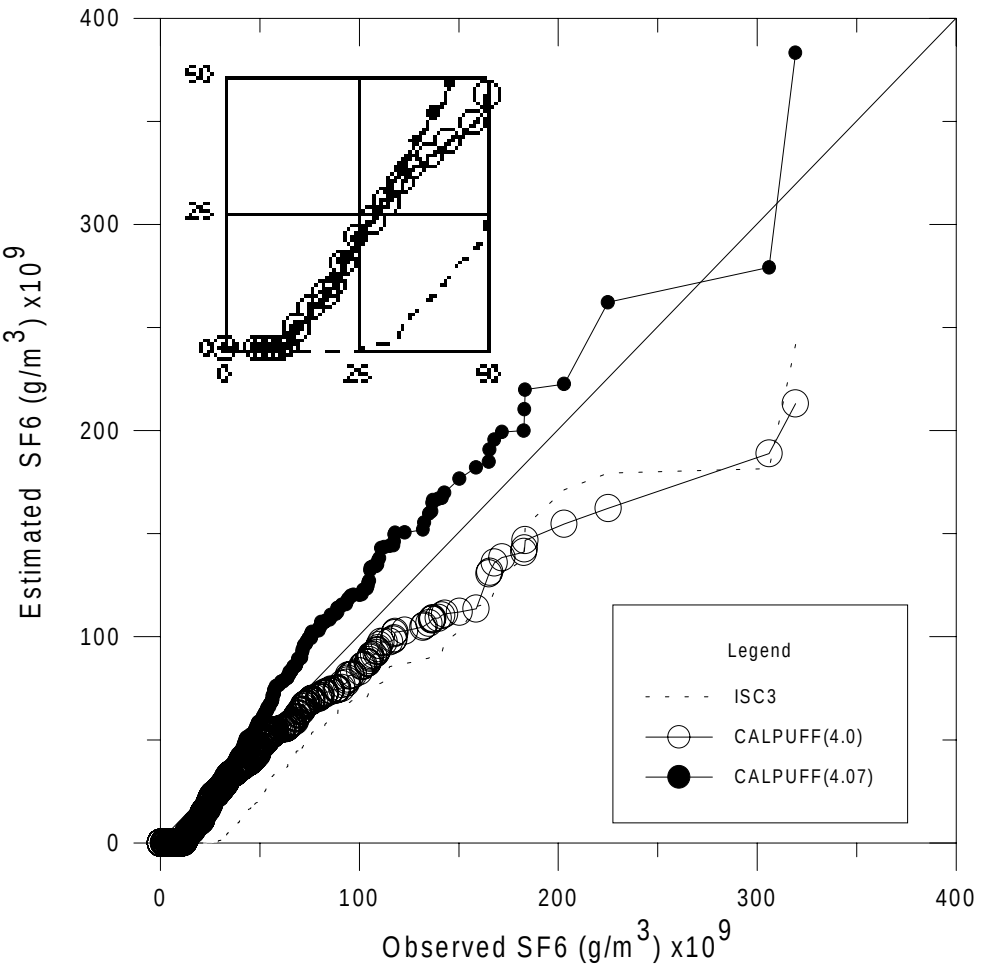


Figure 26. Q-Q plots for Kincaid, comparing observed surface concentration values of SF_6 with simulation results by CALPUFF(4.0), CALPUFF(4.07) and ISC3 for Quality 2 and 3 data.

Figure 26 shows the Quantile-Quantile (Q-Q) plots for CALPUFF(4.07), CALPUFF(4.0) and ISCST3 compared to the observations, for data of quality 2 and 3. Although all models display a tendency to predict more zero-impacts (see inset) than is observed, both versions of CALPUFF predict fewer zeros than ISCST3. This is traceable to the fact that for all CALPUFF model runs, the option for partial plume penetration was enabled. ISC3 sets all surface concentrations to zero whenever the computed centerline of the plume is detected to be above the mixing height. CALPUFF would do the same, except when the partial plume penetration option is enabled. When this option is enabled, a computation is made based on the size of the dispersing plume, and any mass below the mixing height is allowed to continue to disperse and possibly impact surface receptors. While fewer observed concentrations are underpredicted by both versions of CALPUFF (106 out of 586 values) than are

underpredicted by ISCST3 (236 out of 586 values), there remains a substantial number of large observed concentrations for which both models miss (zero is predicted)

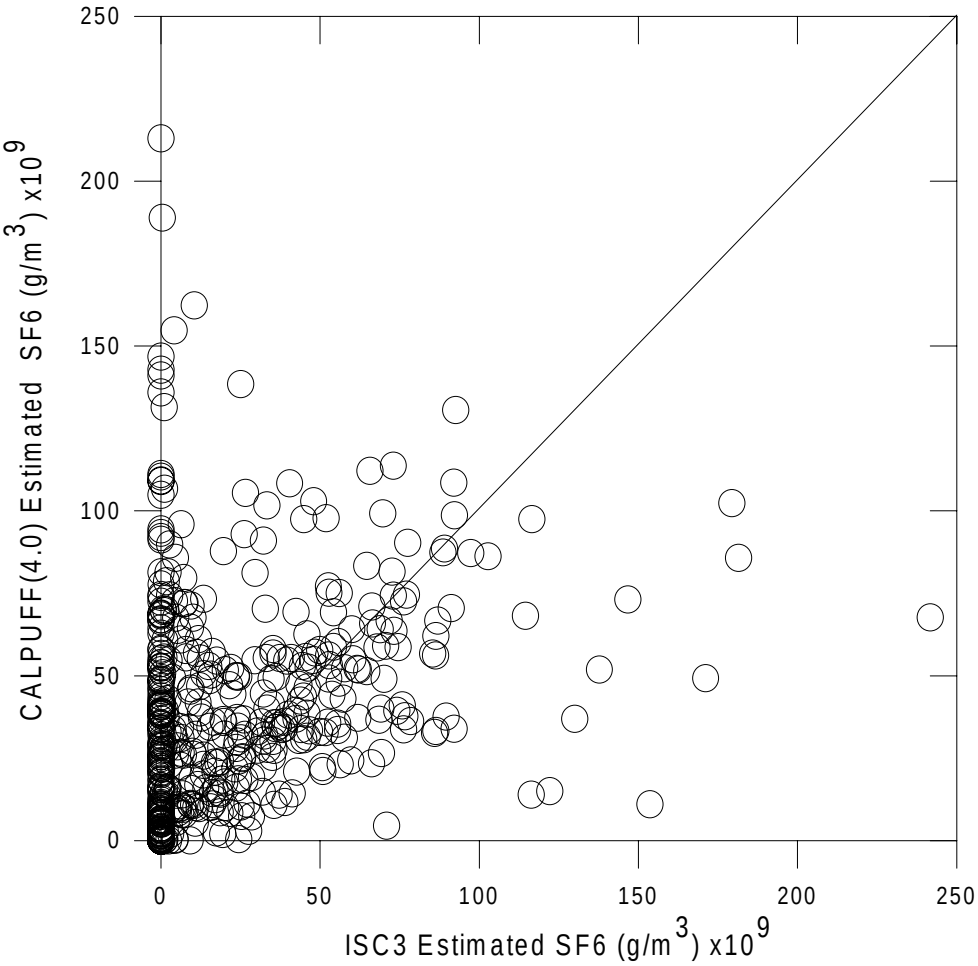


Figure 27. Scatter plot for Kincaid, comparing CALPUFF(4.0) and ISC3 simulation results for surface concentration values of SF_6 for Quality 2 and 3 data.

The CALPUFF(4.0) results in Figure 26 appear to be similar to the ISC3 results. This is true in the sense that the computed maxima are of a similar value. But the CALPUFF(4.0) runs were conducted using dispersion parameters based on similarity theory, and a scatter plot of CALPUFF(4.0) versus ISC3, Figure 27, reveals that the two models are not providing as similar of results as might be deduced from inspection of Figure 26.

CALPUFF(4.07) is seen to overpredict the upper range of observed concentrations, while CALPUFF(4.0) and ISCST3 underpredict throughout, and the ranked distribution for CALPUFF(4.07) lies nearer the 1:1 line in Figure 26. How much of this improved performance might be attributed to the p.d.f. algorithms for the CBL?

As can be seen in Figure 26, the lower end of the ranked distributions for both versions of CALPUFF appear to coincide, which implies that reasons for the elevated frequency of zero-impact predictions are not related to the treatment of dispersion in the CBL. The character of the higher end is quite different, with CALPUFF(4.0) producing concentrations more like ISCST3 than CALPUFF(4.07). This suggests that the p.d.f. is responsible for the improvements at the high end noted in Figure 26.

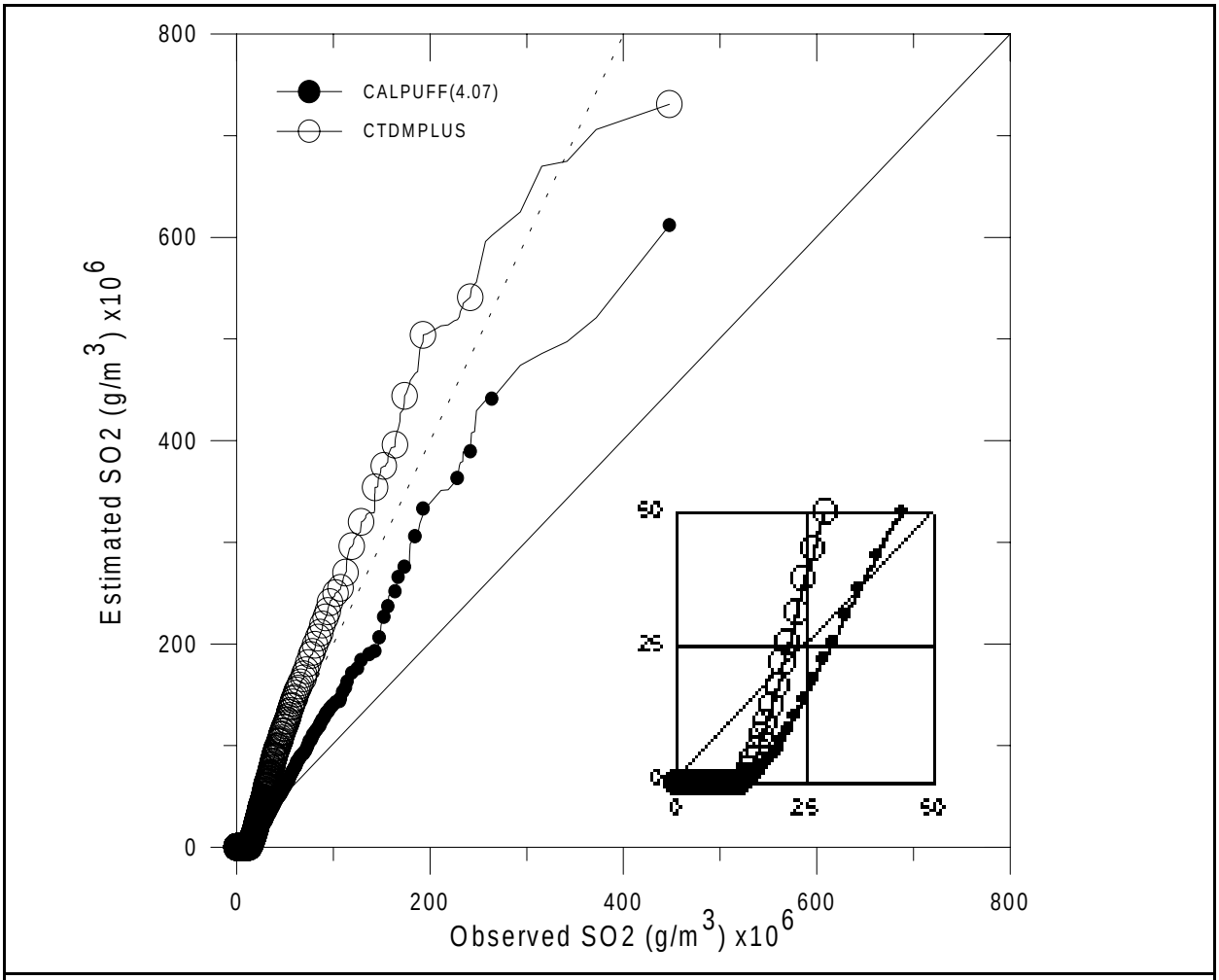


Figure 28. Q-Q plots for Lovett, comparing observed surface concentration values of SO_2 with simulation results CALPUFF(4.07) and CTDMPLUS

For the Lovett data set, Paumier et al. (1992) found that CTDMPLUS and RTDM predictions were poorly correlated with the observed peak hourly concentrations. Given that CALPUFF was applied with the same meteorological data, similar results were expected and found. Figure 28 shows the Q-Q plot for CALPUFF(4.07) and CTDMPLUS compared to the observations. Although both models tend to overpredict the observed ranked distribution, CALPUFF predictions lie nearer the 1:1 line. The

dashed line in Figure 28 indicates an overprediction of two, which is close to the results depicted for CTDMPLUS.

The evaluation results presented suggests that the p.d.f. formulations tested in CALPUFF(4.07) eliminates the tendency seen in the CALPUFF(4.0) and ISC3 to underestimate the surface concentration values for the Kincaid data set, and CALPUFF(4.07) overpredicts surface concentration values less than CTDMPLUS for the Lovett data set. Correlation of hourly predicted and observed concentrations for the Lovett data set are poor for both CALPUFF(4.07) and CTDMPLUS, suggesting that more diagnostic analyses of this data set may be fruitful. For the Kincaid data, CALPUFF (4.0) performance is similar to ISC3's. And for the Kincaid evaluation, performance during periods with observed mixing heights less that about 600m suggests that more mass remains in the mixed layer than is predicted by the models, even with partial penetration enabled.

5.0 CONCLUSIONS

This report provides a summary and status report of the activities sponsored and initiated by the Interagency Workgroup on Air Quality Modeling (IWAQM). The IWAQM was formed to provide a focus for development of air quality models for assessment of pollutant source impacts on Federal Class I areas and wilderness areas. In particular, IWAQM has focused attention on providing modeling techniques for assessing possible adverse air quality impacts resulting from long-range transport of pollutants, as required by the prevention of significant deterioration (PSD) program.

In 1993, IWAQM provided interim Phase 1 recommendations that provided the best approach from existing "off-the-shelf-techniques." The MESOPUFF II puff modeling system was recommended for use. This model provided the ability to simulate the influence of time and space varying meteorological conditions on transport and dispersion. It provided a first-order approximate characterization of the formation of sulfate and nitrate during transport downwind. It provided characterizations for the removal of pollutants by dry and wet deposition. The meteorology processing had limited capabilities, as it was not able to characterize geographical terrain slope flows. The puff dispersion model had no capabilities to address effects associated with variation of terrain heights. Furthermore, due to limitations in the dispersion treatments, the puff model was not considered appropriate for use in characterizing impacts associated with transport distances of less than 50 km.

As discussed in Appendix D, IWAQM provided a status report of ongoing activities at the Sixth Modeling Conference, which was held in Washington, D.C. August 9-10, 1995. As a result of comments received, a series of investigations were undertaken. Comparisons were made of CALPUFF simulated dispersion with near-surface concentrations collected during several tracer field studies, where the transport distances were of the order 50 to 300 km. Comparisons were made of CALPUFF simulated dispersion with simulation results obtained using the Industrial Source Complex (ISC3) plume dispersion model. Initially, the focus was on whether CALPUFF and ISC3 gave similar results for steady-state meteorological conditions. Once this was confirmed, the focus shifted to investigating what difference might result between a puff and plume model, having identical meteorology and dispersion. It became clear that wind reversals and buildup of pollutant mass during calm wind conditions could result in large differences in simulation results. As a consequence of comments received and of the puff/plume model comparisons, a new screening analysis was tested that relied on use of the CALPUFF dispersion model with a greatly simplified characterization of the hourly meteorological conditions.

Based on the findings of the various investigations summarized in Section 4, IWAQM is providing a Phase 2 recommendation to replace the interim Phase 1 recommendation. The CALPUFF modeling system is recommended in place of the MESOPUFF II modeling system for a number of reasons. A primary consideration is that the CALMET meteorological processor is capable of diagnostically characterizing

geographic terrain slope flows, and has been updated to allow use of sophisticated output from modern mesoscale meteorological processors. Another important consideration is that the CALPUFF puff dispersion algorithms have been fashioned to allow characterization of both local-scale and long-range transport and dispersion. This allows use of one model for all sources with a consistent treatment of the chemistry and fate of the pollutants. Using CALPUFF within the new screening analysis provides consistent treatment of the chemistry and fate, and some of the 'causality' effects of hourly varying meteorology that a puff dispersion model can treat more directly and easily than a standard plume dispersion model.

This Phase 2 recommendation provides a major improvement in the treatment and characterization of the meteorological conditions and the mesoscale transport. There is yet room for improvement in the characterization of the chemistry and fate of the pollutants. The CALPUFF dispersion model represents a major improvement over the MESOPUFF II model in its flexibility for treating a variety of source types, time varying emission rates, and of dispersion situations. The IWAQM recommends the CALPUFF modeling system for use as a refined long-range transport and dispersion modeling technique for characterizing reasonably attributable pollutant impacts from one or a few sources.

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APPENDIX A
CALMET RECOMMENDATIONS

In the following, a listing is provided of the defaults currently assumed in CALMET for long-range transport analyses in involving assessments of not on concentration impacts, but also deposition flux impacts and visibility impacts. Some of the variables have the 'Value' is listed in bold. This is meant to indicate that these likely will need to be tailored for a given application.

Variable	Description	Value
GEO.DAT	Name of Geophysical data file	GEO.DAT
SURF.DAT	Name of Surface data file	SURF.DAT
PRECIP.DAT	Name of Precipitation data file	PRECIP.DAT
NUSTA	Number of upper air data sites	User Defined
UPn.DAT	Names of NUSTA upper air data files	UPn.DAT
IBYR	Beginning year	User Defines
IBMO	Beginning month	User Defines
IBDY	Beginning day	User Defines
IBHR	Beginning hour	User Defines
IBTZ	Base time zone	User Defines
IRLG	Number of hours to simulate	User Defines
IRTYPE	Output file type to create (must be 1 for CALPUFF)	1
LCALGRD	Are w-components and temperature needed?	T
NX	Number of east-west grid cells	**User Defines**
NY	Number of north-south grid cells	**User Defines**
DGRIDKM	Grid spacing	**User Defines**
XORIGKM	Southwest grid cell X coordinate	User Defines
YORIGKM	Southwest grid cell Y coordinate	User Defines
XLAT0	Southwest grid cell latitude	User Defines
YLON0	Southwest grid cell longitude	User Defines
IUTMZN	UTM Zone	User Defines
LLCONF	When using Lambert Conformal map coordinates, rotate winds from true north to map north?	F
XLAT1	Latitude of 1st standard parallel	**30**
XLAT2	Latitude of 2nd standard parallel	**60**

Variable	Description	Value
RLON0	Longitude used if LLCONF = T	**90**
RLAT0	Latitude used if LLCONF = T	**40**
NZ	Number of vertical layers	**User Defines**
ZFACE	Vertical cell face heights (NZ+1 values)	**User Defines**
LSAVE	Save met. data fields in an unformatted file?	T
IFORMO	Format of unformatted file (1 for CALPUFF)	1
NSSTA	Number of stations in SURF.DAT file	User Defines
NPSTA	Number of stations in PRECIP.DAT	User Defines
ICLOUD	Is cloud data to be input as gridded fields? (0 = No)	0
IFORMS	Format of surface data (2 = formatted)	2
IFORMP	Format of precipitation data (2 = formatted)	2
IFORMC	Format of cloud data (2 = formatted)	2
IWFCOD	Generate winds by diagnostic wind module? (1 = Yes)	1
IFRADJ	Adjust winds using Froude number effects? (1 = Yes)	1
IKINE	Adjust winds using kinematic effects? (1 = Yes)	0
IOBR	Use O'Brien procedure for vertical winds? (0 = No)	0
ISLOPE	Compute slope flows? (1 = Yes)	1
IEXTRP	Extrapolate surface winds to upper layers? (-4 = use similarity theory and ignore layer 1 of upper air station data)	-4
ICALM	Extrapolate surface calms to upper layers? (0 = No)	0
BIAS	Surface/upper-air weighting factors (NZ values)	NZ*0

Variable	Description	Value
IPROG	Using prognostic or MM-FDDA data? (0 = No)	0
LVARY	Use varying radius to develop surface winds?	**F**
RMAX1	Max surface over-land extrapolation radius (km)	**User Defines**
RMAX2	Max aloft over-land extrapolation radius (km)	**User Defines**
RMAX3	Maximum over-water extrapolation radius (km)	**User Defines**
RMIN	Minimum extrapolation radius (km)	0.1
RMIN2	Distance (km) around an upper air site where vertical extrapolation is excluded (Set to -1 if IEXTRP = ±4)	4
TERRAD	Radius of influence of terrain features (km)	**User Defined**
R1	Relative weight at surface of Step 1 field and obs	**User Defines**
R2	Relative weight aloft of Step 1 field and obs	**User Defines**
DIVLIM	Maximum acceptable divergence	5.E-6
NITER	Max number of passes in divergence minimization	50
NSMTH	Number of passes in smoothing (NZ values)	2, 4*(NZ-1)
NINTR2	Max number of stations for interpolations (NA values)	**99**
CRITFN	Critical Froude number	1
ALPHA	Empirical factor triggering kinematic effects	0.1
IDIOPT1	Compute temperatures from observations (0 = True)	0
ISURFT	Surface station to use for surface temperature (between 1 and NSSTA)	**User Defines**
IDIOPT2	Compute domain-average lapse rates? (0 = True)	0
IUPT	Station for lapse rates (between 1 and NUSTA)	**User Defines**
ZUPT	Depth of domain-average lapse rate (m)	200

Variable	Description	Value
IDIOPT3	Compute internally inital guess winds? (0 = True)	0
IUPWND	Upper air station for domain winds (-1 = 1/r**2 interpolation of all stations)	-1
ZUPWND	Bottom and top of layer for 1st guess winds (m)	1, 1000
IDIOPT4	Read surface winds from SURF.DAT? (0 = True)	0
IDIOPT5	Read aloft winds from UPn.DAT? (0 = True)	0
CONSTB	Neutral mixing height B constant	1.41
CONSTE	Convective mixing height E constant	0.15
CONSTN	Stable mixing height N constant	2400
CONSTW	Over-water mixing height W constant	0.16
FCORIOL	Absolute value of Coriolis parameter	1.E-4
IAVEXZI	Spatial averaging of mixing heights? (1 = True)	1
MNMDAV	Max averaging radius (number of grid cells)	1
HAFANG	Half-angle for looking upwind (degrees)	30
ILEVZI	Layer to use in upwind averaging (between 1 and NZ)	**1**
DPTMIN	Minimum capping potential temperature lapse rate	0.001
DZZI	Depth for computing capping lapse rate (m)	200
ZIMIN	Minimum over-land mixing height (m)	50
ZIMAX	Maximum over-land mixing height (m)	3000
ZIMINW	Minimum over-water mixing height (m)	50
ZIMAXW	Maximum over-water mixing heigh (m)	3000
IRAD	Form of temperature interpolation (1 = 1/r)	1
TRADKM	Radius of temperature interpolation (km)	500

Variable	Description	Value
NUMTS	Max number of stations in temperature interpolations	5
IAVET	Conduct spatial averaging of temperature? (1 = True)	1
TGDEFB	Default over-water mixed layer lapse rate (K/m)	-0.0098
TGDEFA	Default over-water capping lapse rate (K/m)	-0.0045
JWAT1	Beginning landuse type defining water	999
JWAT2	Ending landuse type defining water	999
NFLAGP	Method for precipitation interpolation (2 = 1/r**2)	2
SIGMAP	Precip radius for interpolations (km)	100
CUTP	Minimum cut off precip rate (mm/hr)	0.01
SSn	NSSTA input records for surface stations	User Defines
USn	NUSTA input records for upper-air stations	User Defines
PSn	NPSTA input records for precipitation stations	User Defines

APPENDIX B
CALPUFF RECOMMENDATIONS

In the following, a listing is provided of the defaults currently assumed in CALPUFF for long-range transport analyses in involving assessments of not on concentration impacts, but also deposition flux impacts and visibility impacts. Some of the variables have the 'Value' is listed in bold. This is meant to indicate that these likely will need to be tailored for a given application.

Variable	Description	Value
METDAT	CALMET input data filename	CALMET.DAT
PUFLST	Filename for general output from CALPUFF	CALPUFF.LST
CONDAT	Filename for output concentration data	CONC.DAT
DFDAT	Filename for output dry deposition fluxes	DFLX.DAT
WFDAT	Filename for output wet deposition fluxes	WFLX.DAT
VISDAT	Filename for output relative humidities (for visibility)	VISB.DAT
METRUN	Do we run all periods (1) or a subset (0)?	0
IBYR	Beginning year	User Defined
IBMO	Beginning month	User Defined
IBDY	Beginning day	User Defined
IBHR	Beginning hour	User Defined
IRLG	Length of run (hours)	User Defined
NSPEC	Number of species modeled (for MESOPUFF II chemistry)	5
NSE	Number of species emitted	3
MRESTART	Restart options (0 = no restart), allows splitting runs into smaller segments	**0**
METFM	Format of input meteorology (1 = CALMET)	1
AVET	Averaging time lateral dispersion parameters (minutes)	60
MGAUSS	Near-field vertical distribution (1 = Gaussian)	1
MCTADJ	Terrain adjustments to plume path (3 = Plume path)	**3**
MCTSG	Do we have subgrid hills? (0 = No), allows CTDM-like treatment for subgrid scale hills	**0**
MSLUG	Near-field puff treatment (0 = No slugs)	0

Variable	Description	Value
MTRANS	Model transitional plume rise? (1 = Yes)	1
MTIP	Treat stack tip downwash? (1 = Yes)	1
MSHEAR	Treat vertical wind shear? (0 = No)	0
MSPLIT	Allow puffs to split? (0 = No)	**0**
MCHEM	MESOPUFF-II Chemistry? (1 = Yes)	1
MWET	Model wet deposition? (1 = Yes)	1
MDRY	Model dry deposition? (1 = Yes)	1
MDISP	Method for dispersion coefficients (3 = PG & MP)	3
MTURBVW	Turbulence characterization? (Only if MDISP = 1 or 5)	3
MDISP2	Backup coefficients (Only if MDISP = 1 or 5)	3
MROUGH	Adjust PG for surface roughness? (0 = No)	0
MPARTL	Model partial plume penetration? (0 = No)	1
MTINV	Elevated inversion strength (0 = compute from data)	0
MPDF	Use PDF for convective dispersion? (0 = No)	0
MSGTIBL	Use TIBL module? (0 = No) allows treatment of subgrid scale coastal areas	0
MREG	Regulatory default checks? (1 = Yes)	1
CSPECn	Names of species modeled (for MESOPUFF II, must be SO2, SO4, NOX, HNO3, NO3)	**User Defined**
Specie Names	Manner species will be modeled	**User Defined**
Specie Groups	Grouping of species, if any.	**User Defined**
NX	Number of east-west grids of input meteorology	User Defined
NY	Number of north-south grids of input meteorology	User Defined
NZ	Number of vertical layers of input meteorology	User Defined

Variable	Description	Value
DGRIDKM	Meteorology grid spacing (km)	User Defined
ZFACE	Vertical cell face heights of input meteorology	User Defined
XORIGKM	Southwest corner (east-west) of input meteorology	User Defined
YORIGIM	Southwest corner (north-south) of input meteorology	User Defined
IUTMZN	UTM zone	User Defined
XLAT	Latitude of center of meteorology domain	User Defined
XLONG	Longitude of center of meteorology domain	User Defined
XTZ	Base time zone of input meteorology	User Defined
IBCOMP	Southwest X-index of computational domain	**User Defined**
JBCOMP	Southwest Y-index of computational domain	**User Defined**
IECOMP	Northeast X-index of computational domain	**User Defined**
JECOMP	Northeast Y-index of computational domain	**User Defined**
LSAMP	Use gridded receptors? (T = Yes)	F
IBSAMP	Southwest X-index of receptor grid	User Defined
JBSAMP	Southwest Y-index of receptor grid	User Defined
IESAMP	Northeast X-index of receptor grid	User Defined
JESAMP	Northeast Y-index of receptor grid	User Defined
MESHDN	Gridded recpetor spacing = DGRIDKM/MESHDN	1
ICON	Output concentrations? (1 = Yes)	1
IDRY	Output dry deposition flux? (1 = Yes)	1
IWET	Output west deposition flux? (1 = Yes)	1
IVIS	Output RH for visibility calculations (1 = Yes)	1
LCOMPRS	Use compression option in output? (T = Yes)	T

Variable	Description	Value
ICPRT	Print concentrations? (0 = No)	0
IDPRT	Print dry deposition fluxes (0 = No)	0
IWPRT	Print wet deposition fluxes (0 = No)	0
ICFRQ	Concentration print interval (1 = hourly)	1
IDFRQ	Dry deposition flux print interval (1 = hourly)	1
IWFRQ	West deposition flux print interval (1 = hourly)	1
IPRTU	Print output units (1 = g/m**3; g/m**2/s)	1
IMESG	Status messages to screen? (1 = Yes)	1
Output Species	Where to output various species	**User Defined**
LDEBUG	Turn on debug tracking? (F = No)	F
Dry Gas Dep	Chemical parameters of gaseous deposition species	**User Defined**
Dry Part. Dep	Chemical parameters of particulate deposition species	**User Defined**
RCUTR	Reference cuticle resistance (s/cm)	30.
RGR	Reference ground resistance (s/cm)	10.
REACTR	Reference reactivity	8
NINT	Number of particle-size intervals	9
IVEG	Vegetative state (1 = active and unstressed)	1
Wet Dep	Wet deposition parameters	**User Defined**
MOZ	Ozone background? (1 = read from ozone.dat)	1
BCKO3	Ozone default (ppb) (Use only for missing data)	**80**
BCKNH3	Ammonia background (ppb)	**10**
RNITE1	Nighttime SO2 loss rate (%/hr)	0.2
RNITE2	Nighttime NOx loss rate (%/hr)	2
RNITE3	Nighttime HNO3 loss rate (%/hr)	2

Variable	Description	Value
SYTDEP	Horizontal size (m) to switch to time dependence	550.
MHFTSE	Use Heffter for vertical dispersion? (0 = No)	0
JSUP	PG Stability class above mixed layer	5
CONK1	Stable dispersion constant (Eq 2.7-3)	0.01
CONK2	Neutral dispersion constant (Eq 2.7-4)	0.1
TBD	Transition for downwash algorithms (0.5 = ISC)	0.5
IURB1	Beginning urban landuse type	10
IURB2	Ending urban landuse type	19
Use Following Only For Single-Point Meteorological Input (CALPUFF Screen)		
ILANDUIN	Land use type (20 = Unirrigated agricultural land)	20
ZOIN	Roughness length (m)	0.25
XLAIIN	Leaf area index	3
ELEVIN	Met. Station elevation (m above MSL)	0
XLATIN	Met. Station North latitude (degrees)	**User Defined**
XLONIN	Met. Station West longitude (degrees)	**User Defined**
ANEMHT	Anemometer height of ISC meteorological data (m)	10.0
ISIGMAV	Lateral turbulence (Not used with ISC meteorology)	1
IMIXCTDM	Mixing heights (Not used with ISC meteorology)	0
End of Single Point Meteorology Input Variables		
XMXLEN	Maximum slug length in units of DGRIDKM	1
XSAMLEN	Maximum puff travel distance per sampling step (units of DGRIDKM)	1

Variable	Description	Value
MXNEW	Maximum number of puffs per hour	99
MXSAM	Maximum sampling steps per hour	99
SL2PF	Maximum Sy/puff length	10
PLX0	Wind speed power-law exponents	0.07,0.07,0.10,0.15,0.35,0.55
WSCAT	Upper bounds 1st 5 wind speed classes (m/s)	1.54,3.09,5.14,8.23.10.8
PGGO	Potential temperature gradients PG E and F (deg/km)	0.020, 0.035
SYMIN	Minimum lateral dispersion of new puff (m)	1.0
SZMIN	Minimum vertical dispersion of new puff (m)	1.0
SVMIN	Array of minimum lateral turbulence (m/s)	6*0.50
SWMIN	Array of minimum vertical turbulence (m/s)	0.20, 0.12, 0.08, 0.06, 0.03, 0.016
CDIV	Divergence criterion for dw/dz (1/s)	0.01
WSCALM	Minimum non-calm wind speed (m/s)	0.5
XMAXZI	Maximum mixing height (m)	3000
XMINZI	Minimum mixing height (m)	50
PPC	Plume path coefficients (only if MCTADJ = 3)	0.5,0.5,0.5,0.5,0.35,0.35
NSPLIT	Number of puffs when puffs split	3
IRESPLIT	Hours when puff are eligible to split	**User Defined**
ZISPLIT	Previous hour's mixing height (minimum), (m)	100
ROLDMAX	Previous Max mixing height/current mixing height ratio, must be less then this value to allow puff split	0.25

Variable	Description	Value
EPSSLUG	Convergence criterion for slug sampling integration	1.0E-04
PESAREA	Convergence criterion for area source integration	1.0E-06
NPT1	Number of point sources	User Defined
IPTU	Units of emission rates (1 = g/s)	1
NSPT1	Number of point source-species combinations	0
NPT2	Number of point sources with fully variable emission rates	0
Point Sources	Point sources characteristics	User Defined
Area Sources	Area sources characteristics	User Defined
Line Sources	Buoyant lines source characteristics	User Defined
Volume Sources	Volume sources characteristics	User Defined
NREC	Number of user defined receptors	User Defined
Receptor Data	Location and elevation (MSL) of receptors	User Defined

APPENDIX C
COMPACT DISK DATA RESOURCES

Solar and Meteorological Surface Observation Network (SAMSON), 1961 - 1990
Version 1.0, September 1993

Available from U.S. Department of Commerce, National Climatic Data Center, Federal Building, 37 Battery Park Ave., Asheville, NC 28801

Radiosonde Data of North America, 1946 - 1992
Version 1.0, August 1993

Available from U.S. Department of Commerce, National Climatic Data Center, Federal Building, 37 Battery Park Ave., Asheville, NC 28801

CALMET, CALPUFF, and CALPOST Modeling System
Version 1.0

Available from U.S. Department of Commerce, National Technical Information Service, 5285 Port Royal Rd., Springfield, VA 22161. NTIS PB 96-502 083.

Hourly United States Weather Observations (HUSWO) 1990-1995

Available from U.S. Department of Commerce, National Climatic Data Center, Federal Building, 37 Battery Park Ave., Asheville, NC 28801

MM4 - 1990 Meteorological Data, Volumes 1-12

Available from U.S. Department of Commerce, National Climatic Data Center, Federal Building, 37 Battery Park Ave., Asheville, NC 28801

NCDC Precipitation data CD's

Available from U.S. Department of Commerce, National Climatic Data Center, Federal Building, 37 Battery Park Ave., Asheville, NC 28801

APPENDIX D
SIXTH MODELING CONFERENCE

Section 320 of the 1990 CAA amendments requires the EPA to conduct public conferences on air quality modeling at least every three years. These conferences are to give special attention to appropriate modeling necessary for addressing prevention of significant deterioration of air quality. The sixth of these modeling conferences was held August 9-10, 1995 in Washington, D.C. One of the main topics discussed at the sixth conference was a review of the status of work by IWAQM in the development of a Phase 2 recommendation. At the conference comments were presented by several attendees regarding their experiences in applying the Phase 1 interim recommendations, and thoughts and recommendations were presented on future needs. The presentation results, comments received and conclusions reached at the Sixth Modeling Conference are fundamental to the development of the Phase 2 recommendations, and will be discussed in the following sections.

D.1 Presentation Summary

The IWAQM presentation at the Sixth Modeling Conference began with a review of the work plan (U.S. EPA, 1992a) and the Phase 1 interim recommendations (U.S. EPA, 1993), which have briefly been discussed above. The presentation then provided a summary of work accomplishments in five areas: 1) results from a case study conducted using the Phase 1 interim recommendations; 2) adaptations made to a Lagrangian puff modeling system called CALPUFF; 3) MESOPUFF II and CALPUFF simulation results for three of the 1983 Cross APpalachian Tracer EXperiment (CAPTEX) tracer releases; 4) conclusions reached regarding use of sophisticated mesoscale meteorological analyses; 5) a proposed process for modeling specific Class I areas. In the following five subsections, brief summaries are presented for each of the topics listed. More extensive summaries are presented in Section 4.

D.1.1 MESOPUFF II Implementation Assessment

The objective was to learn by experience where the difficulties are in the process of applying the MESOPUFF II air quality modeling system following IWAQM Phase 1 interim recommendations (U.S. EPA, 1993) 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 part of this study 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 (SNP), including the James River Face (JRF) wilderness area. Model simulations were performed using three years of the developed five-year meteorological data set to demonstrate 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.

Several conclusions were reached as a result of the demonstration assessment. First, tailoring a puff simulation analysis to assess PSD and AQRV impacts at SNP and JRF was a difficult task. A primary goal is to develop a reasonably good characterization of the spatially-varying, time-varying three dimensional wind field. This goal alone requires an air pollution modeler with strong dispersion meteorology experience, having expert judgement and finesse. The differing goals between PSD permitting and AQRV assessment required frequent consultation with FLMs. Since the modeling necessarily required case-specific judgement decisions, strong collaboration and review was required by the various regulatory reviewing authorities. All these considerations have caused IWAQM to believe in and recommend a Regional Approach, as discussed in Section 4.5.

Even with anticipated improvements in the software, it is likely that the analyses will require programming special routines to convert data into appropriate formats, or to assist in the analysis and summarization of the data. Also even though the modeling software can be executed on personal computers, it is likely that a workstation would prove more convenient and useful. Thus it is concluded that mesoscale analyses using Lagrangian puff dispersion models must be viewed as more involved and difficult than using conventional plume dispersion models. This is especially true in consideration that most plume dispersion modeling assessments use a single-station’s hourly meteorological observation, whereas puff dispersion modeling is founded on using a three-dimensional wind field, that is consistent with the terrain and land-use.

The PSD and AQRV impacts developed in the demonstration assessment from the ten aggregated sources exhibited strong year-to-year variations. Furthermore, some of the impacts were close to the PSD increments. These results suggest that at least three years of modeling is needed in order to assess the likely maximum impacts. Part of the reason for recommending a Regional Approach is to address concerns that more attention needs to be given to comparing PSD and AQRV impacts generated by all the sources as a the cumulative impact assessment.

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 declined 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. 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.

D.1.2 Revisions to CALMET and CALPUFF

In the course of completing the Phase 1 recommendations, IWAQM became aware of the CALMET/CALPUFF modeling system (Scire et al., 1990ab), which was actively under development. Building from lessons learned from the MESOPAC/MESOPUFF II modeling system, IWAQM felt further enhancements were needed in two areas. With a view towards allowing one model to be used for all sources (which might include source-receptor distances of less than 50 km), the first area for enhancement was to include within CALPUFF dispersion additional algorithms, so that CALPUFF simulation results would be consistent with the Industrial Source Complex (ISC) model and the Complex Terrain Dispersion Model (CTDMPLUS) (Perry et al., 1989) modeling results for steady-state meteorological conditions. Both ISC and CTDMPLUS are recommended in the *Guideline* for use for source-receptor distances of less than 50 km. The second area for enhancement to the CALMET/CALPUFF modeling system was to include provisions within CALMET to allow use of mesoscale meteorological modeling results created using data assimilation techniques, for example Stauffer and Seaman (1989) and Stauffer et al. (1990). The characterization of the time-varying three-dimensional wind field is one of the most challenging issues for long-range transport.

Consistency with local-scale plume dispersion models.

At the Sixth Modeling Conference, IWAQM reported on the inclusion within CALPUFF of dispersion algorithms to provide results consistent with ISC and CTDMPLUS. At the time of the conference, there were only preliminary sensitivity testing results to show that the modifications to CALPUFF would be successful in mimicking ISC. There were no comparison results available showing consistency between CALPUFF and CTDMPLUS. It was recognized and mentioned by IWAQM at the Sixth Modeling Conference that more testing was needed to test whether the code modifications implemented in CALPUFF would replicate dispersion results as would be simulated by ISC and CTDMPLUS.

Enhancement of CALMET for mesoscale applications.

The wind field module in CALMET is based on the Diagnostic Wind Model (DWM). In anticipation of using CALMET and CALPUFF for long-range transport distances, a series of modifications were made (U.S. EPA, 1995b). The DWM in CALMET uses a two step procedure in developing the final wind fields. An initial guess field is developed based on a domain-average wind profile, and this domain-average profile of winds is adjusted for terrain effects and divergence minimization to produce a "Step 1" wind field. The second step in the processing of the wind field is the introduction of the observational data into the terrain adjusted Step 1 wind field.

The adaptations needed to allow use of meteorological wind fields as analyzed by sophisticated mesoscale meteorological models (hereafter referred to as *FDDA-MM data*) involved more than simply providing a new data input option. (For further discussion of Four Dimensional Data Assimilation (FDDA) and how such data sets are constructed, see Section 4.4.) IWAQM was confident that since the surface and upper-air observations are included as part of the data assimilation process, the mesoscale meteorological analyses from such analyses could be treated as data. But IWAQM was aware that inherently such data are representative of a certain scale, as defined by the physics included in the numerical equations and by the grid scale of the results. Therefore, CALMET was modified to allow introduction of the *FDDA-MM data* 1) as input in the creation of the CALMET Step 1 wind fields; 2) as the CALMET Step 1 wind fields; or 3) as input in the creation of the CALMET Step 2 wind fields.

At the Sixth Conference, results from a series of sensitivity analyses were reported investigating how to combine the *FDDA-MM* data with observations, and investigating the impact of *FDDA-MM* data on simulated trajectory results. The sensitivity analyses were conducted for two episodes in eastern United States, one summer episode (August 1-6, 1988) and one winter episode (December 3-10, 1988). The summer episode was characterized by light wind, stagnant conditions. The winter episode was characterized as an active period that included the passage of a front and low-pressure system through the domain. Penn State Mesoscale Meteorological (version 4) modeling results (MM4) were available employing four dimensional data assimilation (Stauffer and Seaman, 1989) for both episodes and for three different grid resolutions, 18-, 54- and 80-km. The CALMET model was run using hourly weather observations from 119 surface stations for both episodes, and used twice-daily observations from 25 upper-air stations for the summer episode and 23 upper-air stations for the winter episode. In general, the introduction of the 80-km MM4 winds improved the ability of CALMET to reproduce the reference 54- and 18-km MM4 wind fields. Slightly better agreement was achieved when the 80-km MM4 winds were brought in after the diagnostic terrain adjustment procedures (i.e., as the Step 1 wind fields or as "observations"). This was conjectured to occur due to the fact that 1) the 80-km MM4 are already close to the 54- and 18-km MM4 results, and 2) the CALMET diagnostic adjustments may duplicate terrain effects that were already accounted for in the development of the 80-km MM4 winds. From the numerical sensitivity tests,

IWAQM concluded that using *FDDA-MM* wind fields adds a noticeable and significant improvement in the characterization of trajectories of the dispersing material within the atmosphere.

D.1.3 Trajectory Comparisons

As discussed in the previous section, modifications were made to CALMET in anticipation of using CALMET and CALPUFF for long-range transport distances (U.S. EPA, 1995b). It was anticipated that use of *FDDA-MM* winds would improve CALPUFF's characterization of trajectories of dispersing pollutants. To further investigate this, two trajectory studies were conducted: 1) comparisons with simulated trajectories, and 2) comparisons with trajectories derived from surface tracer monitoring.

CALMET trajectory comparisons.

Trajectories were computed from four release locations at three levels (10 m, 200 m, and 400 m) for each of the wind fields discussed in Section 4.1.2 for the summer episode (U.S. EPA, 1995b). Trajectories were generated at each location every 4, 6 and 12 hours from the beginning of the simulation, for up to 24 hours before the end of the simulation. A statistical analysis was conducted on the trajectories to assess the effect of the different wind fields.

Trajectory statistics were computed from each release time and for all three levels. In general, the introduction of the 80 km MM4 winds into CALMET to develop either 54 km or 18 km gridded wind fields significantly improved the comparisons with the trajectories developed from the 54 km and 18 km MM4 wind fields directly, versus using only the routine hourly weather observations and twice-daily upper air observations as input to CALMET.

CAPTEX comparisons

One of the primary objectives of this study was to assess whether use of mesoscale dynamic wind fields developed using *FDDA-MM* data exhibited improved spatial and temporal resolution versus typical mesoscale wind fields determined diagnostically from the available hourly surface and twice-daily upper air observations, would improve the quality of the characterization of the transport and dispersion. Results were presented for CAPTEX releases 3, 5 and 7 (Irwin et al., 1996). The Cross-APpalachian Tracer EXperiment (CAPTEX) is a unique series of tracer releases which, besides testing a particular tracer technology, was conducted for the purpose of providing insight into the mechanisms involved in long-range transport and dispersion (Ferber et al., 1986). A three-hour ground-level release of perfluoromonomethyl-cyclohexan (C_7H_{14}, PMCH) was made five times near Dayton, Ohio and twice from near Sudbury, Ontario when winds were expected to transport the tracer over the ground-level sampling network. Samplers were operated at 86 sites in Ohio, Pennsylvania,

New Jersey, New York, New England and southern Canada at distances from 300 to 1100 km from the release site. Air concentrations were collected for 3 and 6 hour durations for several days following each release.

Meteorological data available for use in developing the CAPTEX wind fields consisted of 122 National Weather Service (NWS) surface locations reporting hourly and 13 upper-air locations reporting twice-daily (0000 GMT and 1200 GMT) throughout the region. Furthermore, mesoscale wind fields developed using Version 8 of the Penn State/NCAR Mesoscale Model - Generation 4 (MM4) were available on an 80-km grid. Three wind field models were used to obtain a gridded field of meteorological data with a horizontal resolution of 18-km: MESOPAC II, CALMET, and CALMET using the mesoscale wind fields as STEP-1 inputs. The latter modeled wind fields were developed using FDDA and are referred to as CALMET/MM4.

The comparison results presented were conducted with simplified puff dispersion model assumptions, hence the model-to-model differences were minimized. It was concluded there was a noticeable improvement in the simulation of the puff centroid trajectories, when the wind fields were developed using *FDDA-MM* data, versus developing the wind fields diagnostically from the available hourly surface and twice-daily upper air observations. The analysis of the concentration maxima and lateral dispersion values suggest that the simulation assumptions employed in these results consistently underestimate the horizontal extent of the tracer puff as it is transported downwind. The centroid maximum surface concentration was found to be correspondingly overestimated and relatively insensitive to the mesoscale wind characterization. In these simulations, no provisions were made to address delayed shear enhancement of the dispersion as described by Moran and Pielke (1994) and Shi et al. (1990). Inclusion of some sort of puff splitting is obviously warranted, but the computational demands are not trivial if one is attempting to develop an operational model for routine use. Furthermore, in those cases where the puff model dynamics have been enhanced, for example Draxler (1987) and Davis et al. (1986), there was a tendency to underestimate the surface maximum concentrations.

D.1.4 Constructing *FDDA-MM* Data Sets Assessment

To foster use of mesoscale meteorological (MM) data processed using Four Dimensional Data Assimilation (FDDA) in routine air pollution modeling assessments and to learn what problems might be associated with such a project, a one-year meteorological data set for 1990 was fabricated that spans the contiguous United States, southern Canada and northern Mexico. The 1990 data set (NCDC, 1995) was somewhat dated when it was discussed at the Sixth Modeling Conference. Yet it still represents a significant advancement to meteorological characterizations employed in many current routine air pollution assessments. These data were made available to allow investigators to have access to this type of data that they might otherwise not have access to (NCDC, 1995), with the hope that this would stimulate investigations, exploring the strengths and weaknesses of these data in a variety of ways.

The 1990 data set consist of hourly profiles of wind, temperature and moisture at 23 levels in the atmosphere on an 80-km grid spacing. The Penn State mesoscale meteorological model (MM4) with FDDA was used in developing these data. The horizontal grid spacing of the MM4 simulation was 80 km in both dimensions, with a grid array size of 85 by 56 centered on 90 W longitude and 40 N latitude to cover most of the North American continent and adjacent oceanic areas (Bullock, 1993). The domain of the model's vertical coordinate system extended from the earth's surface to the 100 millibar pressure level (approximately 15 km above sea level). It's 15-level structure provides height-resolved information similar to that routinely obtained by the National Weather Service at 12-hour intervals from approximately 80 rawinsonde balloon sounding locations across North America. However, the data set obtained from the MM4 simulation provides synthetic soundings at 1-hour intervals for 4080 model grid-point locations, or about 600 times more information than is available from routine observational networks. The 1990 data set is comprized of over 20 billion bytes of information.

One of the lessons learned in developing the 1990 data set was that the science of mesoscale analysis using data assimilation is rapidly developing. Major advancements have been occurring every several months during the period from 1995 through 1997. There are various research groups with active development programs investigating mesoscale meteorological modeling employing data assimilation, e.g. Pielke et al., (1997). This suggests that developing and maintaining a multi-year data set would likely involve a substantial committment in resources. An alternative to commissioning special one-year runs would be to use results from an existing operational ongoing activity (Pielke and Uliasz, 1997). One such activity is a product that currently is under development and refinement by the NOAA Environmental Modeling Center Mesoscale Modeling Branch. They are employing a mesoscale numerical weather prediction model, known as the NCEP ETA Model, with data assimilation. This mesoscale meteorological model produces analyses of the vertical profiles of wind, temperature, pressure and moisture on a 48 km grid resolution that covers a very large domain (e.g., as far west as the Hawaiian Islands, all of the contiguous United States, as far north as all of Alaska). The current operational output provides information for 38 layers in the vertical. The model employs a surface moisture balance model (Chen et al., 1997), and hence is capable of reporting the surface heat and moisture fluxes, soil moisture, and precipitation (amounts for both wet, frozen and snow).

The Environmental Modeling Center (EMC) Home Page is: http://nic.fb4.noaa.gov:8000/. The ETA model outputs are produced by the Mesoscale Modeling Branch (MMB). The Mesoscale Modeling Branch Home Page is: http://nic.fb4.noaa.gov:8000/research/mesoscale2.html.

A major obstacle is access to these data. The 1990 MM4 data set in a compressed format (providing only profiles of wind, temperature and moisture) requires 12 Compact Diskettes. An operational means for gaining easy access to

comprehensive mesoscale meteorological data sets, as alluded to here, has yet to be developed. But IWAQM believes that the future of air quality modeling requires a solution being found to gain routine inexpensive access to such data. And IWAQM believes that it is only a matter of time (perhaps less than three years) that such a solution could be found.

D.1.5 Regional Approach

The effective treatment of mesoscale transport of pollutants requires treatment of the time and space variations of the three-dimensional meteorological conditions. This in turn involves consideration of the variations in terrain heights and land-use, and their consequent effects on the dispersive characteristics of the atmosphere. A major issue in assessing mesoscale impacts to specific Class I areas from specific sources is giving due consideration to the proper characterization of the transport (trajectory) of the pollutants. As alluded to in the discussion of Section 4.1, where MESOPUFF II was used to assess impacts on the Shenandoah National Park, and in Section 4.3, where the characterization of the transport trajectories was investigated, this is not a process that lends itself to a cookbook approach. Tailoring the wind field analysis will require technical judgement and discretion, and IWAQM has come to the opinion that these case-specific decisions are best achieved using a team of experts and development of a consensus.

The discretion and case-specific decision making does not apply soley to the implementation of the dispersion modeling. Not all wilderness areas have the same flora and fauna. The AQRVs of interest will be specific to each wilderness area. Developing an inventory with agreed upon emission rates is not trivial. The inventory could differ depending on whether the analysis is addressing NAAQS assessments (which typically address maximum allowable emission rates from PSD sources) versus AQRV assessments (which typically address actual current emission rates from all sources).

Therefore at the Sixth Modeling Conference, IWAQM suggested that Class I air quality modeling assessments be designed for each Class I area (or cluster of Class I areas), rather than for each permit as is the case for the Class II program. The cornerstone of this approach is an up-front comprehensive increment and AQRV analysis of the area. This "initialization" study would be accomplished outside the context of a permit application, and could involve technical experts from private and public groups. Perhaps most importantly, it provides future applicants with up-front information needed for planning and assurance of what is expected for the given situation.

D.1.6 Sixth Modeling Conference IWAQM Recommendations

At the Sixth Modeling Conference, IWAQM recommended that the CALPUFF modeling system (Scire et al., 1995a,b) replace the MESOPUFF II modeling system.

Based on sensitivity studies and the CAPTEX comparisons of results obtained by the two modeling systems, IWAQM had concluded that the CALPUFF modeling system was at least as good as the MESOPUFF II modeling system, and offered several improvements. For one, the CALPUFF modeling system code was better documented and was believed to be better engineered. Graphical User Interface (GUI) applications were under development to assist and make easier the use of the CALPUFF modeling system. CALMET had been enhanced to allow use of *FDDA-MM* mesoscale meteorology. CALPUFF had been enhanced to allow better correspondence with local-scale (less than 50 km transport) models recommended for use in the *Guideline*. These latter enhancements provided the basis for allowing one model to be used for all sources in a mesoscale assessment, even though for some of the sources the transport might be less than 50 km. At the time of the Sixth Modeling Conference, the CALPUFF modeling system was not available from the EPA Support Center for Regulatory Models (SCRAM) electronic Bulletin Board Service (BBS), but it was anticipated that it would soon be available in an area designated "Topics for Review and Comment."

Even though such data were not available, nor was it likely that IWAQM would be able to develop such data, IWAQM recommended that use of *FDDA-MM* mesoscale meteorological data be approved in regulatory assessments. The comparisons between alternative methods for developing CALMET wind fields, and the comparisons of the resulting trajectories, suggested to IWAQM that the added skill in the assessment was dramatic and desirable. There were (and still remain) serious logistical issues to development and use of such data. But in each case where such data have been used, the characterization of the trajectories has improved.

Finally, given the myriad of decisions needing to be made in most mesoscale assessments of transport and dispersion impacting Class I areas, IWAQM recommended that a Regional Approach be used to resolve the various decisions. This involves assembling a committee of the various public and private stakeholders, and gaining consensus that the committee will be proactive in developing a plan to chart a course through the specific decisions needing to be made for the Class I area they are concerned with, and following the developed plan. For those seeking permits, being able to go to such a committee for information is of great benefit. It insures that all applicants are treated equitably, and it allows packaging of the results from each applicant in a manner that supports cumulative impact tracking and assessment. If the committee sponsors development of meteorological data sets, these can be made available to the applicants to save costs and time.

D.2 Summary Of Sixth Modeling Conference Comments

One commenter pointed out the practical deficiencies with straight line plume transport models and strongly urged the development and adoption of a trajectory model. Another commenter pointed out the technical superiority of CALPUFF over the best Gaussian models EPA supports. The commenter urged that the advantages and applicability of CALPUFF be discussed among state and regional modeling contacts,

that evaluation and comparison data be amassed, and that early consideration be given to case-by-case regulatory applications of CALPUFF.

Another commenter noted that "[The IWAQM] apparently did not address the question of whether or not [an air quality analysis beyond 50 km] can be done with the hope of reaching any reasonable answer." The commenter argued that there is no accurate way to do this. The commenter also noted that IWAQM did not address the accuracy of the Phase I screening analysis (Level I) or refined analysis (Level II). Also, the results were not qualified (i.e., level of conservatism was not stipulated). It was recommended that IWAQM qualify the accuracy of the results. For Level I analyses, it was recommended that IWAQM remove the stagnation and recirculation wording and that IWAQM specify with "reasonable particularity" the *Guideline* models to be used, that some reasonable yet conservative and consistent conversion rates for both visibility and deposition be assumed, and that the Level I analysis be a true screen. For Level II analyses, the commenter recommended that, if a preapproved protocol is required, the regulatory and FLM agencies must agree to abide by the results and that on-site meteorological data not be required. The commenter believes that in some cases the regulatory need to analyze long-range impacts is beyond the state-of-the-practice, and that IWAQM failed to portray how conservative such calculations really may be. Several figures were included to illustrate the commenter's contention that CALPUFF would have severe difficulty simulating accurate concentrations on the back side of terrain along certain transects near the Rockies.

Aside from the more specific comments mentioned above, the commenters all seemed in agreement that the Regional Approach outlined by IWAQM was desirous. There seemed general agreement that the Level I screen suggested in the Phase I interim recommendations was not working well and needed to be improved. There was also general agreement that the CAPTEX comparisons were for transport distances of 300 to 1000 km, well beyond the anticipated range of PSD Class I impact assessments. Therefore, more comparisons with tracer data studies for transport distances of order 50 to 200 km were needed. Finally, although only mentioned by the last commenter, there was a sense that mesoscale transport assessments may be very difficult analyses, involving discretion and expert judgment. In some instances, the modeling results would be so uncertain as to preclude them of being any use.

D.3 Response to Sixth Modeling Conference Comments

The comments received at the Sixth Modeling Conference can be summarized into several general areas: 1) there seemed to be agreement that the Regional Approach outlined by IWAQM was desirous; 2) there was general agreement that as the CAPTEX comparisons were for transport distances of 300 to 1000 km, well beyond the anticipated range of PSD Class I impact assessments, that more comparisons with tracer data studies for transport distances of order 50 to 200 km were needed; 3) there was general agreement that the Level I screen suggested in the Phase I interim recommendations was not working well and needed to be improved; 4) there was

agreement that comparisons were needed to assess whether CALPUFF can provide results similar to ISC and CTDMPLUS for steady-state meteorological conditions; and 5) finally there was a sense that mesoscale transport assessments may be difficult analyses (perhaps impossible in some cases), requiring discretion and expert judgment.

Regional Approach

It has been IWAQM's experience that most long-range transport dispersion assessments involve expert judgement and finesse in order to provide a reasonable characterization of the transport and dispersion with the information and resources available. The process has yet to be successfully accomplished using "cookbook" procedures. To further complicate matters, the AQRV's of interest are typically specific to the Class I area and climate, and thus the modeling endpoints need to be customized to address the site-specific issues of concern. It is therefore understandable that most people concur with the recommendation by IWAQM to employ committees of technical experts, whenever possible, to sort through the various decisions and tradeoffs. It also understandable that most people would endorse having a panel of experts dedicated to a particular Class I area (or areas) that could provide some consistency in the modeling assessments and assist in addressing site-specific questions as they arise. But just as some of the options in an air quality modeling system can not be automatically prescribed, the same can be said for use of technical committees. Hence, while IWAQM endorses use of such committees, IWAQM does not recommend Federal agencies mandate or require their use.

Model evaluations for the 50 to 200 km range

There are very few tracer dispersion field studies with sufficient sampling to depict with some certainty the relative location of the receptors to the puff of dispersing tracer as it was transported downwind. In fact, the number of studies is so small that comparison results that can be developed only provide anecdotal evidence regarding model performance. In response to the suggestion that comparison results be developed for transport of order 50 to 200 km, IWAQM commissioned studies for four tracer dispersion experiments. A summary of the findings for each of the four tracer studies is provided in Section 4.6. Three of these field studies involved 3 to 4 hour releases that were then sampled along arcs of receptors downwind. In some cases, shorter-term concentration values were available, such that the transport of the puff past an arc could be seen. Differences on the order of 10 to 20 degrees were seen between the simulated and observed center of mass of the puff as it passed the receptor arc. Most of the simulated centerline concentration maxima along each arc were within a factor of two of those observed. In those instances when large over- or underpredictions occurred, there was insufficient information available to ascertain the physical processes that resulted in the observed concentration values. Without a better understanding of the physical dispersion processes affecting these instances, no simulation has (or likely will) show skill.

It was concluded from these admittedly anecdotal case studies, that CALPUFF is performing in a reasonable manner, and has no apparent bias towards over- or under-prediction. This is in contrast to the CALPUFF comparison results with the CAPTEX tracer field data, where CALPUFF consistently underestimated the 'footprint' of the puff in contact with the surface, and correspondingly overestimated the puff concentration maxima by a factor of 2 or more. This suggests CALPUFF (as configured for the CAPTEX comparisons) was poorly characterizing dispersion processes (such as delayed shear enhancement) which become important for transport distances of order 300 km or more. It is concluded that CALPUFF will need to be further developed before it can more realistically characterize transport and dispersion for more than one diurnal cycle.

The IWAQM concludes that CALPUFF can be recommended as providing unbiased estimates of concentration impacts for transport distances of order 200 km or less, and for transport times of order 12 hours or less. For larger transport times and distances, our experience thus far is that CALPUFF tends to underestimate the horizontal extent of the dispersion and hence tends to overestimate the surface-level concentration maxima. This does not preclude the use of CALPUFF for transport beyond 300 km, but it does suggest that results in such instances be used cautiously and with some understanding.

Comparisons with ISC and CTDMPLUS

At the time of the Sixth Modeling Conference, the algorithms installed in CALPUFF to allow it to mimic ISC and CTDMPLUS had not been thoroughly tested. In response to the need for further comparisons, a thorough investigation and comparison with ISC was completed. A similar investigation is needed but has yet to be accomplished with CTDMPLUS. A summary of the comparison results with ISC is presented in Section 4.7.

As expected, when the meteorological conditions were steady-state (fixed wind direction, wind speed, mixing height, and stability), there were only minor differences seen between ISC and CALPUFF. For all of the point source and volume source comparisons, the differences seen between ISC and CALPUFF were less than one percent. The largest differences were seen for receptors within and near the downwind edge of a simulated area source. For the area source comparisons, the differences on average were less than four percent, but individual cases were seen with larger differences. These larger differences seen with the area source are traceable to the difficulty of efficiently replicating the plume model's characterization of an area source. The IWAQM concluded that, for all practical purposes, although improvements might be made, the algorithms within CALPUFF are capable of replicating the results of ISC for steady-state meteorological conditions.

When the meteorology was allowed to vary from one hour to the next, but not in space, large differences were seen in the simulated highest and second-highest

concentrations for all averaging times examined (1-hour, 3-hour, 24-hour, and annual) and for all distances downwind out to 300 km. In general, CALPUFF was seen to provide higher surface-level concentration impacts than ISC in those special situations where the preceding hours had several hours of calm winds, or involved a dramatic wind reversal and caused previously released material to be simulated to combine with newly released material. Given that ISC ignores impacts during calm wind conditions, and can not characterize the 'causality' resulting from a buildup of material during an extended period of calm winds or a reversal in the transport winds, such differences were expected.

The IWAQM concludes that CALPUFF does reproduce, for all practical purposes, the results that would be obtained using the ISC plume dispersion model, when the meteorological conditions are steady-state. For situations involving complex winds conditions (frequent periods of extended calms, routine and periodic wind reversals, complex topographical wind effects and channeling, etc.), where a local-scale plume dispersion model (such as ISC) is the recommended modeling approach, IWAQM recommends acceptance on a case-by-case basis the results obtained using the CALPUFF modeling system. In these situations, the three-dimensional time-varying wind field and the 'causality' from one hour to the next are most important in deriving an assessment of the impacts associated with the transport and dispersion of pollutants.

In conducting the comparisons of CALPUFF with ISC, minor inconsistencies were found and corrections were made to the CALPUFF algorithms, so that the CALPUFF results would replicate (to the extent a puff model can) the results that would be obtained by a plume model for steady-state meteorological conditions. A similar intensive inspection of the CTDMPLUS algorithms within CALPUFF has yet to be accomplished. Once such an investigation has been completed (assuming that CALPUFF can be made to provide results acceptably similar to those obtained with CTDMPLUS for steady-state meteorological conditions), then IWAQM would endorse use of results from the CALPUFF modeling system on a case-by-case basis, in lieu of those obtained from the CTDMPLUS model, for complex wind situations.

Develop a better screen technique

At the Sixth Modeling Conference, the 'Level I' technique suggested in IWAQM Phase I interim recommendations (EPA, 1993), of using as a screening model results for the ISC dispersion model, was generally considered inadequate. The Level I screening estimates of the AQRV impacts were considered so conservative that only sources with very small emissions were 'screened' from further consideration. In response to these comments, a study was conducted in an attempt to construct a more meaningful and useful screening technique, a summary of which is presented in Section 4.8.

By far the most demanding task to successfully accomplish is to develop a valid time and space varying characterization of the meteorological conditions for use by the

CALPUFF puff dispersion model. Thus IWAQM concluded that if a simplification could be made in specifying the meteorological conditions, perhaps CALPUFF could be used to develop the screening estimates of pollutant impacts. This would allow the chemistry and fate to be appropriately characterized, and at least some of the 'causality' effects would be captured. It was with this background and understanding that IWAQM investigated developing a screening estimate using CALPUFF with a highly simplified characterization of the meteorological conditions.

In the course of the development of the CALPUFF modeling system, options were implemented that allow the meteorological conditions to be specified using either the meteorological input required for the ISC model, or the meteorological input required for the CTDMPLUS model. These optional formats for specifying the meteorology to CALPUFF were implemented initially to facilitate testing of ISC and CTDMPLUS algorithms in CALPUFF. The IWAQM decided to pursue development of a screening estimate that could be made using the meteorological input for the ISC model, as input to CALPUFF.

One of the consequences of simplifying the meteorological input to that of the ISC model, is all terrain effects (channeling, slope flows, etc.) are lost. The consequence of these effects can become important in assessing pollutant impacts for specific source-receptor combinations. To counter for the loss of properly characterizing the spatial variations in the meteorological conditions, it was decided that rings of receptors would be used that completely surround the source under analysis. The rings would be placed to pass through the Class I area(s) of concern, and would be spaced to provide suitable coverage, using expert judgement and in agreement with applicable reviewing authorities. The maximum pollutant impacts (increment, AQRV, etc.) found anywhere on any of the rings of receptors would be used as the screening impact estimate of the pollutant impact. Selecting only receptors within the particular Class I area(s) is not appropriate, as the screening analysis as designed does not address the spatial variations in the meteorological conditions.

As summarized in Section 4.7, use of ISC meteorological input does not guarantee that the maximum SO_2 concentration found on a ring of receptors is consistently estimated to be larger than what would be found if a complete three-dimensional time-varying wind field and meteorological conditions were used, all other factors being equal. In the sensitivity tests conducted, the longer the averaging time of the SO_2 concentration, the more likely the maximum for a ring of receptors will be similar, whether ISC or CALMET meteorology input is used. The CALPUFF screening estimates of sulfate concentrations and deposition were consistently much less than would be estimated using IWAQM Phase 1 Level 1 ISC procedures. The CALPUFF screening estimates of sulfate concentrations and deposition were sometimes higher and sometimes lower than that seen using full CALMET input to CALPUFF.

It is concluded by IWAQM that using five years of ISC meteorology as input to CALPUFF, and selecting the maximum concentration from rings of receptors that

completely surround the source under analysis, provides a reasonable basis for developing screening estimates. There is a finite possibility that using fully developed CALMET input to CALPUFF, somewhat higher maxima might be simulated, but whether these would be at receptors of interest in the Class I area(s) is considered less likely. In fact, it is considered highly likely that lower pollutant impacts would be simulated if use was made of fully developed CALMET input to CALPUFF, and only impacts to receptors in the Class I area(s) were considered. The IWAQM recommends use of the new screening technique, as it provides a more realistic assessment of the fate and transport of the pollutants than the Phase 1 screening (Level 1) technique. The new screening technique provides estimates of maximum impacts, that are similar to those derived using fully developed CALMET input. Although, the air dispersion modeling community has less experience using the CALPUFF puff dispersion model than the ISC plume dispersion model, the operation of CALPUFF (with ISC meteorological input) is not anticipated to be unduly difficult or onerous.

Realistic expectations

At the Sixth Modeling Conference, some of the concerns expressed were that estimating pollutant impacts is so uncertain in some circumstances to perhaps preclude meaningful use of the estimated impacts. An example that was used to illustrate this point was described where the source emissions being characterized were separated from the receptors of interest by two mountain ridges, whose tops exceeded the effective release height of the example source. The situation described was neither impossible nor unrealistic. The IWAQM agrees with the commenter's conclusion that in such a situation highly uncertain pollutant impacts would be generated, regardless of the air quality model employed. Whether such estimates would be of little practical use would depend on the exact nature of the assessment being attempted. Even though the estimates might be uncertain and depend on the physics incorporated in the air dispersion model simulations, inspection of the simulation results might suggest that impacts from the source in question could reasonably be argued to be inconsequential or highly unlikely. As in any air quality simulation, the usefulness of the results obtained depends mostly on the expertise brought to the analysis in characterizing the situation, and on the experience applied in interpreting the results obtained. The IWAQM agrees with the sentiments of the commenters at the Sixth Modeling Conference, that as the terrain and land-use induced mesoscale circulations become more dominant, the expertise and integrity of the modeler will define the usefulness of the results.

It would be convenient if objective criteria could be developed that would identify when air quality simulation results are of questionable integrity. It would be convenient if objective criteria and "cookbook" procedures could be constructed that would preclude inappropriate application of air dispersion models. This has proved to be troublesome for local-scale modeling, and even more problematic for mesoscale and long-range transport modeling.

In response to the comments received, IWAQM has attempted to warn the modeling community in the summary of its Phase 2 recommendations (Section 2), that conducting a long-range transport assessment requires competent individuals. The IWAQM have also tried to warn the modeling community that application of the CALPUFF modeling system to any situation will require expert judgment, it will likely involve site-specific decisions, and it will require strong interaction and coordination with the applicable reviewing authorities.

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This Phase 2 Report is published by the Interagency Workgroup on Air Quality Modeling (IWAQM) in an effort to provide the sponsoring agencies and other interested parties information on appropriate “off-the-shelf” methods for estimating long range transport impacts of air pollutants on Federal Class I areas.

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