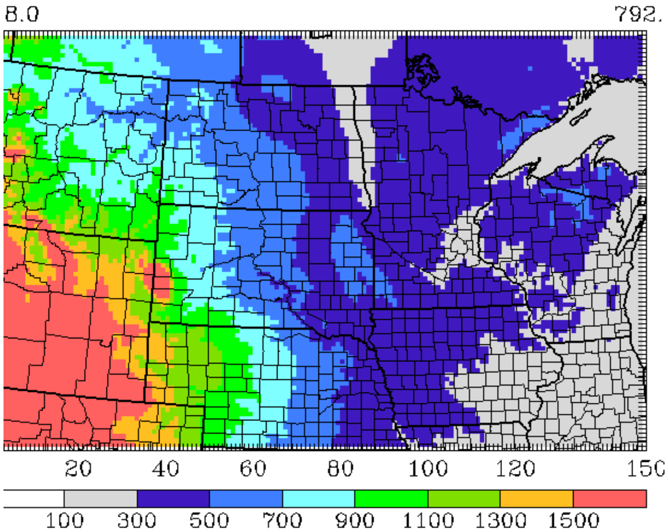
CENRAP BART MODELING GUIDELINES



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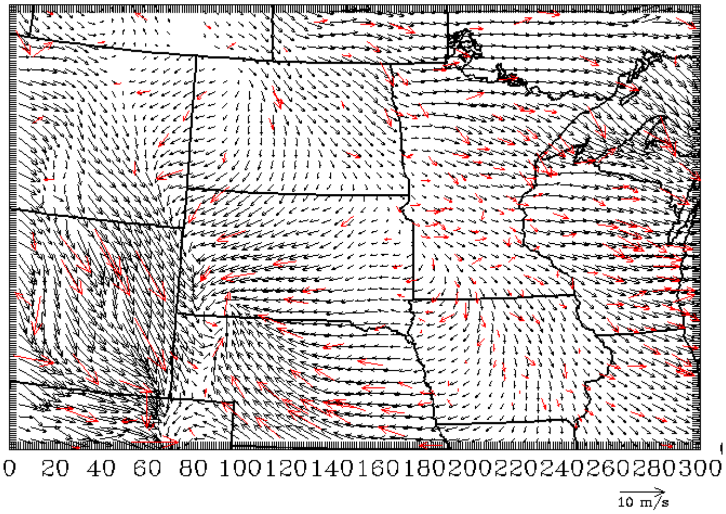

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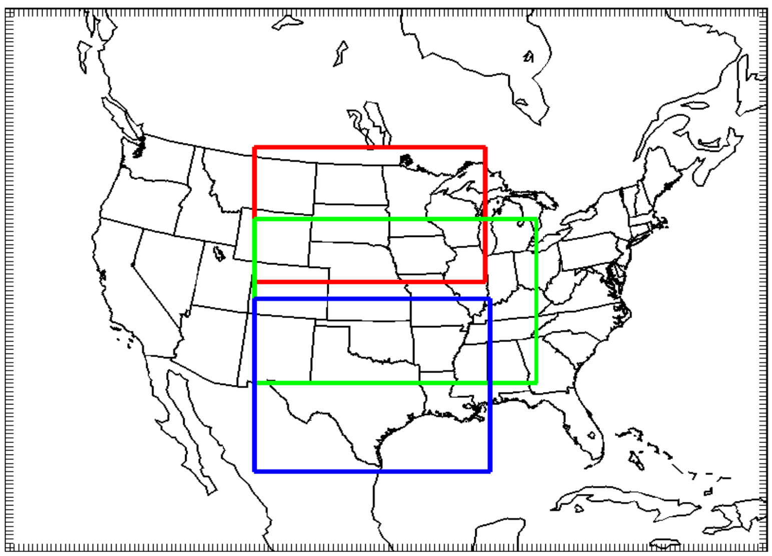

Three CALMET Modeling Domains

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PREFACE

On 6 July 2005, the U.S. Environmental Protection Agency (EPA) published final amendments to its 1999 Regional Haze Rule in the Federal Register, including Appendix Y, the final guidance for Best Available Retrofit Technology (BART) determinations (70 FR 39104-39172).). The BART rule requires the installation of BART on emission sources that fit specific criteria and "may reasonably be anticipated to cause or contribute" to visibility impairment in any Class I area. Air quality modeling is the preferred method for determining which emission sources cause or contribute to visibility impairment.

This document establishes guidelines for performing dispersion modeling analyses in support of BART determinations for sources located within the CENRAP domain. Largely consistent with EPA guidelines, these CENRAP BART Modeling Guidelines cover the many assumptions, data base elements, model configurations and analytical methods that CENRAP states and/or source operators should consider using in their assessments of whether BART eligible sources are indeed 'subject to BART', or may be exempted. For those sources determined to be subject to BART, these guidelines provide for a common and consistent methodology for estimating the visibility improvements associated with BART emissions reductions.

Each state is required to develop a BART Modeling Protocol setting forth the required steps in assessing the levels of controls needed on sources subject to BART. At the same time, the five (5) Regional Planning Organizations (RPOs) are addressing the requirement of the Regional Haze Rule in a generally consistent manner, with some exceptions for how BART is treated. The Midwest RPO for example, is expected to conduct most of the BART modeling for sources within its region. In the VISTAS states, the BART modeling is expected to be a shared exercise between VISTAS and the states. In the central states, the states themselves will take the lead in the BART modeling, but CENRAP will provide assistance in the form of modeling guidance (this document) and readily-available modeling data bases (delivered separately) that can be used by states and/or source operators to conduct their analyses.

Deferring to the states and RPO's, EPA has placed the responsibility of preparing modeling protocols with the groups who will actually be performing the modeling, rather than developing a prescriptive protocol covering all states and sources. EPA has provided so-called BART modeling guidelines (EPA, 2005) which set for the general framework for performing the analyses. It is up to the states and RPO's to develop the modeling protocols governing the BART modeling activities within their jurisdictions.

Several BART modeling protocols have been developed within the past year prior to and in parallel with these CENRAP BART Modeling Guidelines. In the interest of providing consistency in the selection, use, and interpretation of models and analytical methods, we have attempted to synthesize key unifying elements of these protocols and weave them into a consistent set of modeling procedures for the CENRAP region, paying attention to the unique characteristics of this region and the sources located within. At the same time, EPA guidance on how the BART modeling analyses will be judged has evolved and many protocols as well as this guideline document have been refined to reflect EPA's clarifications.

Several modeling protocols developed by other RPOs and State agencies are particularly relevant to CENRAP's effort to develop consistent guidelines for the Central states. Six BART protocols are especially significant:

> *"VISTAS Protocol for the Application of the CALPUFF Model for Analyses of Best Available Retrofit Technology (BART)"*, (VISTAS, 2005). Prepared by the Visibility Improvement State and Tribal Association of the Southeast (VISTAS) Technical Analysis Work Group (TAWG), and Earth Tech, Inc.

> *"CALPUFF Modeling Protocol in Support of Best Available Retrofit Technology Determinations"*, (Johnson, 2005). Prepared by the Iowa Department of Natural Resources, Air Quality Bureau, Des Moines, IA.

> *"Best Available Retrofit Technology (BART) Modeling Protocol to Determine Sources Subject to BART in the State of Minnesota"*, (MPCA, 2005). Prepared by the Minnesota Pollution Control Agency, St. Paul, MN.

> *"Modeling to Support BART"*, (Baker, 2005). Prepared by the Midwest Regional Planning Organization and the Lake Michigan Air Directors Consortium, Des Plaines, IL.

> *"CALMET/CALPUFF BART Protocol for Class I Federal Area Individual Source Attribution Visibility Impairment Modeling Analysis"*, (CDPHE, 2005). Prepared by the Air Pollution Control Division, Colorado Department of Public Health and Environment, Denver, CO.

> *"Screening Analysis of Potentially BART-eligible Sources in Texas"*, (ENVIRON, 2005). Prepared for the Texas Commission on Air Quality, Austin, TX.

All of these protocols address a common subject; thus, there is substantial overlap in the discussions of numerous topics such as Federal requirements, EPA guidance, CALMET/CALPUFF model descriptions, and recommended modeling procedures and so on. There are differences, of course, due to local meteorology, topography, location of Class I areas, the mix of BART-eligible sources, and established modeling procedures within the state, local and federal land manager (FLM) groups.

To promote consistency in BART modeling applications across the central and eastern U.S., in preparing these CENRAP Guidelines, we have incorporated common elements of existing protocols where possible. The VISTAS protocol deserves special mention. It was prepared jointly by members of the VISTAS Technical Analysis Work Group (TAWG) led by Ms. Pat Brewer, VISTAS' Technical Advisor Dr. Ivar Tombach, and Mr. Joe Scire of Earth Tech, Inc. The VISTAS protocol represents the culmination of several draft versions and considerable public discussion and input. At least two public workshops were convened in the autumn of 2005 to solicit comments and suggestions on draft versions and to receive input from EPA staff on evolving agency guidance. Details of these public discussions may be found at: http://www.vistas-sesarm.org/BART/BARTComments.asp. Because the VISTAS protocol reflects the work of a large number of organizations, we have incorporated a number of the recommendations set for the therein..

In summary the CENRAP BART Modeling Guidelines presented in this document represent the integrated writing efforts of many groups, especially the modelers and regulatory decision-makers instrumental in developing the VISTAS, MRPO, Iowa, Minnesota, Texas, and Colorado BART Modeling Protocols. The authors are indebted to the contributions of these groups, and assume responsibility for any misstatements or errors in incorporating written descriptions from the aforementioned documents.

ACKNOWLEDGMENTS

The authors wish to acknowledge specifically the assistance and, in several cases, written contributions by the following individuals in the preparation of this guidance document:

> Mr. Chris Arrington, West Virginia Department of Environmental Protection; Mr. Bret Anderson, U.S. EPA; Dr. Kirk Baker, Lake Michigan Air Directors Consortium; Ms. Pat Brewer, VISTAS Technical Coordinator; Mr. Chad Daniels, Iowa Department of Natural Resources; Dr. Bright Dornblaser, Texas Commission on Environmental Quality; Mr. Todd Hawes, EPA/OAQPS; Ms. Cyndi Huber, U.S. Forest Service; Mr. Matthew Johnson, Iowa Department of Natural Resources; Ms. Margaret McCourtney, Minnesota Pollution Control Agency; Mr. Bruce Polkowsky, National Park Service; Mr. Tom Rodgers, Florida Department of Environmental Protection; Ms. Rosalina Rodriguez, North Carolina Department of Natural Resources; Mr. Joe Scire, Earth Tech, Inc.; Dr. Ivar Tombach, VISTAS Technical Advisor; Mr. John Vimont, National Park Service; and Ms. Lee Warden, Oklahoma Department of Environmental Quality.

Particular recognition is due Mr. Ralph Morris of ENVIRON International Corporation who served as an independent technical reviewer throughout the course of this study and provided many useful suggestions, insightful recommendations and key text.

1.0 INTRODUCTION

On 6 July 2005, the U.S. Environmental Protection Agency (EPA) published final amendments to its 1999 Regional Haze Rule (RHR) in the Federal Register, including Appendix Y, the final guidance for Best Available Retrofit Technology (BART) determinations (70 FR 39104-39172). The rule applies to any BART-eligible source that ‘‘emits any air pollutant which may reasonably be anticipated to cause or contribute to any impairment of visibility” in any mandatory Class I federal area (Figures 1-1 through 1-4). States retain the authority to exempt certain BART-eligible sources based on dispersion modeling demonstrating that the source cannot reasonably be anticipated to cause or contribute to visibility impairment in a Class I area. States also have the authority to define the modeling procedures used to establish BART emissions limits on those sources for which controls are required. To assist the states, the EPA has offered guidelines for how BART modeling should be conducted (EPA, 2005). Although the Federal regulations implementing the BART requirement afford States latitude in establishing criteria for BART-exemptions and for determining levels of BART controls required on specific sources, the dispersion modeling analyses must either conform to established EPA guidance for regulatory modeling or demonstrate, through an acceptable modeling protocol, that alternative modeling methods are equally consistent with the overall aim of the RHR.

States have the responsibility for preparing modeling protocols that describe both the modeling analyses for the ‘subject to BART’ test and the visibility improvement analyses as part of the BART determination. In developing modeling protocols, states are expected to collaborate with all stakeholders including Tribes, EPA, Federal Land Managers (FLMs), Regional Planning Organizations (RPOs) and the various source operators. Ultimately, EPA has the authority to approve or disapprove a state’s State Implementation Plan (SIP). A flawed BART modeling analysis, including deviations from an agreed upon protocol, would be considered in the SIP approval process.

At least three CENRAP States (Iowa, Minnesota, and Texas) have already developed BART modeling protocols:

- *“CALPUFF Modeling Protocol in Support of Best Available Retrofit Technology Determinations”*, (Johnson, 2005). Prepared by the Iowa Department of Natural Resources, Air Quality Bureau, Des Moines, IA

- *“Best Available Retrofit Technology (BART) Modeling Protocol to Determine Sources Subject to BART in the State of Minnesota”*, (MPCA, 2005), prepared by the Minnesota Pollution Control Agency, St. Paul, MN.

- *“Screening Analysis of Potentially BART-eligible Sources in Texas”*, (ENVIRON, 2005), prepared for the Texas Commission on Air Quality, Austin, TX.

Protocols may be under development in other States as well. To promote consistency between states in the development of BART modeling protocols and to harmonize the approaches between adjacent RPOs, CENRAP commissioned the development of the BART Modeling Guidelines set forth in this document. These guidelines are intended to assist CENRAP states and source operators in the development of state-wide and source-specific modeling protocols specifically tailored to the needs and requirements of a given facility and Class I area(s).

In addition to the Iowa, Minnesota, and Texas protocols, the states of Colorado (CDPHE, 2005) and North Dakota (NDDH, 2005), VISTAS (VISTAS, 2005), the Midwest RPO (Baker, 2005;

LADCo, 2005) have also developed BART protocols. Since they all address a common subject, there is substantial overlap in the discussions of numerous topics such as Federal requirements, EPA guidance, CALMET/CALPUFF model descriptions, and recommended modeling procedures. Differences among the protocols exist, of course, due to local meteorology, topography, the location of Class I areas, the mix of BART-eligible sources, and established modeling procedures within the state, local and FLM groups. For consistency in BART modeling applications across the central U.S., in preparing these CENRAP Guidelines we have utilized relevant elements of each of these protocols.

The VISTAS protocol deserves special mention. It was prepared by members of the VISTAS Technical Analysis Work Group led by Ms. Pat Brewer, VISTAS's Technical Advisor Dr. Ivar Tombach and Mr. Joe Scire of Earth Tech, Inc. The VISTAS BART protocol represents the culmination of several draft versions and considerable public discussion and input. At least two public workshops were convened in the autumn of 2005 to solicit comments and suggestions on draft versions and to receive input from EPA and FLM staff on evolving agency guidance. See full comments at: http://www.vistas-sesarm.org/BART/BARTComments.asp. Thus, element of the VISTAS protocol, reflecting the work of a very large number of organizations, were incorporated as appropriate into the CENRAP modeling recommendations.

The guidelines presented in this document therefore represent the integrated writing efforts of many groups, especially the modelers and regulatory decision-makers instrumental in developing the VISTAS, MRPO, Iowa, Minnesota, Colorado and North Dakota protocols.

1.1 Overview

EPA's BART requirements (70 FR, 39104-39172) are mandatory for electric generation units (EGUs) $\geq$ 750 MW capacity. States are not required to follow the EPA BART guidelines for all sources, but are encouraged to apply the guideline concepts to all sources. States have the authority to make any or all aspects of the EPA BART guidelines mandatory for all BART determinations.

Sources are BART-eligible if they meet three specific criteria including (a) emissions of at least 250 tons per year of a visibility-impairing pollutant, (b) begin operation between 7 August 1962 and 7 August 1977, and (c) are listed as one of the 26 listed source categories in the guidance. BART controls are required for any BART-eligible source that can be reasonably expected to "cause" or "contribute" to impairment of visibility in any of the 156 federal parks and wilderness (Class I) areas protected under the regional haze rule. Air quality modeling is an important tool available to the States in determining whether a source can be reasonably expected to contribute to visibility impairment in a Class I area.

A "BART-eligible emission unit" is defined as any single emission unit that meets the BART criteria described above. A "BART-eligible source" is defined as the total of all BART-eligible emission units at a single facility. If a source has several emission units, only those that meet the BART-eligible criteria are included in the definition "BART-eligible source".

1.2. Objectives of These Guidelines

Overall compliance with RHR visibility improvement goals in the CENRAP region entails four phases of visibility modeling:

> Single-source modeling to determine which BART-eligible sources are ‘subject to BART’;

> Single-source modeling to determine the degree of visibility improvement attributable to proposed BART controls for each source subject to BART;

> Cumulative modeling to determine the combined effect of proposed BART controls for sources subject to BART in each CENRAP state; and

> Regional-scale modeling to determine if the combined effect of proposed BART controls for all CENRAP states ultimately satisfy the RHR visibility improvement goals.

The responsibility for the first three modeling analyses belong to the individual states. CENRAP’s mandate is to assess the aggregate effects of controls on progress toward attaining the visibility goals across the domain. Tables 1-1 and 1-2 identify the Class I areas in and adjacent to the CENRAP domain. Figures 1-2 through 1-4 indicate the location of Class I areas by federal land manager. Figure 1-5 identifies where visibility monitoring is currently occurring in the CENRAP region.

This document applies only to the first two phases involving single-source modeling (i.e., screening to determine which BART-eligible sources are subject to BART, and single-source modeling to determine the degree of improvement related to the proposed BART control). The third phase will be addressed by the states in their Regional Haze SIPs due in 2008 and will most likely use the same or similar full-science modeling tools (CAMx or CMAQ) being used by the various RPOs dealing with the fourth phase. Individual CENRAP states will most likely conduct most, if not all, visibility modeling to determine which BART-eligible sources are subject to BART. Operators of sources determined to be ‘subject to BART’ may wish to conduct their own single-source modeling to determine the degree of visibility improvement, as they consider a variety of BART control options. The division of BART modeling between state and source operators will likely vary widely across the CENRAP states. Ultimately, it is the state’s responsibility to review and verify all single-source visibility modeling analyses. Note that all BART modeling for sources in the CENRAP states must follow a written and approved protocol either developed by the state for general application or by the source operator for a source-specific analysis. Thus, depending upon the state in which they operate, BART-eligible sources may or may not have to develop individual protocols. This issue must be worked out with the state and cognizant FLM.

Given the focus on the first two visibility assessment phases, these guidelines focus on common procedures for air quality modeling in support of BART determinations, consistent with the EPA guidelines and harmonized with the methods employed by other RPOs. (Figure 1-6 depicts this process). The guidelines are intended to provide a common understanding among the organizations performing or reviewing BART analyses – CENRAP state and local air agencies, EPA, FLMs, source operators, and contractors. Each state retains responsibility for the processes and procedures it will follow in satisfying the requirements of the RHR. Nothing in the CENRAP process replaces States’ responsibility to determine BART controls. Therefore, this document describes suitable BART modeling systems and their application to two situations:

> Air quality modeling to determine whether a BART-eligible source is “subject to BART” and therefore the BART analysis process must be applied to its operations.

> Air quality modeling of emissions from sources that have been found to be subject to BART, to evaluate regional haze benefits of alternative control options and to document the benefits of the preferred option.

These guidelines incorporate EPA final guidance and results of extensive public comments on BART modeling procedures recently proposed by several organizations.

1.3 Overview of Recommended BART Modeling Procedures

States must determine whether a source in their jurisdiction emits any air pollutant (SO_2, NO_x, PM, VOC) that "may reasonably be anticipated to cause or contribute to any impairment of visibility" in a Class I area. EPA identifies three options for the states to consider. First, a state might conclude that all BART-eligible sources are subject to BART. Alternatively, a state might demonstrate that all BART-eligible sources together do not cause or contribute to any visibility impairment. Finally, a state may seek to determine if the impact from each individual BART-eligible source on any day is greater than a threshold value. If so, then the source is subject to BART.

The CENRAP states intend to pursue the third option, utilizing dispersion modeling to calculate impacts from individual sources with respect to a prescribed visibility threshold in Class I areas. This section discusses how the CALPUFF modeling system can be used to: (a) evaluate whether a BART-eligible source is exempt from BART controls, or to (b) quantify the visibility benefits of control options for sources that are determined to be subject to BART.

1.3.1 Three BART Modeling Approaches

The visibility modeling methods described in these guidelines are grouped into three categories:

> **Screening Modeling**: The *screening* analysis uses the CALPUFF modeling system in default mode with pre-prepared modeling domains and model-ready meteorological inputs. This simple methodology, described in detail in Chapter 6, is intended to quickly distinguish between sources that have no significant impacts on Class I area visibility and those sources for which impacts are demonstrable or for which source-specific analyses are warranted.

> **Source-Specific Modeling** : A *source-specific* CALPUFF analysis (the subject of Chapter 7) is intended to remove some of the conservatism of the screening approach and bring more realism to bear in the analysis of a specific BART-eligible source. Here, the state or source operator may elect to introduce greater source specificity into the modeling through the use of variable background ammonia, ozone, and visibility levels; puff-splitting; finer horizontal grid meshes in the meteorological and air quality modeling, and so on.

> **Alternative Modeling**: Refined *full-science modeling* is available to states or source operators on a case-by-case basis. Described in Chapter 8, this entails the application of a state-of-the-science regional modeling system and readily available RPO visibility data bases for either single source or cumulative source impact assessments.

For most sources in the CENRAP region, the use of the screening or source-specific approaches will satisfy the BART regulatory requirements. Separate chapters of this protocol are devoted to each of these BART modeling approaches. Regardless of the approach, exemption modeling is the initial task at hand, followed if necessary by visibility impact modeling.

1.3.2 Exemption Modeling

Exemption modeling is intended as a definitive test of whether a source is subject to BART. A state and/or source operator may use one or more of three modeling approaches just introduced in performing exemption modeling. For most sources, an initial screening assessment with CALPUFF should be considered to assess whether a BART-eligible source is subject to BART. As described in Chapter 6, a screening CALPUFF dispersion modeling analysis is performed to assess whether a particular source is exempt from BART, obviously ‘subject to BART’, or should consider additional source-specific modeling analyses to explore further its exemption status. Assumptions for the screening assessment are purposefully conservative so that a source that contributes to visibility impairment is not inadvertently exempted. If a source is shown not to contribute to visibility impairment using the CALPUFF screening assessment, the state may choose to exempt the source from BART or to require additional source-specific modeling to confirm it is not subject to BART.

If a source is shown to contribute to visibility impairment in the screening assessment, the source has the option to undertake source-specific CALPUFF modeling to evaluate further whether it is subject to BART (see Chapter 7). Source-specific exemption modeling analysis can be used for sources that do not pass the screening analysis above or for which a more detailed modeling investigation is warranted. These analyses would typically include exercising CALPUFF with finer grid resolution (e.g., 1-2 km), more realistic estimates of background pollutant concentrations, site-specific estimates of background natural visibility conditions, and so on.

In some circumstances, a state or source operator may wish to apply full-science modeling methods to overcome CALPUFF’s inherent limitations (see Chapter 8). For example, sources close to Class I areas, sources located in proximity to other large industrial or urban source complexes, or sources located great distances from a Class I area may be better treated by a comprehensive full-science modeling system. If alternative modeling is pursued, the requirements of the modeling protocol are increased. An alternative modeling protocol must justify the need for more advanced modeling methods, identify the availability of pertinent data sets, address model selection and configuration issues, and describe the methods to be used in applying the model to estimate visibility impacts. Discussions with state, EPA and FLM representatives should be conducted prior to development of an alternative modeling protocol to ensure all of the relevant issues are addressed in the document.

1.3.3 Modeling the Effects of BART Controls on Visibility

For sources determined to be ‘subject to BART’, the next step involves estimating the visibility benefits of possible BART control measures. These benefits are determined by re-running the dispersion model using the screening modeling procedures or more resolved source-specific inputs. A key difference from the exemption modeling is that the source terms and/or emissions data are modified to reflect the BART control measures being evaluated. The base case to which the effectiveness of BART controls is compared is the “current emissions” scenario for which the exemption modeling analysis was performed. The post processing steps and procedures are the same. Side-by-side comparison of the visibility impacts provides a direct estimate of the effectiveness of each control scenario relative to the base case.

1.3.4 Modeling Protocols

Regardless of the BART modeling approach (e.g., screening, source-specific, or alternative modeling), a formal modeling protocol is required. A modeling protocol should be submitted for all modeling demonstrations regardless of the distance from the BART-eligible source to the Class I area. The protocol is typically written by the state or the source operator and then reviewed with state, EPA, and the FLM. EPA's role in the development of the protocol is advisory only as the "States better understand the BART-eligible source configurations" and factors affecting their particular Class I areas (70 FR 39126).

A protocol consists of many elements but mainly serves as a means for planning and communicating how a BART modeling study will be performed *before* it occurs. Examples of required elements in the modeling protocol:

> The meteorological and terrain data that will be used;

> The source-specific information (stack height, temperature, exit velocity, elevation, and emission rates, speciation and size fractionization of applicable pollutants); and

> Receptor data from appropriate Class I areas.

The protocol guides the technical details of a modeling study and provides a formal framework for reviewing technical assumptions, operational details, commitments and expectations of the participants. It also provides means for resolution of potential differences of technical and policy opinion in an open process within prescribed time and budget constraints.

Modeling protocols all too often fall short of providing sufficient detail in the description of the modeling assumptions and procedures to be employed (Roth et al., 2005). To assist the states and source operators in development of a protocol specific to a particular facility, protocol templates are given in Chapters 6 and 7 containing key elements that should be include in screening and source-specific applications, respectively. Of course, each protocol will have some unique features depending on the nature of the sources(s) and the Class I area(s) of interest. Also, the requirements for technical detail escalate from a screening application to source-specific application and this should be reflected in the content of the protocol.

1.4 Organization of this Document

The remainder of this document describes available models and data bases and the recommended procedures for their application. Chapter 2 reviews EPA's guidance for regional haze BART analysis modeling, as outlined in the 6 July 2005 Federal Register notice. Readers already familiar with the BART Rule may wish to skip to Chapter 3 where the CALPUFF model, EPA's preferred tool for BART analyses, is introduced and its characteristics and limitations discussed. EPA's guidance allows for the use of appropriate alternative models and Chapter 4 gives an overview of pertinent state-of-science regional photochemical/aerosol models and currently available data bases. However, these CENRAP guidelines focus primarily on the application the CALPUFF modeling system. Chapter 5 identifies existing data bases developed by CENRAP and others to support BART modeling. Then, Chapters 6, 7 and 8 present the three BART modeling approaches.

Chapter 6 discusses the specific steps needed to determine whether a BART-eligible source is subject to BART using the CALPUFF model in the *screening* mode using pre-compiled regional meteorological modeling data sets and CALPUFF run in a conservative mode. Procedures are also identified for evaluating the effects of BART controls on those sources that are identified as 'subject to BART. For sources determined to be subject to BART based on screening analyses, additional *source-specific* CALPUFF modeling might be performed as described in Chapter 7. In a limited number of cases, it may be appropriate to use a full-science modeling system to develop more accurate estimates of a sources' BART eligibility and/or to assess the effects of BART controls. Chapter 8 discusses the applications of state-of-science alternative models for this purpose. For each modeling approach described in Chapters 6 through 8, information regarding protocol development is provided as a template. Finally, a quality assurance methodology for CALMET/CALPUFF BART modeling is outlined in Chapter 9.

Figure 1-1. Federal Class I Areas in the United States.

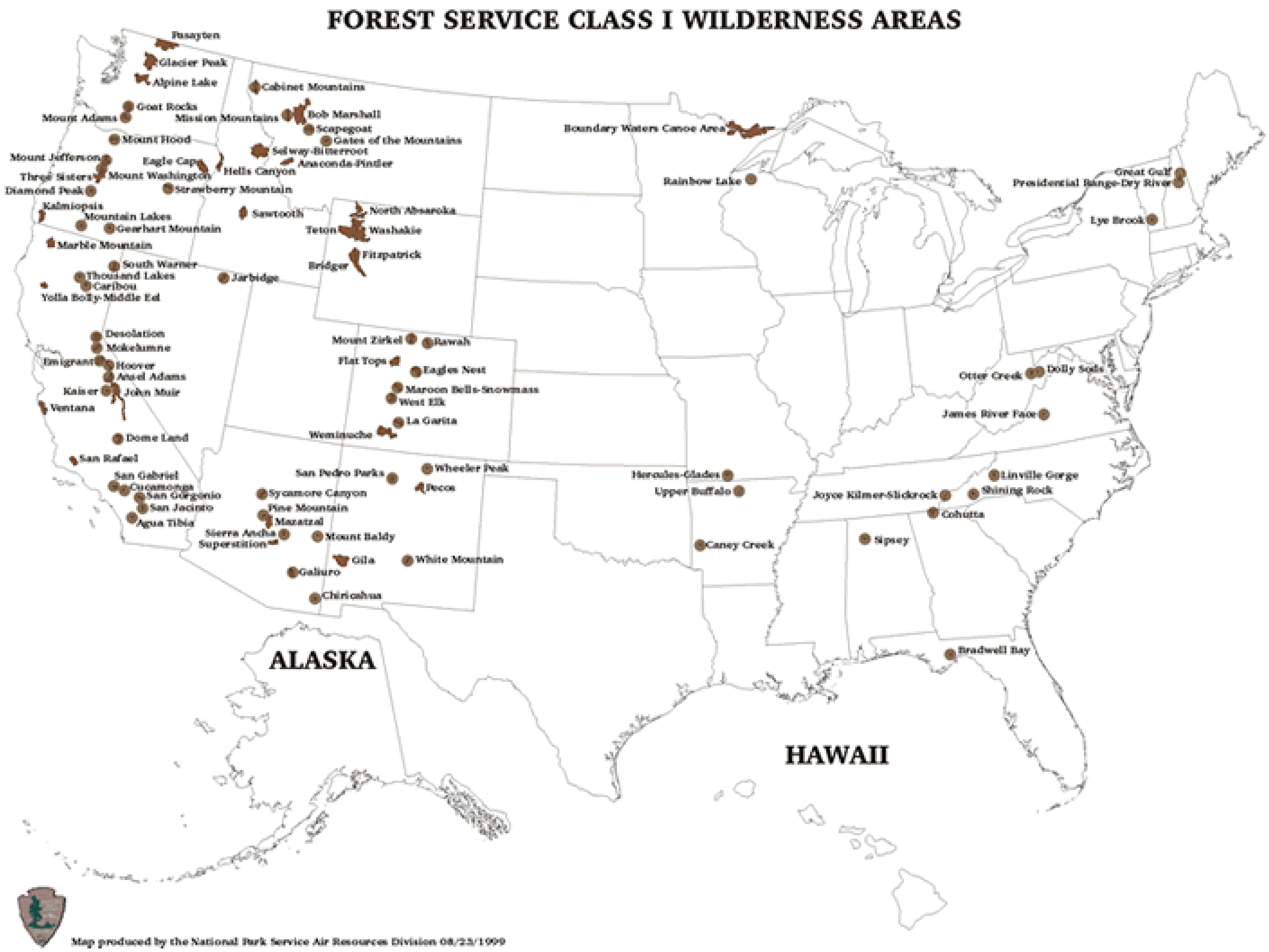

Figure 1-2. U.S. Forest Service Class I Areas.

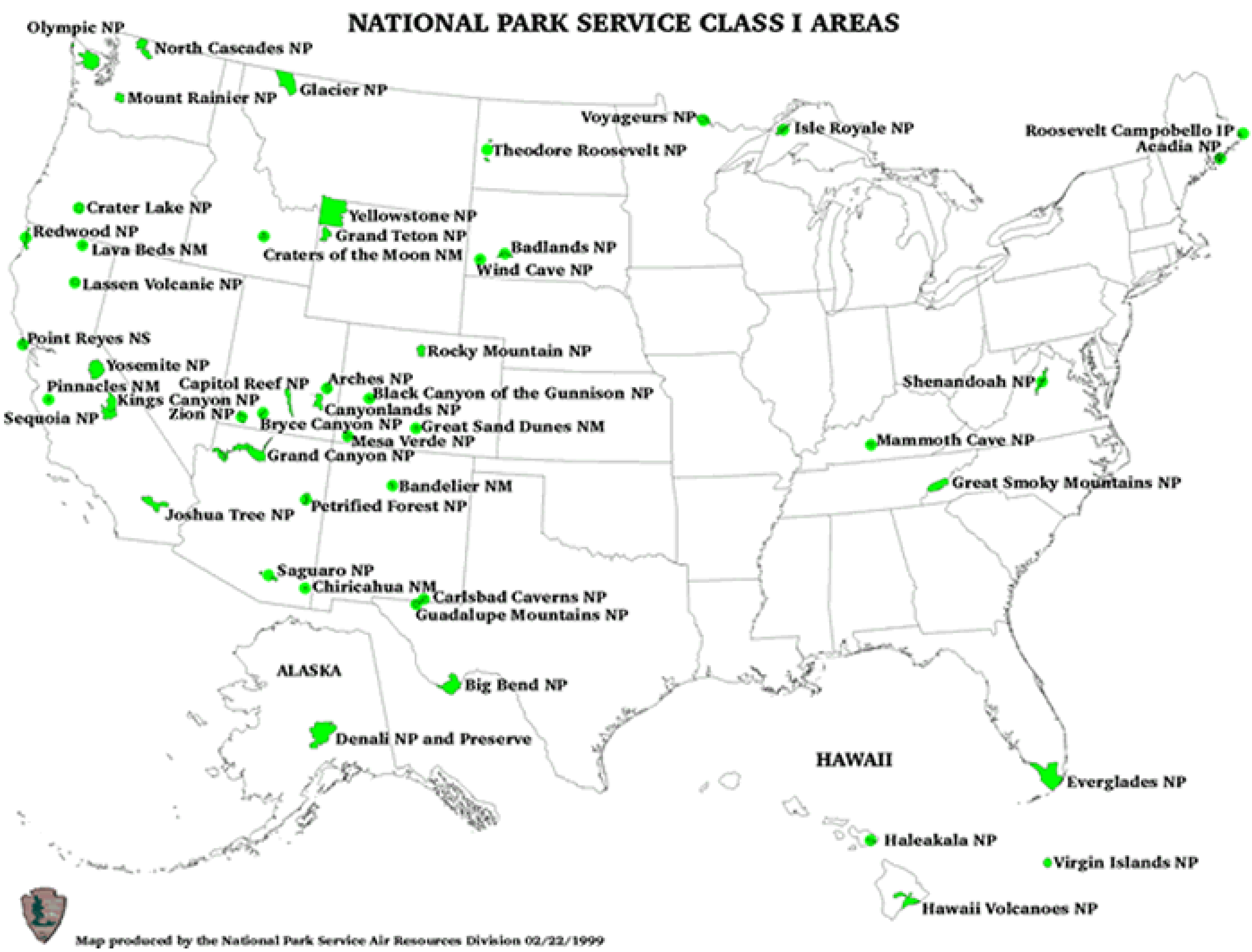

Figure 1-3. National Park Service Class I Areas.

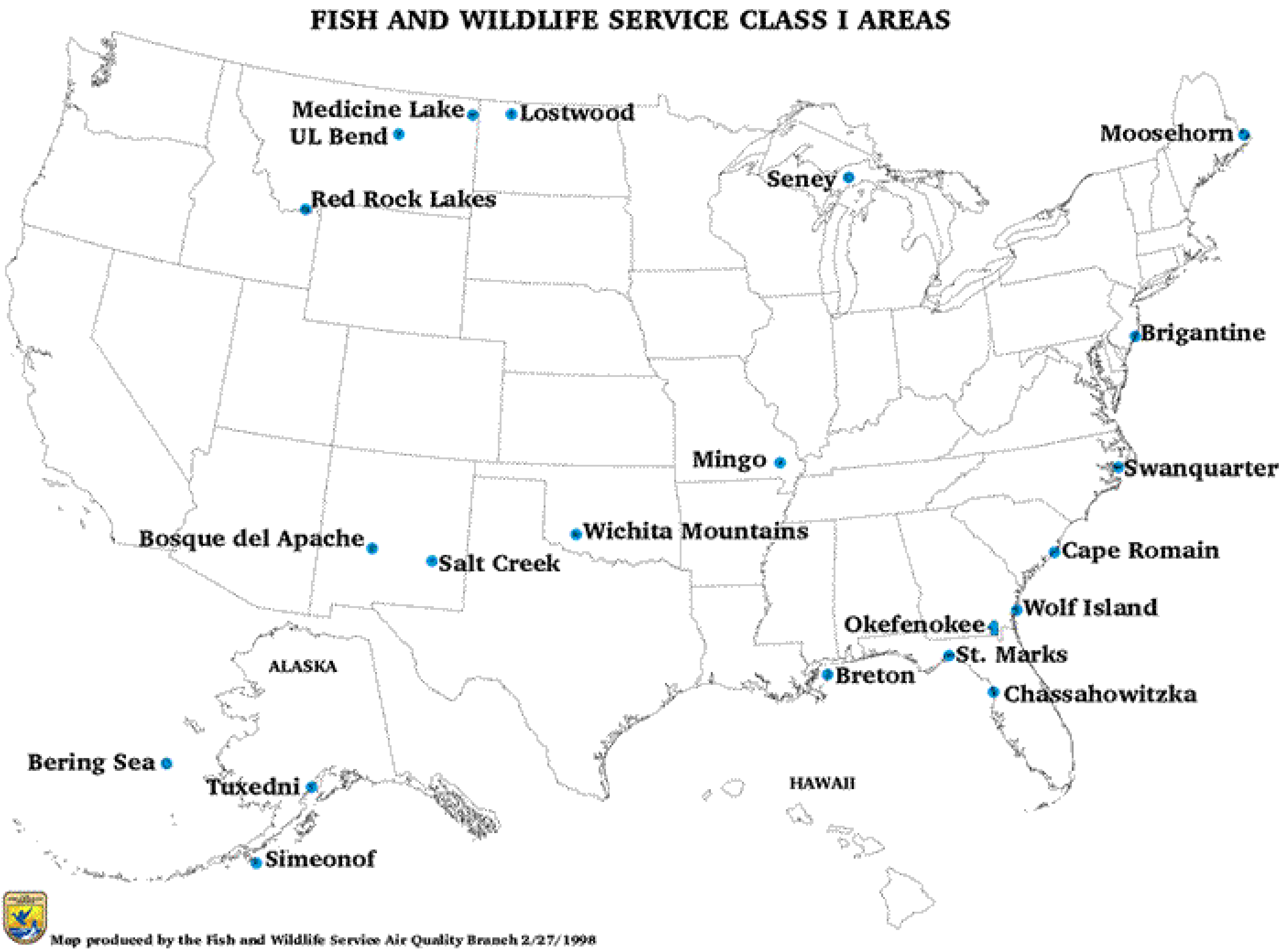

Figure 1-4. Fish and Wildlife Service Class I Areas.

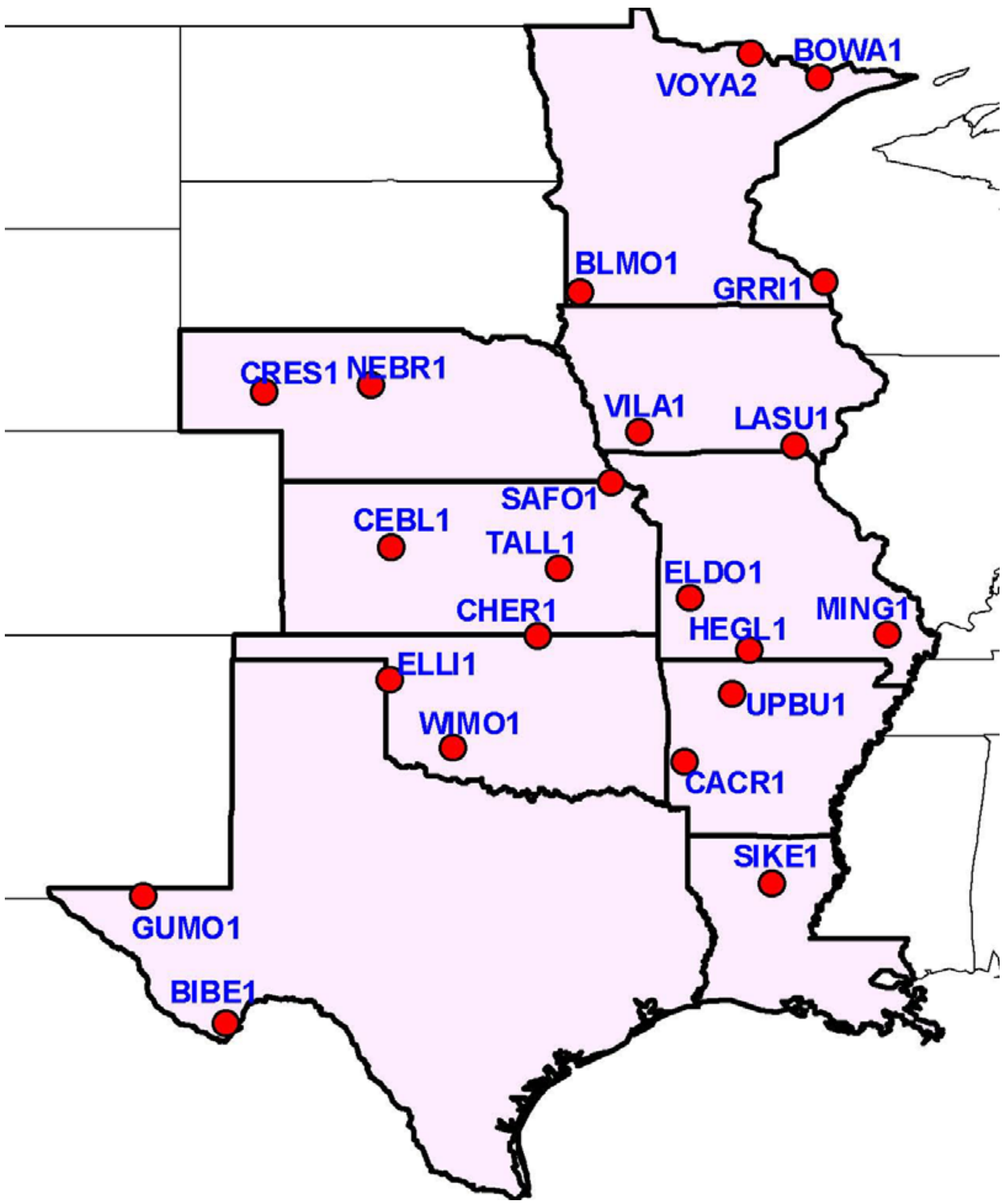

Figure 1-5. Location of Visibility Monitoring Sites in the CENRAP Domain.

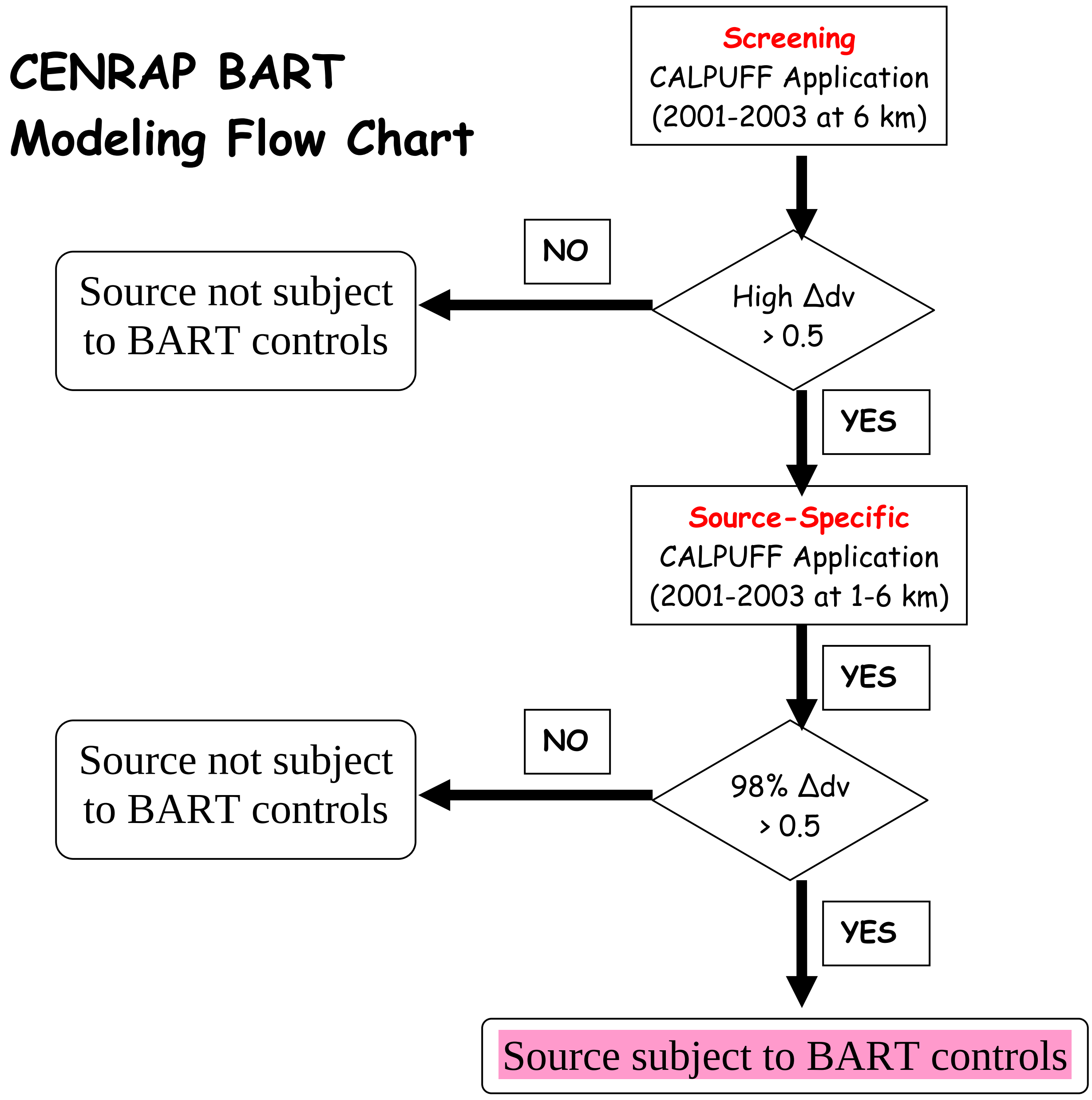

Figure 1-6. CANRAP BART Modeling Flow Chart.

Table 1-1. Federally Mandated Class I Areas in the CENRAP States.

U. S. Forest Service
- Caney Creek Wilderness (AR)
- Upper Buffalo Wilderness (AR)
- Boundary Waters Canoe Area (MN)
- Hercules - Glades Wilderness (MO)

National Park Service
- Big Bend National Park (TX)
- Guadalupe Mountains National Park (TX)
- Voyageurs National Park (MN)

U.S. Fish and Wildlife Service
- Wichita Mountains Wilderness (OK)
- Mingo Wilderness (MO)
- Breton Wilderness (LA)

Table 1-2. Federally Mandated Class I Areas Near the CENRAP States.

U.S. Forest Service
- Eagles Nest Wilderness (CO)
- Rawah Wilderness (CO)
- Pecos Wilderness (NM)
- Wheeler Peak Wilderness (NM)
- White Mountain Wilderness (NM)
- Sipsey Wilderness (AL)
- Rainbow Lakes Wilderness (WI)

National Park Service
- Arches National Park (CO)
- Bandelier National Monument (NM)
- Carlsbad Caverns National Park (NM)
- Chiricahua National Monument (NM)
- Great Sand Dunes National Monument (CO)
- Rocky Mountain National Park (CO)
- Badlands National Park (SD)
- Isle Royale National Park (MI)
- Theodore Roosevelt National Park (ND)
- Wind Cave National Park (SD)
- Mammoth Cave National Park (KY)

U.S. Fish and Wildlife Service
- Bosque Del Apache Wilderness (NM)
- Salt Creek Wilderness (NM)
- Seney Wilderness (MI)
- St. Marks Wilderness (FL)
- Lostwood Wilderness (ND)

2.0 BART MODELING REQUIREMENTS

The final version of EPA's Regional Haze Regulations was published in the Federal Register on 6 July 2005 (70 FR 39104). One of the provisions of the program is the requirement that certain existing stationary sources emitting visibility-impairing air pollutants install and operate the Best Available Retrofit Technology (BART). The regulations require case-by-case BART determination to define specific emissions limitations representing BART and schedules for compliance for each source 'subject to BART'. These requirements would be part of the SIP revisions that each State must submit to EPA by 17 December 2007. This chapter summarizes the requirements of EPA's BART Rule, particularly with respect to the modeling analyses that are required to determine (a) if a source is 'subject to BART', and (b) what levels of emissions controls might be necessary for sources shown to cause or contribute to visibility impairment at federally-protected Class I areas.

2.1 Regional Haze Rule and BART Guidelines

Section 169A of the Clean Air Act (CCA) sets forth a national goal for visibility which is the "prevention of any future, and the remedying of any existing, impairment of visibility in Class I areas which impairment results from manmade air pollution." In 1999, EPA published a final rule to address a type of visibility impairment known as regional haze (64 FR 35714). The Regional Haze Rule (RHR) requires States to submit implementation plans (SIPs) to address regional haze visibility impairment in 156 federally-protected parks and wilderness areas (i.e., the Class I scenic areas identified in the Clean Air Act). The 1999 rule was issued to fulfill a long-standing EPA commitment to address regional haze under the authority and requirements of sections 169A and 169B of the CAA. As required by the CAA, the final RHR included a requirement for Best Available Retrofit Technology (BART) for certain large stationary sources that were put in place between 1962 and 1977. The regional haze rule addresses visibility impairment resulting from emissions from a multitude of sources located across a wide geographic area. Because the problem of regional haze is believed to be caused in large measure by long-range transport of emissions from multiple sources, EPA adopted an approach that requires states to look at the contribution of all BART sources to the problem of regional haze in determining both applicability and the appropriate level of control. If a source potentially subject to BART is located in an area from which pollutants may be transported to a Class I area, that source ''may reasonably be anticipated to cause or contribute'' to visibility impairment in the Class I area.

The BART guidelines were written primarily for the benefit of state, local and Tribal agencies, and describe a process for making the BART determinations and establishing the emission limitations that must be included in their SIPs or Tribal implementation plans (TIPs). Because the individual states have the authority to require source operators to assume part of the analytical burden in the BART analysis, there may be some differences in how the analyses are carried out across the CENRAP region. The BART guidelines also recognize that data collection, analysis, and rule development may be performed by Regional Planning Organizations, for adoption within each SIP or TIP.

The BART guidelines provide a process for making BART determinations that states can use in implementing the regional haze requirements on a source-by-source basis. States must follow the guidelines in making BART determinations on a source-by-source basis for > 750 megawatt (MW) power plants but are not required to use the process in the guidelines when making BART determinations for other types of sources, i.e., states retain the discretion to adopt approaches that differ from the guidelines.

Sources are BART-eligible if they meet three criteria: (a) emissions of at least 250 tons per year of a visibility-impairing pollutant, (b) in operation between 7 August 1962 and 7 August 1977, and (c) one of 26 listed source categories in the guidance. BART controls are required for any BART-eligible source which can be reasonably expected to cause or contribute to impairment of visibility in any of the 156 federal parks and wilderness (Class I) areas protected under the regional haze rule. Air quality modeling is an important tool available to the States in determining whether a source can be reasonably expected to contribute to visibility impairment in a Class I area.

In EPA's recent 1 August 2005 proposed rulemaking (70 FR 44154) entitled "Revisions to Provisions Governing Alternative to Source-Specific Best Available Retrofit Technology Determinations" the agency addressed BART for electric generating units (EGUs). Theses newly-proposed guidelines establish certain control levels or emission rates as presumptive standards for facilities of greater than 200 MW capacity at plants with total generating capacity in excess of 750 MW. These presumptive levels, developed through a formal rulemaking process, are to be applied on a source-specific basis. EPA believes that it appropriate to apply them in a trading context where the burden to meet BART-equivalent reductions may be shared among non-BART eligible sources as well. Thus, when states estimate emissions reductions achievable from source-by-source BART, they must assume that all EGUs which would otherwise be subject to BART will control at the presumptive level, unless they demonstrate such presumptions are not appropriate at particular units.

2.2 Role of Air Quality Models

The EPA guidelines present several options for assessing whether or not sources are subject to BART. The options, relying on different modeling and/or emissions analysis approaches, are provided as guidance and the states are entitled to use other reasonable approaches for analyzing the visibility impacts of an individual source or group of sources. The options are:

Option 1: Individual Source Attribution. States can use dispersion modeling to determine that an individual source cannot reasonably be anticipated to cause or contribute to visibility impairment in a Class I area and thus is not subject to BART. Under this option, states can analyze an individual source's impact on visibility as a result of its emissions of SO_2, NOx and direct PM emissions. Because EPA's recommended CALPUFF dispersion model cannot currently be used to reliably estimate the predicted impacts on visibility from an individual source's emissions of VOC or ammonia, states may elect to use a more qualitative assessment to determine on a case-by-case basis which sources of VOC or ammonia emissions may be likely to impair visibility and should therefore be subject to BART review. EPA approved models should be used to predict the visibility impacts from a single source at a Class I area.

Option 2: Use of 'Model' Plants. Under this option, analysis of model (or prototypical) plants could be used to exempt certain BART-eligible sources that share specific characteristics. EPA (2005) provides a model plant analysis assuming potential emissions as an example of how states might use this approach. The plume and stack characteristics of the model plants were developed considering a broad range of sources, and the analysis was based on impacts at two hypothetical Class I areas. States may develop their own model plant analyses to account for the meteorology and terrain in their region. Alternatively, a state could determine that the assumptions in EPA's model plant analyses accurately reflect the characteristics of the sources and region at issue and no further analysis would be necessary. Because PM was not evaluated in EPA's model plant analysis, states must determine whether PM emissions are significant enough to warrant further analysis.

> It may be most useful to use this type of analysis to identify the types of small sources that do not cause or contribute to visibility impairment for purposes of BART, and thus should not be subject to a BART review. Different Class I areas may have different characteristics, however, so care must be taken to ensure that the criteria developed are appropriate for the applicable cases. States could use modeling analyses of representative plants to reflect groupings of specific sources with important common characteristics. Based on these analyses, states may find that certain types of sources are clearly anticipated to cause or contribute to visibility impairment. States can then choose to categorically require those types of sources to undergo a BART determination.
>
> **Option 3: Cumulative Modeling**. States may also submit to EPA a demonstration, based on an analysis of overall visibility impacts, that emissions from BART-eligible sources in a state, considered together, are not reasonably anticipated to cause or contribute to any visibility impairment in a Class I area and thus no source should be subject to BART. States may do this on a pollutant-by-pollutant basis or for all visibility-impairing pollutants to determine if emissions from these sources contribute to visibility impairment.

While EPA identifies several options for determining whether a source is "subject to BART", the most credible method is the use of dispersion modeling. Air quality modeling allows a state or source operator to analyze an individual source's impact on visibility as a result of its gaseous SO_2, NOx and direct PM emissions.

EPA assumes in the BART guidance that dispersion modeling cannot currently be used to estimate the predicted impacts on visibility from an individual source's emissions of VOC or ammonia owing to uncertainties in the ammonia inventories[1]. Presumably, EPA believes that the uncertainty in current biogenic and anthropogenic ammonia inventories are sufficiently large that dispersion modeling of such sources would not provide meaningful results. However, this view does not comport with EPA's CAIR modeling or ongoing RPO regional haze visibility modeling in which existing ammonia inventories are indeed used to calculate daily and annual $PM_{2.5}$ and visibility impact assessments. EPA suggests a more qualitative assessment to determine on a case-by-case basis which sources of VOC or ammonia emissions may be likely to impair visibility and should therefore be subject to BART review. CENRAP is considering the use of advanced one-atmosphere models (CAMx) to investigate whether VOC and ammonia emissions from BART eligible sources in the region constitute a problem. Findings from these CENRAP modeling studies are expected to provide information helpful to the States or source operators in deciding whether and to what extent ammonia and VOCs need to be considered in the BART modeling.

2.3 EPA Guidance on Air Quality Models

The BART determination under the Regional Haze Rule seeks to quantify the impact of source emissions of SO_2, NOx, and direct PM ($PM_{2.5}$ and/or PM_{10}) on 24-hr visibility impairment at receptors located within downwind Class I areas. Since visibility is defined in the context of light extinction, which itself is determined by atmospheric concentrations of specific fine particulate species --

[1] We believe this viewpoint is outdated, give recent improvements in modeling data bases and one-atmosphere models by EPA ORD/OAQPS and others (Seigneur et al., 2000; Arnold et al., 2003; Morris et al., 2005a,b; Tesche et al, 2005).

ammonium, sulfate, nitrate, organic carbonaceous matter, elemental carbon, and coarse mass – logic dictates that the modeling method(s) used must be capable of simulating these components reliably.

EPA's position on recommended models for fine particulate and visibility estimation *from single point sources* is clearly set out in the Final BART Rule and in the BART Modeling guidance document. The Final BART Rule (pg 101) states "Because the air quality model CALPUFF is currently the best application available to predict the impact of a single source on visibility in a Class I area, we proposed that CALPUFF assessment be used as the preferred approach first, for determining whether an individual source is subject to BART, and second, in the BART determination process. CALPUFF can be used to estimate not only the effects of directly emitted $PM_{2.5}$ emissions from a source, but also to predict the visibility impacts from the transport and chemical transformation of fine particle precursors." The Rule goes on to state (pg 110) that "regional scale modeling typically involves use of a photochemical grid model that is capable of simulating aerosol chemistry, transport, and deposition of airborne pollutants, including particulate matter and ozone. Regional scale air quality models are generally applied for geographic scales ranging from a multi-state to the continental scale. Because of the design and intended applications of grid models, they may not be appropriate for BART assessments, so States should consult with the appropriate EPA Regional Office prior to carrying out any such modeling".

In contrast, EPA's "Guidance for Demonstrating Attainment of the Air Quality Goals for $PM_{2.5}$ and Regional Haze" (EPA, 2001) sets forth the types of models that should be used for simulating secondary fine particulate and visibility for SIPs. EPA states (pg 169): "States should use a regional scale photochemical grid model to estimate the effects if a control strategy on secondary components of PM. Changes in primary components may be estimated using a numerical grid model (with no chemistry), a Lagrangian model, or in some cases a receptor model". Thus, in its Regional Haze and $PM_{2.5}$ SIP modeling guidance, EPA indicates that CALPUFF (a Lagrangian non-steady-state Gaussian puff model) should not be used for secondary PM and visibility impacts at Class I areas, but rather is relegated to the category of estimating primary species.

So, on the one hand, EPA maintains that CALPUFF is the "best regulatory modeling application currently available for predicting a single source's contribution to visibility impairment" and notes that "it is the only EPA-approved model for use in estimating single source pollutant concentrations resulting from the long range transport of primary pollutants". On the other hand, only regional grid models with appropriate chemistry are to be used in developing $PM_{2.5}$ and Regional Haze SIPs. EPA attempted to reconcile these two positions in the Final BART Rule by asserting that (a) regional models were not developed to treat individual point sources and (b) CALPUFF's secondary aerosol chemistry is adequate for estimating relative benefits of controls on BART sources. The first point ignores the significant amount of advanced plume-in-grid model development carried out at EPA and elsewhere over the past 20 years, while the second point is the focus of continuing debate in the scientific modeling community. Regardless, the BART modeling guidance stands and CALPUFF is the recommended model for BART determinations. EPA does allow for the use of alternative models on a case-by-case basis. Thus, this guidance addresses both approaches with CALPUFF being the primary tool for most BART visibility assessments.

2.4 Steps in the BART Modeling Process

The BART guidelines identify four steps required to determine emission limitations for affected sources.

Identify BART-Eligible Sources. The first step is to identify whether a source is "BART-eligible" based on its source category, when it was put in service, and the magnitude of its emissions of one or more "visibility-impairing" air pollutants. The BART guidelines list 26 source categories of stationary sources that are BART-eligible. Sources must have been put in service between 7 August 1962 and 7 August 177 in order to be BART-eligible. Potential emissions of 250 tons per year or more of a visibility-impairing air pollutant are required to make a source eligible for BART. Qualifying pollutants include primary particulate matter (PM_{10}) and gaseous precursors to secondary fine particulate matter such as SO_2 and NOx. Whether ammonia and VOCs should be included as visibility-impairing pollutants for BART eligibility is left for the states to determine on a case-by-case basis. The guidance states that high molecular weight VOCs with 25 or more carbon atoms and low vapor pressure should be considered as primary $PM_{2.5}$ emissions and not VOCs for BART purposes.

Determine Sources Subject to BART. To determine whether a source or facility is 'subject to BART', EPA recommends modeling all units and all pollutants together. This entails using plant-wide emissions and considering the effect of all pollutants combined for comparison to the visibility threshold. EGUs participating in the CAIR program may be BART-eligible for PM if plant wide potential emissions of PM are greater than *de minimus.* If the EGU is BART-eligible for PM and if the source emissions result in impairment above the state-determined threshold, the source may be deemed subject to BART.

To determine whether a BART-eligible source can be excluded from BART controls, a modeling demonstration is required. EPA's preferred approach is an assessment with CALPUFF followed by comparison of the estimated 24-hr visibility impacts against a threshold above estimated natural conditions to be determined by the states. The threshold to determine whether a single source "causes" visibility impairment is set at 1.0 deciview change from natural conditions over a 24-hour averaging period. Any exceedance of this threshold would trigger a BART review. The guidance also states that the proposed threshold at which a source may "contribute" to visibility impairment should not be higher than 0.5 deciviews, although depending on factors affecting a specific Class I area, it may be set lower than 0.5 deciviews.

EPA's guidance builds upon the 1990 National Acid Precipitation Assessment Program (NAPAP) that found that a 5% change in light extinction will evoke a just noticeable change in most landscapes. Converting the 5% change in light extinction to a change in deciviews yields a change of approximately 0.5 deciviews. EPA believes that this is a natural breakpoint at which to set the BART exemption levels. Since visibility degradation may begin to be recognized by a human observer at this extinction level, the guidance uses a 0.5 deciview change on a 24-hour average basis for determining that an individual source is causing visibility impairment at a Class I area. This level would be calculated by comparing the air quality model's results for an individual source against' natural visibility' conditions. A source's impact is assessed by comparing the 98^{th} percentile modeled value (8^{th} highest day annually at a receptor or 22^{nd} highest over 3-years) with the 0.5 deciview threshold. An impact is declared if the source contributes to visibility impairment. If so, it is 'subject to BART'.

If individual BART-eligible units at a facility have impacts that are less than 0.5 dv but in aggregate with other BART eligible sources at the facility are greater than 0.5 dv, the source is 'subject to BART'. In other words, if the combined impact of all units is greater than the threshold for contribution determined by the state (such as 0.5 dv), the source is declared 'subject to BART'. This does not imply that controls are necessary for each unit; the control technology analysis, which follows the 'subject to BART' test, can be a unit-by-unit evaluation and a visibility analysis can be conducted for single units and individual pollutants.

Determine Appropriate Types and Levels of Control. The third step is to determine BART for the source by considering various control options and selecting the "best" alternative, taking into consideration: (a) any pollution control equipment in use at the source which affects the availability of options and their impacts, (b) the costs of compliance with control options, (c) the remaining useful life of the facility, (d) the energy and non air-quality environmental impacts of compliance, and (e) the degree of improvement in visibility that may reasonably be anticipated to result from the use of such technology.

Incorporate BART-Determinations into the State's Regional Haze SIP. Results of the BART determinations must be incorporated into the state's regional haze SIP which is due 17 December 2007. Instead of applying BART on a source-by-source basis, a state (or a group of states) has the option of implementing an emissions trading program designed to achieve regional haze improvements that are greater than the visibility improvements that could be expected from BART[2] alone. If the geographic distributions of emissions under the two approaches are similar, determining whether trading is "better than BART" may be possible by simply comparing emissions expected under the trading program against the emissions that could be expected if BART was applied to eligible sources. If the geographic distributions of emissions are likely to be different, however, regional air quality modeling comparing the expected improvements in visibility from the trading program and from BART would be required.

According to the BART guidance, a modeling protocol should be submitted for all modeling demonstrations regardless of the distance from the BART-eligible source to the Class I area. EPA's role in the development of the protocol is only advisory as the "States better understand the BART-eligible source configurations" and factors affecting their particular Class I areas.

2.5 CALPUFF Modeling Recommendations

To evaluate the visibility impacts of a BART-eligible source at Class I areas beyond 50 km from the source, the EPA guidance recommends the use of the CALPUFF model. For modeling sources closer than 50 km to a Class I area, the guidance recommends that expert modeling judgment be used "giving consideration to both CALPUFF and other methods." While the PLUVUE-II model is mentioned as a possible tool to consider in addition to CALPUFF within 50 km of a source, it seems unlikely this technique would be any more credible than CALPUFF. The EPA guidance notes that regional scale photochemical grid models may have merit, but such models are resource intensive relative to CALPUFF. Photochemical grid models are clearly more appropriate than CALPUFF for cumulative modeling options such as in the determination of the aggregate contribution of all-BART-eligible sources to visibility impairment, but such use should involve consultation with the appropriate EPA Regional Office.

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[2] EPA's BART guidance suggests that CAIR would satisfy the BART requirements for affected EGUs, which could affect the modeling efforts a State would need to undertake.

For both BART exemption and BART determination modeling with CALPUFF, emissions reflecting periods of start-up, shutdown and malfunction are not to be considered in determining the appropriate emission rates. The EPA recommends that the states use the highest 24-hour average actual emission rate for the most recent five-year period (excluding periods with start-up, shutdown and malfunctions). Visibility improvements may be evaluated on a pollutant-specific basis. States are "encouraged to account for the magnitude, frequency, and duration of the contributions to visibility impairment caused by the source based on the natural variability of meteorology.

EPA does not recommend CALPUFF for addressing visibility impacts from VOCs because its capability to simulate secondary organic aerosol formation from VOC emissions is deficient, especially for anthropogenic emissions. Currently, VISTAS is performing a weight-of-evidence analysis using EPA's CMAQ regional air quality model to assess whether VOC emissions from all BART-eligible and non-BART point sources in each VISTAS State contribute to visibility impairment. If the impact of eliminating all VOC emissions from all point sources in a VISTAS state is shown to be less than 0.5 dv, then, logically, the impact of any one BART-eligible source would be less than 0.5 dv. If the VISTAS regional modeling analysis confirms this expectation, the CENRAP States might argue similarly that VOC emissions should not be subject to BART.

EPA has given states the option to address ammonia (NH_3) emissions from BART-eligible sources. VISTAS weight-of-evidence modeling with CMAQ is also addressing ammonia in the same way VOCs are being examined. If the CMAQ sensitivity evaluations shows that the collective impact of all point NH_3 emissions in a state is less than 0.5 dv, then the impact of a single BART eligible source would be less than 0.5 dv. Should the VISTAS modeling confirm the expected insignificant role of direct NH_3 emissions on Class 1 area visibility, the CENRAP States might argue similarly that VOC emissions should not be subject to BART. CENRAP is presently considering similar modeling for both ammonia and VOCs. If the VISTAS modeling demonstrates the importance of VOCs and/or NH_3 emissions on Class I area visibility, then CENRAP will need to consider the use of advanced regional models to assist the States in establishing BART controls for these pollutants.

2.6 Alternative Models for BART Analyses

All air quality models share a common foundation: the species-conservation (or atmospheric diffusion) equation. Source-oriented air quality models including CALPUFF derive from this equation (Tesche, 1983) which applies equally to one source or a million or more sources. The distinction lies in how the various terms are treated (CAMx, CMAQ) or neglected (CALPUFF) in the governing equations and the choice of coordinate system (Lagrangian or Eulerian). As shown in the next Chapter, much of the simplicity of the CALPUFF model derives from the fact that many chemical and physical processes known to influence visibility are simply ignored. More sophisticated plume models such as SCIPUFF and SCICHEM (Karamchandani et al., 2000) rely on a second order closure treatment of turbulent mixing and detailed photochemical reaction schemes and to provide more realistic simulations than simpler approaches such as CALPUFF. Full-science regional models such as CAMx and CMAQ treat the various physical and chemical processes in detail, albeit at the expense of greater computer resources. Furthermore, detailed plume-in-grid treatment is available in several regional scale models, at least in CAMx, it is now possible to perform particulate and gas-phase source apportionment within the plume-in-grid formulation. Because EPA allows the use of alternative models on a case-by-case basis, these CENRAP guidelines include descriptions of these models and how they can be used.

EPA essentially dismisses the use of regional scale models because they are "generally applied for geographic scales ranging from a multi-state to the continental scale and that by design they may not be appropriate for simulating individual point sources". This posture ignores a very substantial body of research and model development carried out at the agency and elsewhere in the U.S. over the past 20 years. Modern one-atmospheric regional photochemical grid models, employing multi-scale nested grids (Kumar and Russell, 1996) and plume-in-grid techniques (Karamanchandani et al., 2002), are fully applicable to the analysis of point source plumes, most especially when reactive atmospheric chemistry occurs. If they were not, then they would not be reliable in simulating the combined effects of the wide array of anthropogenic and biogenic emissions that cause gas phase, particulate, secondary aerosol, and visibility air pollution problems—precisely the problem currently being addressed by all five RPOs. Furthermore, the convergence of fast commodity-based Linux computer clusters and the recently-developed RPO regional modeling emissions, meteorological, and air quality data bases make application of these comprehensive models no longer a research or academic exercise. While regional scale modeling clearly requires expertise to perform properly, the actual program costs to conduct a CMAQ or CAMx regional modeling study are today quite comparable with and occasionally less that a traditional PSD modeling study using ISC, CALPUFF, or AERMOD. Given grid nesting and plume-in-grid technology, modern regional models are applicable to a very broad range of scales from 10-20 km to continental scale. Regional photochemical grid models are clearly more appropriate than CALPUFF for cumulative modeling requirements such as in the determination of the aggregate contribution of all-BART-eligible sources to visibility impairment.

States may elect to perform cumulative modeling in order to examine the feasibility of exempting BART-eligible sources, but this is certainly not an EPA or BART Rule requirement. The regional haze rule requires States to consider the degree of visibility improvement resulting from a source's installation and operation of retrofit technology, along with the other statutory factors when making a BART determination. However, there is no longer a cumulative modeling requirement in determining the degree of visibility improvement.

For the vast majority of potential BART-eligible sources in the CENRAP domain, application of the CALPUFF modeling system will in all likelihood be sufficient to address the needs of the source operator, the state, EPA and the FLM. For those special cases where more accurate modeling results are required, appropriate full-science modeling systems and supporting RPO data bases are available. Their broad use by the five RPOs in the past three years amply demonstrate that these comprehensive models are no longer arcane academic/research institution projects but applications-ready tools suitable for regulatory decision-making.

3.0 CALPUFF FORMULATION AND IMPLEMENTATION

The RHR relates visibility attenuation to extinction coefficient (b_{ext}) which is a measure of light scattering and absorption due to atmospheric constituents. Values for b_{ext} are estimated using an empirically derived equation which relates the extinction coefficient to relative humidity and the following components of particulate matter mass: (a) sulfates (SO_4); (b) nitrates (NO_3); (c) organic carbon (OC); (d) elemental carbon (EC); (f) particulate matter (IP) ("crustal material"); and (g) coarse mass (CM) (i.e., PM_{10} – $PM_{2.5}$). The BART guidance requires the use of modeled concentrations of these components, together with a "humidity correction factor", to estimate values for b_{ext} on all days within a three year period. These estimates, when compared with naturally occurring background extinction, are used to determine whether a source is causing or contributing to visibility impairment and also to measure the effectiveness of emissions controls on the source aimed at mitigating such effects. EPA notes that secondary particulate matter constitutes an important fraction of $PM_{2.5}$ and that the modeling requirements for secondary and primary particulate matter differ in their need to consider atmospheric chemistry and in the degree of spatial resolution needed for the modeling (EPA, 2001, pg 22).

This chapter introduces the formulation of the CALPUFF modeling system. We summarize the model capabilities as described in the user's manuals (Scire et al., 2000a,b) and discuss the capabilities and limitations of the model. Equipped with this information, states and source operators can identify those situations for which screening and/or source-specific applications of CALPUFF are appropriate.

In most cases, we expect that application of the CALPUFF system will be sufficient to meet the BART Rule requirements. For that subset of conditions requiring advanced methods, Chapter 5 provides details on full-science alternative models and available data bases for BART modeling. Such conditions might include a situation where the default modeling shows that a source just barely causes or contributes to visibility degradation or in negotiations over the final BART determination that weighs technical and economic feasibility against expected air quality benefits. In both situations, a more accurate estimate of a source's impacts may be very important to source operators.

3.1 Original Model Development

The CALPUFF modeling system was originally developed as a component of a three-part modeling system sponsored by the California Air Resources Board (ARB) in the mid-1980s. The ARB sought to develop a new puff-based model, a new grid-based model and an improved meteorological processor that would support application of the two. CALGRID was the urban-scale photochemical grid model resulting from the project (Yamartino et al., 1992) comparable in science and capabilities to the Urban Airshed Model (UAM-IV) (Scheffe and Morris, 1993). The model formulation was aimed at overcoming the deficiencies in EPA's steady-state Gaussian plume models that were routinely used in California for inert and linearly reactive materials (principally SO_2) from elevated point sources. Thus, the CALGRID model was designed to treat the complexities of urban-scale photochemical processes while CALPUFF was formulated to treat the non-steady state transport, diffusion, linear reaction, and deposition of primary pollutants from point sources. CALPUFF was not designed to address photochemical oxidants or and secondary aerosol formation production processes in a scientifically rigorous manner.

In recent years, CALPUFF and its meteorological pre-processor (CALMET) have been used in a range of regulatory modeling studies to address point source issues that include complexities posed by complex terrain, large source-receptor distances, parameterized chemical transformation and deposition, and issues related to Class I visibility impacts. These applications are more complex than the California ARB's non-steady-state, linear chemistry formulation of the mid-1980s.

The CALPUFF modeling system has been adopted by the EPA as a guideline model for source-receptor distances greater than 50 km, and for use on a case-by-case basis in complex flow situations for shorter distances. It was recommended for Class I impact assessments by the FLM Workgroup (FLAG, 2000) and the Interagency Workgroup on Air Quality Modeling (IWAQM) (EPA, 1998). As directed in the BART guidance, CALPUFF is the primary modeling system for screening and source-specific BART applications in the CENRAP region. Thus, examination of the model's formulation provides the context for assessing the extent to which it suitable for simulating the various physical processes and gas-phase, aerosol, and aqueous-phase chemical processes that influences visibility.

3.2 CALPUFF Model Formulation

The CALPUFF user's guide (Scire et al., 2000a) depicts the modeling system as shown in Figure 3-1. CALMET is a diagnostic/interpolation model that provides meteorological inputs to CALPUFF. These fields include hourly-averaged three-dimensional wind and temperature fields and two-dimensional fields of mixing heights and other meteorological parameters. CALMET uses routine surface and aloft meteorological observations and/or three-dimensional output from prognostic numerical models such as MM5 (Grell et al., 1995) or RUC (Benjamin et al., 2004) to construct the meteorological inputs. Other inputs to the air quality program include emissions information, receptor locations, ancillary geophysical information, and estimated concentrations of ambient pollutants that are entrained by the modeled puffs as each is carried downwind. Tables 3-1 and 3-2 summarize the key features of the CALMET/CALPUFF models as described in the user's guides.

Two post-processor routines are included to facilitate cumulative source impacts (POSTUTIL) and estimates of light extinction and visibility attenuation at Class I receptors of interest (CALPOST). In particular, CALPOST contains several options for computing change in extinction and deciviews for visibility assessments while the POSTUTIL postprocessor includes options for summing contributions of individual sources or groups of sources to assess cumulative impacts. POSTUTIL also contains an empirical nitric acid-nitrate chemical equilibrium module to estimate the cumulative effects of ammonia consumption by background sources once the simulation is completed.

3.2.1 Model Concept and Governing Equations

The starting point for the CALPUFF development was the choice of the fundamental reference system of which there are two: Eulerian and Lagrangian. Consistent with the original ARB design criteria, the Lagrangian (moving puff) reference system was chosen for CALPUFF. In the Eulerian approach, the behavior of pollutants is described relative to a fixed coordinate system. The Lagrangian reference frame, in contrast, relates the behavior of pollutants relative to a coordinate system that moves with the average wind. These two approaches yield different mathematical relationships for pollutant concentrations *that are equally valid*. The choice of which approach to adopt depends upon the specific design goals of the modeling system.

The advantages and drawbacks of each approach are thoroughly discussed in the literature (Tesche, 1983; Seinfeld and Pandis, 1998; Jacobson, 1999; Russell and Dennis, 2000). One of the criticisms of early Eulerian grid models was their 'over-dilution' of point source emissions into the fixed grid cells; but for the past twenty years, this limitation has been overcome through with the development of sub-grid-scale, plume-in-grid algorithms (Seigneur, et al., 1981; Godowitch, 2004;

Karamchandani et al., 2005; Emery and Yarwood, 2005) and the use of multi-scale nested grids (Russell and Dennis, 2000). While the Lagrangian approach is conceptually simple, flexible, and computationally inexpensive, the governing equations are not directly applicable to situations involving non-linear chemical reactions (Seinfeld and Pandis, (1998) and it is awkward to handle a large number of sources realistically.

3.2.2 Transport and Dispersion

Adopting the Lagrangian concept, CALPUFF simulates the transport, dispersion, linear chemical transformation, and deposition of individual puffs carried downwind by the three-dimensional fields generated by CALMET. The model's implementation follows puffs from the near source region (a few tens of meters) to hundreds of kilometers downwind. Its puff-based formulation, in conjunction with three-dimensional hourly meteorological data, allow CALPUFF to simulate the effects of time- and space-varying meteorological conditions on pollutants emitted from a variety of source types. The major features and options of the CALPUFF model are summarized below:

Building Downwash: The Huber-Snyder and Schulman-Scire downwash models are both incorporated into CALPUFF. An option is provided to use either model for all stacks, or make the choice on a stack-by-stack and wind sector-by-wind sector basis. Both algorithms have been implemented in such a way as to allow the use of wind direction specific building dimensions. The PRIME building downwash model (Schulman et al., 2000) is also included in CALPUFF as an option.

Dispersion Coefficients: Turbulent dispersion in CALPUFF is treated with the K-theory (flux-gradient) closure scheme, defined for a Lagrangian frame of reference. Several options are provided in CALPUFF for the computation of dispersion coefficients, including the use of turbulence measurements (σ_v and σ_w), the use of similarity theory to estimate σ_v and σ_w from modeled surface heat and momentum fluxes, or the use of Pasquill-Gifford (PG) or McElroy-Pooler (MP) dispersion coefficients, or dispersion equations based on the CTDM. Options are provided to apply an averaging time correction or surface roughness length adjustments to the PG coefficients. Recently, the EPA AERMOD dispersion parameters have been included in CALPUFF and are used regularly.

Puff Sampling Functions: Puff sampling routines are included in CALPUFF to address computational difficulties encountered when applying a puff model to near-field releases. For near-field applications during rapidly-varying meteorological conditions, an elongated puff (slug) sampling function may be used. An integrated puff approach may be used during less demanding conditions. Both techniques reproduce continuous plume results under the appropriate steady state conditions.

Wind Shear Effects: A key underpinning of the Lagrangian concept is that the modeled puffs retain their identity over the time- and spatial-scale associated with the effects the model is attempting to predict (i.e., visibility impairment at 200 km or beyond) While discrete puffs emitted from a source retain their physical integrity for a period of time, at some point the action of horizontal and vertical variations in wind speed and direction (i.e. 'wind shear') shred the puff into multiple elements. These new puff parcels, composed of remnants of the old puff, continue to be diffused and dispersed by the wind. The point where significant puff shredding occurs is difficult to define since it depends substantially upon the complexity of the meteorological conditions and the underlying terrain. But when shredding occurs, the Lagrangian concept in CALPUFF breaks down. By ignoring puff shredding (i.e., by keeping puffs intact), the model will systematically over-predict pollutant concentrations.

To deal with this conceptual limitation, CALPUFF contains an optional puff splitting algorithm to simulate vertical wind shear effects across individual puffs. Differential rates of dispersion and transport among the "new" puffs generated from the original, well-mixed puff act to increase the effective rate of horizontal spread of the material as would be expected in the real atmosphere. Puffs may also be split in the horizontal when the puff size becomes large relative to the grid size to account for wind shear across the puffs. Detailed guidance on when and how the puff-splitting algorithm should be used and actual verification studies demonstrating that the technique operates as intended are not discussed in the model documentation or presented in the science literature.

Complex Terrain: Effects of complex terrain on puff transport are derived from the CALMET winds. In addition, puff-terrain interactions at gridded and discrete receptor locations are simulated using one of two algorithms that modify the puff-height (either that of ISCST3 or a general "plume path coefficient" adjustment), or an algorithm that simulates enhanced vertical dispersion derived from the weakly-stratified flow and dispersion module of the Complex Terrain Dispersion Model (CTDMPLUS) (Perry et al., 1989). The puff-height adjustment algorithms rely on the receptor elevation (relative to the elevation at the source) and the height of the puff above the surface. The enhanced dispersion adjustment relies on the slope of the gridded terrain in the direction of transport during the time step.

Subgrid Scale Complex Terrain (CTSG): An optional module, CTSG treats terrain features that are not resolved by the gridded terrain field, and is based on the CTDMPLUS (Perry et al., 1989). Plume impingement on subgrid-scale hills is evaluated at the CTSG subgroup of receptors using a dividing streamline height (H_d) to determine which pollutant material is deflected around the sides of a hill (below H_d) and which material is advected over the hill (above H_d). The local flow (near the feature) used to define H_d is taken from the gridded CALMET fields. As in CTDMPLUS, each feature is modeled in isolation with its own set of receptors.

Overwater and Coastal Interaction Effects: The CALMET processor contains overwater and overland boundary layer parameterizations allowing certain of the effects of water bodies on plume transport, dispersion, and deposition to be estimated. In a sense, CALPUFF operates as a hybrid model, by utilizing gridded fields of meteorology and dispersion conditions as well as grid-based descriptions of underlying land use. This includes the abrupt changes that occur at the coastline of a major body of water.

Dry Deposition: A resistance model is used for the computation of dry deposition rates of gases and particulate matter as a function of geophysical parameters, meteorological conditions, and pollutant species. For particles, source-specific mass distributions may be provided for use in the resistance model. Of particular interest for BART analyses is the ability to separately model the deposition of fine particulate matter (< 2.5 μm diameter) from coarse particulate matter (2.5-10 μm diameter).

Wet Deposition: An empirical scavenging coefficient approach is used to compute the depletion and wet deposition fluxes due to precipitation scavenging. The scavenging coefficients are specified as a function of the pollutant and precipitation type (i.e., frozen vs. liquid precipitation).

3.2.3 Primary Particulates

CALPUFF is designed to simulate PM_{10} or $PM_{2.5}$ or other user defined size distributions of particles. The smaller the particles, the more they disperse like an inert gas. In most cases, the dispersion of inert $PM_{2.5}$ particles will differ only slightly from that of an inert gas. A key primary

$PM_{2.5}$ emission from coal-fired electric generating units (EGUs) of relevance to visibility calculations is particulate sulfate. Although primary sulfate emissions account for only a small fraction of the total sulfur emissions from such sources, it is appropriate to include their effect if reasonable estimates of primary sulfate emissions from the source are available. Treating primary sulfate emissions is likely to be most important at short distances from the stack before significant SO_2 to secondary sulfate conversion has taken place.

3.2.4 Gas-Phase Chemistry

Chemical reactions in the gas-phase play an important role in secondary aerosol formation by generating radical concentrations (e.g., the hydroxyl radical). These radical species oxidize SO_2 and NOx, providing the precursors to aqueous–phase chemistry (i.e., chemistry in liquid water droplets) that convert SO_2 to sulfate (e.g., H_2O_2 and O_3), and form condensable gases from some volatile organic compounds (VOCs) that can then condense into particulate secondary organic aerosols (SOA). The levels of NOx, VOC, and O_3 concentrations along with the reactivity of the VOCs, sunlight, temperature, and water vapor are all key variables that influence the radical cycle and consequent sulfate and nitrate formation rates.

CALPUFF neglects realistic gas-phase processes entirely. The chemistry in CALPUFF parameterizes chemical transformation effects using five species (SO_2, $SO_4^{=}$, NO_x, HNO_3, and NO_3^-) via a set of user-specified, diurnally-varying transformation rates. The model estimates secondary fine particulate matter (sulfate and nitrate) from emissions of gas-phase SO_2 and NO_x. Rather than simulating important non-linear gas phase oxidant chemistry, the model employs a user-supplied hourly ozone concentration as a surrogate for the hydroxyl radical and other oxidizing radical species. Ambient ammonia concentrations are also a user input along with temperature and relative humidity.

Although simplifications of photochemistry have been attempted in the past, correct representation of the gas-phase photochemistry and the radical cycles are critically important in order to properly characterize sulfate and nitrate formation in the real atmosphere. Seigneur et al., (2000) demonstrated this fact in their evaluation of full-science representations of photochemistry against simplified representations (but more advanced than CALPUFF). They concluded that simplified linearized transformation schemes are inadequate for describing sulfate and nitrate formation processes:

> "These results indicate that the accurate prediction of source-receptor relationships for $PM_{2.5}$ requires a comprehensive treatment of $PM_{2.5}$ formation from gaseous precursors for the secondary components of $PM_{2.5}$ and a spatially resolved treatment of transport processes for primary $PM_{2.5}$. Simplified treatments of either atmospheric chemistry or transport are appropriate only when the secondary or primary components of $PM_{2.5}$, respectively, are not significant. Therefore, the development of source-receptor relationships for $PM_{2.5}$ should be based on air quality models that provide comprehensive descriptions of atmospheric chemistry and transport."

Morris et al., (1998) also compared the sulfate and nitrate particulate estimates from a comprehensive full-science regional model with those from a model incorporating a simplified empirical chemical mechanism developed in a manner similar to the mechanism in CALPUFF. Evaluating the full-science and empirical chemistry models against observed concentrations, Morris and co-workers concluded:

> "Given the importance of the radical cycle for determining secondary PM formation rates, it appears that empirical gas-phase algorithms are inadequate for determining secondary PM formation."

The uncertainty and potential biases introduced into the CALPUFF visibility estimates due to neglect of gas phase oxidant chemistry remain unknown.

3.2.5 Aerosol Chemistry

Formation of secondary fine particulate matter (e. g., nitrates, sulfates, organic aerosols) in point source plumes is strongly dependent on the rate of mixing with ambient (background) air and the chemical composition of this background. The rates of oxidation of sulfur dioxide (SO_2) and nitrogen dioxide (NO_2) to sulfate and nitric acid can be very different within a power plant or industrial plume compared to that in the background air (Gillani and Godowitch, 1999; Karamchandani et al., 2000). Similarly, the formation of secondary organic aerosols from emitted VOCs and those from other anthropogenic and biogenic sources, adds yet another pathway in the formation of visibility-impairing aerosols. The presence of atmospheric ammonia introduces further nonlinearities into the gas phase and aerosol reactions. Accordingly, for a model to realistically simulate the production of secondary particulate sulfate, nitrate, and organic aerosols from a potential BART source, the mixing processes and chemical reactions within and outside of the plume must be treated realistically. If the chemical interactions between these two fundamentally different and interactive chemical environments are overly-simplified or neglected altogether, the ability of the model to correctly calculate plume concentrations, deposition, or visibility impacts is lost.

Sulfate and Nitrate Formation. Two SO_2 and NOx chemical transformation schemes are available in CALPUFF: the MESOPUFF-II algorithm (Scire et al., 1983; Atkinson et al., 1982) and the RIVAD algorithm (Latimer et al., 1986). These algorithms calculate sulfate and nitrate formation rates based on the puff concentrations, background environmental parameters provided by CALMET, and background ozone and ammonia concentrations provided as input by the user. SOA particulates are not treated by either mechanism. The parameters used are as follows (note that each method does not use all of these parameters).

Puff Average Concentrations (from CALPUFF)

- NOx concentration
- SO_2 concentration

Environmental Parameters (from CALMET)

- Temperature
- Surface Relative Humidity (RH)
- Atmospheric Stability
- Solar Radiation

Background Concentrations (User Input)

- Ozone (O_3)
- Ammonia (NH_3)

The MESOPUFF-II chemical transformation scheme is EPA's recommended approach for Class I area impact assessment (IWAQM, 1998). It entails pathways for five active pollutants (SO_2, SO_4, NOx, HNO_3, and NO_3) as follows:

$$SO_2 \xrightarrow{k_1} SO_4$$

$$NOx \xrightarrow{k_2} HNO_3\ (+RNO_3)$$

$$NOx \xrightarrow{k_3} HNO_3$$

$$HNO_3\ (g) \overset{NH_3}{\leftrightarrow} NO_3\ (PM)$$

where,

SO_2 is the puff average sulfur dioxide concentration;
NOx is the puff average oxides of nitrogen concentrations;
SO_4 is sulfate concentrations formed from the SO_2;
HNO_3 is the nitric acid formed from the NOx;
NO_3 is the particulate nitrate that is in equilibrium with the nitric acid; and
NH_3 is the background ammonia concentration.

Daytime Rates

$k_1 = 36 \times R^{0.55} \times [O_3]^{0.71} \times S^{-1.29} + k_{1(aq)}$

$k_{1(aq)} = 3 \times 10^{-8} \times RH^4$ (added to k_1 above during the day)

$k_2 = 1206 \times [O_3]^{1.5} \times S^{-1.41} \times [NOx]^{-0.33}$

$k_3 = 1261 \times [O_3]^{1.45} \times S^{-1.34} \times [NOx]^{-0.12}$

Nighttime Rates

k_1 = 0.20 (%/hr)
k_2 = 0.00 (%/hr)
k_3 = 2.00 (%/hr)

with,

k_1 is the SO_2 to SO_4 gas-phase transformation rate (%/hr)
$k_{1(aq)}$ is the SO_2 to SO_4 aqueous-phase transformation rate (%/hr)
k_2 is the NOx to HNO_3+RNO_3 transformation rate (%/hr)
k_3 is the NOx to HNO_3 (only) transformation rate (%/hr)
S is the stability index ranging from 2 to 6 (PGT class A&B=2, C=3, D=4, E=5, F=6)
R is the total solar radiation intensity (kw/m^2)
RH is the relative humidity (%)
$[O_3]$ is the user provided background ozone concentrations (ppm)
[NOx] is the plume average NOx concentration (ppm)
NH_3 is the user provided background ammonia concentrations

Daytime chemical transformations are based on statistically analyzed hourly transformation rates (Scire et al., 1983) obtained from box model simulations using the Atkinson et al., (1982) photochemical mechanism. In this scheme, gas-phase oxidation of SO_2 and NOx depends on the hydroxyl (OH) radical concentrations for which background ozone, solar intensity (R), and stability index are used as surrogates. At night, OH concentrations are much lower and default SO_2 and NOx oxidation rates of 0.2 %/hr and 2.0 %/hr are assumed. The $k_{1(aq)}$ sulfate formation rate is added to the k_1 rate during the day as a surrogate for aqueous-phase sulfate formation which begins to assume importance above approximately 50% RH (~0.2 %/hr sulfate formation rate) and peaks at 100% RH (3%/hr sulfate formation rate).

The sulfate and nitrate formation rate equations used in the MESOPUFF II scheme were originally generated by developing regression equations for a few key variables on the results of 144 box model simulations that used the 1982 photochemical mechanism of Atkinson et al. These box model simulations varied ambient temperature, ozone concentration, sunlight intensity, VOC concentrations, atmospheric stability, and plume NOx concentrations as shown in Table 3-1. The actual environmental conditions used to generate the sulfate and nitrate transformation equations were extremely limited. For example, the transformation rates did not cover temperatures below 10 deg C (50 deg F) or cleaner rural atmospheric conditions with VOC concentrations less than 50 ppbC.

The CALPUFF MESOPUFF-II chemistry clearly neglects several environmental parameters and chemical processes that are important in simulating sulfate and nitrate formation in NO_X/SO_2 emissions source plumes. In many cases these deficiencies lead to an overestimation bias of the source's sulfate and nitrate impacts. Factors that lead such a bias include:

Lack of Temperature Effects: Photochemistry is known to be highly temperature sensitive, as evidenced by the fact that elevated ozone concentrations tend to occur on hot summer days. Lower temperatures produce lower OH and other radical concentrations and consequently lower sulfate and nitrate formation rates. The CALPUFF sulfate and nitrate formation rates, however, do not adequately incorporate temperature effects. The MESOPUFF-II chemical transformation algorithm was developed under conditions with a minimum temperature of only 10° C (50° F). Thus, under conditions colder than 10° C, CALPUFF will overpredict sulfate and nitrate formation rates and impacts. CALPUFF typically estimates maximum sulfate and visibility impacts during the late fall/early spring and winter months; these are the same months when the CALPUFF overestimation bias from not considering temperature effects will be greatest. In addition, under colder temperatures, NOx will be converted to peroxyacetyl nitrate (PAN) so that the NOx is no longer available to be converted to nitrate. Since the CALPUFF chemistry ignores the PAN sink for NOx, it will systematically overpredict nitrate impacts.

Effects of NOx Emissions on Sulfate Chemistry: Downwind of a point source with significant NOx/SO_2 emissions, high NOx and SO_2 concentrations co-exist. Under high NOx concentrations, radical concentrations are greatly reduced, resulting in very low ozone, sulfate, and nitrate formation rates. This is due to the NOx inhibition effect on photochemistry whereby: (1) the titration of NO with ozone eliminates ozone and its source as a radical generator; and (2) the high NO_2 concentrations eliminate the OH radical via the NO_2 + OH reaction thereby effectively shutting down photochemistry. Thus, in a NOx/SO_2 point source plume near the source, there will be very low OH radical and ozone concentrations and consequently very low sulfate and nitrate formation. Since the simple MESOPUFF-II transformation equations cannot account for the NOx effect on the sulfate formation, CALPUFF will tend to over-predict sulfate formation rate in a NOx/SO_2 point source plume near the source, which in turn leads to overstating the sulfate formation rate. Because NOx/SO_2 point sources are typically buoyant, they are frequently be emitted aloft in a stable layer where the high NOx concentrations and inhibited sulfate and nitrate formation rates could persist 100 km or more downwind.

Aqueous-Phase Sulfate Formation Algorithm. CALPUFF's MESOPUFF-II chemistry treats aqueous-phase sulfate formation solely as a function of relative humidity (RH), which actually has no direct affect on aqueous-phase sulfate formation chemistry. The CALPUFF MESOPUFF-II aqueous-phase sulfate formation rate ranges from values of approximately 0.2 %/hr at 50% RH to 3.0 %/hr at 100% RH. Relative humidity (RH) is a measure of the content of water vapor in the atmosphere. However, in reality aqueous-phase sulfate formation will depend on the amount of atmospheric liquid water content (LWC) in cloud or fog droplets, the pH of the water droplets, and the level of H_2O_2, ozone, and SO_2 concentrations. Accordingly, in the atmosphere, aqueous-phase sulfate formation chemistry is not affected by RH. Thus, the CALPUFF aqueous-phase chemistry parameterization is incorrect. Although under conditions of clouds and fog there will be high RH, the occurrence of high RH with very little or no clouds or fog can be quite frequent.

In a liquid water droplet, the reaction of SO_2 with H_2O_2 to form sulfate is essentially instantaneous and is usually limited by the amount of H_2O_2 present (i.e., oxidant limited) for a NOx/SO_2 point source. Once the H_2O_2 is reacted away within the water droplet, sulfate formation via this pathway slows to the rate of H_2O_2 formation, which would be extremely slow to nonexistent in a large point source plume due to the scavenging of radicals by the high NOx concentrations. This introduces an inaccurate representation of sulfate formation in CALPUFF that creates uncertainties and bias in modeled visibility impacts. Whether this uncertainty results in an under- or overestimate of sulfate formation is difficult to determine since the approach is scientifically invalid. Under conditions of high RH and little clouds or little plume interaction with clouds, it will clearly overstate sulfate formation. However, under conditions of cloudy conditions with available photochemical oxidants (i.e., H_2O_2 and O_3) and a dilute NOx/Sox point source plume, it may understate sulfate formation. Near large NOx/SO_2 point source where the elevated NOx concentrations scavenge and limit photochemical oxidants, the MESOPUFF-II algorithm will likely overstates sulfate formation.

Thus, the CALPUFF aerosol chemistry fails to account for many environmental parameters that are necessary to simulate sulfate and nitrate formation rates, including VOCs and their reactivity, temperature, liquid water content, and NOx concentrations. In their evaluations against full-science PM models and observations, Seigneur et al., (2000) and Morris et al., (1998) both independently found that the empirical chemistry modules, such as employed by CALPUFF, are inadequate for estimating sulfate and nitrate formation. These findings are supported by EPA's $PM_{2.5}$ and Regional Haze SIP modeling guidance (EPA, 2001) that recommends against using Lagrangian models such as CALPUFF for simulating secondary PM.

From the foregoing, it is clear that the CALPUFF chemical transformation algorithms neglect important chemical processes necessary to accurately estimate the sulfate and nitrate impacts due to SO_2 and NO_X emissions. Given that EPA recommends the model for BART determinations, a key question is "What is the influence of the simplified chemistry on modeled estimates of visibility impacts from BART sources? In some cases, the inadequacies in the CALPUFF chemistry algorithms may simply introduce broader uncertainties into the calculation of estimated sulfate and nitrate impacts. In many cases, however, the simplifications made in the CALPUFF description of chemical processes result in a systematic bias in the estimated concentrations and visibility impacts due to SO_2 and NO_X emissions sources. For large point sources that emit SO_2 and NOx emissions, such as EGUs, petrochemical process heaters, cement plant kilns, etc., many of the limitations in the CALPUFF MESOPUFF-II SO_2 and NOx transformation algorithms would result in an overestimation bias. While models that are systematically biased high (i.e., over-predict impacts) may be appealing to regulatory decision-makers because they are 'conservative', the overprediction tendency may well lead to unwarranted and excessive control of emissions from some sources. Thus, the tradeoff between simplicity and conservativism on the one hand and technical credibility and unbiased answers on the other is a key element in the negotiation of modeling protocols developed by the states or source operators.

3.2.6 Surface Removal

An especially important contributor to particulate concentrations is the rate of deposition to the surface. $PM_{2.5}$ particles, which have a mass median diameter around 0.5 µm, have an average net deposition velocity of about 1 cm/min (or about 14 m/day) and thus the deposition of fine particles is not usually significant except for ground-level emissions. On the other hand, coarse particles (those PM_{10} particles larger than $PM_{2.5}$) have an average deposition velocity of more than 1 m/min (or 1440 m/day), which is significant, even for emissions from elevated stacks.

CALPUFF includes parametric representations of particle and gas deposition in terms of atmospheric, deposition layer, and vegetation layer "resistances" and, for particles, the gravitational settling speed. Gravitational settling, which is of particular importance for the coarse fraction of PM_{10}, is accounted for in the calculation of the deposition velocity. Effects of inertial impaction (important for the upper part of the PM_{10} distribution) and Brownian motion (important for small, sub-micron particles) and wet scavenging are also addressed. The BART guidance recommends that fine particulate matter (less than 2.5 µm diameter), which has higher light extinction efficiency than coarse particulate matter (2.5-10 µm diameters), should be treated separately in the model. CALPUFF allows for user-specified size categories to be treated as separate species, which includes calculating size-specific dry deposition velocities for each size category.

3.3 CALMET Meteorological Preprocessor

The CALMET meteorological model consists of a diagnostic wind field module and micrometeorological modules for over-water and overland boundary layers. When modeling a large geographical area such as the CENRAP domain, the user has the option to use a Lambert Conformal Projection coordinate system to account for Earth's curvature. The major features and options of the meteorological model are summarized in Table 3-1. The techniques used in the CALMET model are briefly described below.

3.3.1 Boundary Layer Modules

The CALMET processor contains two boundary layer modules for application to overland and overwater grid cells.

<u>*Overland Boundary Layer Module*</u>: Over land surfaces, the energy balance method of Holtslag and van Ulden (1983) is used to compute hourly gridded fields of the sensible heat flux, surface friction velocity, Monin-Obukhov length, and convective velocity scale. Mixing heights are determined from the computed hourly surface heat fluxes and observed temperature soundings using a modified Carson (1973) method based on Maul (1980). The module also determines gridded fields of PGT stability class and hourly precipitation rates.

Overwater Boundary Layer Module: The aerodynamic and thermal properties of water surfaces suggest that a different method is needed for estimating boundary layer parameters in the marine environment. A profile technique, using air-sea temperature differences, is used in CALMET to compute the micro-meteorological parameters in the marine boundary layer. An upwind-looking spatial averaging scheme is optionally applied to the mixing heights and three-dimensional temperature fields in order to account for important advective effects.

3.3.2 CALMET Diagnostic Wind Field Module

The CALMET wind model was constructed from two other meteorological models used in California in the late 1970s. One was the California Institute of Technology (CIT) mass consistent interpolation model described by Goodin et al., (1980). The other was the Complex Terrain Wind Model (CTWM) developed at Systems Applications, Inc. (Tesche and Yocke, 1978; Yocke and Liu, 1978). The CTWM terrain adjustments used to modify the flow fields were assembled in the 1970s as part of research into fire spread and avalanche forecasting in mountainous regions of California. Various heuristic algorithms were developed to approximate down slope drainage flows, terrain blocking and channeling (Geiger, 1965), thermal heat islands (Stern and Malkus, 1953), surface friction retardation, capping by an elevated inversion and so on. These algorithms were based on empirical studies in wind tunnels, numerical modeling experiments, and field studies in the Alps, some dating back to the 1930s (Defant, 1933). Later work by Tesche et al., (1986), Kessler et al., (1987) and Douglas and Kessler (1988) integrated the CIT and CTWM modeling system into a single meteorological model that included algorithms to blend observational data with prognostic meteorological model output. The combined model was used extensively for urban-scale ozone studies throughout the U.S. prior to the switch to MM5 as the preferred meteorological model for SIP studies in the mid-1990s.

The CALMET model development incorporated the main features of the CTWM and CIT wind model and significantly updated the physical parameterizations and improved model input/output (I/O) schemes (Scire et al., 2000a). Today, CALMET uses the CTWM two-step approach to the computation of the wind fields. In the first step, an ‘initial-guess’ wind field is constructed and then adjusted to approximate the kinematic effects of terrain, slope flows, and terrain blocking. Currently, the gridded MM5 field is used as the initial guess prior to terrain-perturbation. The second step consists of an objective analysis procedure to blend the MM5 field with observational data to produce a final wind field. This introduction of observational data in the second step of the CALMET wind field development is optional. It is also possible to run the model in “no observations” (No-Obs) mode, which involves the use only of MM5 gridded data for the initial guess field followed by fine-scale terrain adjustments on the scale of the CALMET domain.

Normally, the CALMET computational domain is specified to be at smaller grid spacing than the MM5 dataset used to initialize the initial guess field. For example, 36/12 km MM5 data sets available for 2000-2003 over the CENRAP domain have been used to develop the 6 km CALMET grids shown in Figures 5-1 through 5-4.

The current thermal, kinematic, and dynamic effects parameterized in CALMET, used in the first step of the windfield development, are as follows:

Kinematic Effects of Terrain: The CTWM algorithms for kinematic effects (Liu and Yocke, 1980) is used to evaluate the influence of the terrain on the wind field. The initial guess field winds are used to compute a terrain-forced vertical velocity, subject to an exponential, stability-dependent decay function. The effects of terrain on the horizontal wind components are evaluated by applying a divergence-minimization scheme to the initial guess wind field. The divergence minimization scheme is applied iteratively until the three-dimensional divergence is less than a threshold value.

Slope Flows: The original slope flow algorithm (Defant, 1933) has been upgraded (Scire and Robe, 1997) based on the shooting flow algorithm of Mahrt (1982). This scheme includes both advective-gravity and equilibrium flow regimes. At night, the slope flow model parameterizes the flow down the sides of the valley walls into the floor of the valley, and during the day, upslope flows are parameterized. The magnitude of the slope flow depends on the local surface sensible heat flux and local terrain gradients. The slope flow wind components are added to the wind field adjusted for kinematic effects.

Blocking Effects: The thermodynamic blocking effects of terrain on the wind flow are parameterized in terms of the local Froude number (Allwine and Whiteman, 1985). If the Froude number at a particular grid point is less than a critical value and the wind has an uphill component, the wind direction is adjusted to be tangent to the terrain.

3.4 Estimation of Regional Haze Contributions

The default procedure for quantifying visibility impacts is described in several documents (IWAQM, 1998; FLAG, 2000). Implementation of these procedures in CALPUFF is described in the user's documentation (Scire et al., 2000b). Generally, 'visibility' may be quantified either by visual range (the greatest distance that a large object can be seen) or by the light extinction coefficient, which is a measure of the light attenuation per unit distance due to scattering and absorption by gases and particles. Visibility is impaired when light is scattered in and out of the line of sight and by light absorbed along the line of sight. The light extinction coefficient (b_{ext}) considers light extinction by scattering (b_{scat}) and absorption (b_{abs}):

$$b_{ext} = b_{scat} + b_{abs}$$

The scattering components of extinction (b_{scat}) are represented by light scattering due to air molecules (i.e., Rayleigh scattering, $b_{rayleigh}$) and light scattering due to particles, b_{sp}. The absorption components of extinction (b_{abs}) include light absorption due to gases (b_{ag}) and particles (b_{ap}). Furthermore, particle scattering, b_{sp}, can be expressed by its components:

$$b_{sp} = b_{SO4} + b_{NO3} + b_{OC} + b_{SOIL} + b_{Coarse}$$

where the chemical species and soot scattering coefficients are given as:

$$b_{SO4} = 3\,[(NH_4)_2SO_4]\,f(RH)$$

$$b_{NO3} = 3\,[NH_4NO_3]f(RH)$$

b_{OC} = 4 [OC]

b_{SOIL} = [Soil]

b_{Coarse} = 0.6 [Coarse Mass]

b_{ap} = 10 [EC]

The numeric coefficient at the beginning of each equation is the dry scattering or absorption efficiency in meters-squared per gram. The f(RH) term is a monthly-average relative humidity adjustment factor. The terms in the brackets are the estimated concentrations fro CALPUFF (or other model) in micrograms per cubic meter ($\mu g/m^3$).

Finally, the total atmospheric extinction is estimated as:

$$b_{ext} = b_{SO4} + b_{NO3} + b_{OC} + b_{SOIL} + b_{Coarse} + b_{ap} + b_{rayleigh}$$

or, substituting in the above terms,

$$b_{ext} = 3\ f(RH)\ [(NH_4)_2SO_4] + 3\ f(RH)\ [NH_4NO_3] + 4[OC] + 1[Soil] + + 0.6[Coarse\ Mass] + 10[EC] + b_{Ray} \quad (3\text{-}1)$$

This is the so-called IMPROVE extinction equation currently recommended by EPA (2003). Note that the sulfate (SO_4) and nitrate (NO_3) components are hygroscopic because their extinction coefficients depend upon relative humidity. The concentrations, in square brackets, are in $\mu g/m^3$ and b_{ext} is in units of Mm^{-1}. The Rayleigh scattering term (b_{Ray}) has a default value of 10 Mm^{-1}, as recommended in EPA guidance for tracking reasonable progress (EPA, 2003a). The effect of relative humidity variability on the extinction coefficients for SO_4 and NO_3 can be estimated in several ways, but following the EPA BART guidelines, the Class I area-specific monthly f(RH) values shown in Table 6-1 should be used.

Modeled ground level concentrations of each of the above visibility impairing pollutants are used with the IMPROVE equation to deduce the extinction coefficient. The change in visibility (measured in terms of 'deciviews') is compared against background conditions. The delta-deciview, Δdv, value is calculated from the source's contribution to extinction, b_{source}, and background extinction, $b_{background}$, as follows:

$$\Delta dv = 10\ ln((b_{background} + b_{source}) / b_{background})$$

The impact of a source is determined by comparing the Δdv, or haze index (HI), for estimated natural background conditions with the impact of the source and without the impact of the source. *If the Δdv value is greater than the 0.5 dv threshold the source is said to contribute to visibility impairment and is thus subject to BART controls.*

CALPOST uses a previous IMPROVE *f(RH)* curve (FLAG, 2000) which differs slightly from the *f(RH)* now used by IMPROVE and EPA (2003), mainly at high relative humidity. Also, CALPOST sets the maximum *RH* at 98% by default (although the user can change it), while the EPA's guidance now caps it at 95% (easily modified in the CALPUFF input file).

For regional haze light extinction calculations, use of a plume-simulating model such as CALPUFF is appropriate only when the plume is sufficiently diffuse that it is not visually discernible as a plume *per se*, but nevertheless its presence could alter the visibility through the background haze. The IWAQM Phase 2 report states that such conditions occur starting 30 to 50 km from a source. This is consistent with the BART guidance recommendation for using CALPUFF for source-receptor distances greater than 50 km. But, CALPUFF is also recommended by EPA as an option that can be considered for shorter transport distances when the plume may in fact be discernible from the background haze.

Apart from the chemistry issues discussed previously, there do not appear to be any major reasons why CALPUFF cannot be used for even shorter transport distances than 30 km, as long as the scale of the plume is larger than the scale of the output grid so that the maximum concentrations and the width of the plume are adequately represented and so that the sub-grid details of plume structure can be ignored when estimating effects on light extinction. The standard 1-km output grid that has been established for Class I area analyses should serve down to source-receptor distances somewhat under 30 km; how much closer than 30 km will depend on the topography and meteorology of the area and should be evaluated on a case-by-case basis with individual CENRAP State modelers. (For reference, the width of a Gaussian plume, $2\sigma_y$, is roughly 1 km after 10 km of travel distance, assuming Pasquill-Gifford dispersion rates under neutral conditions.)

3.4.1 CALPOST Methods

Calculation of the impact of the simulated plume particulate matter component concentrations on light extinction is carried out in the CALPOST postprocessor. For BART applications, this processor is of considerable importance.

CALPOST is used to process the CALPUFF outputs, producing tabulations that summarize the results of the simulations, identifying for example, the highest and second-highest hourly-average concentrations at each receptor. When performing visibility-related modeling, CALPOST uses concentrations from CALPUFF to compute light extinction and related measures of visibility (deciviews), reporting these for a 24-hour averaging time. The CALPOST processor contains several options for evaluating visibility impacts, including the method described in the BART guidance, which uses monthly average relative humidity values. CALPOST contains implementations of the IWAQM-recommended and FLAG-recommended visibility techniques and additional options to evaluate the impact of natural weather events (fog, rain and snow) on background visibility and visibility impacts from modeled sources. CALPOST uses Equation 3-1 to calculate the extinction increment due to the source of interest and provides various methods for estimating the background extinction against which the increment is compared in terms of percent or deciviews.

For background extinction, the CALPOST processor contains seven techniques for computing the change in light extinction due to a source or group of sources (i.e., Methods 1 through 7). These are usually reported as 24-hour average values, consistent with EPA and FLM guidance. In addition, there are two techniques for computing the 24-hour average change in extinction (i.e., as the ratio of 24-hour average extinctions, or as the average of 24-hour ratios). Method 2 is the current default, recommended by both IWAQM (EPA, 1998) and FLAG (2000) for source-specific. Method 6 is recommended by EPA's BART guidance (70 FR 39162).

In Method 2, user-specified, speciated monthly concentration values are used to describe the background. When applied to natural conditions, for which EPA's default natural conditions concentrations are annual averages, the same component concentrations would have to be used throughout the year (unless potential refinements to those default values resulted in concentrations that vary during the year). Hourly background extinction is then calculated using these concentrations and hourly, site-specific *f(RH)* from a 1993 IWAQM curve or, optionally, the EPA regional haze f(RH) curve.[1] Again the *RH* is capped at either 98% (default) or a user-selected value (most commonly at 95%).

Method 6 is similar to Method 2, except monthly f(RH) values (e.g., EPA's monthly climatologically representative values) are used in place of hourly values for calculating both the extinction impact of the source emissions and the background conditions extinction. Hourly source impacts, with the effect on extinction due to sulfates and nitrates calculated using the monthly-average relative humidity in f(RH), are compared against the monthly default natural background concentrations. Thus the monthly-averaged relative humidity is applied to the hygroscopic components (i.e., sulfate and nitrate) of both the source impact and the background extinction with Method 6.

3.4.2 POSTUTIL

The POSTUTIL processor allows the cumulative impacts of multiple sources from different simulations to be summed, including computing the difference between two sets of predicted impacts (useful for evaluating the benefits of BART controls). It also contains a chemistry module to evaluate the equilibrium relationship between nitric acid and nitrate aerosols. This capability allows the potential non-linear effects of ammonia scavenging by background sulfate and nitrate sources to be approximated in the formation of nitrate from an individual source. The processor can compute the impacts of individual sources or groups of sources on sulfur and nitrogen deposition into aquatic, forest and coastal ecosystems, thereby allowing changes in deposition fluxes resulting from changes in emissions to be quantified.

The POSTUTIL processor attempts to overcome the bias introduced when CALPUFF assumes that the full background ammonia concentration is entrained into each discrete puff. For a single puff, this may be satisfactory, but the model overestimates the production of ammonium nitrate when multiple puffs co-exist and overlap. The POSTUTIL processor re-partitions the ammonia and nitric acid concentrations to conform to the ammonia-limiting processes influencing nitrate formation. Though based on recognized science, this approximate post-processing method is fundamentally dependent on reliable estimates of ambient NH_3 at the Class I receptor of interest.

3.4.3 Refined Extinction and Background Visibility Estimates

EPA, the IMPROVE Steering Committee, and the RPOs are evaluating whether refinements are warranted to the methods recommended for calculating extinction and the default estimate of natural background visibility. Whether EPA will approve of any changes to the IMPROVE equation is uncertain at this time. Also, the responsibility for incorporating any changes to the algorithms in CALPUFF (e.g., new f(RH) curves) is unclear. If changes to these methods are recommended by EPA, CENRAP is encouraged to adopt them. However, details of the process for incorporation of any

[1] Note that the hourly-varying natural background extinction here is not consistent with that prescribed by the EPA's natural conditions guidance (EPA, 2003b), for which a "climatologically-representative" f(RH) that only varies monthly is to be used. Method 6 uses these monthly average humidity values.

refinements to the IMPROVE equations in the CALPUFF system should be addressed in the State's or source operators modeling protocol.

3.5 Model Availability

The EPA-approved version of the CALPUFF modeling system is available from Earth Tech, Inc., (http://www.src.com/calpuff/calpuff1.htm). The main models (CALMET, CALPUFF, and CALPOST), their GUIs, and many of the processors are available to download. One may also register to receive notices of model updates. The most recent update to the system (25 May 2005) is a new version of CALMM5 (MM5 V3) that has been added to the Download BETA-Test page. This version of CALMM5 processes MM5 Version 3 output data directly.

Earth Tech offers CALPUFF training courses that include a description of the technical formulation of the models, overviews of each of the processor programs, and hands-on application of the models to several case study data sets. Attendees of the course receive a training notebook, a workbook of case study problems, exercises, and data sets, updates on recent and future model enhancements, and the latest (proprietary) versions of the models and Graphical User Interfaces (GUIs). Other third-party training courses and materials are also available.

3.6 CALPUFF Evaluation Studies

Tesche (2002, 2003) reviewed results of various CALPUFF evaluation studies and reached the following conclusions:

> There is a paucity of model evaluation information for CALPUFF at scales of 50 to 200 km and beyond;

> Based on the limited information available, CALPUFF may be able to give unbiased estimates of short-term (i.e., 3-10 hr) concentrations of *non-reactive contaminants* to within a factor of two (e.g. 200%) out to distances of about 200 km from a source. This level or uncertainty in a 200 km radius around a source is increased if one examines CALPUFF's predictions in a particular modeling cell (e.g., one containing a population center) at a specific hour as opposed to considering the question of bias generally over the entire 200 km region irrespective of location and time of occurrence;

> For time periods of a day or less, CALPUFF is unable to produce reliable predictions of non-reactive concentrations at a specific location and time;

> What limited experimental data do exist suggest that the accuracy and reliability of the model's predictions degrade as the distance scale increases;

> While the IWAQM recommendations on the range of applicability of the CALPUFF model (50 to 200 km) rests on very sparse model evaluation information, EPA's suggestion that the model can be used for scales beyond 200 km, even with case-by-case approval, is not based on model evaluation data; and

> For chemically reactive pollutants such as SO_2, NO_x, sulfate, nitrate, nitric acid, and other secondary reaction products, the testing of CALPUFF model over extended spatial scales (50 km and beyond) has not been attempted in a rigorous manner.

Scire et al., (2001) report an evaluation of CALPUFF sulfate, nitrate, light extinction, and sulfur and nitrogen deposition at a Class I areas over a range of source-receptor distances. In this study, in which a large number of sources were modeled simultaneously, sulfate and nitrate predictions at the CASTNet monitoring site in Pinedale, Wyoming were evaluated against observations, and light extinction predictions were evaluated using transmissometer measurements. Wet sulfur and nitrogen predictions were compared to observations at several acid deposition monitoring sites. This study is especially relevant because it evaluates the performance of the model to predict variables of direct interest in Class I visibility analyses, such as sulfate and nitrate concentrations and light extinction coefficients

More recently, Chang et al., (2003) reported an intercomparison of CALPUFF with two other transport and dispersion models with high resolution field data. CALPUFF predictions for inert SF_6 were compared using two recent mesoscale field datasets: the Dipole Pride 26 (DP26) and the Overland Along-wind Dispersion (OLAD). Both field experiments involved instantaneous releases of sulfur hexafluoride tracer gas in a mesoscale region with desert basins and mountains. Tracer concentrations were observed along lines of samplers at distances up to 20 km. CALPUFF predictions were evaluated using the maximum 3-h dosage (concentration integrated over time) along a sampling line. At the DP26 sampler array, CALPUFF had mean biases within 35% and random scatters of about a factor of 3–4. About 50%–60% of the CALPUFF predictions were within a factor of 2 of the observations. At the OLAD site, the model underpredicted by a factor of 2–3, on average, with random scatters of a factor of 3–7. Only about 25%–30% of the CALPUFF predictions of inert SF_6 were within a factor of 2 of observations.

The tracer studies with which CALPUFF transport and diffusion capabilities were evaluated in the IWAQM Phase 2 report were generally over distances greater than 50 km. More recently, model performance has been performed at shorter distances including a power plant in Illinois in simple terrain at source-receptor distances in arcs ranging from 0.5 km to 50 km from the stack (Strimaitis et al., 1998). Another CALPUFF evaluation study over short-distances is reported by Morrison et al. (2003). These studies address model performance over source-receptor distances from a few hundred meters to 50 km.

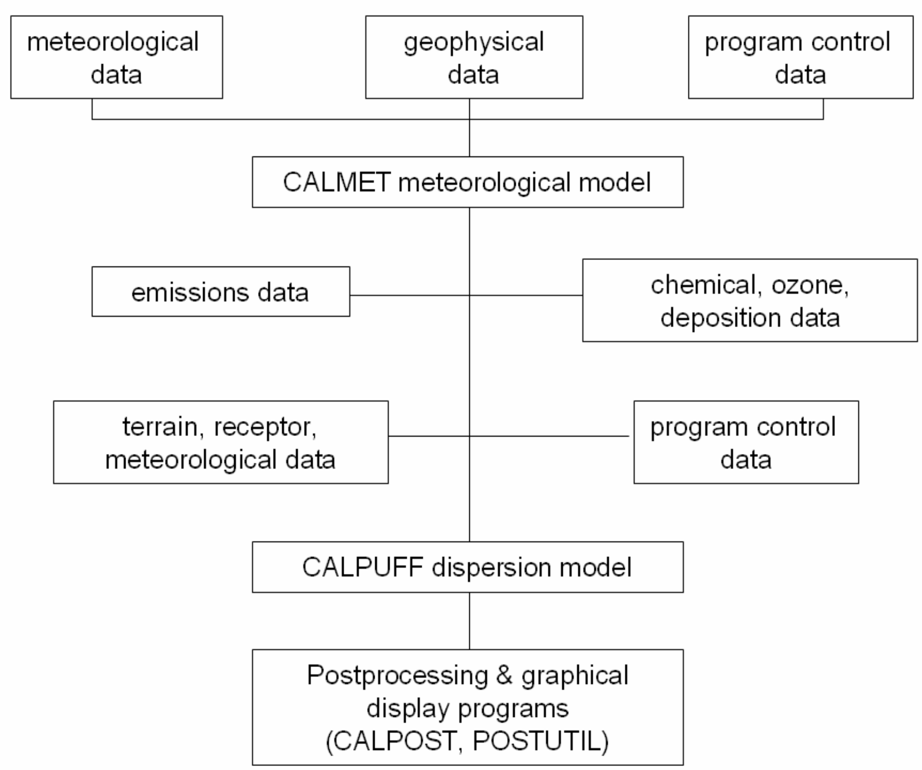

Figure 3-1. CALPUFF Modeling System Components. (Scire et al., 2000a)

Table 3-1. Major Features of the CALMET Meteorological Model. (Scire et al., 2000b)

- **Boundary Layer Modules of CALMET**
  - Overland Boundary Layer - Energy Balance Method
  - Overwater Boundary Layer - Profile Method
  - Produces Gridded Fields of:
    - -- Surface Friction Velocity
    - -- Convective Velocity Scale
    - -- Monin-Obukhov Length
    - -- Mixing Height
    - -- PGT Stability Class
    - -- Air Temperature (3-D)
    - -- Precipitation Rate

- **Diagnostic Wind Field Module of CALMET**
  - Slope Flows
  - Kinematic Terrain Effects
  - Terrain Blocking Effects
  - Divergence Minimization
  - Produces Gridded Fields of U, V, W Wind Components
  - Inputs Include Domain-Scale Winds, Observations, and (optionally) Coarse-Grid Prognostic Model Winds
  - Lambert Conformal Projection Capability

Table 3-2. Major Features of the CALPUFF Dispersion Model (Scire et al., 2000a)

- **Source types**
  - Point sources (constant or variable emissions)
  - Line sources (constant or variable emissions)
  - Volume sources (constant or variable emissions)
  - Area sources (constant or variable emissions)

- **Non-steady-state emissions and meteorological conditions**
  - Gridded 3-D fields of meteorological variables (winds, temperature)
  - Spatially-variable fields of mixing height, friction velocity, convective velocity scale,
    Monin-Obukhov length, precipitation rate
  - Vertically and horizontally-varying turbulence and dispersion rates
  - Time-dependent source and emissions data for point, area, and volume sources
  - Temporal or wind-dependent scaling factors for emission rates, for all source types

- **Interface to the Emissions Production Model (EPM)**
  - Time-varying heat flux and emissions from controlled burns and wildfires

- **Efficient sampling functions**
  - Integrated puff formulation
  - Elongated puff (slug) formulation

- **Dispersion coefficient (σ_y, σ_z) options**
  - Direct measurements of σ_v and σ_w
  - Estimated values of σ_v and σ_w based on similarity theory
  - Pasquill-Gifford (PG) dispersion coefficients (rural areas)
  - McElroy-Pooler (MP) dispersion coefficients (urban areas)
  - CTDM dispersion coefficients (neutral/stable)

- **Vertical wind shear**
  - Puff splitting
  - Differential advection and dispersion

- **Plume rise**
  - Buoyant and momentum rise
  - Stack tip effects
  - Building downwash effects
  - Partial penetration
  - Vertical wind shear

- **Building downwash**
  - Huber-Snyder method
  - Schulman-Scire method
  - PRIME method

Table 3-2. Major Features of the CALPUFF Dispersion Model (Concluded).

- **Complex terrain**
  - Steering effects in CALMET wind field
  - Optional puff height adjustment: ISC3 or "plume path coefficient"
  - Optional enhanced vertical dispersion (neutral/weakly stable flow in CTDMPLUS)

- **Subgrid scale complex terrain (CTSG option)**
  - Dividing streamline, H_d, as in CTDMPLUS:
    - Above H_d, material flows over the hill and experiences altered diffusion rates
    - Below H_d, material deflects around the hill, splits, and wraps around the hill

- **Dry Deposition**
  - Gases and particulate matter
  - Three options:
    - Full treatment of space and time variations of deposition with a resistance model
    - User-specified diurnal cycles for each pollutant
    - No dry deposition

- **Overwater and coastal interaction effects**
  - Overwater boundary layer parameters
  - Abrupt change in meteorological conditions, plume dispersion at coastal boundary
  - Plume fumigation

- **Chemical transformation options**
  - Pseudo-first-order chemical mechanism for SO_2, $SO_4^{=}$, NO_x, HNO_3, and NO_3^- (MESOPUFF II method)
  - Pseudo-first-order chemical mechanism for SO_2, $SO_4^{=}$, NO, NO_2 HNO_3, and NO_3^- (RIVAD/ARM3 method)
  - User-specified diurnal cycles of transformation rates
  - No chemical conversion

- **Wet Removal**
  - Scavenging coefficient approach
  - Removal rate a function of precipitation intensity and precipitation type

Table 3-3. Parameter Variations in Box Model Simulations Used to Develop the CALPUFF Sulfate and Nitrate Formation Algorithms. (Morris et al., 2003).

<table>
<tr><th>Surrogate Parameter</th><th>Number of Variations</th><th>Model Input Parameters And Variations</th></tr>
<tr><td>Season</td><td>3</td><td>Temperatures of 30, 20 and 10 °C were used for the, respectively, summer, fall and winter seasons. Diurnally varying clear skies solar radiation was assumed for each season corresponding to a latitude of 40°.</td></tr>
<tr><td>Background Air Reactivity</td><td>4</td><td>For the summer season the following four levels of background ozone and VOCs were used:
<table>
<tr><th>Ozone (ppb)</th><th>VOC (ppbC)</th></tr>
<tr><td>20</td><td>50</td></tr>
<tr><td>50</td><td>250</td></tr>
<tr><td>80</td><td>500</td></tr>
<tr><td>200</td><td>2,000</td></tr>
</table>
For fall and winter the ozone concentrations were assumed to be 75% and 50% of the summer levels.</td></tr>
<tr><td>Dispersion</td><td>2</td><td>Two different rates of plume dispersion were used: (1) a stable case with a wind speed of 1.5 m/s and; (2) a slightly unstable case with a wind speed of 5.0 m/s.</td></tr>
<tr><td>Release Time</td><td>2</td><td>Photochemical box model simulations were performed with release times of sunrise and noon.</td></tr>
<tr><td>Plume NOx Concentration</td><td>3</td><td>Initial plume NOx concentrations of 7, 350 and 1400 ppb were used.</td></tr>
</table>

4.0 ALTERNATIVE MODELING

In some situations, the modeling of a BART-eligible source may require more rigorous simulation tools in order to adequately estimate the potential that the source adversely impacts a Class I receptor or to develop reasonable, cost effective controls on BART sources. Situations where more comprehensive fine particulate/visibility modeling might be required might include:

> The source's plume traverses over other strong discrete sources of visibility-reducing emissions (e.g., SO_2, NOx);

> Co-mingling of the sources plume with emissions from one or more urban or metropolitan areas;

> Complex meteorological flows entailing significant lateral and/or vertical wind shear or stagnation; and

> Extensive transport distance between source location and the nearest Class I area (e.g., > 300 km).

Another significant motivation for some BART sources may be the need to develop more accurate, less biased estimates of the source's impact on the Class I area given the propensity of CALPUFF to over-predict fine particulate aerosol concentrations and attendant visibility effects. In these or other situations, alternative full-science modeling systems and associated regional data bases are available and allowed by EPA on a case-by-case basis. Though somewhat more costly than routine CALPUFF modeling, the potential costs savings associated with more reasoned BART control requirements may prompt some states or BART source operators to pursue alternative modeling.

This chapter summarizes these tools and provides an assessment of their accuracy and reliability in estimating the impacts of BART-eligible sources on visibility in Class I areas. Of course, use of a more advanced modeling framework would necessitate a detailed 'source-specific' modeling protocol and discussions with the state, EPA and FLM.

4.1 Overview

All source-oriented models, including CALPUFF, are derived from the fundamental atmospheric species conservation equation (Tesche, 1983). Much of the difference between simple and comprehensive models stems from the extent to which the various chemical and physical atmospheric processes are treated: rigorously, heuristically, in a highly parameterized fashion, or neglected altogether. Model developers must choose what pollutants and processes need to be treated rigorously and which ones may be parameterized or neglected altogether when constructing a model to fulfill its design objectives. Simple screening tools such as the Gaussian Plume model neglect a host of atmospheric processes for the sake of providing solutions on a hand-held calculator or nomograph. As noted in Chapter 3, CALPUFF entails a number of simplifications in atmospheric chemistry and transport and dispersion in order to yield a system that runs swiftly on a PC with minimal data requirements.

At the other end of the spectrum, full-science photochemical dispersion models rigorously treat the major processes that govern the formation, transport, gas-phase and secondary aerosol chemical transformation and removal of atmospheric gas phase and aerosol species and their precursors. These state-of-science 'one-atmosphere' models include five basic components: a chemical kinetic mechanism, an emissions model(s), a meteorological model of pollutant transport, a model for pollutant removal at the earth's surface, and a set of numerical algorithms for integrating the governing species conservation equations. The scientific rigor in the development, testing, and peer-review of one-atmosphere models is well-described in a recent annual report by the National Oceanic and Atmospheric Administration (NOAA, 2005) to the EPA. Other in-depth reviews of photochemical and meteorological models, chemical kinetic mechanisms, emissions inventorying techniques, deposition modules, numerical methods, and data base preparation procedures appear extensively in the literature (see, for example: http://www.cmascenter.org/index.html).

One-atmosphere photochemical dispersion models employ nested, stationary three-dimensional arrays of grid cells within which pollutants are emitted, transported from cell to cell, diffused by turbulence, undergo chemical reactions, and are removed from the grid region by precipitation, adsorption on the ground, and other means. This Eulerian grid model concept has been usefully applied and tested across a large range of domain scales, from microscale to regional and continental scales. Current generation 'one-atmosphere' models estimate concentrations of VOCs, NO, NO_2, NOx, O_3, fine particulate aerosol including sulfate, nitrate, ammonium, elemental and organic species, and product species such as HNO_3 and PAN. Model predictions are generated at roughly 6 to 10 minute intervals and then hourly averaged for each grid cell in the three-dimensional computational domain. Current regional models are operated for episodes of several weeks duration up to a year or more. Model output is displayed as time series plots at all monitoring stations and as two-dimensional 'tile' plots that show the hourly modeled concentrations for each species across the full domain. Comparisons between hourly model estimates of gas phase (e.g., ozone, NOx, VOCs, PAN) and particulate (sulfate, nitrate, ammonium, organic and elemental carbon, etc.) species and observations are readily made.

One-atmosphere models offer numerous advantages for certain BART analyses:

- They include detailed characterization of all relevant man-made and natural sources of NOx, VOCs, SOx, and primary particulates (e.g., sulfate, nitrate, ammonia, carbon) across the entire modeling domain on an hourly basis for the entire year.

- They include state-of-science treatment of the coupled non-linear atmospheric chemistry of gas phase photochemical and secondary aerosol species within comprehensive, tested and documented chemical mechanism packages.

- They include detailed characterization of three-dimensional meteorological processes in each grid cell of the modeling domain, account for wind speed and direction shears, turbulent mixing, precipitation processes, solar radiation, and pressure variations;

- They contain modern procedures for specifically treating the near source plume chemical and transport dynamics in the near-field before the plume grows to the size of the finest Eulerian grid nest (typically 4-12 km). Elimination of the over-dilution problem in the original grid models is accomplished through use of high resolution multi-scale nested grids and integrated plume-in-grid (PiG) sub-grid-scale (SGS) modules that simulate the full interactive dynamics and chemistry of point source plumes until they are assimilated into the grid nest;

> As the result of detailed mulsti-scale nesting or plume-in-grid treatment and accounting for *all* manmade and natural source emissions in the entire region, one-atmosphere models are well suited to the analysis of single BART sources and especially the combination of BART sources in a region, a state, or the entire CENRAP domain;

> They can evaluate relative benefits of actual control measures on various man-made sources that might influence the fate of BART-eligible plumes, including differences in location, source type, and composition;

> The results provide complete spatial and temporal mapping of concentration fields (with and without the BART-eligible source included) that can be used for direct plume impact assessment; there is no need to compute or estimate an artificial 'natural background extinction' level since the base case model simulation (without BART sources) produces this automatically. Furthermore, these background estimates can be rigorously evaluated using existing CASTNet, IMPROVE, SEARCH, and related aerosol data sets;

> They have been widely applied by state and federal regulatory agencies, industrial organizations and academic/consulting organizations worldwide;

> They are accompanied by in-depth EPA regulatory guidance documents (for 8-hr ozone, $PM_{2.5}$, and Regional Haze) specifying regarding procedures for justifying model usage in a protocol; developing emissions, meteorological, and air quality inputs; evaluating model performance; and usage in control strategy and SIP development:

> There now exist up-to-date, detailed regional date bases for the entire U.S. (plus northern Mexico and southern Canada) to support model applications, including high resolution 36/12 km data bases over the CENRAP region;

While these science advantages over CALPUFF are substantial, they come at a price. One-atmosphere models are (a) computationally intensive relative to puff models, (b) they have significant data requirements, and (c) they require a high level of expertise in their use. However, for some BART sources in the CENRAP region, these drawbacks may not dissuade source operators from considering their use. When compared to the likely cost of BART controls, the marginal increased cost of an alternative modeling study is modest indeed. In fact, recent experience in the RPO modeling programs suggests that application of 'one-atmosphere' regional models with existing annual regional haze data sets can be roughly equivalent to the costs of a typical PSD modeling exercise using CALPUFF. The regional models run on inexpensive clusters of Linux PCs. Furthermore, in the U.S. today there are over a hundred agency, industry, academic, government laboratory, and consulting groups using one-atmosphere models, providing an ample resource base for on-line help, training, development assistance, documentation, data bases (e.g., the CMAS clearing house) and so on.

Several questions need to be addressed in determining whether use of a one-atmosphere model is preferred over EPA's default CALPUFF modeling system:

> What alternative models are available?

> How do the models treat the sub-grid-scale interaction of BART plumes with the surrounding atmosphere containing emissions from other man-made and biogenic emissions sources?

> What are the steps in using an alternative model?

> What are the performance capabilities of alternative models for gas phase and fine particulate concentrations and visibility impacts?

> What data bases are available in the CENRAP domain to support full-science modeling?

> What are the computational requirements?

> What are the schedule implications of using an alternative model?

> What is the approval process for an alternative model?

> What are the costs of using an alternative model instead of CALPUFF?

Each of these questions is addressed in the following section.

4.2 Available Alternative Models

Though no atmospheric model is wholly accurate and reliable in estimating visibility and fine particulate impacts, two models clearly constitute the state-of-science in modeling fine particulate aerosol and visibility:

> **CMAQ:** EPA's Models-3/Community Multiscale Air Quality (CMAQ) modeling system is a 'one-atmosphere' photochemical grid model capable of addressing ozone, particulate matter (PM), visibility and acid deposition at regional scale for periods up to one year (Byun and Ching, 1999). Developed by EPA over a 12 year period, the CMAQ modeling system is designed to address air quality as a whole by including state-of-the-science capabilities for modeling multiple air quality issues, including tropospheric ozone, fine particles, toxics, acid deposition, and visibility degradation. As with CAMx, CMAQ was designed to have multi-scale capabilities so that separate models were not needed for urban and regional scale air quality modeling. The CMAQ modeling system contains three types of modeling components: (a) a meteorological module for the description of atmospheric states and motions, (b) an emission models for man-made and natural emissions that are injected into the atmosphere, and (c) a chemistry-transport modeling system for simulation of the chemical transformation and fate.

> **CAMx:** The Comprehensive Air Quality Model with Extensions (CAMx) modeling system is a second state-of-science 'one-atmosphere' photochemical grid model capable of addressing ozone, particulate matter (PM), visibility and acid deposition at regional scale for periods up to one year (ENVIRON, 2004). CAMx is a publicly available open-source computer modeling system for the integrated assessment of gaseous and particulate air pollution. CAMx is designed to (a) simulate air quality over many geographic scales, (b) treat a wide variety of inert and chemically active pollutants including ozone, inorganic and organic $PM_{2.5}$ and PM_{10} and mercury and toxics, (c) provide source-receptor, sensitivity, and process analyses and (d) be computationally efficient and easy to use. EPA has approved the use of CAMx for numerous ozone and

PM SIPs throughout the U.S, and has used both CAMx and CMAQ to evaluate regional ozone and fine particulate strategies (e.g., CAIR, CAMR).

Each of these models have been shown to be significantly more accurate and free from systematic bias in estimating visibility reducing air pollutants when compared with CALPUFF (Tesche, 2002; Morris et al., 2003, 2005a,b; Tesche et al., 2005).

A potential compromise between the CMAQ/CAMx comprehensive three-dimensional photochemical grid grids with full-science that simulates all sources and the single-source CALPUFF Lagrangian model with simplified chemistry is the SCICHEM model (Karamchandani et al., 2000), which is also a Lagrangian model designed to treat a single source but uses full-science chemistry:

> **SCICHEM:** SCICHEM is the reactive chemistry version of SCIPUFF, which stands for Second-Order-Closure (SOC) Integrated Puff, and includes comprehensive treatment of gas-phase and aqueous-phase chemistry and aerosol processes. SCIPUFF simulates plume transport and dispersion using a second-order closure approach to solve the turbulent diffusion equations (Sykes et al., 1988, 1993; Sykes and Henn, 1995). SCIPUFF represents a plume by a collection of three-dimensional puffs that are advected and dispersed according to the local meteorological and micrometeorological characteristics. Each puff has a Gaussian representation of the concentrations of emitted inert species. The overall plume, however, can have any spatial distribution of these concentrations, since it consists of a multitude of puffs that are independently affected by the transport and dispersion characteristics of the atmosphere. The turbulent diffusion parameterization used in SCIPUFF is based on the second-order turbulence closure theories of Donaldson (1973) and Lewellen (1977), providing a direct connection between measurable velocity statistics and predicted dispersion rates. The closure model has been applied on local scales up to 50 km range (Sykes et al., 1988) and also on continental scales up to 3000 km range (Sykes et al., 1993c). Gabruk et al. (1999) have shown that the second-order closure algorithm provides better model performance than both empirical algorithms such as the Pasquill-Gifford-Turner (PGT) method or first-order closure algorithms that use similarity theory to relate the dispersion coefficients to micrometeorological variables (e.g., as used in CALPUFF).

SCICHEM can simulate the effect of wind shear since individual puffs will evolve according to their respective locations in an inhomogeneous velocity field. As puffs grow larger, they may encompass a volume that cannot be considered homogenous in terms of the meteorological variables. A puff splitting algorithm accounts for such conditions by dividing puffs that have become too large into a number of smaller puffs. Conversely, puffs may overlap significantly, thereby leading to an excessive computational burden. A puff merging algorithm allows individual puffs that are affected by the same (or very similar) micro-scale meteorology to combine into a single puff. Also, the effects of buoyancy on plume rise and initial dispersion are simulated by solving the conservation equations for mass, heat, and momentum. The gas-phase chemical reactions within the puffs are simulated using a general framework that allows any chemical kinetic mechanism (e.g., CB-IV, SAPRC) to be treated. SCICHEM includes an aqueous-phase chemistry module based on Walcek and Taylor (1986). The module includes the major pathways for aqueous-phase conversion of SO_2 to sulfate. A pathway is also included for the heterogeneous production of nitrate from N_2O_5 hydrolysis in the presence of cloud or fog droplets. For $PM_{2.5}$ calculations, SCICHEM includes modules to simulate the partitioning of species among the gas, aqueous, and solid phases. Particle size distribution is simulated using a sectional representation with 2 size sections.

In the 1 August 2005 Federal Register notice (70 FR, 44154), EPA invited comments on the use of CMAQ or CAMx in estimating the BART ``benchmarks'' for controls on sources subject to BART. For example, regional scale models can be used to inform BART determinations at many sources simultaneously through the use of source apportionment techniques which track multiple single source contributions of individual pollutant species that combine to reduce visibility. EPA notes that this "benchmark" modeling is different from the traditional use of regional scale models like CMAQ and/or CAMx to assess the cumulative impact on visibility after controls on all "subject to BART" sources have been made. Indeed, this usage is consistent with EPA's application of CMAQ and CAMx in support of the Clean Air Interstate Rule (CAIR) and of the most-stringent-case BART for EGUs.

What EPA has not addressed, both in the BART Rule and the BART Modeling Guidelines, is the capability of full-science models such as CMAQ and CAMx to reliably model the photochemical and aerosol processes in individual plumes. EPA's characterization of regional models in the BART Rule and the *Guidelines on Air Quality Models* makes no mention of the substantial body of model research and development performed at EPA and elsewhere over the past 10-20 years in extending grid model to treat sub-grid-scale reactive point source plumes. Below, we summarize highlights of the model development activities at EPA and other organizations that have resulted in full-science models that are indeed capable of simulating the fine details of BART plumes within the context of a regional-scale domain.

4.3 Treatment of Sub-Grid-Scale Plumes

The Plume-in-Grid (PiG) technique constitutes an attempt to account rigorously for the sub-grid-scale treatment of the dynamic and chemical processes governing gas-phase and aerosol species concentrations in isolated, major point source plumes within the grid-based (Eulerian) modeling system. Since the original PiG model formulation and atmospheric testing in the 1970s sponsored by the Electric Power Research Institute (Seigneur et al., 1981; Tesche et al., 1981), there have been sustained research efforts within and outside of EPA to improve the characterization of reactive point source plumes within a variety of host photochemical grid models.

Indeed, development and verification of plume-in-grid (PinG) treatment has been an integral component of EPA's CMAQ modeling system. EPA's PinG approach was specifically developed to simulate the relevant processes governing pollutant concentrations in subgrid scale plumes released from major point sources within the CMAQ grid modeling domain. Since excessive dilution occurs when high NOx or SOx point source emissions are instantly emitted into large volumes of Eulerian grid cells defined for typical regional modeling domains, chemical processes and pollutant concentration levels from point source emissions are greatly impacted. Consequently, the PinG approach models the meteorological, photochemical, and aerosol processes at the appropriate spatial dimension by allowing for the realistic, gradual horizontal/vertical growth of each subgrid scale plume. The PinG treatment has been fully integrated into the CMAQ chemical transport model (CTM)

4.3.1 CMAQ PinG

Godowitch and Young (2005) describe the current status of EPA's program to implement and verify the plume-in-grid (PinG) technique in the CMAQ chemical transport model. As described by Gillani and Godowitch (1999) EPA's original goal was to provide a realistic treatment of the dynamic and chemical/aerosol processes impacting pollutant concentrations in major point source plumes. They formulated the CMAQ/PinG model with an imbedded Lagrangian plume technique to simulate the relevant atmospheric dispersion processes governing vertical and horizontal plume expansion. This more realistic treatment of plume growth allows photochemistry and aerosol formation to evolve at the proper spatial and temporal scales. (Godowitch and Young, 2005). The current PinG module in CMAQ utilizes the same chemical mechanisms (i.e., CB-IV, SAPRC-99) and aerosol modules used by the parent chemical transport model. The updated AE3 aerosol algorithm in CMAQv4.4 was incorporated and successfully tested in the PinG module. The current 2005 public release (CMAQ4.5) contains EPA's most recent PinG module that has significantly improved capability to simulate aerosol species and $PM_{2.5}$ along with gas-phase photochemistry in the subgrid plumes.

During a simulation in which point sources are treated as PinG, CMAQ provides boundary conditions at the plume edges in the PinG model. For example, in Figure 4-1, the five individual plumes embedded in the regional grid all receive gaseous and aerosol boundary condition updates at each integration time step (~6 min). In the PinG model, a continuous plume is simulated by hourly emissions released into a new plume section. The PinG model resolves the detailed horizontal internal structure of each plume section by an attached set of plume cells. Figure 4-2 shows the modeled cross section of a high NOx/ low SO2 industrial plume in the middle Tennessee area. Once a plume section reaches the grid size, its subgrid PinG simulation ceases and a feedback of plume material into the CTM grid is performed. The net impact of a potential source is determined by subtracting a base case simulation (i.e., a NoPinG run) from a full CMAQ-PinG simulation (see Figure 4-3 for example). A full description of the capabilities of EPA's CMAQ-PinG model and its technical formulation were described in EPA's original science document (Gillani and Godowitch, 1999) and more recently by Godowitch (2001, 2004) and NOAA (2005).

4.3.2 CMAQ-APT-PM

Another PinG formulation incorporated into EPA's CMAQ model and evaluated with monitoring program data is described by Vijayaraghavan, et al., (2004). CMAQ-APT-PM consists of the EPA CMAQ model with an embedded reactive plume model, the Second-order Closure Integrated puff model (SCIPUFF) with CHEMistry (SCICHEM). SCICHEM uses a second-order closure approach to solve the turbulent diffusion equations. The plume is represented by a myriad of three-dimensional puffs that are advected and dispersed according to the local micrometeorological characteristics. Each puff has a Gaussian representation of the concentrations of emitted inert species. The overall plume, however, can have any spatial distribution of these concentrations, since it consists of a multitude of puffs that are independently affected by the transport and dispersion characteristics of the atmosphere. SCICHEM can simulate the effect of wind shear since individual puffs will evolve according to their respective locations in an inhomogeneous velocity field. The effects of buoyancy on plume rise and initial dispersion are simulated by solving the conservation equations for mass, heat, and momentum. The formulation of nonlinear chemical kinetics within the puff framework is described by Karamchandani et al. (2000). Chemical species concentrations in the puffs are treated as perturbations from the background concentrations. The chemical reactions within the puffs are simulated using a general framework that allows any chemical kinetic mechanism to be treated. The full CMAQ PM aerosol and aqueous-phase chemistry is included in the PinG formulation of CMAQ-APT-PM (Karamchandani et al., 2005).

4.3.3 CMAQ-MADRID-APT

Karamchandani, et al., (2005) describe another implementation of plume-in-grid technology into the CMAQ framework, but this modeling system used an alternative state-of-science gas-phase and aerosol chemical mechanism. CMAQ-MADRID (CMAQ with the Model of Aerosol Dynamics, Reaction, Ionization and Dissolution, MADRID) is a version of CMAQ that is publicly available and currently distributed by EPA's Community Modeling and Analysis System (CMAS) center. CMAQ-MADRID-APT utilizes the same emissions, meteorological and air quality files as the other CMAQ versions discussed above. It also has been tested with atmospheric data.

4.3.4 CAMx PM IRON PiG

Implementation of plume-in-grid algorithms in CAMx has been underway since the mid 1990s. Emery and Yarwood (2005) and Yarwood et al., (2005) describe the science formulation, implementation and testing of two versions: IRON PiG and PM PiG. The CAMx IRON (Incremental Reactions for Organics and NOx) Plume-in-Grid model features:

> New puff structure and dynamics to better account for deforming shears;
> Second-order closure puff spread calculation following SCIPUFF equations;
> Puff initialization and transport performed on the time step of finest grid;
> Full photochemistry using CB-IV or SAPRC99;
> Revised puff dumping approach for IRON PiG based on comparison to cell area; and
> "Virtual dumping" of puff mass into average output concentration fields for post-processing and analysis.

Implementation of PM chemistry into the IRON PiG closely paralleled the approach for grid chemistry. The PM chemistry modules are used in each puff following the same incremental chemistry approach that IRON PiG uses for the gas-phase ozone chemistry; i.e., by separate integrations for background and puff + background (to determine the evolution of puff incremental concentrations.) The PM PiG updates have been incorporated into CAMxv4.20_PMPiG. Details on the PiG implementations in CAMx are available at www.camx.com)

4.3.5 CAMx Multi-Scale Flexi-nesting

A final procedure for treating sub-grid-scale plume chemistry and physics takes advantage of the 'flexi-nesting' capability of CAMx. In this method, a series of nested grids are defined with successively smaller horizontal grid spacing, provide a cascading multi-scale representation from local plume scale (say a few hundred meters) to regional scale (12 or 36 km). Through careful assessment of the meteorological conditions influencing the BART source and Class I receptor(s), a multi-scale nested grid system can be defined that directly overcomes the plume over-dilution problem of older Eulerian models while retaining manageable computational times over the annual period. CENRAP's existing MM5/CALMET meteorological fields for 2001-2003 can be used to define the sector(s) of greatest concern for the BART plume, thereby allowing the modeler to ensure that the fine grid mesh is used to best effect.

4.4 Steps in an Alternative Modeling Study

The motivation to consider an alternative model to CALPUFF for the BART exemption and/or BART determination analysis would typically come from a State or source operator. The first step in the process would be to discuss the rationale for use of an alternative model with representatives from the state, EPA, and FLM. Since decisions on acceptability of an alternative model is a joint responsibility, it is prudent to engage the EPA and FLM early in this process. Section 4.8 describes the specific steps in the approval process.

Consistent with the approval process and to guide the actual modeling study, a detailed source-specific modeling protocol must be prepared. While this protocol would generally follow the content of the source-specific CALPUFF protocol (see Chapter 7), additional technical details would be required in the description of the model configuration, model-set up procedures, data bases to be employed, model evaluation and sensitivity tests, and procedures for application.

Once the alternative modeling protocol is approved, the state or source operator (or consultant) would implement the procedures set forth in the document. Typically, these would include: selection of appropriate emissions, meteorological, and air quality models; selection of modeling year(s) to use; selection and acquisition of pertinent regional modeling data bases (e.g., from CENRAP, VISTAS, MRPO, or WRAP); base case model simulation; model performance evaluation and sensitivity testing; modeling of BART source(s) with appropriate sub-grid-scale plume technology; calculation of background visibility; comparison of BART source plume increment relative to background visibility; uncertainty analysis; reporting; and modeling data archival and distribution.

4.5 Accuracy of Regional PM and Visibility Models

A major motivation for using full-science models for BART analysis is the expectation that they provide more accurate and less biased predictions of visibility reducing fine particulate aerosols than CALPUFF. While this likelihood is easily seen in comparative evaluations of CALPUFF and one-atmosphere model science formulations (e.g., Morris et al., 2003), a comparison of model performance against actual gas-phase, fine particulate aerosol, and visibility measurements is also instructive. Indeed, as noted in Section 4.8 below, one of the factors influencing EPA and FLM assessment of an alternative model is whether it performs better for the application than CALPUFF and better satisfies the BART Rule regulatory requirements.

Unfortunately, it is not possible to carry out a clean, head-to-head comparative model evaluation between CALPUFF and full-science models for their ability to simulate fine particulate species and visibility. First, there simply are no detailed atmospheric plume data bases that record the chemical evolution of point source plumes at numerous downwind locations (i.e., from point of emission to downwind distances of 200-400 km where the concentrations of sulfates, nitrates, EC, OC, secondary organic aerosols (SOA), and extinction coefficient are measured.) If such data bases existed, it would be a simple matter to compare alternative modeling platforms. Second, CALPUFF has no *reliable* means for accounting for the effects of all other manmade and natural emissions sources in the region that participate in the chemical transformation of point source emissions. Thus, one cannot evaluate CALPUFF predictions against downwind secondary aerosol measurements or visibility. Measurements reflect the interaction of a variety of upwind sources; CALPUFF outputs principally the fate of emissions from the point source(s) under consideration.

Several evaluations of CALPUFF that have been carried out using inert atmospheric tracers (see Section 3.6). These studies are useful in elucidating the model's ability to simulate the transport and dispersion of non-reactive materials. In contrast, there is a rich and evolving performance evaluation history of regional one-atmosphere models, stimulated in large measure by the CMAQ and/or CAMx modeling being performed by WRAP, CENRAP, MRPO, VISTAS and MANE-VU for regional haze. These regional modeling studies have examined one or both models over grid domains of 36 km and 12 km for the years 2001, 2002, and 2003 (depending upon the RPO). Detailed performance evaluations of the models have been carried out by various groups, focusing on several performance attributes of relevance to BART analyses. For the CENRAP modeling (Morris et al., 2005d), these evaluations, for NO, NO_2, ozone, sulfate, nitrate, ammonium, ammonia, EC, OC, secondary organic aerosol, $PM_{2.5}$, extinction coefficient, and various other species are reported as:

> Daily scatter and time-series plots at each individual site.

> Monthly average model performance metrics. Bar plots for 12 months showing bias and error averaged over all sites in the CENRAP region, providing a quick summary of the variability in seasonal performance.

> Bugle plots grouped both by species and by monitoring network. Monthly average error and bias terms are plotted in a Bugle plot as a function of the species concentration. This helps characterize differences in model performance at clean versus polluted conditions. These plots also include curves showing model benchmarks and performance goals. Benchmark curves indicate the skill of a wide array of previous PM modeling studies. Performance goals are arbitrarily defined based on ozone performance goals.

> Animated spatial plots with data overlaid on the model predictions: These animated, daily average plots show the IMPROVE and AQS data superimposed over the model simulated data. These are useful for showing spatial distributions and instances where poor model performance occurs because the model mis-locates the high concentrations by just a few grid cells from the observed high concentrations.

> Stacked bar time-series plots for each site: These plots show contributions of each PM component to visibility impairment for the daily average for each day with ambient data in one plot, and for each of the 365 modeled days in a second plot.

> Stacked bar plots for the best & worst 20% day average at each site using (1) matched in space & time; (2) relaxed in time; and (3) relaxed in both space and time: These comparisons show whether the model is capable of simulating the full range of clean to polluted conditions seen in the ambient data at the individual sites. It increases confidence in the model as a "reasonable version of reality" if it can simulate the range of clean to polluted conditions.

Three recent studies summarize the current performance capabilities of the CMAQ and CAMx regional models for aerosol species and visibility. Morris et al., (2005d) summarize the performance of CAMx and CMAQ over the 36 km CENRAP domain for the full calendar year 2002. For VISTAS, Morris et al., (2005a,b) and Tesche et al., (2005a) summarize detailed performance evaluations of CAMx and CMAQ for the VISTAS region, also for 2002.

Boylan and Russell (2005) proposed PM model performance goals (the level of accuracy that is considered to be close to the best a model can be expected to achieve) and criteria (the level of accuracy that is considered to be acceptable for regulatory applications) that vary as a function of concentration and extinction. Specifically, it has been proposed that a model performance goal has been met when both the mean fractional error (MFE) and the mean fractional bias (MFB) are less than or equal to +50% and ±30%, respectively. Additionally, the model performance criteria has been met when both the MFE ≤ +75% and MFB ≤ ±60%. Less abundant species would have less stringent performance goals and criteria. These recommendations are based upon an analysis of numerous PM and visibility modeling studies performed throughout the country.

In particular, Boylan and Russell (2005) tabulated the mean fractional bias and mean fractional error for several recent one-atmosphere modeling studies: SAMI, WRAP, VISTAS, Midwest RPO, and EPRI. The one-atmosphere models evaluated included CAMx, CMAQ, CMAQ-MADRID, and URM. Figure 4-9 presents so-called 'bugle plots' of fractional bias and fractional error for each component of PM as well as PM_{10} and $PM_{2.5}$. Overall model performance for $PM_{2.5}$ is fairly good with about 50% of the points meeting the goals and a large majority meeting the criteria. Sulfate performance is better than most components of $PM_{2.5}$ that were examined, with a majority of the points meeting the goal and only two points falling outside the criteria. This was attributed to good estimates of SO_2 emissions, sulfate chemistry being less complex than other components of PM species, and the high spatial homogeneity of sulfate. On the contrary, nitrate performance is poorer with approximately 40% of the points falling outside the criteria and only values smaller 0.8 μg m^{-3} meeting the goal. As pointed out by recent EPA researchers (Yu et al., 2005) nitrate performance with all atmospheric models continues to be a significant challenge. Ammonium performance falls between that of sulfate and nitrate. Overall, the performance is fairly good because the majority of the ammonium is associated with sulfate which performs well. Less than 40% of the organic performance assessments meet the goal and a fair number fall outside the criteria. The large errors are mainly due to simulated organic levels being lower than observations, especially at the urban STN sites. Elemental carbon concentrations are typically below 1.0 μg m^{-3} and the performance is within the performance goals for all assessments except one, which is just barely outside the goal. Approximately 40% if the soil points meet the goal, while another 45% are outside the criteria. Most of the soil error is caused by large overestimations by the model. Finally, coarse mass performance is poor with only 2 points meeting the goal and a majority falling outside the criteria.

Boylan and Russell (2005) performed an identical analysis for components of light extinction. They report similar performance patterns to those of PM for sulfate, nitrate, ammonium, organics, and elemental carbon. These similarities are due to the fact that each of these components receive multipliers that are on the same order of magnitude as the scale change when converting from mass to light extinction. However, since soils and coarse mass do not get large multipliers due to their minimal impact on visibility, their performance is much improved over that of their PM mass performance. In fact, only a handful of soils and coarse mass points fall outside the criteria lines. Using the identified metrics, sulfate and EC components of $PM_{2.5}$ and light extinction are generally the most accurately simulated, while nitrate and organic carbon performance are poor. Poor soil performance is of concern for $PM_{2.5}$, but not visibility. Poor coarse mass performance does not impact total $PM_{2.5}$ and has minimal impact on total light extinction. Detailed model evaluation results for the CENRAP, MPPO, VISTAS, and WRAP modeling studies may be found at:

CENRAP: http://pah.cert.ucr.edu/aqm/cenrap/cmaq.shtml
MRPO: http://www.ladco.org/

VISTAS: http://pah.cert.ucr.edu/vistas/vistas2/results.shtml
WRAP: http://pah.cert.ucr.edu/aqm/308/cmaq.shtml

In summary, the performance status of current one-atmosphere models such as CMAQ and CAMx reveals that for some species (sulfate, $PM_{2.5}$) the models do quite well while for certain others the models exhibit bias and large uncertainty (e.g., nitrate concentrations, secondary organic aerosols). The models have been tested over a full range of atmospheric conditions covering the CENRAP region and have been evaluated for up to three continuous years (2001, 2002, and 2003). This performance record clearly surpasses – in rigor, scope, and statistics – any evaluation that has been published to date for CALPUFF. The current status of one-atmosphere models in simulating fine particulate aerosols and visibility impairment is thus well established and this information would be quite helpful in supporting discussions with EPA Regional Offices and the FLM on the merits of using full-science visibility models as alternatives to CALPUFF.

4.6 Data Base Requirements

The data sets needed to support the evaluation and application of alternative regional models may be grouped into three general categories: emissions, meteorology, and air quality. Fully developed CAMx and CMAQ modeling data sets at 36/12 km grid scales are available over the CENRAP states and may be obtained from one or more RPOs. Details are described in Chapter 5.

4.7 Resource Requirements

The current availability of RPO-developed regional PM modeling data bases and publicly-available modeling tools and technical support venues now make it feasible to perform a BART visibility impact study in a matter of a few months at a cost that is not too much larger than a traditional PSD modeling exercise. A summary of current computer, staff, and schedule requirements associated with a BART exemption or BART determination study is given below.

4.7.1 Computers

While the computational costs to run CMAQ or CAMx for a typical BART application far exceed those of a guideline CALPUFF analysis, the hardware requirements are still well within the range of modern scientific computing set-ups. Given the availability of model-ready meteorological, emissions, and air quality data bases from the various RPOs, the only significant computational cost in alternative modeling is in running the base case simulation to establish background conditions, and the BART impact cases to assess determine if the source is 'subject to BART' and if so, what appropriate controls might be. As with the CALPUFF applications, there is no need to develop new meteorology. Unlike CALPUFF, there is no need to develop estimates of background emissions, or air quality; these are already compiled in the existing RPO data bases. The only data input development need, common to CALPUFF too, is the characterization of the point source's emissions.

CMAQ and CAMx run efficiently on modern commodity PCs under the Linux operating system. For example, a typical Linux cluster configuration for applying CMAQ in multi-processor mode might include 3 dual Athlon MP 2800+ computers (6 total processors), 1 to 2.5 Gybte RAM for each node, a GigE switch connection, and 1-3 Tbyte external hard disk storage for model input and output files. With four such clusters, an annual CMAQ simulation can be performed by quarter with 15 days spin-up. Four quarters are run in parallel, saving project calendar time. In this example, four (4) sub-clusters of three dual-processor Athlon MP machines would be employed with the 'master" node of each sub-cluster maintaining one 250 Gbyte drive for meteorological data per quarter and one 250 Gbyte drive for output for quarter. Experience shows that using more than 3 nodes (i.e., 6 processors) per quarter does not yield substantial run-time speed up.

CAMx4.2 employs a shared memory scheme rather than a parallel processing scheme, so model simulations are performed on one stand-alone system. Multiple jobs can be run in parallel however. The overall computer run times of a projects do not seem to vary significantly between CMAQ and CAMx platforms.

Finally, EPA provides a website for the community to share different experiences in acquiring, configuring, and applying different hardware solutions for CMAQ and other one-atmosphere tools and data bases. Go to: **http://www.cmascenter.org/html/hardware.html.**

4.7.2 Staff Expertise

Setting up and exercising the CMAQ or CAMx modeling system requires a high level of atmospheric modeling expertise and typically transcends the skill level normally associated with operating EPA guideline models. Particular areas of modeling expertise involve meteorology, atmospheric chemistry, emissions inventory development, regional air quality modeling, data analysis, and computational science. However, there are over 100 groups in the U.S. today that possess this level of expertise; many reside within state agencies, regional EPA offices, governmental laboratories, and academic institutions. There is also a fairly large consultant community with the requisite level of experience. Accordingly, for the limited set of states or source operators for whom alternative regional modeling may be attractive, there should be no shortage of skilled practitioners available to assist with the modeling analyses.

4.7.3 Schedule

Typically a 3 to 4 month time period is required to design, negotiate, implement, and complete CALPUFF modeling for a nominal BART application. Of course, some studies can be performed more quickly and others may take longer than 4 months.

An alternative modeling study will require more time than a CALPUFF application for three reasons. First, because the use of advanced regional models may be somewhat new to some CENRAP state or federal agencies, the length of time to negotiate a consensus CMAQ or CAMx BART Modeling Protocol will take longer. Part of this stems from the requirement to justify the need and appropriateness of alternative models to CALPUFF. In this connection, there are some important decisions to be ratified (calculation of 'natural visibility background', number of years to be modeled, appropriate sub-grid-scale plume technology to be used, etc) and this will require discussion and negotiation with state and federal agencies. Second, the full-science models require a couple of weeks or more to simulate a full calendar year. So, depending on the number of years modeled and the number of BART control strategies examined, computer simulations alone may necessitate two months or more of calendar time.[1] Third, unlike CALPUFF model applications, the alternative model protocol development and annual visibility simulations can not realistically be carried out in parallel. Negotiation of the protocol must first be completed before the commitment to run annual CMAQ or

[1] Most modeling centers operate several clusters of high-speed Linux machines; by configuring the clusters and model simulation jobs thoughtfully, multiple annual CAMx or CMAQ simulations can be carried out in parallel, thus condensing elapsed time for the model applications.

CAMx simulations is actually implemented. Based on these factors, it is reasonable to expect that an alternative BART modeling application would require on the order of 4 to 6 months to complete.

4.8 Approval Process for an Alternative Model

The decision to use a full-science alternative model would typically be made by the State or the particular source. To justify the use of an alternative model, one must follow the procedures set forth in the Guideline on Air Quality Models for obtaining approval for the use of a non guideline models. EPA encourages selection of the best techniques for each individual air quality analysis, but requires that the selection be done in a consistent manner.

Determination of acceptability of an alternative model is a Regional Office responsibility. If it can be demonstrated that in a specific application the alternative model is more appropriate than CALPUFF, the model may be used subject to certain requirements. This demonstration before the Regional Administrator normally requires that the State or the source show that either CALPUFF is not appropriate for the specific application *or* the alternative model is available and is applicable. There are three separate conditions under which an alternative model will normally be approved for use:

> If a demonstration can be made that the model produces concentration estimates equivalent to the estimates obtained using a preferred model;

> If a statistical performance evaluation has been conducted using measured air quality data and the results of that evaluation indicate the alternative model performs better for the application than a comparable model in appendix A; and

> If there is no preferred model for the specific application but a refined model is needed to satisfy regulatory requirements.

Any one of these three separate conditions may warrant use of an alternative model.

The procedures and techniques for determining the acceptability of a model for an individual case based on superior performance is contained in the document entitled "Interim Procedures for Evaluating Air Quality Models" should be followed. Preparation and implementation of an evaluation protocol which is acceptable to both control agencies and regulated industry is an important element in such an evaluation. If it can be shown that CALPUFF is not applicable to the BART source-specific modeling problem at hand, an alternative refined model may be used provided that:

> The model can be demonstrated to be applicable to the problem on a theoretical basis;

> The data bases which are necessary to perform the analysis are available and adequate; and

> Performance evaluations of the model in similar circumstances have shown that the model is not biased toward underestimates.

In short, the guidance requires that the alternative model be evaluated from both a theoretical and a performance perspective.

EPA has prepared a document entitled "Interim Procedures for Evaluating Air Quality Models" to assist in developing a consistent approach when justifying the use of other than the preferred modeling techniques. Another EPA document "Protocol for Determining the Best Performing Model"provides a general framework for objective decision-making on the acceptability of an alternative model for a given regulatory application. These documents contain procedures for conducting both the technical evaluation of the model and the field test or performance evaluation.

Ultimately, the Regional Administrator has the authority to determine whether an alternative model is acceptable for a source-specific BART analysis. However, recognizing the need for assistance and guidance in the selection process so that fairness and consistency in modeling decisions is fostered among the various Regional Offices and the States, EPA's Model Clearinghouse serves as the final authority on modeling issues.

4.9 Cost of Alternative Modeling

The cost of a CALPUFF dispersion modeling study for a source can vary depending upon several factors including: (a) availability of meteorological and air quality data sets, (b) availability of emissions source characterization (especially particulate matter speciation and size fractionization), (c) the number of Class I areas to be examined, (d) the distance(s) from source to Class I area(s), (e) the effort required to prepare and successfully negotiate the modeling protocol with the state, EPA and FLM, and various other factors. Computer costs are minimal since the CALPUFF system runs on personal computers equipped with inexpensive external hard disk drive storage. (Current storage costs run less than $1 per Gigabyte). Experience shows that the cost of a typical CALPUFF modeling exercise for a BART source[2] is in the range of $20,000 to $50,000 depending upon the nature of the problem, the expertise and cost structure of the organization performing the modeling, the modeling experience of the state or source operator, and the extent of interaction required with the reviewing agencies.

An alternative modeling study using CAMx or CMAQ costs more than a CALPUFF BART application but the differential is much less today given the ready availability of applicable regional data sets. Key cost elements in an alternative modeling study include: (a) protocol development and negotiation with the reviewing agencies, (b) obtaining and setting up one or more RPO data bases on the host computer network[3], (c) running the base case regional model simulation to establish 'background visibility conditions, (d) running the regional model with the BART source included, and (e) post processing and reporting the results. Assuming that the alternative modeling was performed for one calendar year (e.g., 2001, 2002, or 2003), the cost range is $50,000 to $75,000.

The greatest cost variable in alternative modeling is whether the state, EPA, and/or FLM will require that more than one calendar year be modeled to establish whether a source is 'subject to BART' and/or the level of BART emissions controls needed. If a full three year CMAQ or CAMx modeling analysis is required, the aforementioned cost range could double. However, even if the reviewing agencies require a full three years of CMAQ or CAMx modeling, there are still several opportunities for cost reduction. Opportunities include:

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2 This exercise would includes analyses to determine whether the source is 'subject to BART', followed by several CALPUFF model runs to estimate the visibility impacts of different levels of BART emissions controls.

3 The computational platform needed to efficiently run the full-science models is a Linux- or Unix-based cluster with multiple nodes and several TBytes of external disk storage.

> If three full years of alternative modeling is performed to confirm that a source is subject to BART, then the BART control modeling can likely focus just on that year for which the maximum visibility impacts were calculated.

> Exercise the CAMx or CMAQ models *in an episodic mode only*, simulating only those infrequent time periods when peak 24-hr average visibility impacts are greatest.

> Invoke the plume-in-grid or multi-scale grid nesting SGS technologies in the regional model only during those episodic periods where peak 24-hr average impacts were estimated in the initial modeling;

> Exercise the CAMx or CMAQ models *in an episodic mode only*, simulating only those infrequent time periods when peak 24-hr average visibility impacts are greatest.

Thoughtful application of alternative models can very likely reduce the overall program cost. The greatest variable in estimating the resources required to employ CAMx or CMAQ in BART modeling is the level of effort required to work with the state, EPA, and FLM to reach a consensus on how the model(s) should be applied. Since this is likely to be 'new territory' for some agency staff, it may require somewhat more effort to reach consensus.

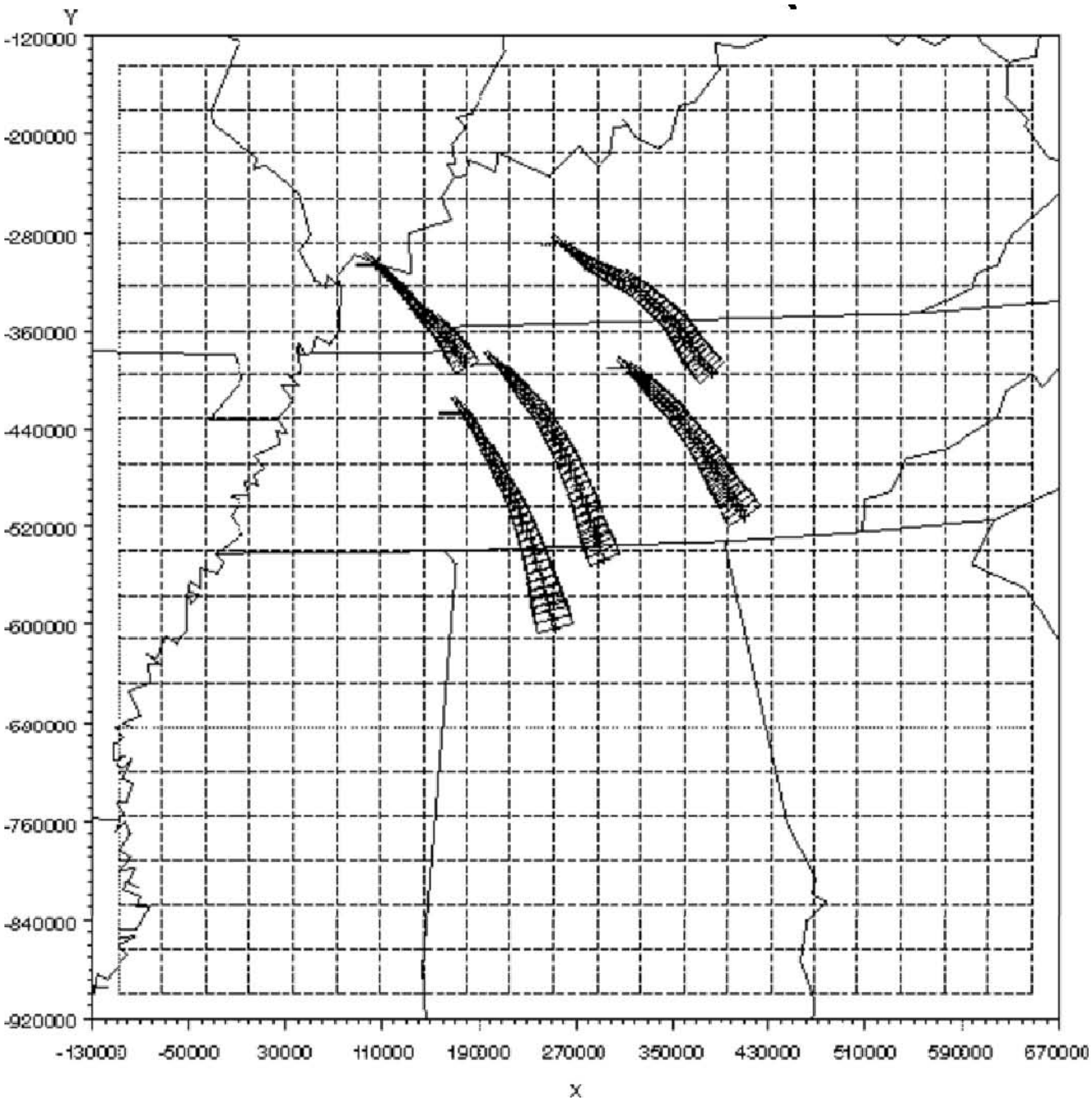


Figure 4-1. Plume Trajectory Paths and Growth Rates of Sub-Grid-Scale Reactive Plumes within the CMAQ-PinG Model Simulation of the July 1995 SOS Field Program in Nashville, TN. Plumes Released at 1500 UTC on 7 July 1995 on the Modeling Domain with the 36 km Grid. (Source: Godowitch, 2004).

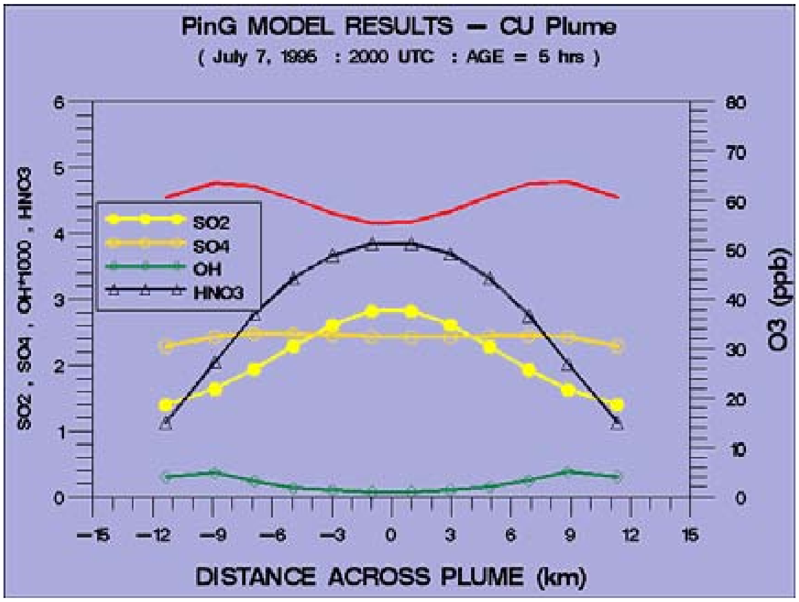


Figure 4-2. Reactive Plume Species Concentrations in the Cross Section from a High NOx/Low SO2 Emissions Source at 5 Hours After Release. Ozone (O_3) is the solid red line. Units: SO4 ($\mu g/m^3$), OH (ppt), SO_2 and HNO_3 (ppb). (Source: Godowitch, 2004).

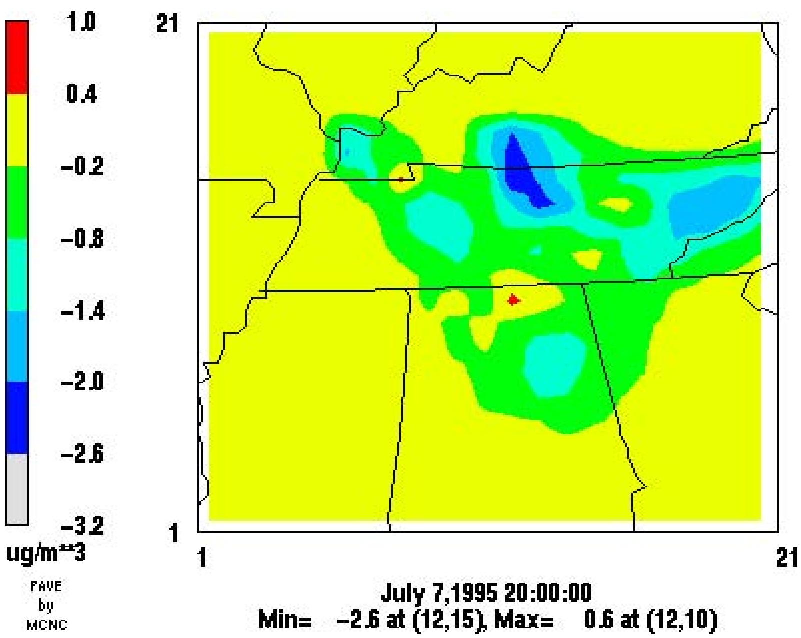


Figure 4-3. Aerosol Sulfate (SO_4) Difference Field Determined by Subtracting the CMAQ-NoPinG Concentrations from the CMAQ-PinG Concentrations at 2 pm EDT on 7 July 1995. (Source: Godowitch, 2004).

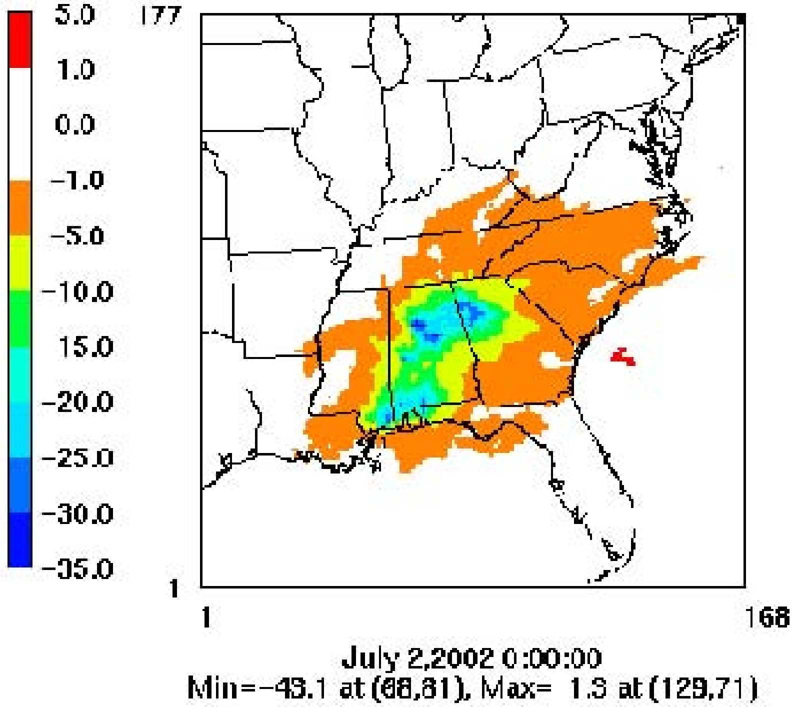


Figure 4-4. Change in the Contributions of Fourteen (14) EGUs to Local Sulfate (SO_4) Concentrations When the CMAQ-APT-PM Plume-in-Grid Approach is Used. (Source: Karamchandani et al., 2005).

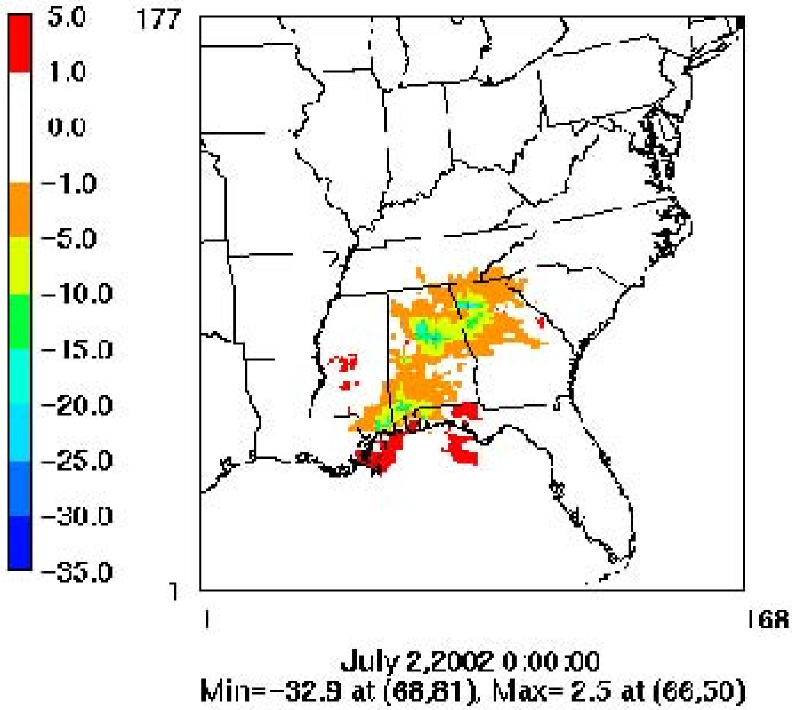


Figure 4-5. Change in the Contributions of Fourteen (14) EGUs to Local Nitrate (NO_3) Concentrations When the CMAQ-APT-PM Plume-in-Grid Approach is Used. (Source: Karamchandani et al., 2005).

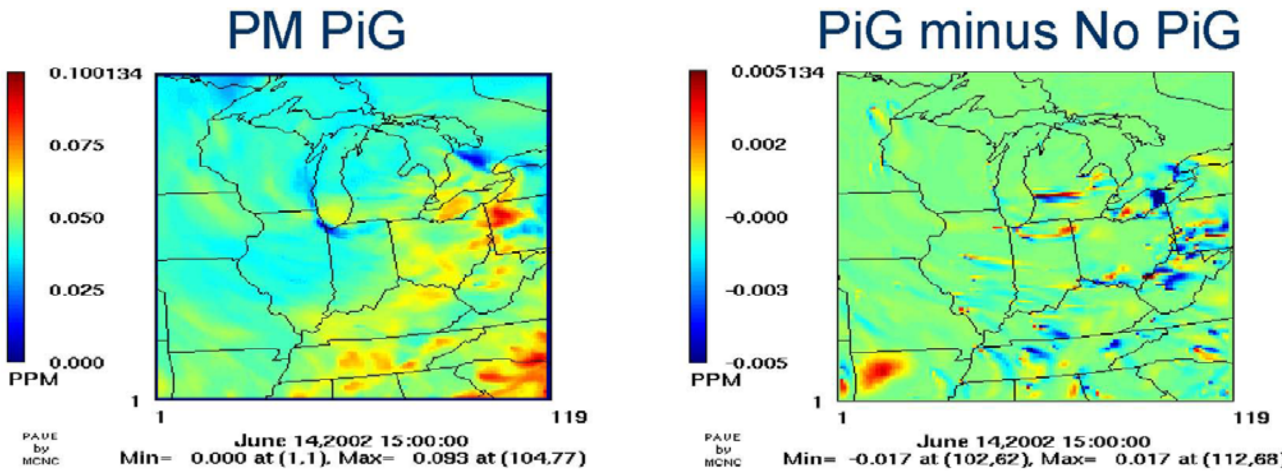


Figure 4-6. CAMx PM PiG Simulation of Ozone Over the Upper Midwest on 14 June 2002: Plot on Right Reveals the Ozone Increments Associated with Sub-Grid-Scale Treatment of Reactive Plumes. (Source: Yarwood et al., 2005).

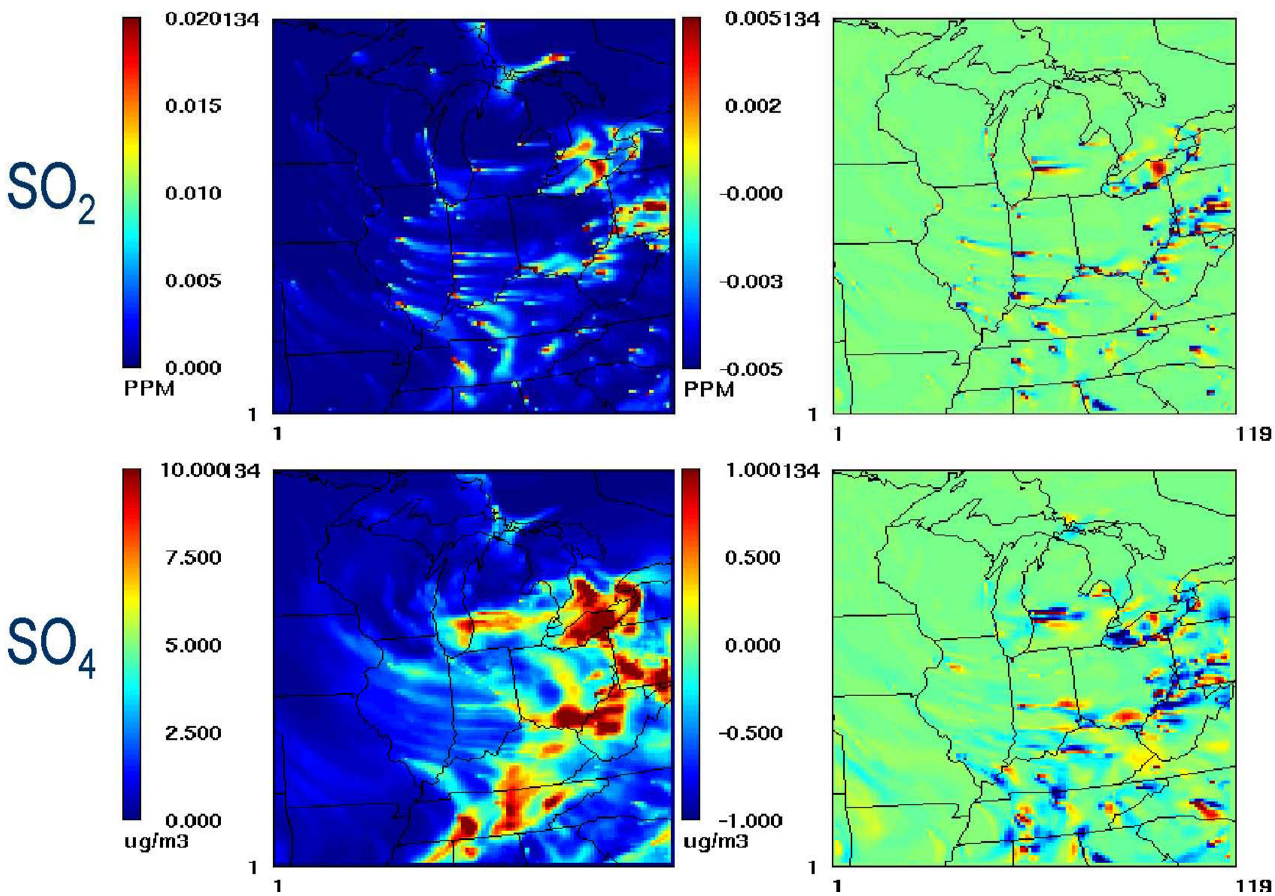


Figure 4-7. CAMx PM PiG Simulation of SO_2 and Sulfate Over the Upper Midwest on 14 June 2002: Plot on Right Reveals the SO_2 and SO_4 Increments Associated with Sub-Grid-Scale Treatment of Reactive Plumes. (Source: Yarwood et al., 2005).

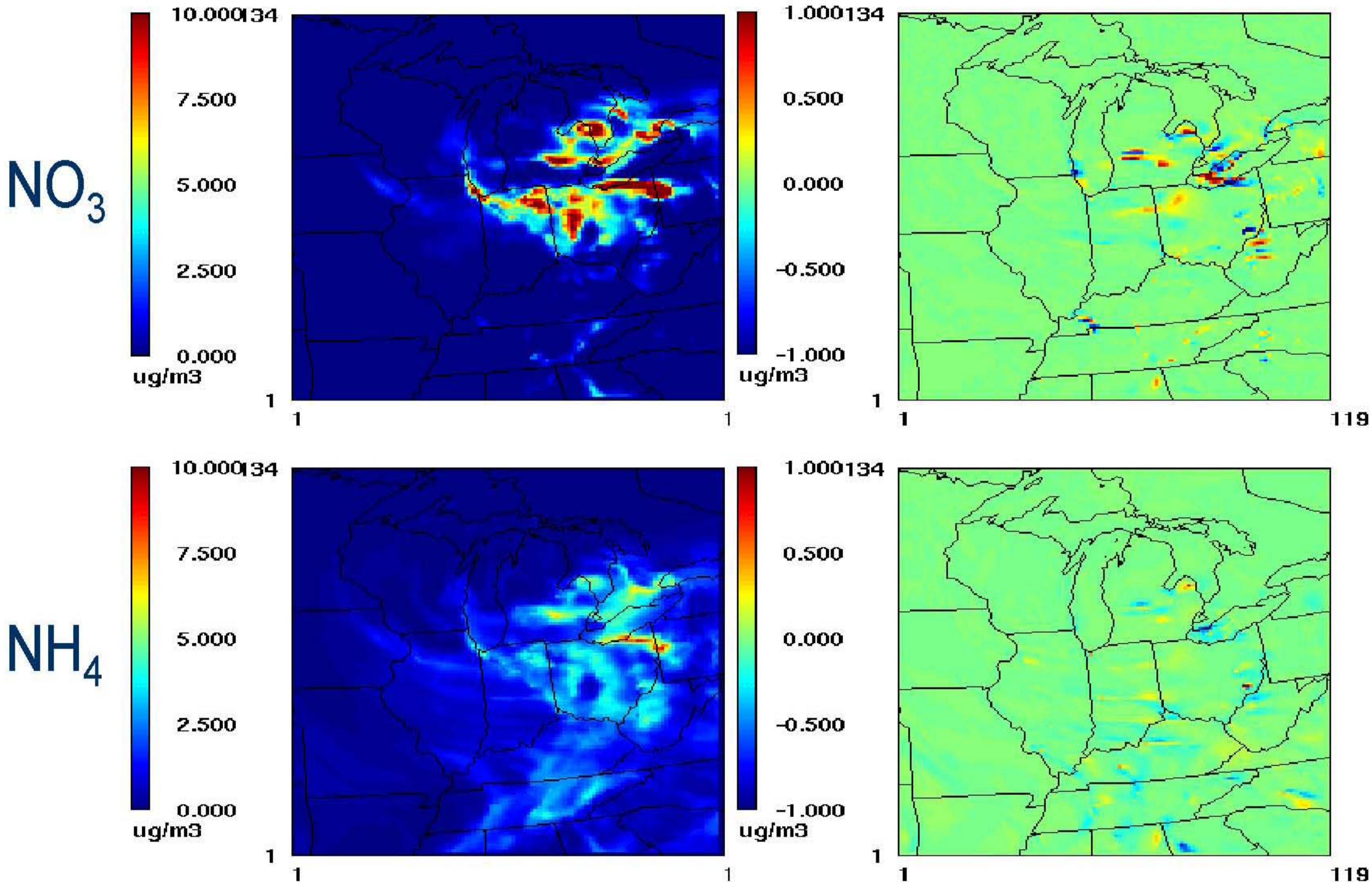
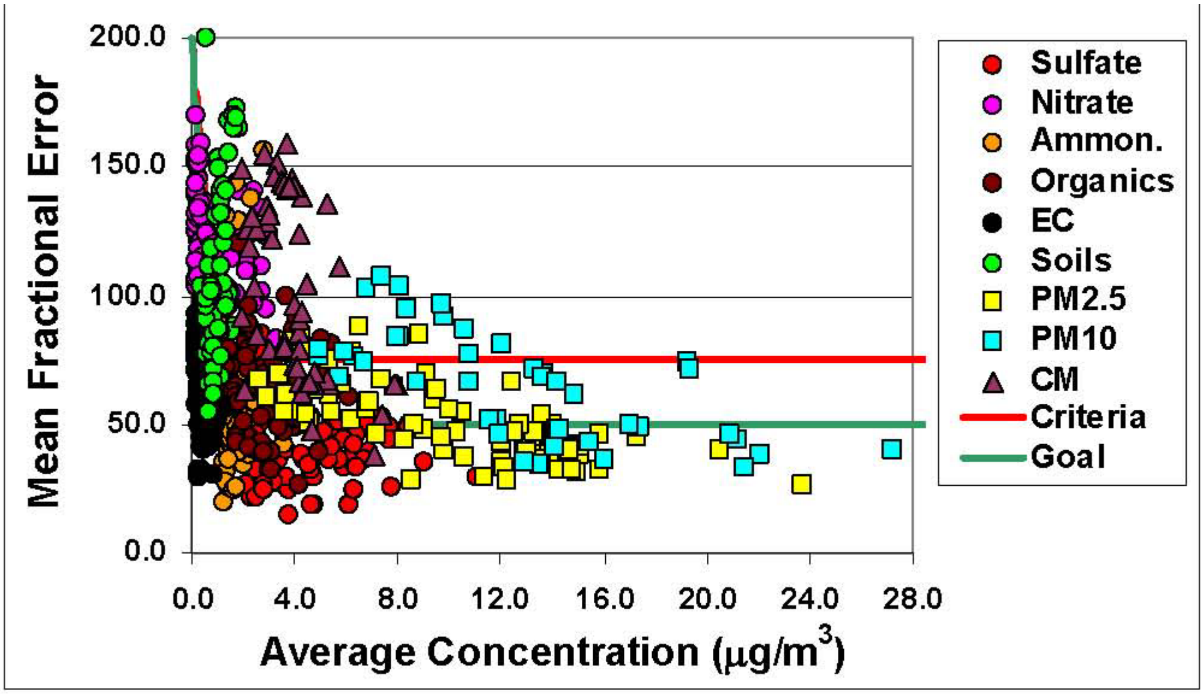
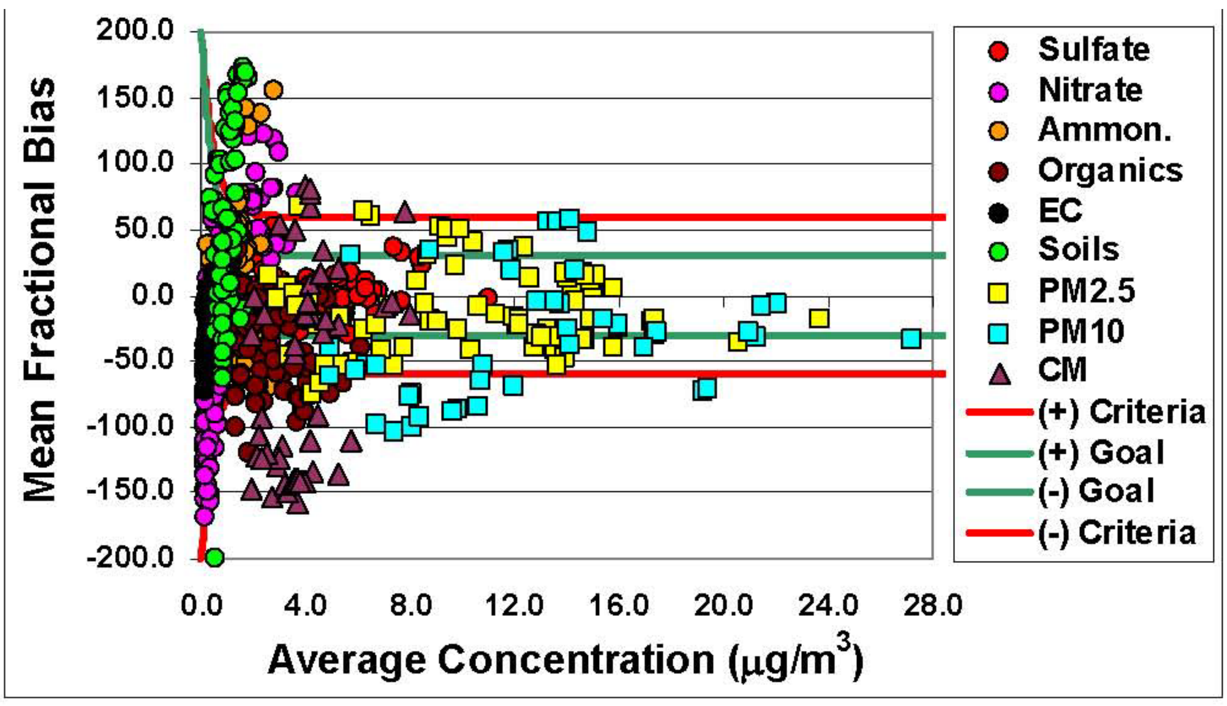


Figure 4-8. CAMx PM PiG Simulation of NO_3 and NH_4 Over the Upper Midwest on 14 June 2002: Plot on Right Reveals the NO_3 and NH_4 Increments Associated with Sub-Grid-Scale Treatment of Reactive Plumes. (Source: Yarwood et al., 2005).



(a) Mean Fractional Bias in 24-hr Average Model Predictions



(b) Mean Fractional Error in 24-hr Average Model Predictions

Figure 4-9. Mean Fractional Bias and Error in Fine Particulate Species Predictions from the CAMx, CMAQ, URM, and CMAQ-MADRID Models over Several Regional PM and Visibility Model Evaluation Studies. (Source: Boylan and Russell, 2005).

5.0 DATA BASES FOR CALPUFF MODELING

To support BART modeling by the states and source operators, both meteorological and aerometric data sets are required. Regional meteorological data sets generated by the CALMET model suitable for direct input to the CALPUFF modeling system have been developed and archived. These data sets cover calendar years 2001, 2002, and 2003 for three sub-regional grid domains shown in Figures 5-1 through 5-4. The procedures used in developing the CALMET data sets generally follow the IWAQM recommendations (EPA, 1998), except for a few notable refinements. *The processed CALMET files, in CALPUFF-ready input format, are available from CENRAP on hard disk drives to interested states and stakeholders.*

This chapter describes how these meteorological modeling sets were developed and evaluated. The basic CALMET model configuration used to generate the three years of CALPUFF-ready meteorology is described in detail so that users of this information have a clear understanding of the data sets and their applicability. In addition, for those states or source operators who elect to conduct more source-specific CALMET/CALPUFF modeling, the information in this chapter may be helpful in guiding specification of revised CALMET model inputs and generation of revised CALMET data sets.

Also included in Section 5 .2 is a discussion of routinely available air quality monitoring data sets available to the states and source operators in support of screening and source-specific BART modeling exercises.

5.1 Development of CALMET Meteorological Files

5.1.1 MM5 Data Sets

Alpine Geophysics developed a consistent set of CALMET regional meteorological modeling data sets for use by the CENRAP States, BART eligible sources within the region and others. These meteorological modeling data sets were constructed through the joint use of the CALMET processor and results from existing annual three-dimensional MM5 meteorological simulations. The specific annual prognostic model simulations available for CENRAP BART modeling included:

> 2001 MM5 data set at 36/12 km resolution developed for EPA by Alpine Geophysics (McNally and Tesche, 2002; McNally 2003);

> 2002 MM5 data set at 36 km resolution developed for CENRAP by Iowa DNR (Johnson, 2003a,b),

> 2003 MM5 data set at 36 km resolution developed for the Midwest RPO (Baker, 2005; Baker et al., 2004; Kembell-Cook et al., 2005)

Each of these studies included a performance evaluation of the MM5 generated data sets against surface meteorological observations and the results of these evaluations are contained in the reports or presentations cited above. While there exists a set of annual 12 km MM5 meteorology for 2002, this data set was developed by four independent CENRAP modeling centers and these data sets have not been concatenated into one master data base. More importantly, there has been no systematic, rigorous model performance evaluation performed on the CENRAP 2002 12 km MM5 data yet. Accordingly, until such time as the 2002 12 km data set has been evaluated and shown to be of comparable reliability as the aforementioned MM5 data sets, it's use is contraindicated.

5.1.2 CALMET Model Configuration

The CALMET modeling procedures used to construct meteorological inputs to CALPUFF for visibility screening of BART eligible sources generally follows the IWAQM recommendations (EPA, 1998), except as noted below.

CALMET Model Options. The CALMET model has a number of user-selected options, parameter settings, and 'switches' that must be defined prior to exercising the processing system. These options and settings are well-described in the CALMET User's Guide (Scire et al., 2000a) and in the CALMET input file to the executable code. Appendix A of this protocol summarizes the CALMET configurations used in developing the processed 6 km meteorological fields over the three CENRAP BART modeling domains. Also included in the tables in Appendix A are the default CALMET options and parameter settings recommended in the IWAQM Phase 2 Report (EPA, 1998).

CALMET Domain. Three slightly overlapping modeling domains were defined by CENRAP to support BART modeling. These domains are shown in Figures 5-1 through 5-4 and Table 5-1. The processors used to generate the domain, land use, and elevation data for the CALMET/CALPUFF system include TERREL, CTGPROC, and MAKEGEO, as described below.

> TERREL is the terrain pre-processor that averages terrain features to the modeling grid resolution; TERREL constructs the basic properties of the gridded domain and defines the coordinates upon which meteorological data are stored. Key parameters include specification of grid type, location, resolution and terrain elevation.

> CTGPROC computes the fractional land use for the modeling grid resolution. Land use characteristics for each grid cell are assigned using CTGPROC. The primary variable adjustment associated with CTGRPOC is selection of an appropriate land use database. Version 2.0 of the North American Land Cover Characteristics database is used.

> MAKEGEO is the final pre-processor that combines the terrain and land use data for input to CALMET. Generating the appropriate MAKEGEO.INP control file requires only minimal alteration of the default assignments. Key modifications include specifying domain attributes and ensuring input files are correctly referenced.

Terrain. CALMET requires both terrain height and land use/land cover for the application region. These are generated using the CALMET CTGPROC, TERREL and MAKEGEO processors. The terrain data were created using the TERREL (version 3.311, level 030709) processor and the Shuttle Radar Topography Mission (SRTM)-GTOPO 30 second (~1 km) resolution dataset.

Land Use. The landuse data set was created using the Composite Theme Grid CTGROC processor (version 2.42, level 030709) and the United States Geological Survey (USGS) Global Land Cover Characterization (GLCC) version 2.0 database. The GLCC database is available at 30 second (~1km) resolution. References for these and other modeling datasets can be found at www.src.com.

Vertical Layer Structure. The vertical layer structure for the CALMET/CALPUFF screening applications is more refined than the general suggestions of IWAQM. The CENRAP vertical structure was designed to reduce the need for vertical interpolation while simultaneously improving vertical resolution within the planetary boundary layer (PBL). Table 5-2 identifies the 11 layer interfaces required to define the 10 layer vertical CALMET grid structure. The top interface in the CALMET simulation is 4000 meters.

*Use of Observations***.** Based on considerable discussions with State and Federal managers and agency personnel, CENRAP has elected to use the No-Obs mode in CALMET for constructing the 6 km meteorological fields for CALPUFF screening exercises. The three annual MM5 simulations (2001, 2002, and 2003) will be used as the sole source for meteorological data within CALMET. Blending observational data with the MM5 data within CALMET (i.e., use of the "OBS" option is essentially a redundant use of the same data. Substantial improvement in the MM5 initialization data and in the use of four dimensional data assimilation (FDDA) has been achieved in recent years using observational data. The ETA analysis data used in initial and boundary conditions estimates as well as within the FDDA fields derive from 3-hourly, 40 km objective analysis fields computed using an extensive supply of observational data (National Weather Service surface and upper air data, GOES satellite precipitable water; VAD wind profiles from NEXRAD; ACARS aircraft temperature data; SSM/I oceanic surface winds; daily NESDIS snow cover and sea-ice analysis data; RAOB balloon drift; GOES and TOVS-1B radiance data; 2D-VAR SST from NCEP Ocean Modeling Branch; radar estimated rainfall; and surface rainfall). The complexity, resolution, and accuracy of the ETA data that is used to initialize and 'nudge' the MM5 forecasts is extensive indeed. Particularly at the 12-36 km horizontal grid scales over the flat to modestly rolling topography of the CENRAP domain, there is no need to introduce local meteorological observations in order to retrieve local terrain effects, for example. Thus, mesoscale wind patterns are likely to be adequately characterized by the MM5 simulations.

Many observations, especially surface observations, reflect local conditions on a scale smaller than the 6 km CENRAP CALMET fields. The introduction of the local observations into the regional modeling domain may extend the influence of the observational data beyond its true representativeness and result in internally inconsistent flow features. In particular the time interpolation of the 12-hourly upper air sounding data may wash out structure in the MM5 fields that are appropriate to retain. Given that the CENRAP domain as a whole includes areas of moderately rolling terrain, coastal regions and relatively flat terrain, a single set of representative weights[1] that allows significant influence of the observations where appropriate, will involve a considerable effort and substantial testing. The internally consistent MM5 fields are considered likely to be appropriate for the regional simulations, and the incremental benefit of adding the observational data into the regional CALMET simulations is not considered worthwhile.

However, on the smaller domains likely to be considered in source-specific modeling (e.g., 1-4 km in scale) with the higher CALMET grid resolution and the smaller domain size, more control over the region of influence of the meteorological observations can be achieved. It is easier for the diagnostic model to allow the local flow observations to have appropriate influence in the vicinity of the observation, but allow terrain-adjusted flow to dominate away from the observations. Given that the fine scale source-specific domains will be used especially in irregular and/or meteorologically complex settings, the relatively coarser-scale MM5 simulations are less likely to be fully adequate, and the introduction observational data into CALMET is more likely to achieve improvements in the resulting meteorological fields.

Diagnostic Model Settings

A number of diagnostic model settings must be selected for CALMET to properly process representative diagnostic meteorological data sets. These are summarized in Appendix A, compared to the default CALMET settings, and discussed in the following:

[1] Weights are assigned in CALMET to control the 'blending' of observations and MM5 predictions**.**

> CALMET options dealing with radius of influence parameters (R1, R2, RMAX1, RMAX2, RMAX3), BIAS, ICALM parameters are not used in No-Observations mode;

> Gridded cloud data were inferred from the MM5 relative humidity fields (ICLOUD=3);

> Given that all state variables are MM5-derived (IPROG=14; ITPROG=2), surface layer winds were not extrapolated to the upper layers (IEXTRP = -1);

> The IWAQM recommendation for disabling the computation of kinematic effects in the wind field options and parameters was selected. This was selected in light of the very modest elevated terrain in the CENRAP domain, relative to the mountainous regions in the U.S. and Alps where the kinematic parameterizations were originally developed. Thus, the option for computing kinematic effects was disabled (IKINE = 0).

> The BIAS array was set to 0. in the CALMET control file because surface and upper air data were not used (NOOBS = 2);

> Because the MM5 wind fields supply CALMET with the initial guess fields to the diagnostic wind model (IWFCOD =1, IPROG = 14) and observational data are not reintroduced, the following variables were set to nominal values:

- The minimum distance for which extrapolation of surface winds should occur was set to -1 (RMIN2 = -1.).
- RMIN was left at the IWAQM recommendation of 0.1 km.
- RMAX1 and RMAX2 were each assigned a value of 30 km. RMAX3 was assigned a value of 50 km.
- R1 and R2 were each assigned the value of 1.0.
- ISURFT and IUPT were assigned placeholder values of 4 and 2, respectively.

> The radius of influence regarding terrain features is comparable to the resolution of the processed terrain data: 12 km.

> The radius of influence for temperature interpolation is set to 36 km (TRADKM), a value considered appropriate given the 6 km CALMET domain and 36/12 km MM5 domain.

> The beginning/ending land use categories for temperature interpolation over water are assigned category 55: (JWAT1 = JWAT2 = 55).

> SIGMAP was set to 50 km, while the IWAQM recommendation is 100 km, but with no supporting documentation. Because precipitation rates are explicitly incorporated from the MM5 data, a lower radius of influence was deemed appropriate.

> Diagnostic options: IWAQM default values were used (see Appendix A);

> TERRAD (terrain scale) is required for runs with diagnostic terrain adjustments (i.e., the 2003 simulations). Values of ~10-20 km were tested, and an appropriate value determined.

> Land use defining water: JWAT1 = 55, JWAT2 = 55 (large bodies of water). This feature allows the temperature field over large bodies of water such as the Gulf of Mexico and the Great lakes to be properly characterized by buoy observations.

> Mixing height averaging parameter (MNMDAV) were determined sensitivity tests. The purpose of the testing is to optimize the variable to allow spatial variability in the mixing height field, but without excessive noise.

Obviously, there are some instances where more advanced and/or recently developed procedures for constructing the CALMET fields have been used compared with the IWAQM (1998) guidance. For example, one agency expressed concern about the choice to employ prognostic model-derived gridded cloud cover data in CALMET (ICLOUD = 3). While this is admittedly a ‘non-guideline’ option, in our view it represents the best science option currently available. In particular, the EPA CAIR and CAMR rulemaking modeling and the CAMx/CMAQ modeling being performed by the RPOs for regional haze all utilize the gridded moisture fields in the MM5 model as a basis for estimating cloud. Presumably, if the method is suitable for such advanced visibility modeling, it is adequate for CALPUFF modeling. Of course, in the protocol negotiation, the States, source operators, and regulatory agencies have an opportunity to re-examine the CALMET diagnostic model settings used in creating the CENRAP gridded fields and modify them if warranted.

In summary, the development of the regional CALMET meteorological fields from MM5 data was conducted in No-Observations (“No-Obs”) mode. CALMET’s boundary layer modules were used to compute mixing heights, turbulence coefficients and other meteorological parameters required as input to CALPUFF.

5.1.3 MM5/CALMET Processing

Construction of the CALPUFF-ready meteorological fields entails a two-step process. First, the MM5 prognostic model output fields are extracted and processed for input to CALMET. This step entails running various extraction software routines followed by the CALMM5 code. Then, CALMET is exercised for the full three year period over each sub-regional CENRAP domain.

CALMM5. Previous applications of the prognostic Mesoscale Meteorological model version 5 (MM5) served as the source of the gridded meteorological fields for calendar years 2001, 2002, and 2003. The actual CALMM5 configuration entailed modification of a few user-specified variables. However, two setting are of primary importance:

> All vertical layers from MM5 were extracted, providing CALMET configuration flexibility, and

> Vertical velocity, relative humidity, cloud/rain fields, and ice/snow fields were extracted. (Graupel was extracted for 2001, the only year where the data were available in the MM5 datasets.)

CALMET. CALMET (v5.53a, lev 040716) was applied consistent with CENRAP’s recommendation that the 6 km be generated using the ‘No-Obs’ option. The specific options used have been discussed above and are summarized in Appendix A.

5.1.4 Evaluation of the CALPUFF-Ready Meteorological Data Sets

In typical applications the adequacy of the CALMET fields is seldom evaluated using independent measurements. Often, only cursory visual examination of wind vector plots or time series is considered. This evaluation is important because the CALMET performance analysis gives direct insight into the adequacy of the model-processed fields on a subregional basis. It also serves as an independent quality assurance tool. Alpine's MAPS evaluation software to perform an independent evaluation of the processed CALMET data bases. MAPS was used in conjunction with the NCAR DS472 TDL data sets to evaluate the surface winds and temperatures for 2001-2003 across all three domains. Since only a small portion of the meteorological content of these data were ingested in the MM5 data assimilation routines (see Johnson, 2003a), these data sets are essentially an independent, quantitative means for evaluating the adequacy of the meteorological fields input to CALPUFF.

CALMET Evaluation Methodology

Several statistical measures were calculated as part of the CALMET meteorological evaluation using established procedures (e.g., Tesche et al., 1990; Emery et al., 2001). Additional plots and graphs are used to present these statistics on both hourly and daily time frames over the full annual cycle. For this study, evaluation measures were calculated for wind, temperature, and relative humidity because these parameters are the principal meteorological inputs to CALPUFF. The full set of CALMET evaluation statistics and graphical displays generated with the AG-MAPS software (McNally and Tesche,1994) are contained on a DVD available from CENRAP.

The statistics used to evaluate the meteorological fields for 2001-2003 are generated in both absolute terms (e.g., wind speed error in m/s), and relative terms (percent error) as is commonly done for air quality assessments. Obviously, a very different significance is associated with a given relative error for different meteorological parameters. For example, a 10% error for wind speed measured at 10 m/s is an absolute error of 1 m/s, a minor error. Yet a 10% error for temperature at 300 K is an absolute error of 30 K, a ridiculously large error. On the other hand, pollutant concentration errors of 10% at 1 ppb or 10 ppm carry practically the same significance.

Three key meteorological metrics include the bias, error, and index of agreement (IOA) for wind speed, temperature and relative humidity. These measures are defined as follows:

Bias (B): Calculated as the mean difference in prediction-observation pairings with valid data within a given analysis region and for a given time period (hourly or daily):

$$B = \frac{1}{IJ}\sum_{j=1}^{J}\sum_{i=1}^{I}\left(P_j^i - O_j^i\right)$$

Error (E): Calculated as the mean *absolute* difference in prediction-observation pairings with valid data within a given analysis region and for a given time period (hourly or daily).

$$E = \frac{1}{IJ}\sum_{j=1}^{J}\sum_{i=1}^{I}\left|P_j^i - O_j^i\right|$$

Note that the bias and gross error for winds are calculated from the predicted-observed residuals in speed and direction (not from vector components *u* and *v*). The direction error for a given prediction-observation pairing is limited to range from 0 to ±180°.

Index of Agreement (IOA): calculated following the approach of Willmont (1981). This metric condenses all the differences between model estimates and observations within a given analysis region and for a given time period (hourly and daily) into one statistical quantity. It is the ratio of the total RMSE to the sum of two differences – between each prediction and the observed mean, and each observation and the observed mean:

$$IOA = 1 - \left[\frac{IJ \cdot RMSE^2}{\sum_{j=1}^{J} \sum_{i=1}^{I} \left| P_j^i - M_o \right| + \left| O_j^i - M_o \right|} \right]$$

Viewed from another perspective, the index of agreement is a measure of the match between the departure of each prediction from the observed mean and the departure of each observation from the observed mean. Thus, the correspondence between predicted and observed values across the domain at a given time may be quantified in a single metric and displayed as a time series. The index of agreement has a theoretical range of 0 to 1, the latter score suggesting perfect agreement.

CALMET Evaluation Results

Table 5-5 summarizes the statistical measures, averaged over the month, for temperature, wind speed, and relative humidity for all three years. The CALMET evaluation DVD contains a full compilation of the statistical and graphical results. Figures 5-7 through 5-31 present a variety of graphical displays of processed and observed surface temperature, relative humidity, and wind across the three CENRAP subdomains for the three-year period 2001-2003. Figures 5-28 through 5-31 provide convenient summaries of the bias and error in the relative humidity, temperature, and wind speed fields across the continuous 36 month period by subdomain.

Thorough discussion of the performance findings is beyond the scope of these guidelines. However, a few key findings of the evaluation are worth noting here. From Table 5-5, the wind speed index of agreement, a general measure of correlation between measured and observed winds, is systematically greater than a value of 0.8 for virtually every month. These values are typically better than those generally achieved in urban- and regional-scale model applications for ozone SIPs. For example, the statistical benchmark for IOA suggested by Emery et al., (2001) is IOA > 0.6. Thus, the wind speed agreement for all three domains and all three years appears quite good relative to other MM5/RAMS model applications. From Figure 5-11, the wind speed root mean square error for the Central domain for 2002 is generally below 2.0 m/s, the performance goal for this parameter. From Figure 5-29 (as well as in Table 5-5), the temperature bias results for the 36 month are generally quite close to the ± 0.5 deg C performance goal. As shown in Figure 5-30 the temperature error results are slightly poorer than the 2 deg C performance goal for 2001 and 2003, but are below the 2.0 deg C threshold for 2002. Note that the benchmarks were developed not to provide a pass/fail standard to which all modeling results should be held, but rather to put the results into an historical context.

In summary, we find that:

- Relative Humidity
  - Bias over three-year period near zero all domains
  - For some months over- and under-prediction (up to 10% or more) is evident – no discernable trend

  - Errors typically diminish from 2001 through 2003, and are generally < 12% after 1st quarter of 2001.

- Surface Temperatures
  - Monthly averaged temperatures are systematically biased low (cooler) by 0.25 to 1.25 deg C.
  - The errors in monthly averaged temperatures typically range between 1.8 and 2.6 deg C
  - Average error over all months is about 2.2 deg C.

- Surface Wind Speeds
  - IOA typically between 0.8 0-0.9
  - Seasonally variable
  - Central subdomain gives best correlation

- Results from MM5/CALMET evaluation provide potentially useful information for diagnosing BART visibility modeling analyses

- MM5/CALMET fields exhibit good statistical agreement with observations, in part because observations figure prominently in the construction of the interpolated CALMET fields.

- MM5/CALMET fields for the three CENRAP subdomains are quite sufficient for use in CALPUFF modeling.

5.1.5 Meteorological Data Archive and Distribution

All models, scripts and CALMET data (excepting MM5 outputs) are available from CENRAP on appropriate external combination Firewire/USB drives.

5.2 Aerometric Monitoring Networks

Data from ambient monitoring networks for both gas-phase and aerosol species are available for use in CENRAP BART modeling analyses. Table 5-4 summarizes ambient monitoring networks. Data for 2002 have been compiled for all networks covering the CENRAP domain with the exception of the PAMS and PM Supersites. These data sets may be obtained from CENRAP. Figures 5-5 and 5-6 display the locations of monitoring sites in and near the CENRAP States.

Table 5-1. CENRAP Lambert Conic Conformal Modeling Domain Specifications (40.97 degree projection origin; 33 and 45 degree matching parallels).

Domain	Southwest Coordinate (km)	Number of X grid cells	Number of Y grid cells	Horizontal Resolution
CALMET				
South	-1008, -1620	306	246	6 km
Central	-1008, -864	388	234	6 km
North	-1008, 0	300	193	6 km

Table 5-2. Vertical Layer Structure in CALMET Fields. (Heights are in meters.)

Layer Number	Layer Height	Layer Number	Layer Height
0	0.	6	640.
1	20.	7	1200.
2	40.	8	2000.
3	80.	9	3000.
4	160.	10	4000.
5	320.		

Table 5-3. Meteorological Model File Sizes for CENRAP BART Modeling.

CALMET 6 km File Sizes, (Gbytes)				MM5 File Sizes, (Gbytes)		
Domain	Monthly	Annual	3 Years	Domain	Grid	3 years
North	4.6	55.2	165.6	2001	12 km	1370
Central	6.6	79.2	237.6	2002	36 km	430
South	6.0	72.0	216.0	2003	36 km	430
total	17.2	206.4	619.2	total		2230

Table 5-4. Statistical Evaluation of the CALMET Meteorological Fields for 2001-2003.

CALMET Model Evaluation Statistics for 2001.	Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep	Oct	Nov	Dec	Mean
RH Bias (%)													
North	4.54	3.19	0.17	-14.55	-12.09	-4.35	-0.62	1.17	-2.07	-7.98	-6.62	-4.22	-3.62
Central	-2.60	-7.28	-11.38	-10.69	-8.62	-2.90	0.66	1.07	-1.44	-5.46	-6.16	-7.78	-5.21
South	-10.23	-11.53	-13.78	-4.24	-2.08	0.99	4.12	3.16	-0.12	-2.12	-3.44	-9.76	-4.09
RH Error (%)													
North	10.06	10.31	14.03	18.77	16.28	12.39	11.82	11.76	13.26	15.54	13.53	12.89	13.39
Central	13.32	15.86	17.45	17.05	14.50	11.67	11.52	11.32	12.26	15.52	14.79	14.95	14.18
South	16.22	18.37	18.17	13.26	12.15	11.51	12.09	12.40	11.82	14.85	14.73	16.19	14.31
Temp Bias (^{0}C)													
North	-1.63	-1.23	-1.23	-0.24	0.08	-0.29	-0.23	-0.54	-0.55	-0.09	-0.40	-1.27	-0.64
Central	-0.99	-0.65	-0.54	-0.16	0.13	-0.23	-0.43	-0.54	-0.36	-0.34	-0.30	-0.74	-0.43
South	-0.47	-0.42	0.03	-0.31	-0.33	-0.63	-0.99	-0.85	-0.52	-0.36	-0.19	-0.21	-0.44
Temp Error (^{0}C)													
North	3.10	2.88	2.54	2.49	2.44	2.43	2.42	2.49	2.58	2.48	2.89	2.55	2.61
Central	2.38	2.25	1.99	2.18	1.99	2.01	2.07	2.11	2.21	2.52	2.61	2.42	2.23
South	2.31	2.28	1.92	2.13	2.01	2.17	2.19	2.21	2.19	2.70	2.49	2.50	2.26
Wind Speed IOA													
North	0.79	0.83	0.83	0.87	0.86	0.85	0.81	0.84	0.84	0.82	0.81	0.79	0.83
Central	0.85	0.87	0.88	0.88	0.89	0.86	0.84	0.86	0.87	0.86	0.85	0.84	0.86
South	0.81	0.80	0.85	0.79	0.83	0.83	0.78	0.80	0.82	0.82	0.80	0.82	0.81

CALMET Model Evaluation Statistics for 2002.	Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep	Oct	Nov	Dec	Mean
RH Bias (%)													
North	8.33	9.52	6.63	0.95	-2.42	1.25	2.43	1.60	0.57	0.47	4.47	7.73	3.46
Central	7.43	5.13	4.60	1.65	-1.02	1.52	2.50	1.88	-0.27	-1.40	-0.01	4.35	2.20
South	3.08	-1.19	2.53	2.32	1.26	1.98	2.51	2.62	-0.80	-2.42	-4.45	-1.03	0.53
RH Error (%)													
North	11.85	13.18	11.61	11.13	11.90	10.04	9.54	9.08	10.26	10.26	11.55	11.61	11.00
Central	12.21	12.43	11.26	10.58	10.72	9.89	9.55	9.54	10.22	10.25	11.42	11.26	10.78
South	11.24	11.76	10.34	8.95	9.30	9.49	9.46	9.61	9.68	9.33	11.63	10.95	10.14
Temp Bias (^{0}C)													
North	-0.70	-0.82	-0.96	-0.52	-0.25	-0.36	-0.53	-0.49	-0.44	-0.67	-0.76	-0.69	-0.60
Central	-0.57	-0.65	-0.79	-0.62	-0.41	-0.68	-0.81	-0.74	-0.49	-0.54	-0.55	-0.52	-0.61
South	-0.23	-0.13	-0.52	-0.61	-0.61	-0.94	-0.94	-1.07	-0.65	-0.47	0.04	-0.13	-0.52
Temp Error (^{0}C)													
North	2.15	2.07	2.04	1.89	1.86	1.83	1.86	1.80	1.95	1.78	1.99	2.15	1.95
Central	2.12	2.05	2.14	1.95	1.91	1.93	1.93	1.92	2.02	1.77	2.00	2.00	1.98
South	2.18	2.05	2.17	1.83	1.89	1.91	1.88	2.00	1.92	1.68	2.06	1.93	1.96
Wind Speed IOA													
North	0.82	0.84	0.86	0.88	0.86	0.85	0.85	0.83	0.85	0.85	0.81	0.78	0.84
Central	0.87	0.88	0.90	0.90	0.88	0.87	0.84	0.84	0.87	0.88	0.85	0.85	0.87
South	0.86	0.86	0.85	0.85	0.84	0.82	0.79	0.80	0.83	0.83	0.83	0.82	0.83

CALMET Model Evaluation Statistics for 2003.	Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep	Oct	Nov	Dec	Mean
RH Bias (%)													
North	10.15	7.40	6.01	0.93	-3.76	-0.38	1.38	2.04	-1.66	-1.99	2.96	7.68	2.56
Central	6.94	4.76	4.15	0.42	-2.18	0.17	2.08	2.13	-2.05	-4.13	0.00	5.47	1.48
South	0.00	0.00	0.47	-1.10	-0.37	0.54	1.77	2.89	-3.31	-6.01	-3.66	-0.33	-0.76
RH Error (%)													
North	13.30	11.21	12.32	11.70	11.65	10.03	9.70	9.57	11.13	12.68	11.53	11.85	11.39
Central	12.77	10.95	11.61	11.18	10.33	9.91	9.49	9.50	10.70	12.69	12.10	12.43	11.14
South	11.18	10.00	9.85	10.17	9.20	9.54	8.90	9.91	10.21	12.12	12.15	12.39	10.47
Temp Bias (^{0}C)													
North	-1.24	-0.99	-0.63	-0.29	-0.11	-0.10	-0.22	-0.49	-0.34	0.29	-0.85	-1.34	-0.53
Central	-0.84	-0.80	-0.64	-0.47	-0.27	-0.36	-0.60	-0.66	-0.32	0.30	-0.54	-0.89	-0.51
South	-0.17	-0.27	-0.36	-0.43	-0.46	-0.62	-0.91	-0.98	-0.28	0.53	0.00	-0.03	-0.33
Temp Error (^{0}C)													
North	2.31	2.15	2.14	2.02	1.81	1.77	1.91	1.98	2.25	2.57	2.30	2.67	2.16
Central	2.14	2.03	2.15	2.13	1.80	1.81	1.96	1.99	2.16	2.54	2.31	2.45	2.12
South	2.10	1.90	2.00	2.08	1.84	1.81	1.88	2.06	1.94	2.40	2.28	2.48	2.06
Wind Speed IOA													
North	0.79	0.81	0.83	0.86	0.87	0.85	0.86	0.87	0.84	0.82	0.80	0.82	0.83
Central	0.85	0.88	0.87	0.89	0.90	0.87	0.87	0.86	0.87	0.87	0.86	0.86	0.87
South	0.83	0.83	0.85	0.83	0.85	0.81	0.83	0.82	0.85	0.84	0.82	0.82	0.83

Table 5-5. Overview of Ambient Data Monitoring Networks Covering the CENRAP Domain.

Monitoring Network	Chemical Species Measured	Sampling Period	Data Availability/Source
The Interagency Monitoring of Protected Visual Environments (**IMPROVE**)	Speciated PM25 and PM10 (see species mappings)	1 in 3 days; 24 hr average	http://vista.cira.colostate.edu/improve/Data/IMPROVE/improve_data.htm
Clean Air Status and Trends Network (**CASTNET**)	Speciated PM25, Ozone (see species mappings)	Approximately 1-week average	http://www.epa.gov/castnet/data.html
National Atmospheric Deposition Program (**NADP**)	Wet deposition (hydrogen (acidity as pH), sulfate, nitrate, ammonium, chloride, and base cations (such as calcium, magnesium, potassium and sodium)), Mercury	1-week average	http://nadp.sws.uiuc.edu/
Air Quality System (**AQS**) Aka Aerometric Information Retrieval System (**AIRS**)	CO, NO2, O3, SO2, PM25, PM10, Pb	Typically hourly average	http://www.epa.gov/air/data/
Speciation Trends Network (**STN**)	Speciated PM	24-hour average	http://www.epa.gov/ttn/amtic/amticpm.html
Southeastern Aerosol Research and Characterization (**SEARCH**) (Southeastern US only)	24-hr PM25 (FRM Mass, OC, BC, SO4, NO3, NH4, Elem.); 24-hr PM coarse (SO4, NO3, NH4, elements); Hourly PM2.5 (Mass, SO4, NO3, NH4, EC, TC); Hourly gases (O3, NO, NO2, NOy, HNO3, SO2, CO)	Hourly or 24-hour average, depending on parameter.	Electric Power Research Institute (EPRI), Southern Company, and other companies. http://www.atmospheric-research.com
EPA Particulate Matter Supersites (Includes St. Louis in the CENRAP region)	Speciated PM25		http://www.epa.gov/ttn/amtic/supersites.html
Photochemical Assessment Monitoring Stations (**PAMS**)	Varies for each of 4 station types.		http://www.epa.gov/ttn/amtic/pamsmain.html
National Park Service Gaseous Pollutant Monitoring Network	Acid deposition (Dry; SO4, NO3, HNO3, NH4, SO2), O3, meteorological data	Hourly	http://www2.nature.nps.gov/ard/gas/netdata1.htm

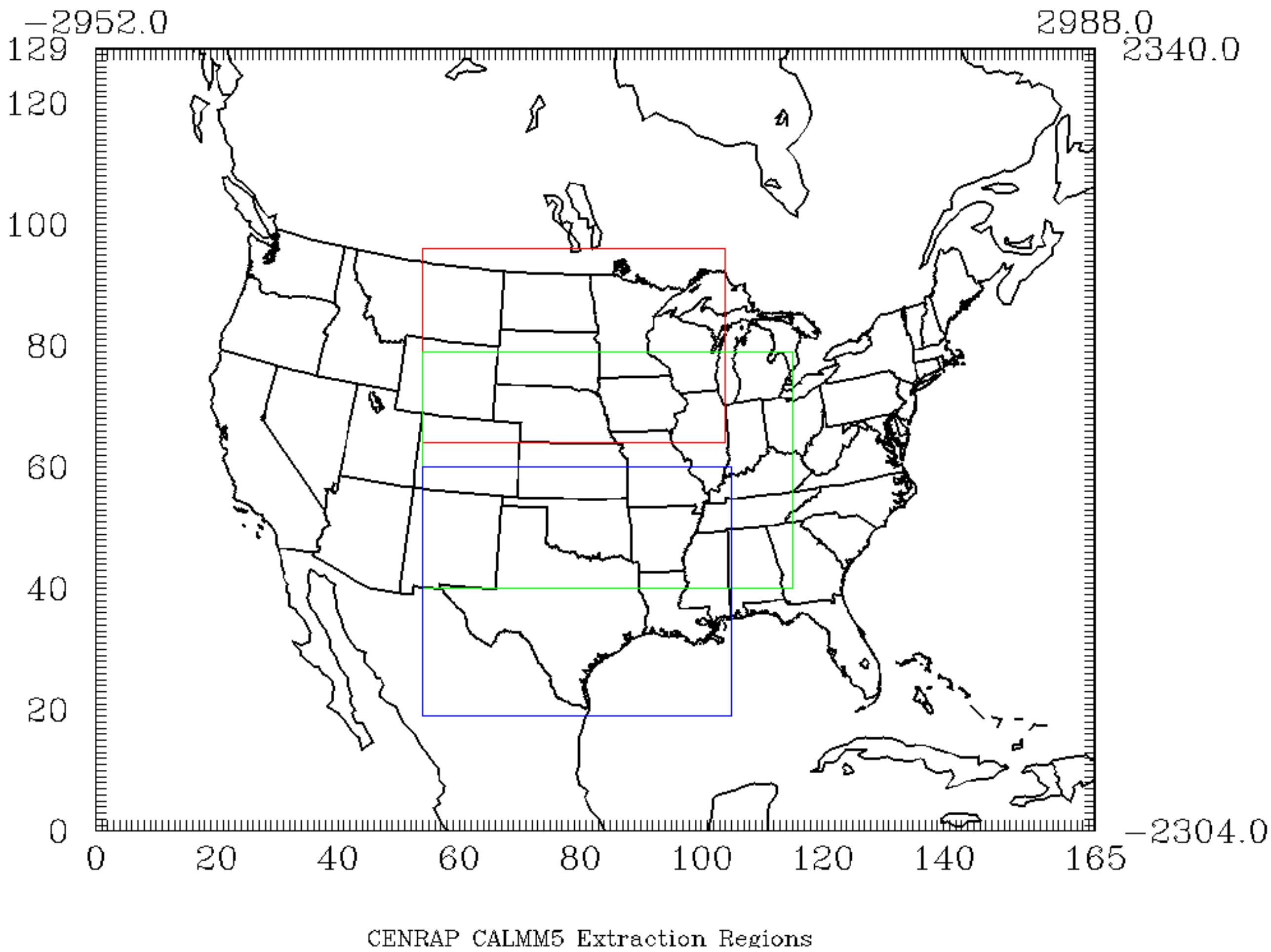


Figure 5-1. CENRAP North, Central, and South 6 km Meteorological Domains.

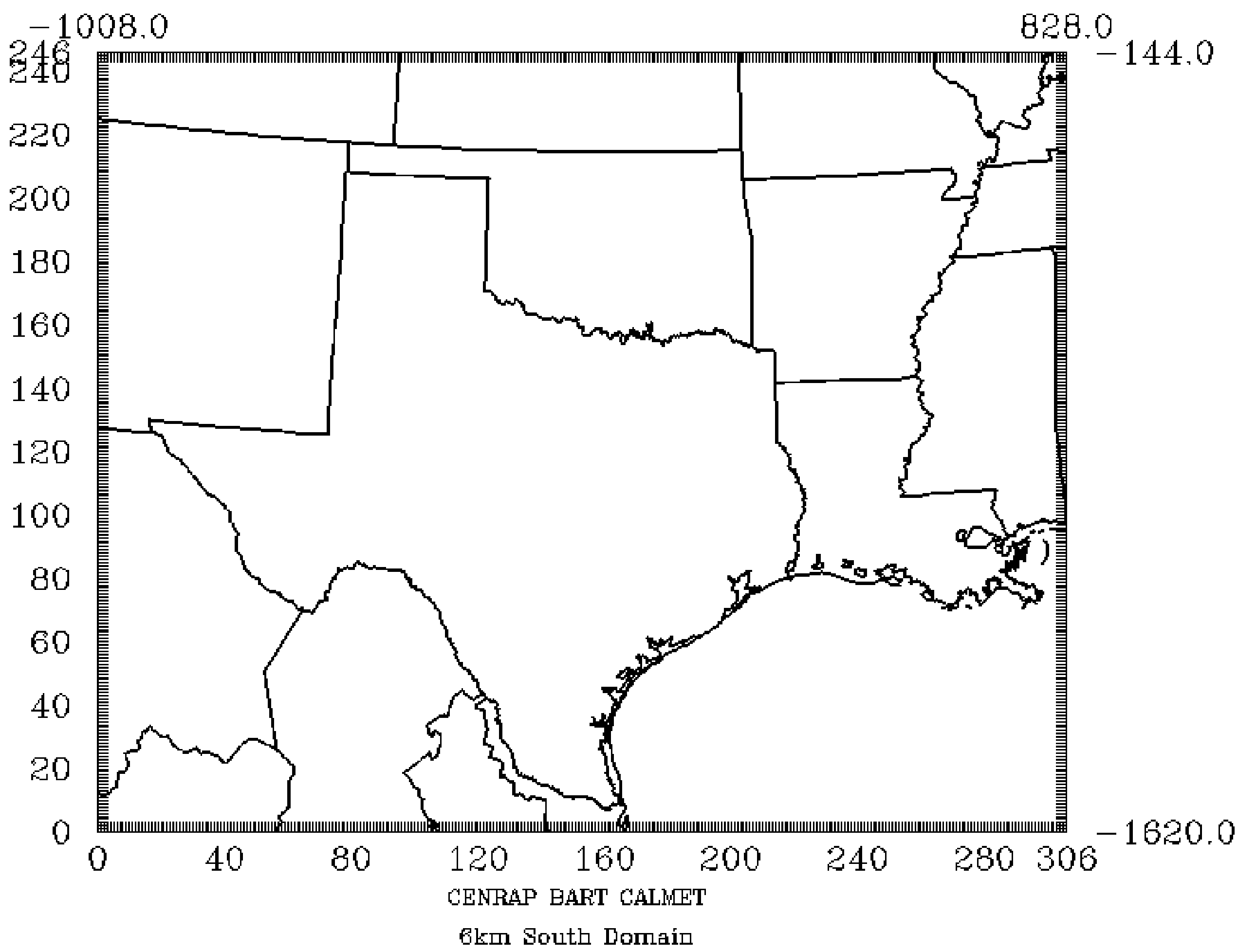


Figure 5-2. CENRAP South Domain.

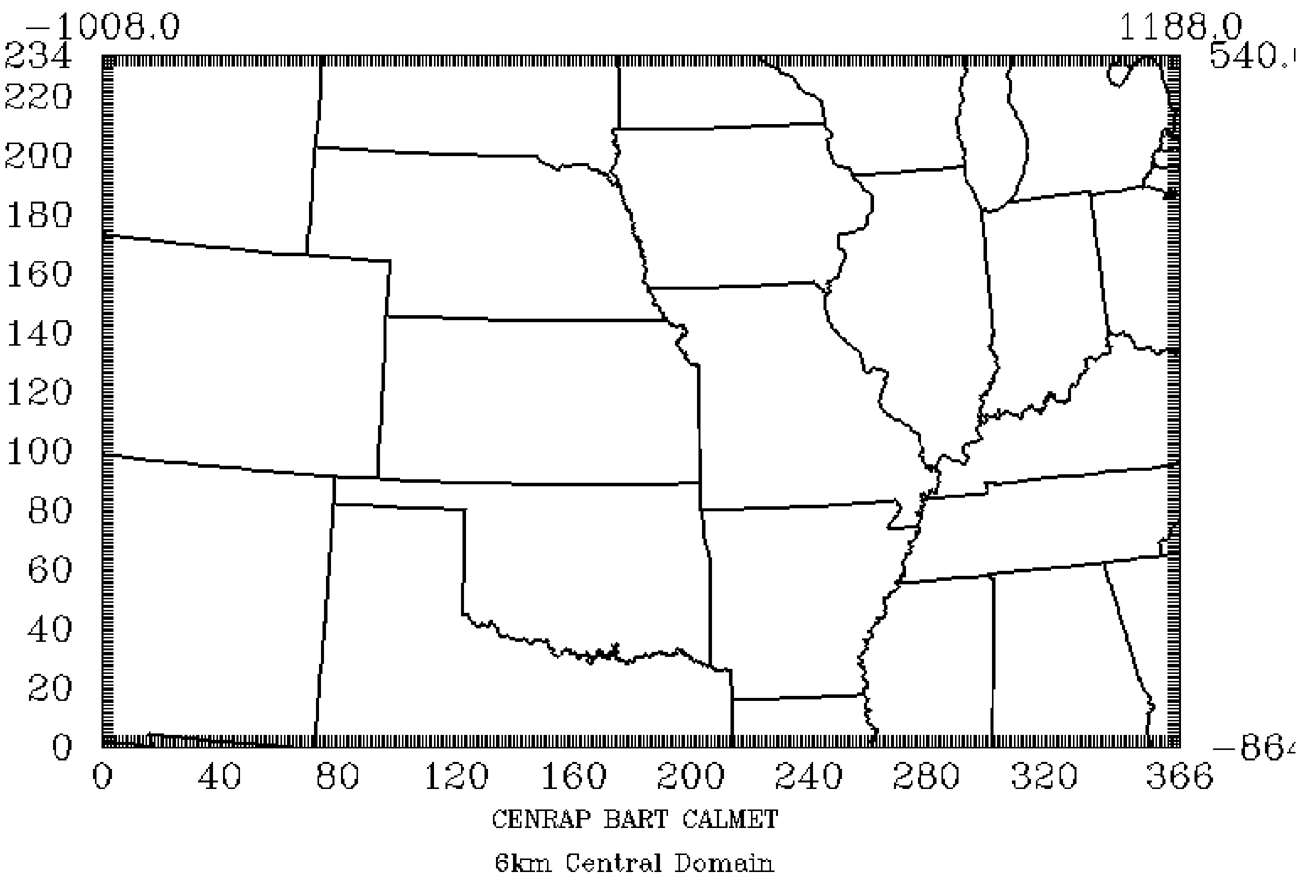


Figure 5-3. CENRAP Central Domain.

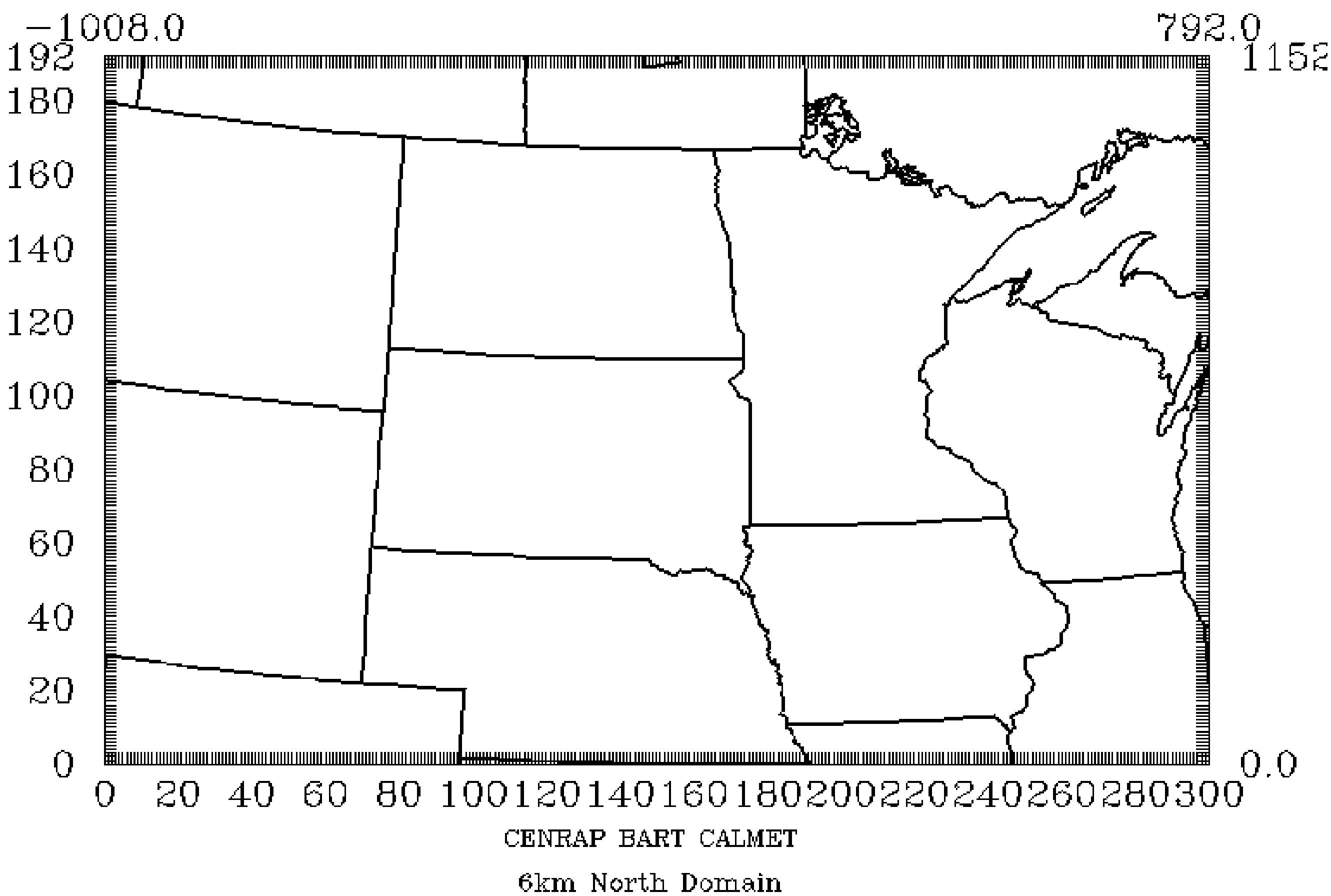


Figure 5-4. CENRAP North Domain.

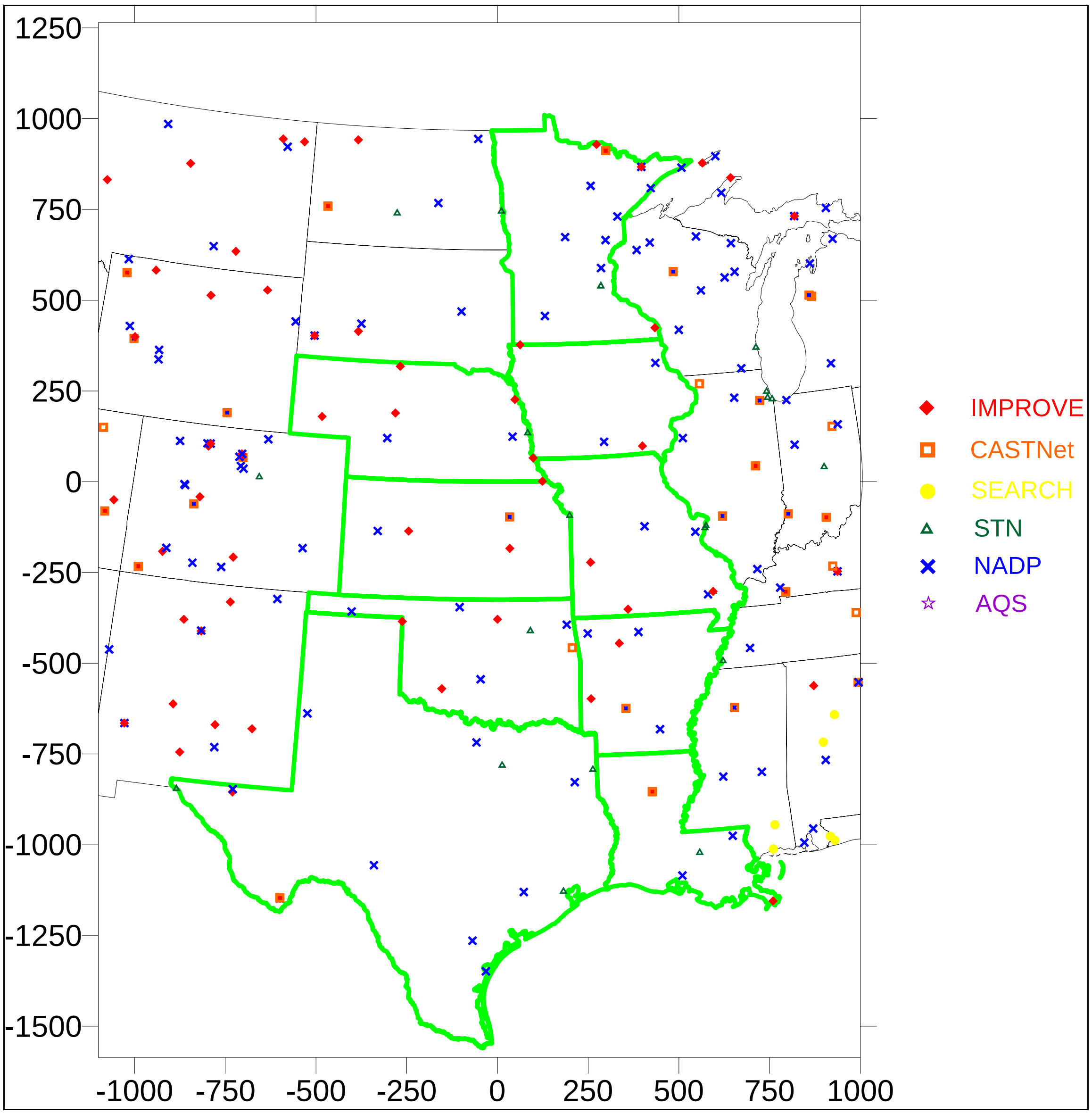


Figure 5-5. Locations of IMPROVE, CASTNet, SEARCH, STN and NADP Monitoring Sites in and Near the CENRAP States.

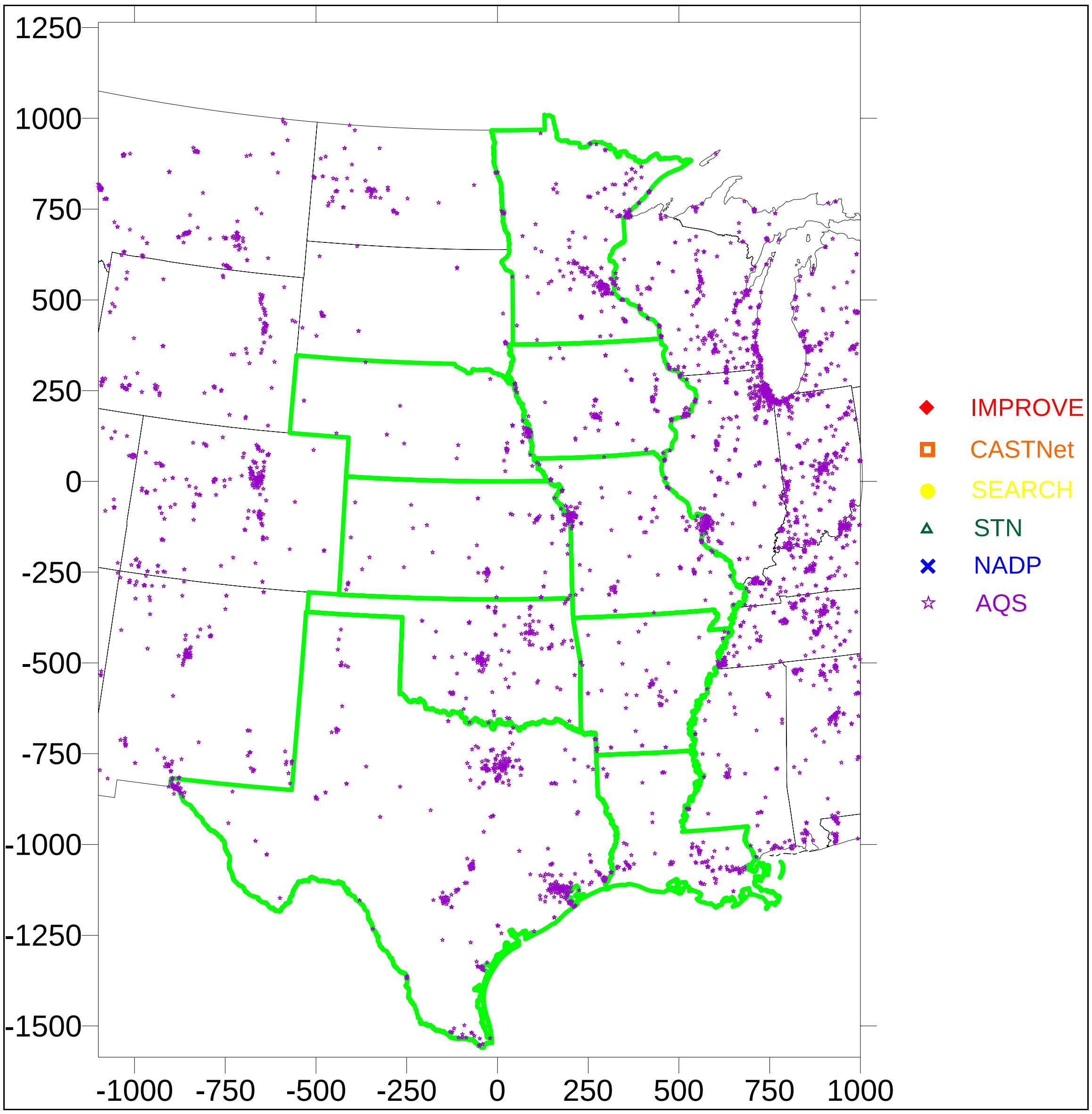


Figure 5-6. Locations of AQS Monitoring Sites in and Near the CENRAP States.

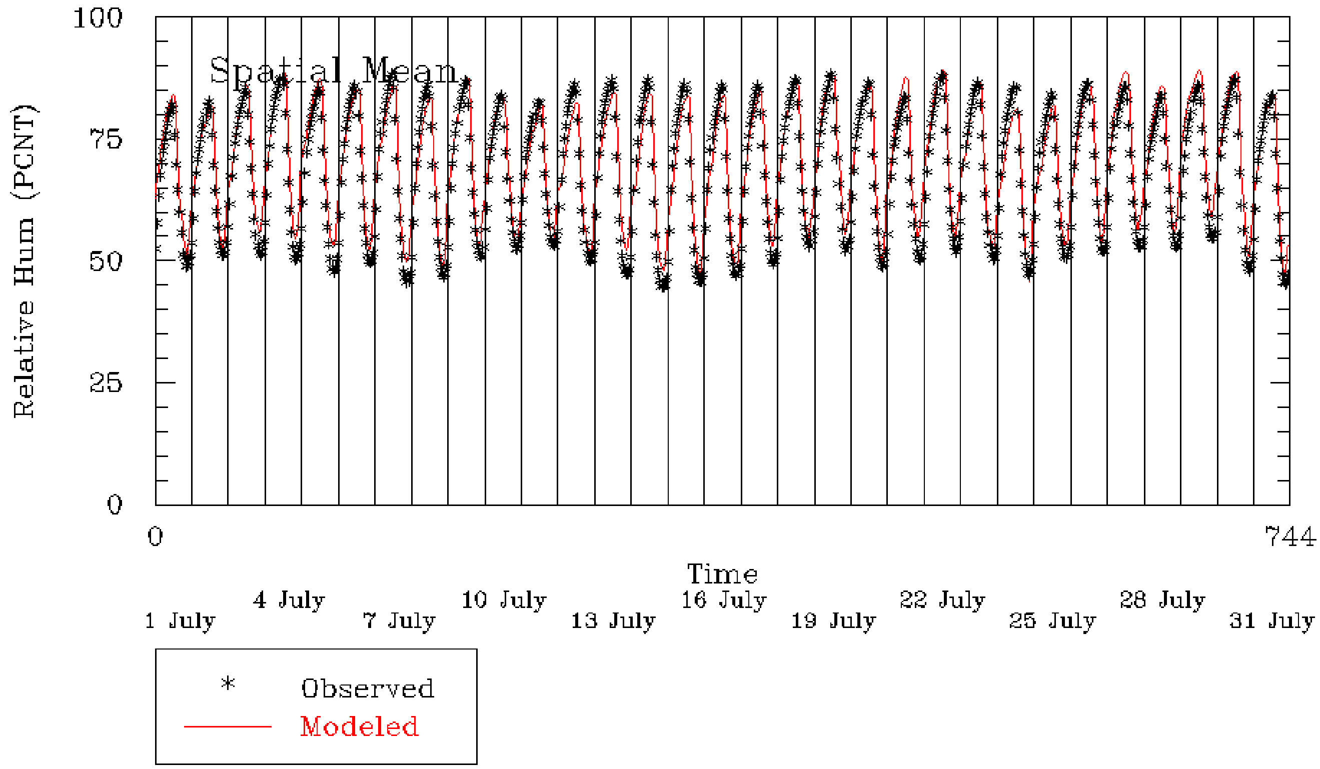


Figure 5-7. Spatial Mean Relative Humidity (%) over the Central Domain: July 2002.

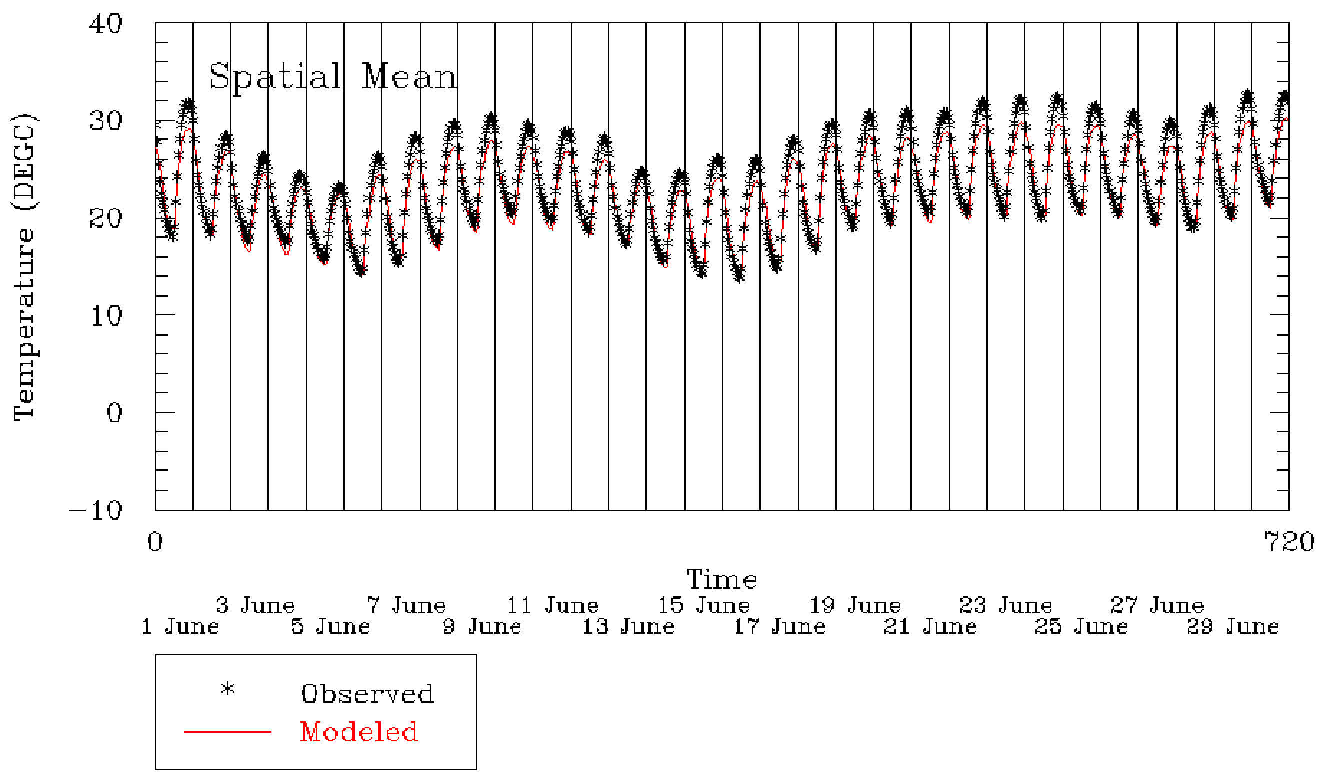


Figure 5-8. Spatial Mean Surface Temperature (deg C) over the Central Domain: July 2002.

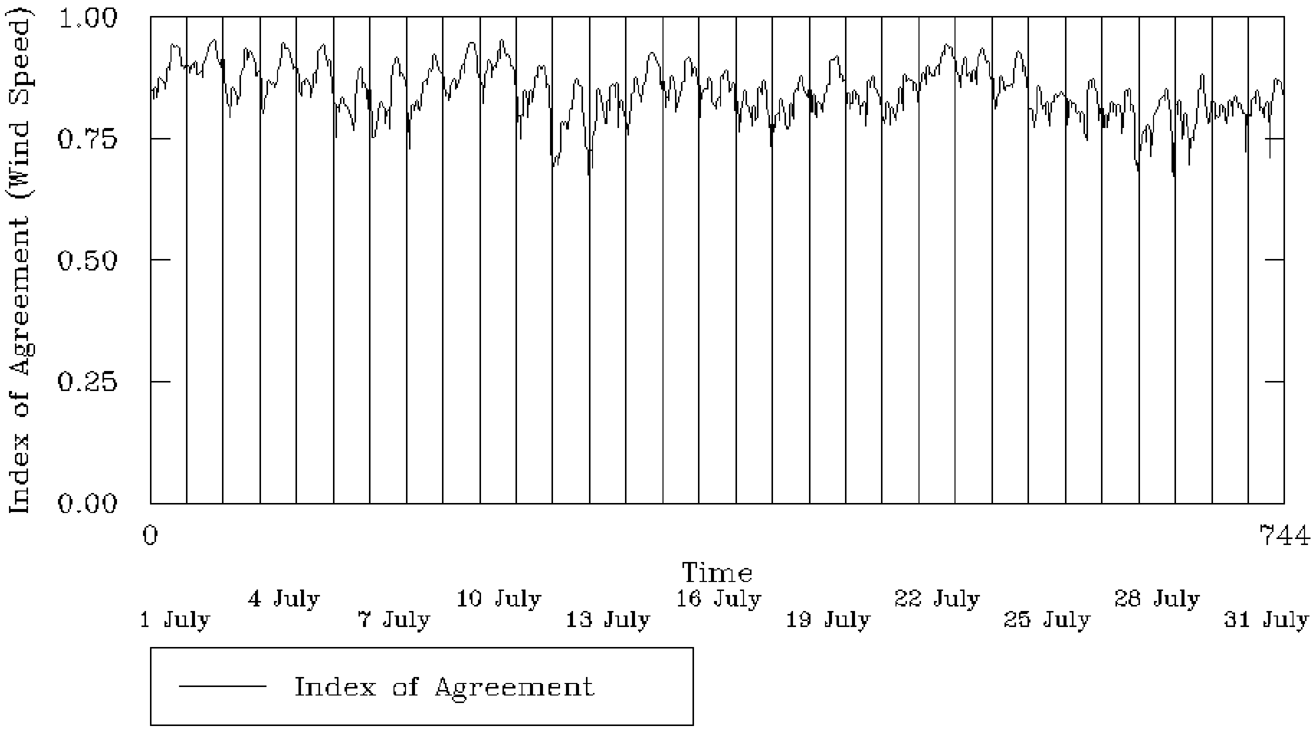


Figure 5-9. Wind Speed Index of Agreement over the Central Domain: July 2002.

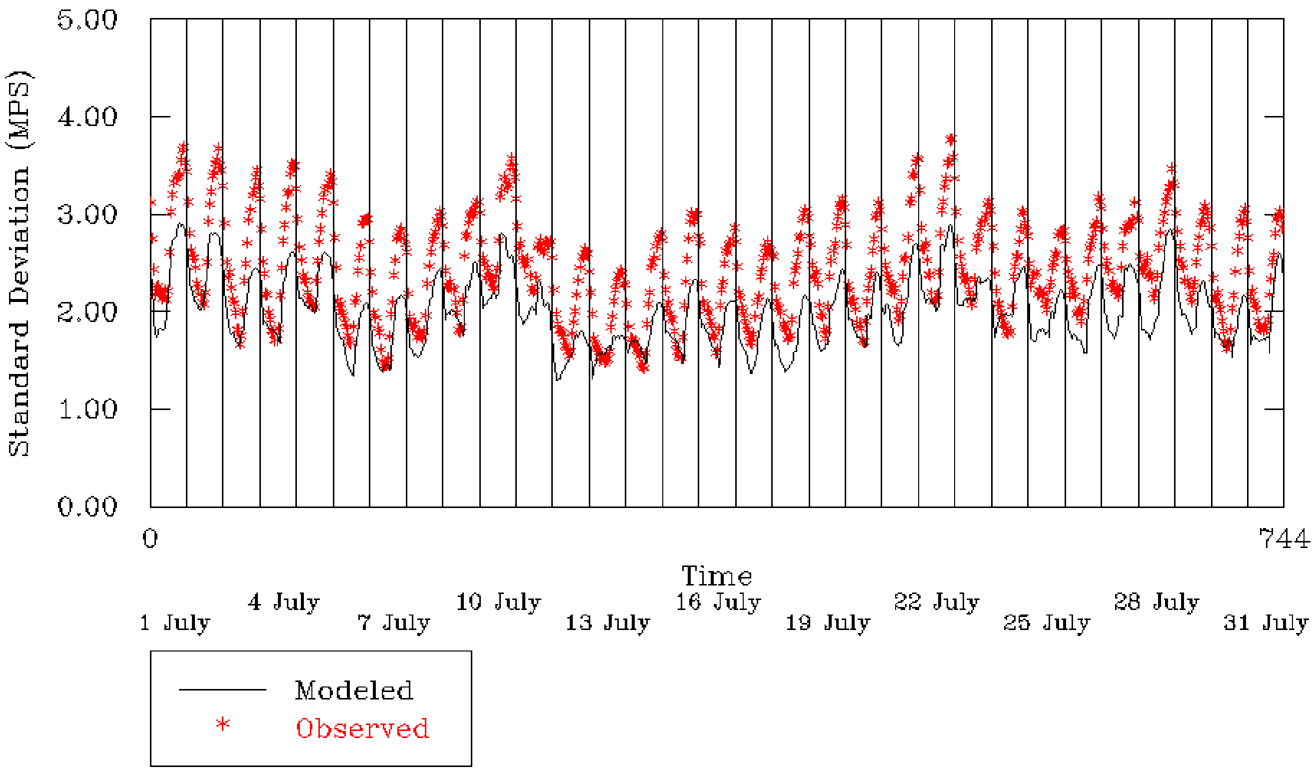


Figure 5-10. Standard Deviation in Wind Speed (m/s) over the Central Domain: July 2002.

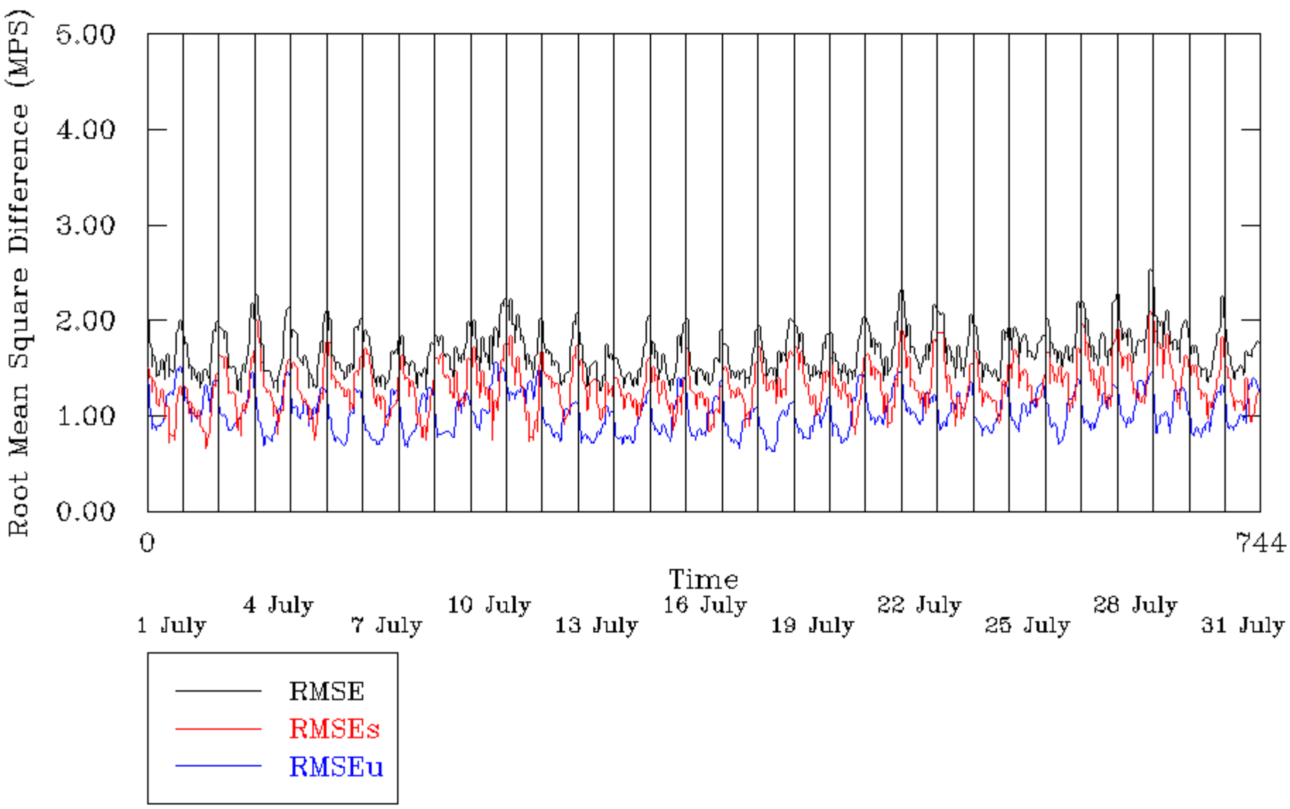


Figure 5-11. Root Mean Square Error in Wind Speed (m/s) over the Central Domain: July 2002.

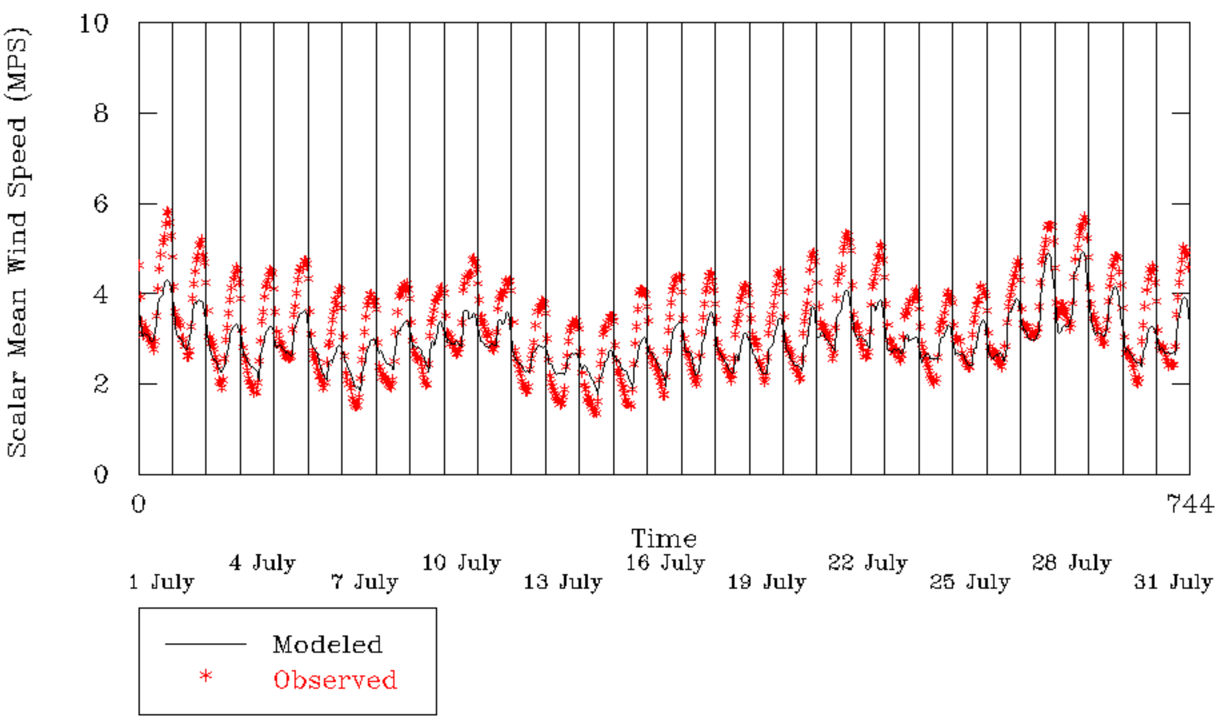


Figure 5-12. Scalar Mean Wind Speed (m/s) over the Central Domain: July 2002.

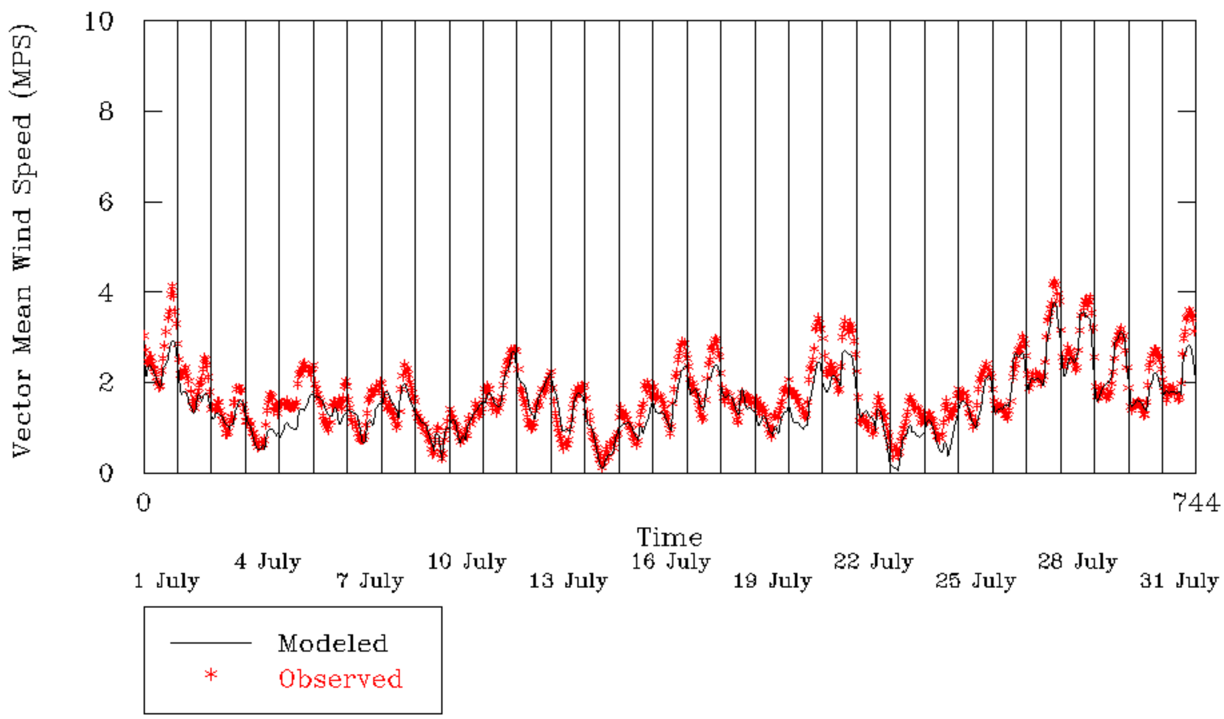


Figure 5-13. Vector Mean Wind Speed (m/s) over the Central Domain: July 2002.

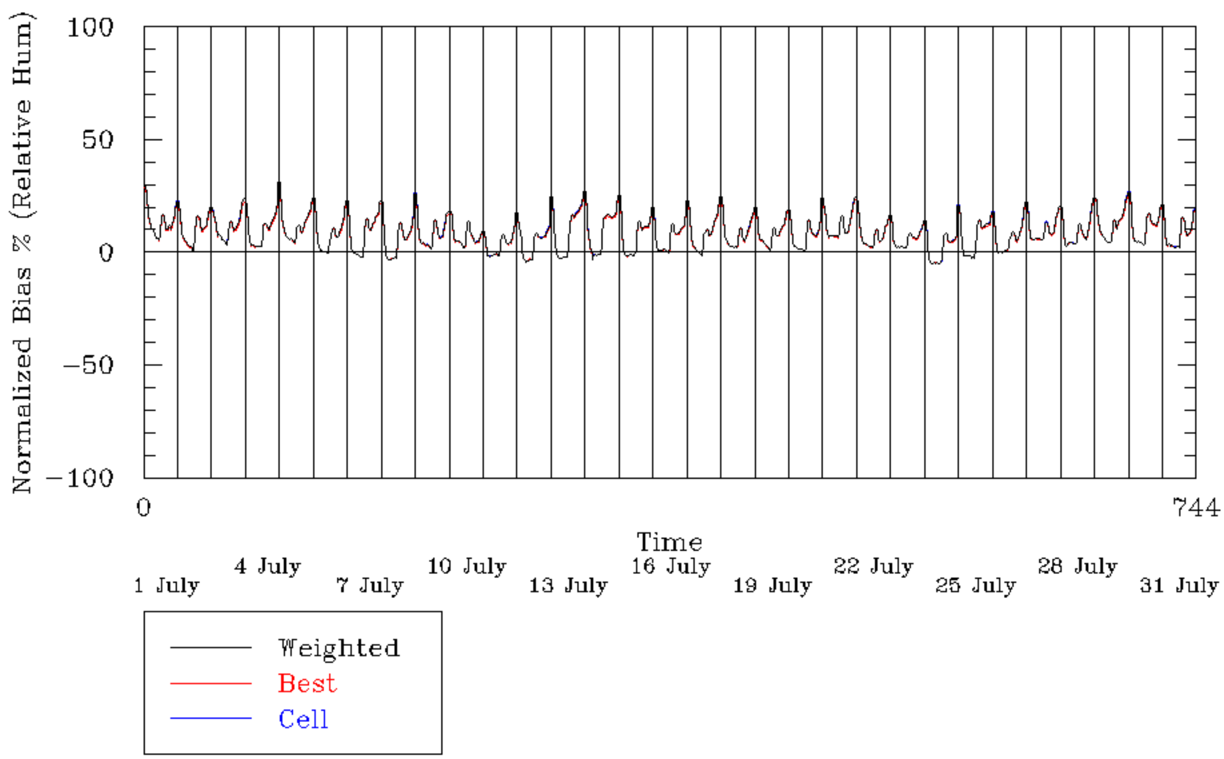


Figure 5-14. Normalized Bias in Relative Humidity (%) over the Central Domain: July 2002.

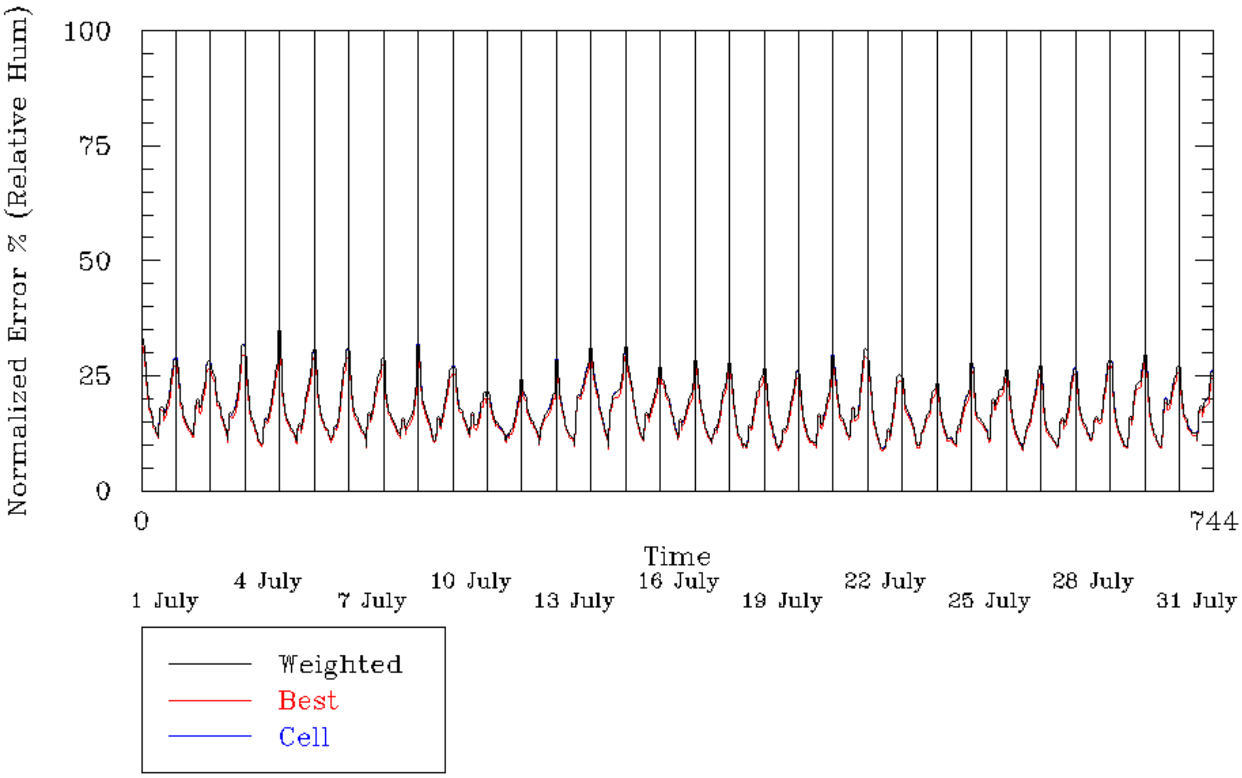


Figure 5-15. Normalized Error in Relative Humidity (%) over the Central Domain: July 2002.

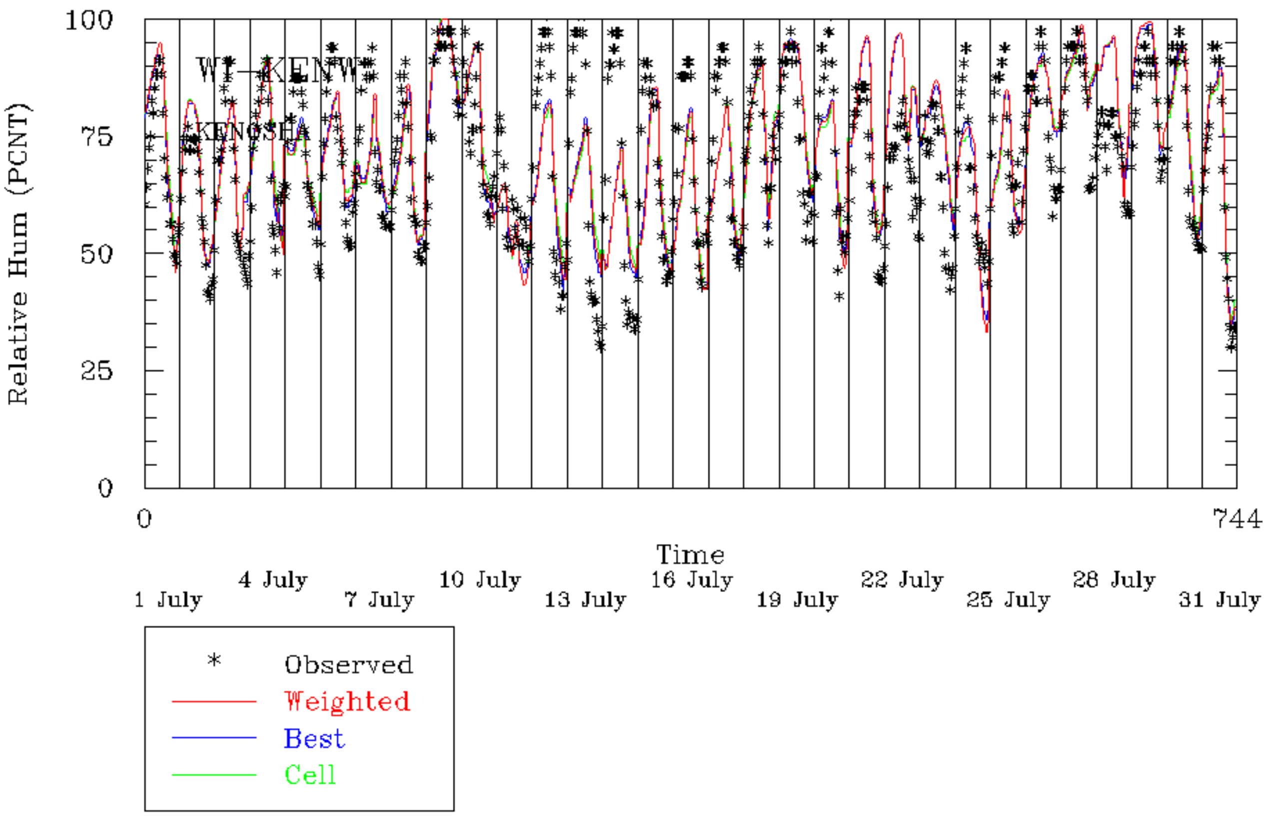


Figure 5-16. Relative Humidity (%) at Kenosha, WI: July 2002.

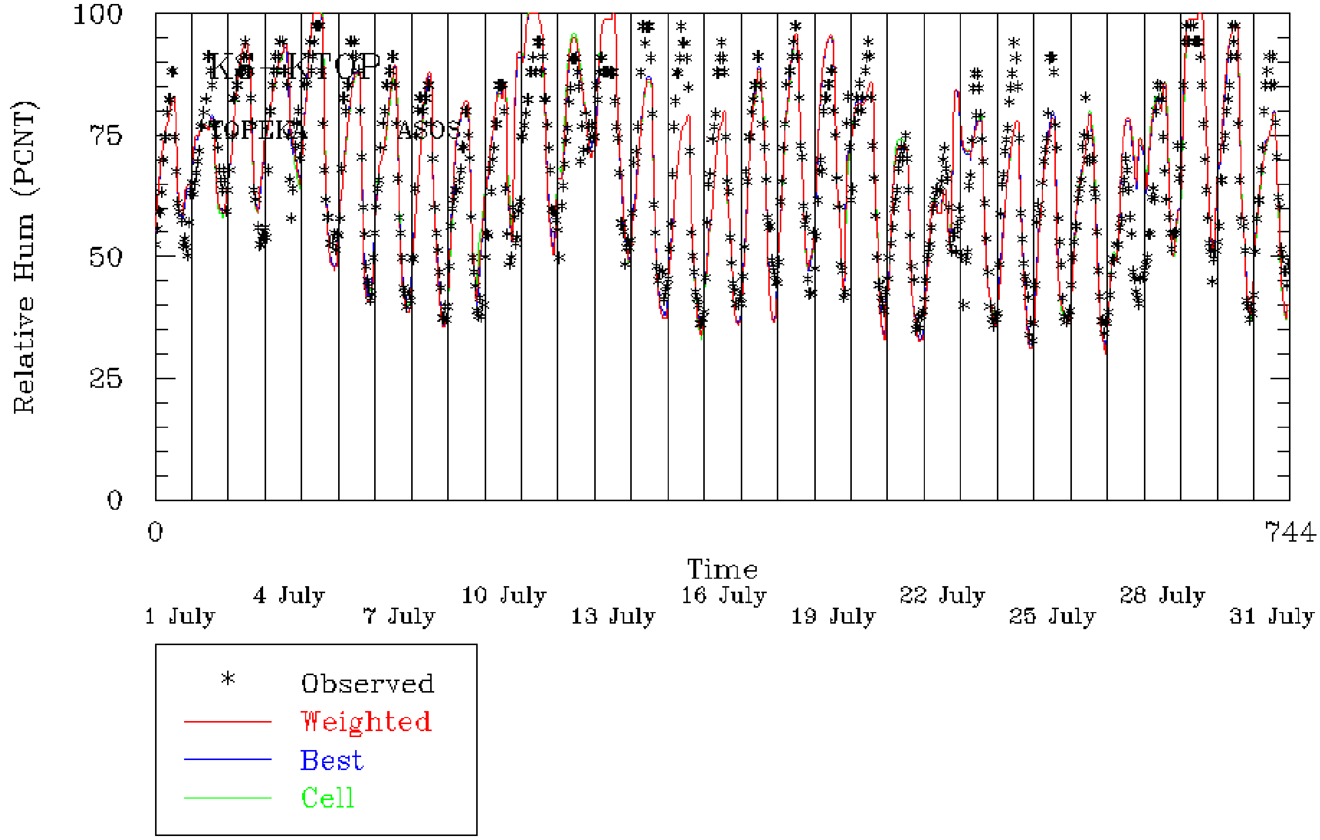


Figure 5-17. Relative Humidity (%) at Topeka, KS: July 2002.

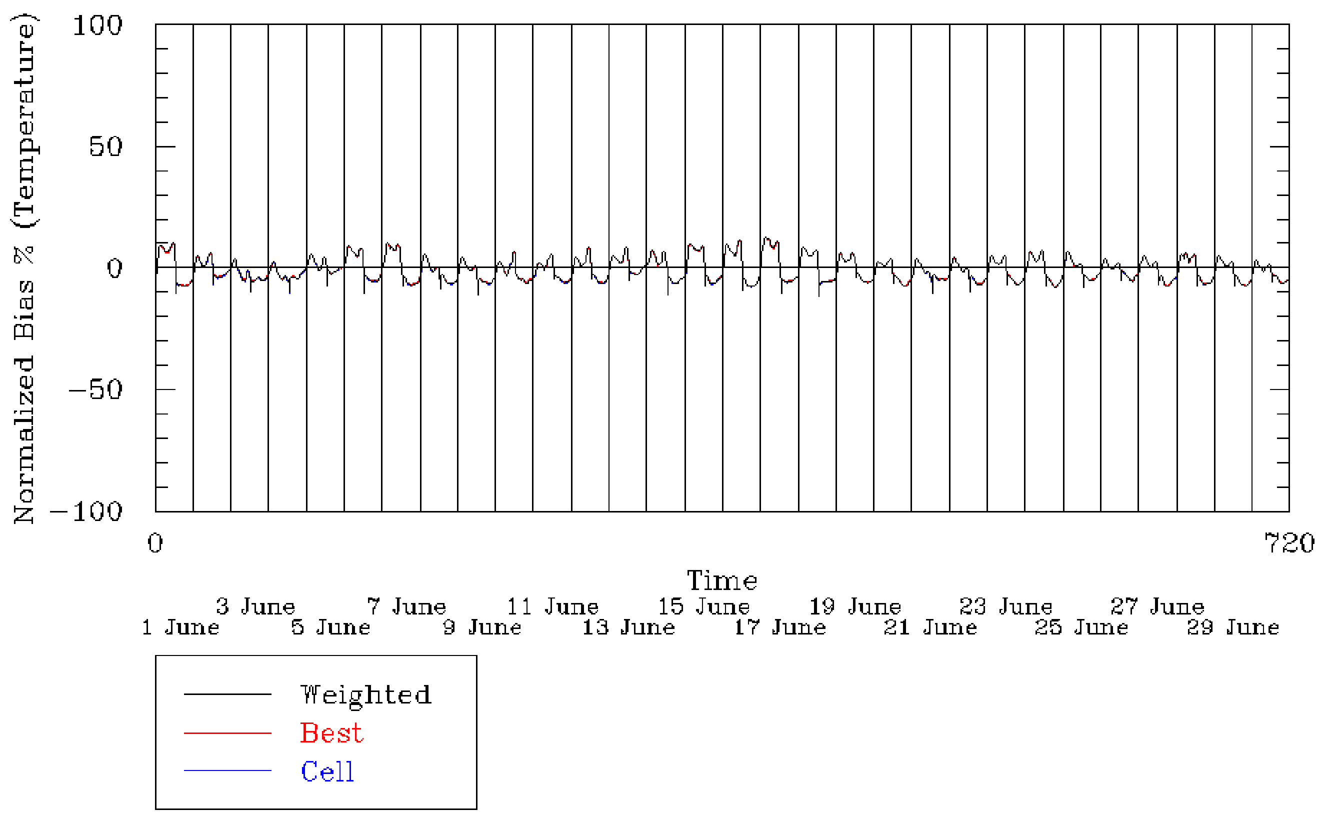


Figure 5-18. Normalized Bias in Surface Temperature (%) over the Central Domain: July 2002.

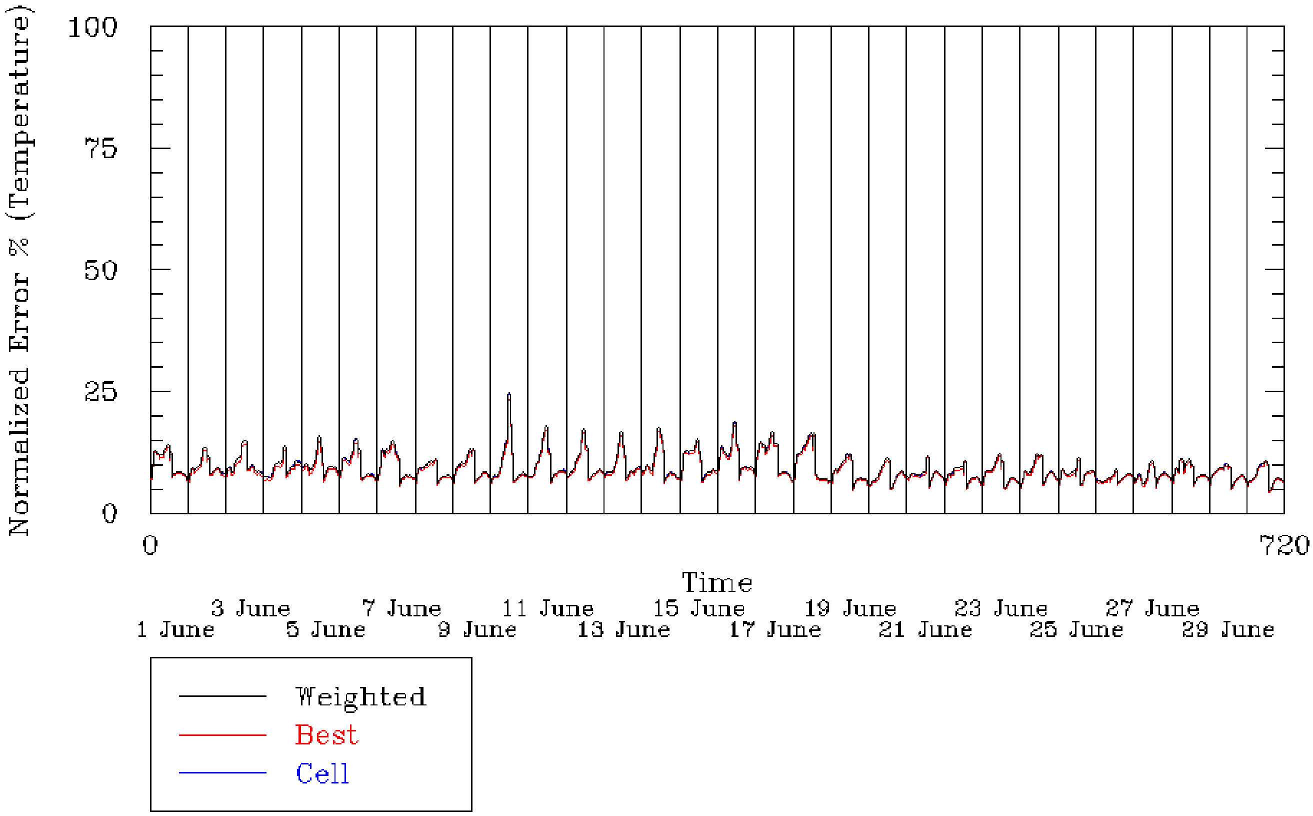


Figure 5-19. Normalized Error in Surface Temperature over the Central Domain: July 2002.

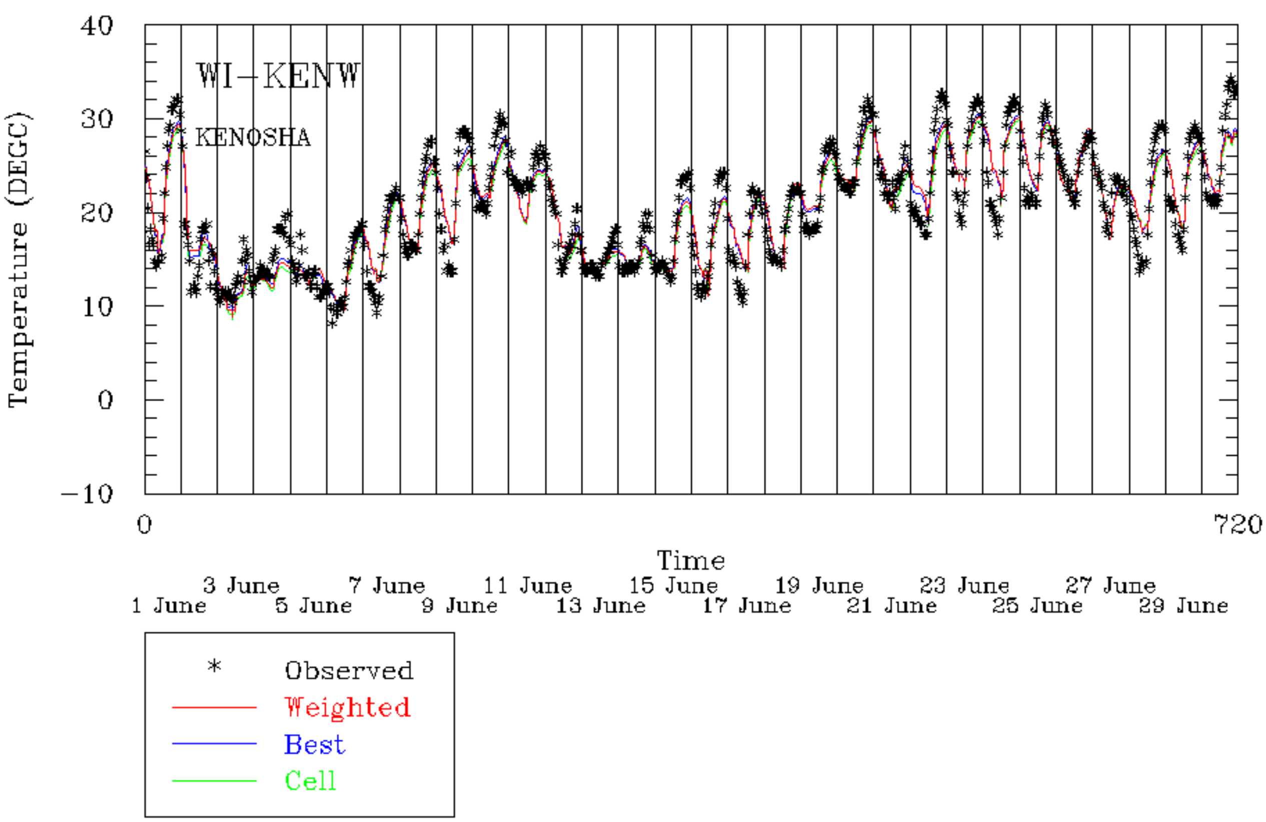


Figure 5-20. Surface Temperature (deg C) at Kenosha, WI: July 2002.

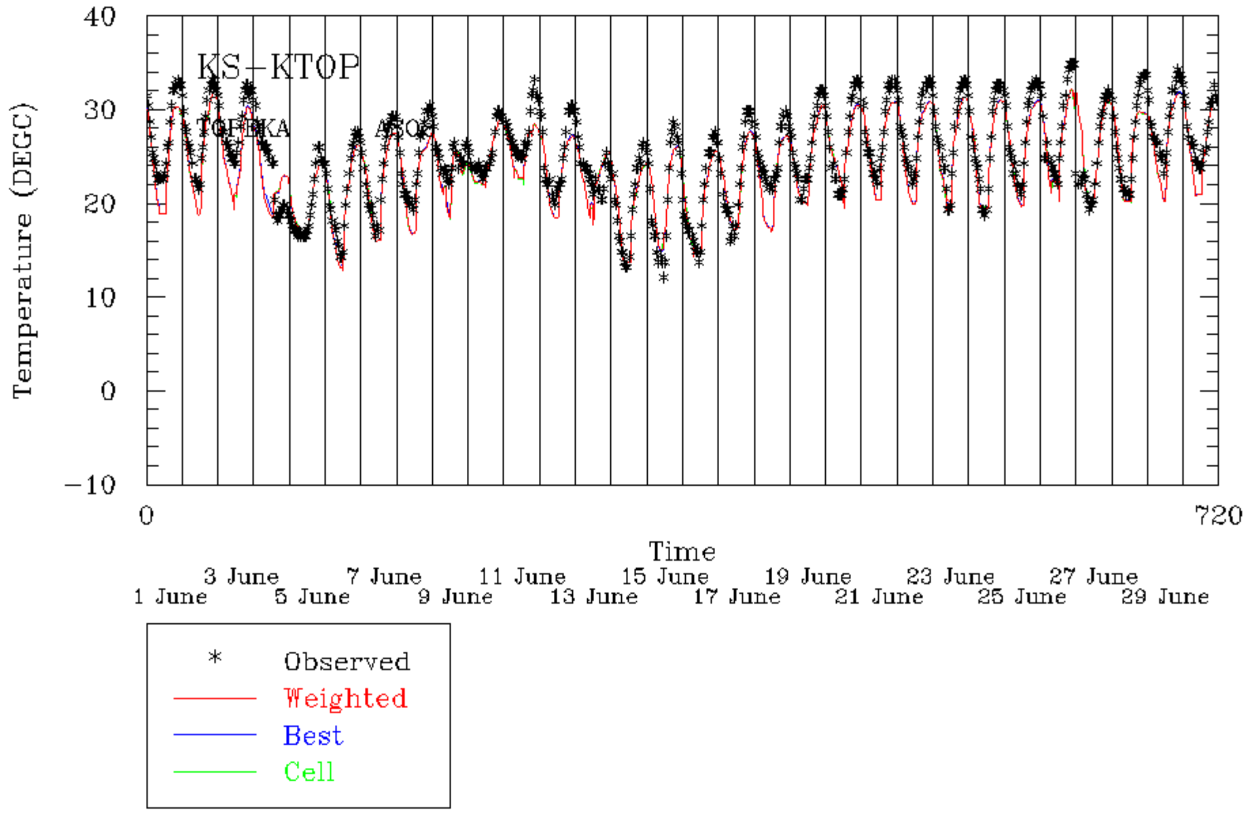


Figure 5-21. Surface Temperature at Topeka, KS: July 2002.

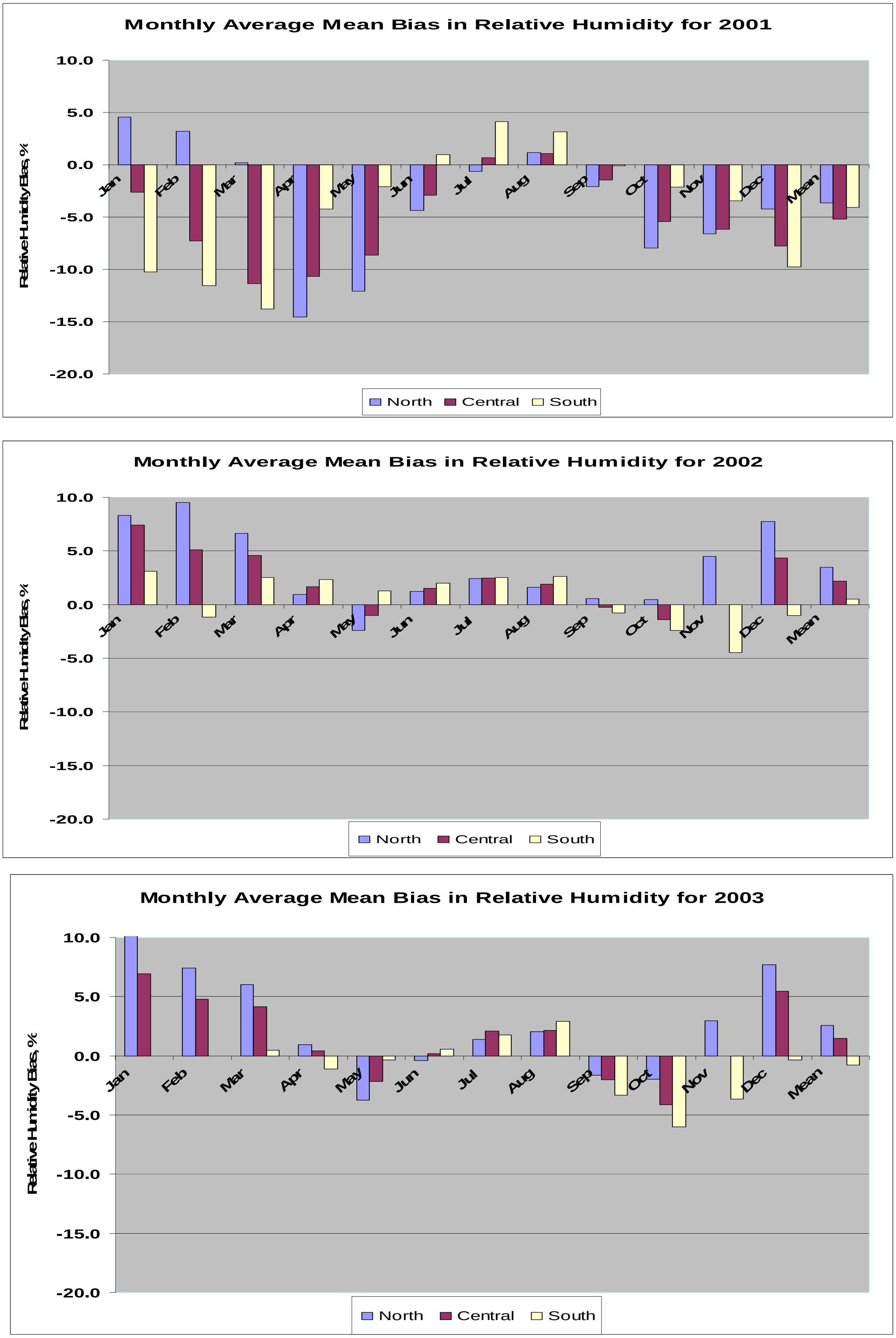
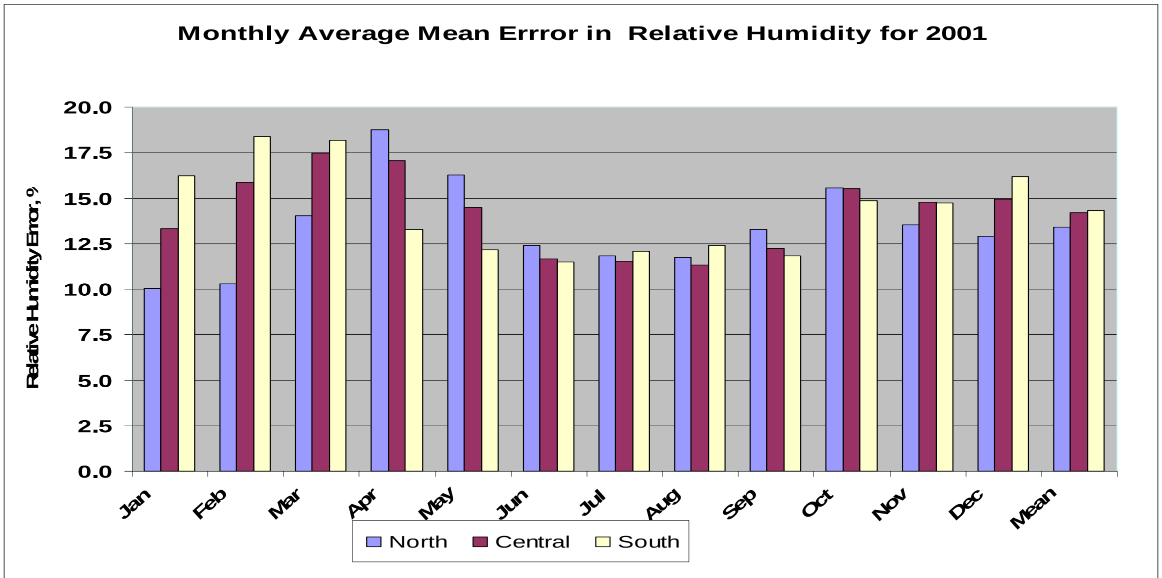
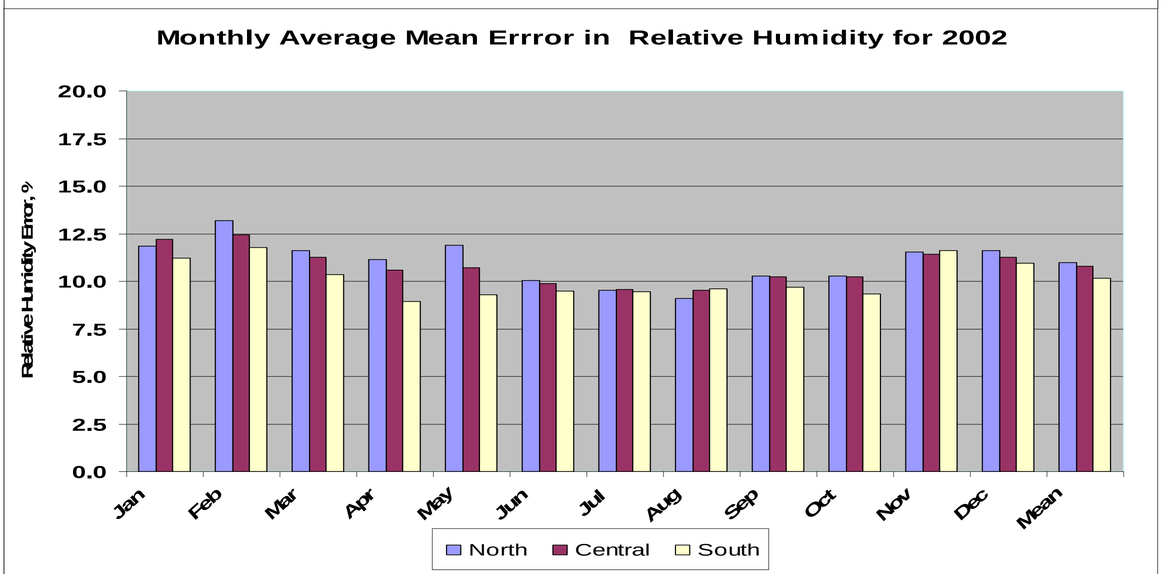


Figure 5-22. MM5/CALMET Relative Humidity Bias (%) by Month for Three BART Modeling Years (2001, 2003, and 2003).





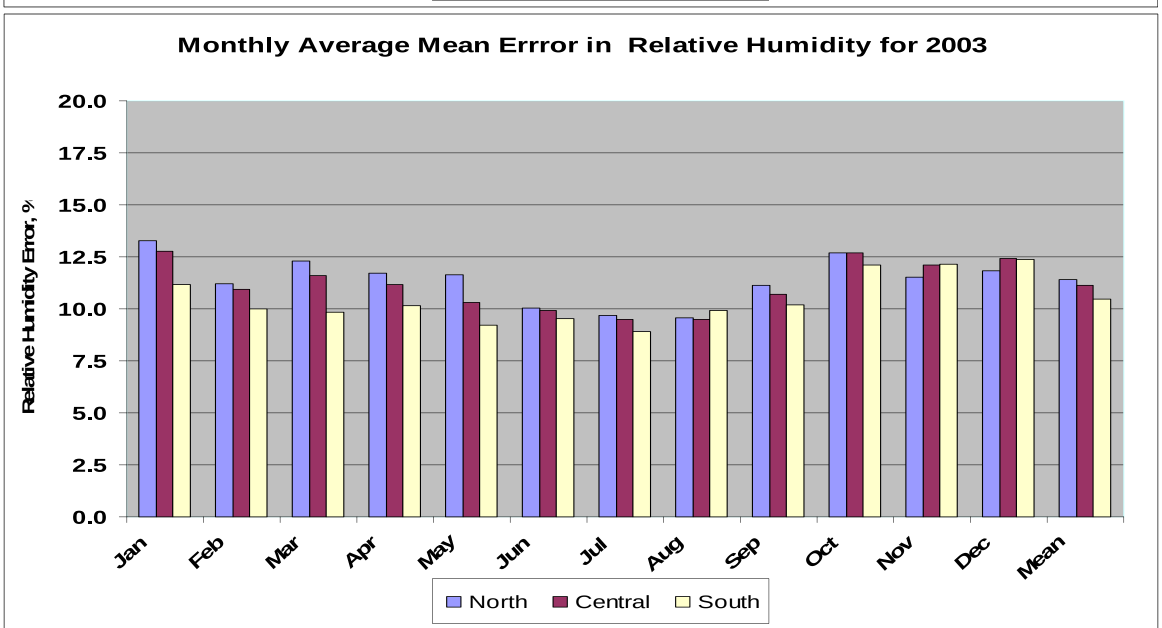


Figure 5-23. MM5/CALMET Relative Humidity Error (%) by Month for Three BART Modeling Years (2001, 2003, and 2003).

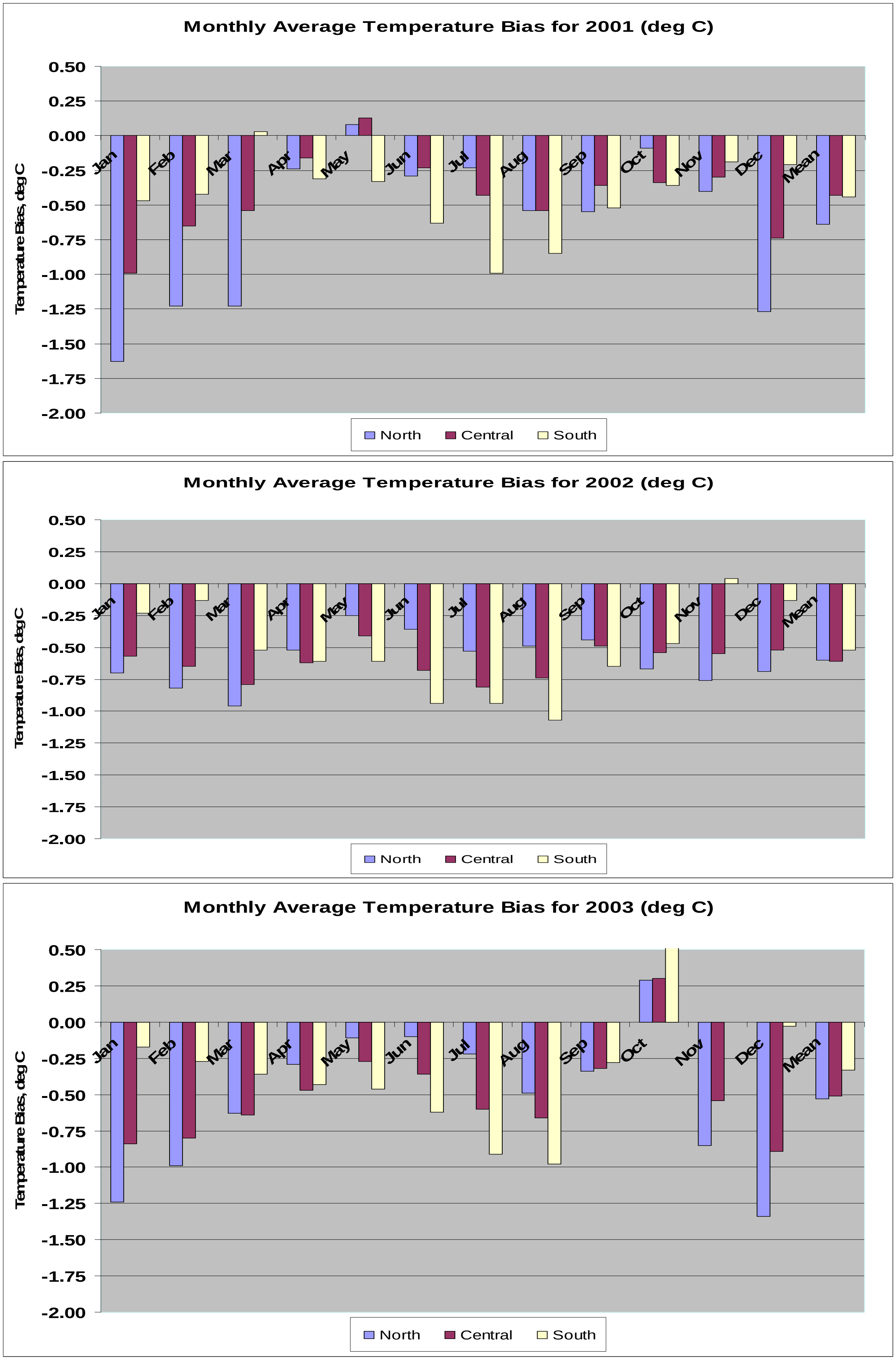
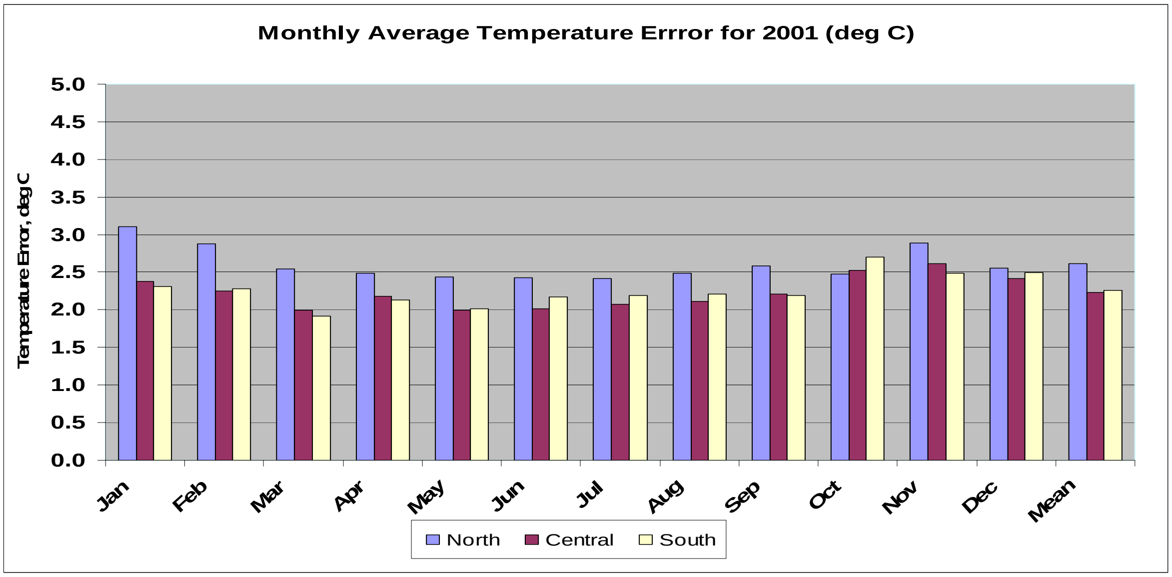
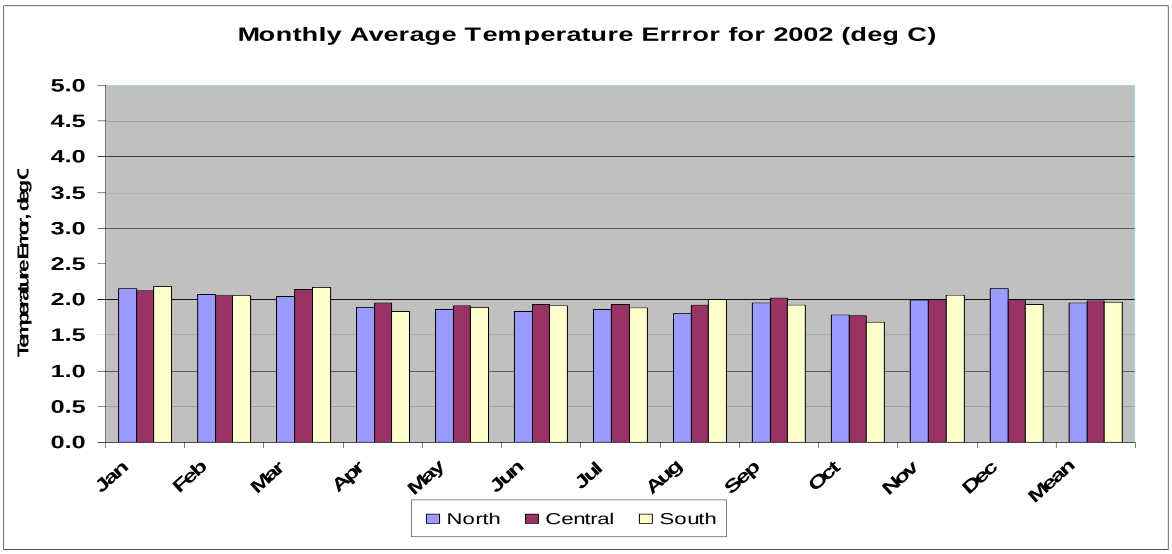


Figure 5-24. MM5/CALMET Temperature Bias (deg C) by Month for Three BART Modeling Years (2001, 2003, and 2003).





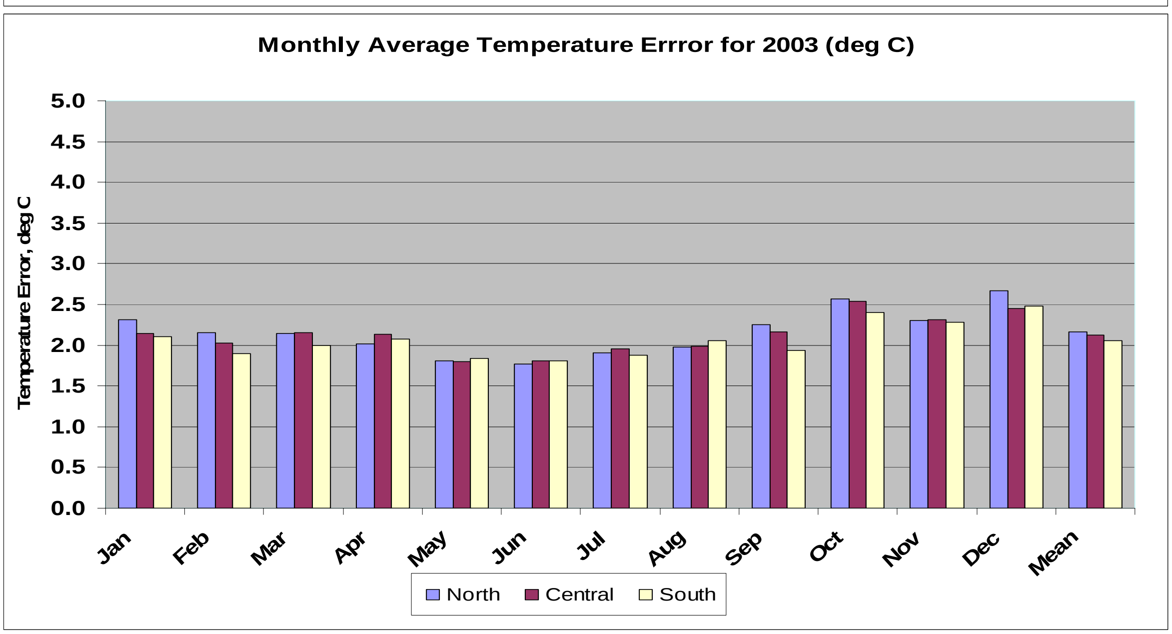
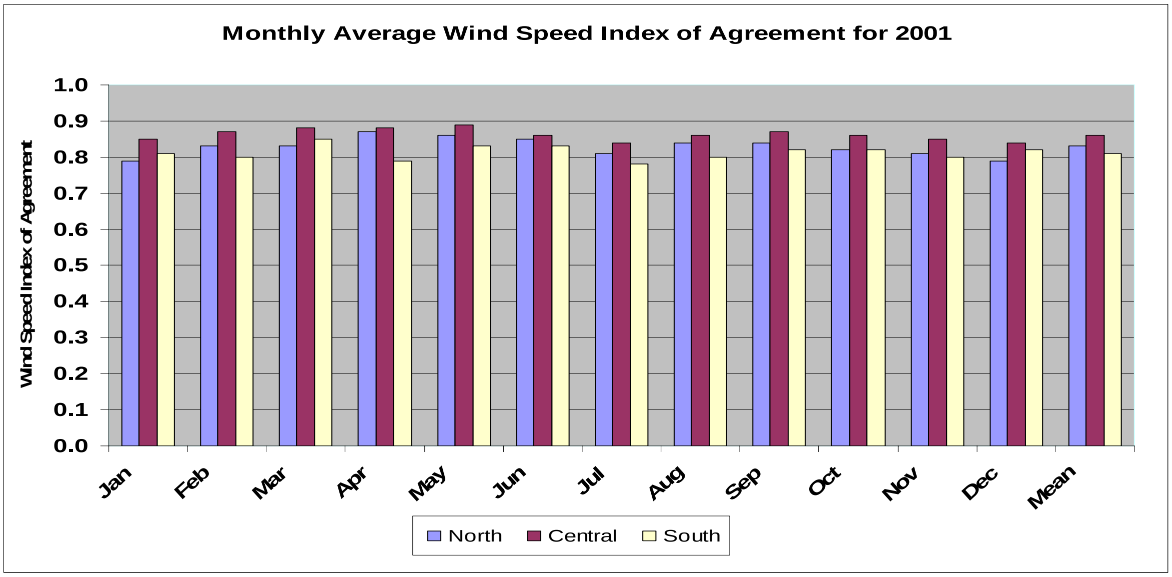
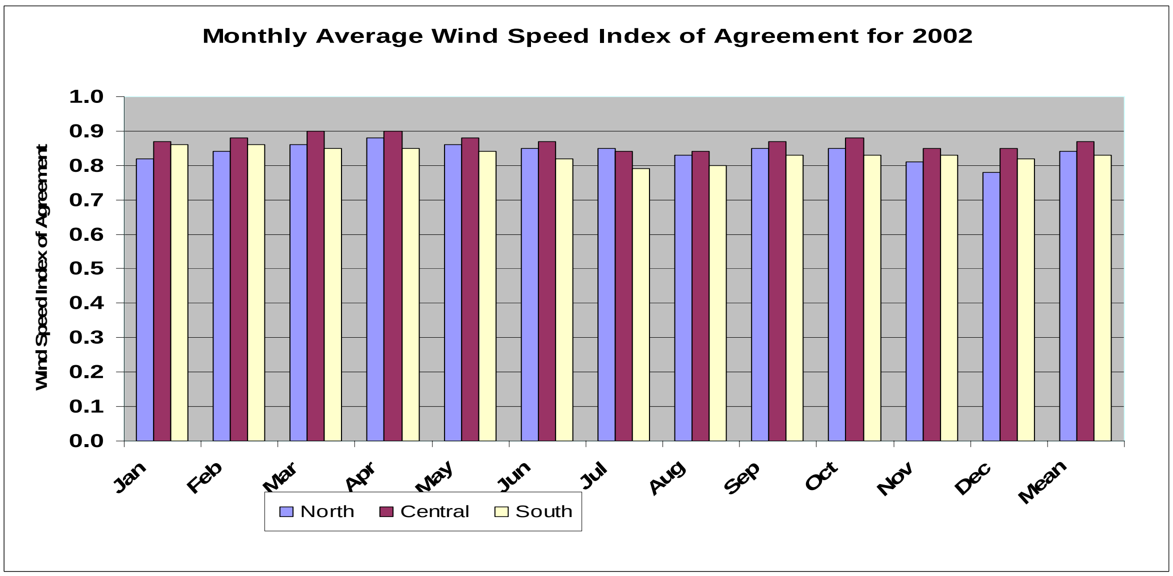


Figure 5-25. MM5/CALMET Temperature Error (deg C) by Month for Three BART Modeling Years (2001, 2003, and 2003).





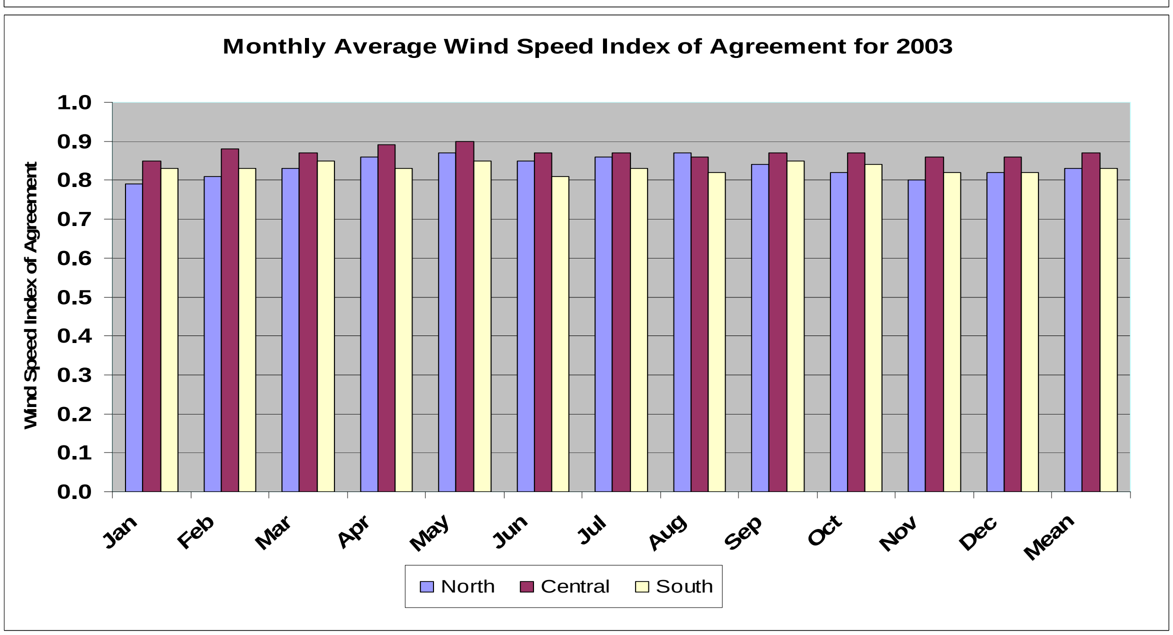


Figure 5-26. MM5/CALMET Wind Speed Index of Agreement by Month for Three BART Modeling Years (2001, 2003, and 2003).

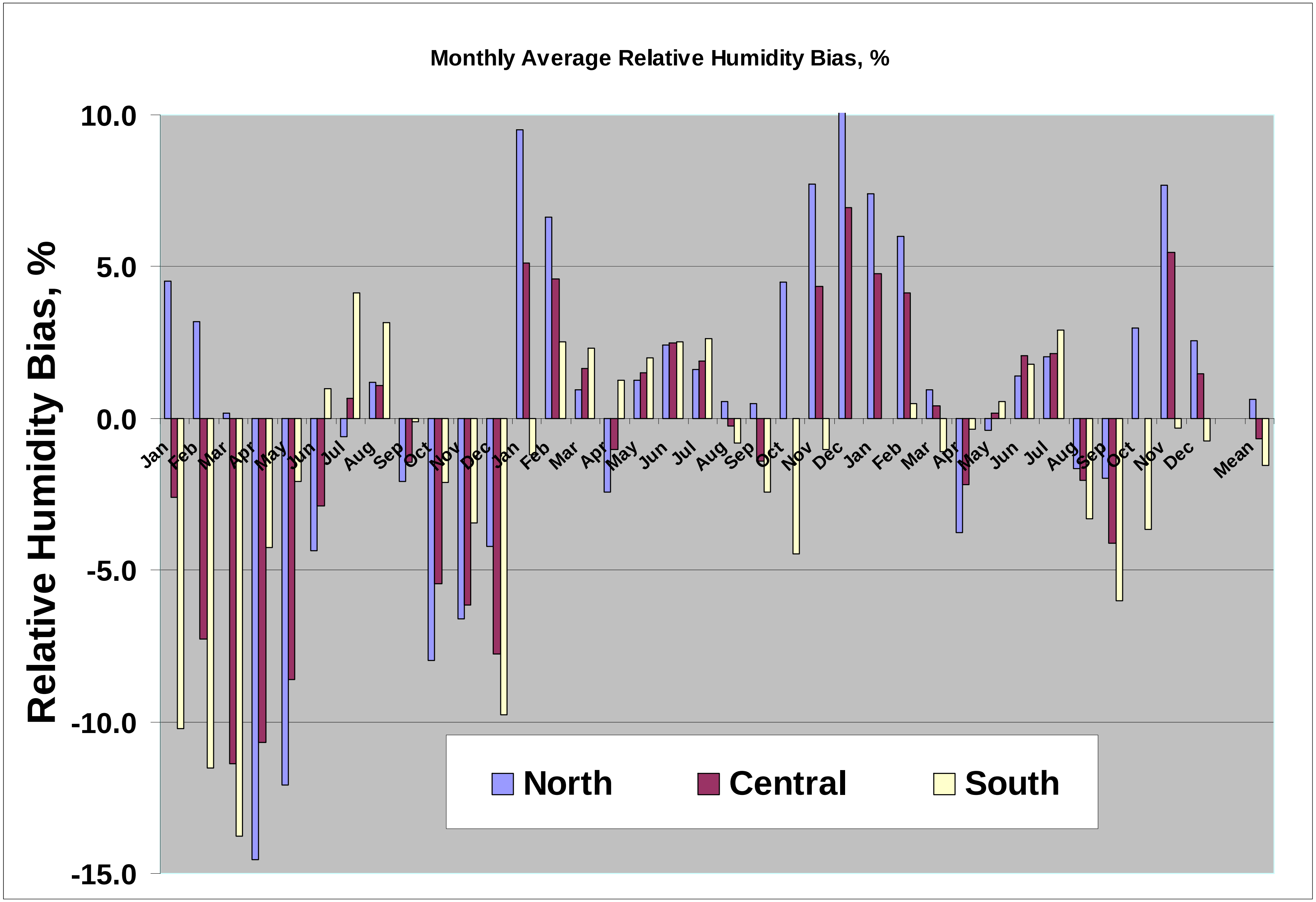


Figure 5-27. MM5/CALMET Relative Humidity Bias (%) over Three Years in All CENRAP Domains.

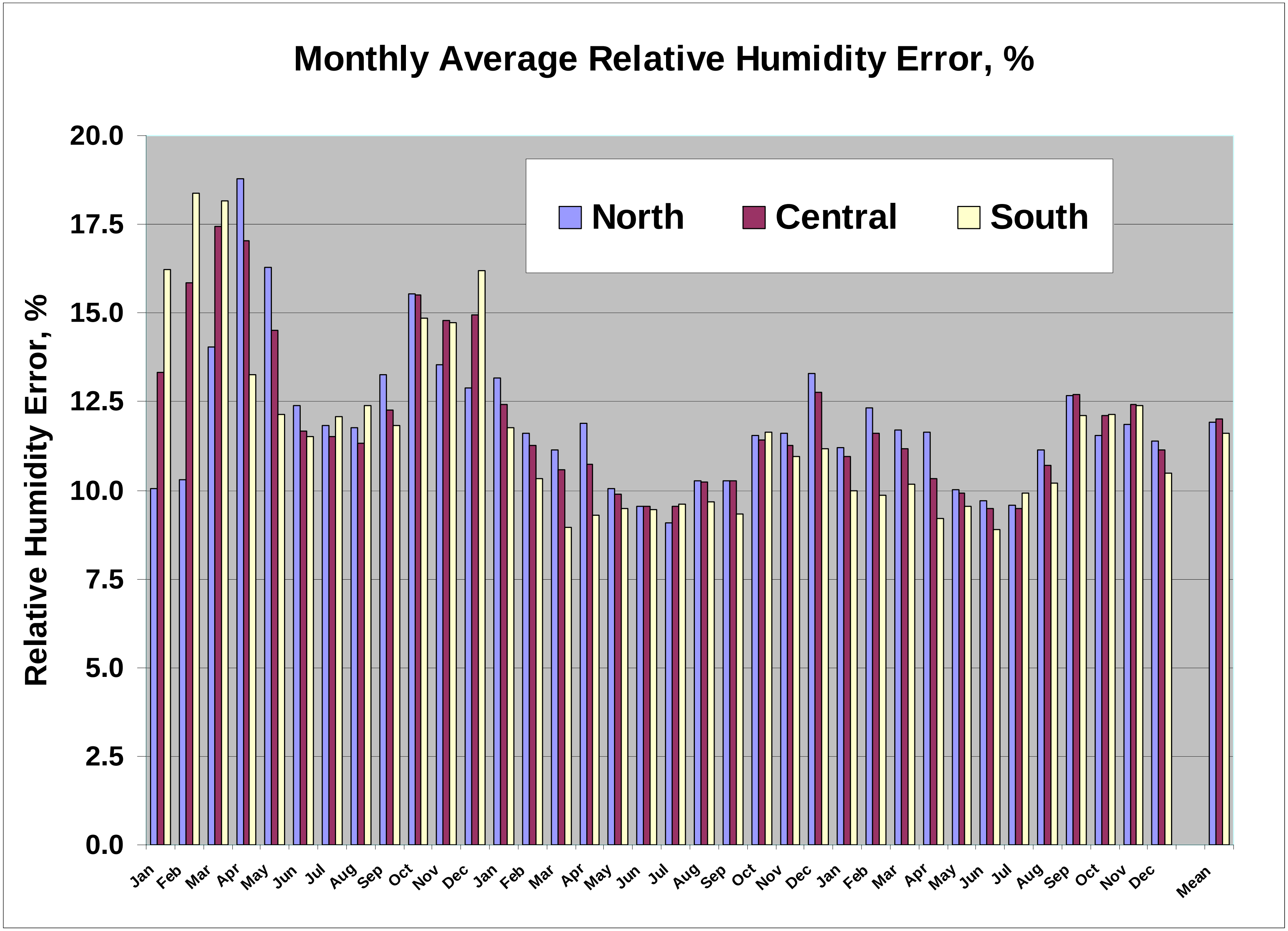


Figure 5-28. MM5/CALMET Relative Humidity Error (%) over Three Years in All CENRAP Domains.

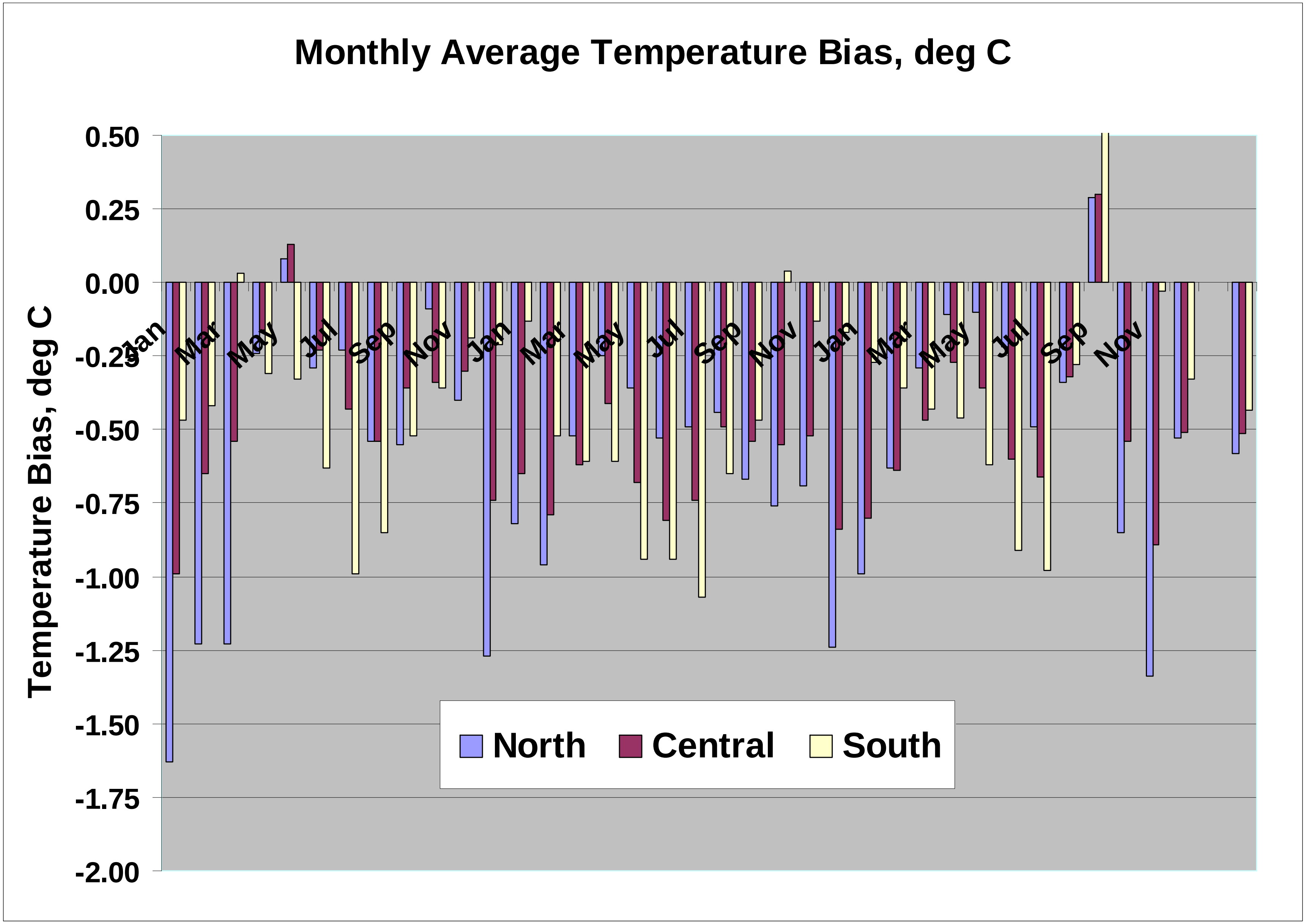


Figure 5-29. MM5/CALMET Surface Temperature Bias (deg C) over Three Years in All CENRAP Domains.

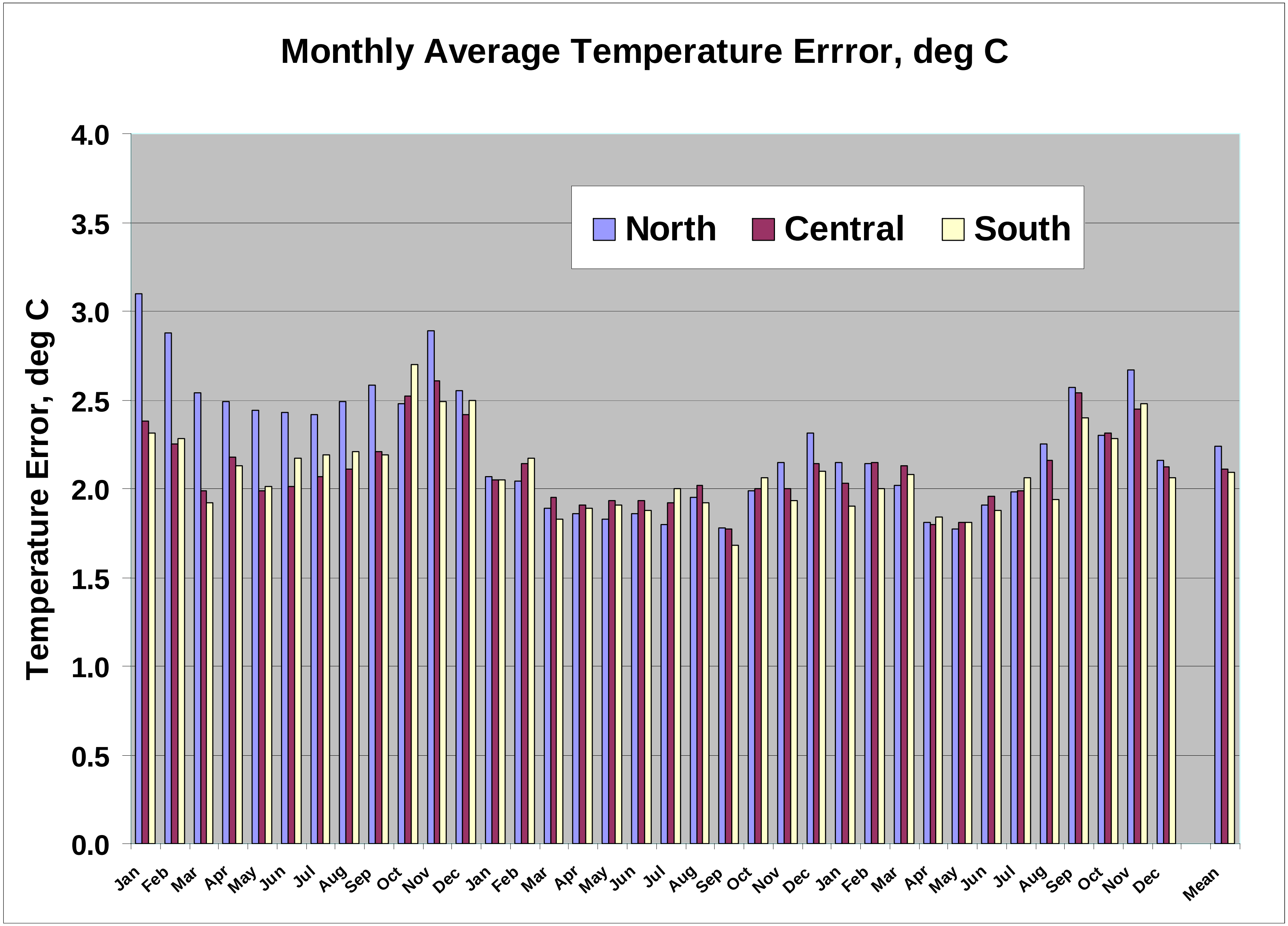


Figure 5-30. MM5/CALMET Surface Temperature Error (deg C) over Three Years in All CENRAP Domains.

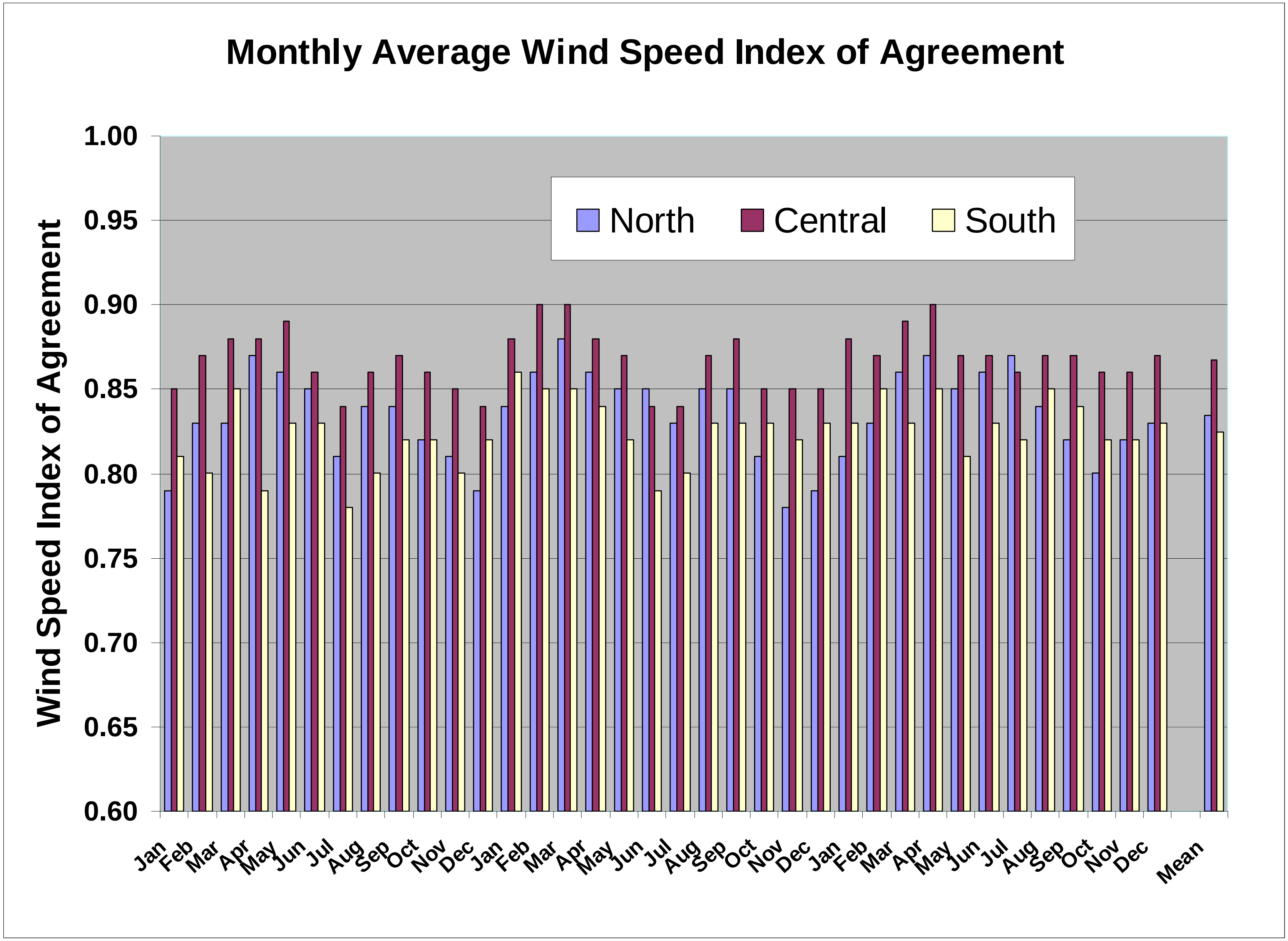


Figure 5-31. MM5/CALMET Wind Speed Index of Agreement over Three Years in All CENRAP Domains.

6.0 CALPUFF SCREENING APPLICATIONS

The objective of the CALPUFF screening approach is to efficiently and conservatively determine whether a source can be exempted from BART controls or whether source-specific modeling is needed. The screening method described in this chapter will also help identify specific Class I areas that might be affected by the source. Should source-specific modeling become necessary, this information will assist the state or source in tailoring the analysis domain and modeling procedures to focus on the area(s) of greatest likely interest. Due to the nonlinearities in the physical and chemical processes governing visibility impairment and the variability in wind and dispersion transport patterns, simple notions about source-receptor relationships (e.g., the closest Class I area will produce the controlling visibility impacts) may not be universally reliable. So the screening analysis may offer some insight here.

CALPUFF screening modeling should be performed consistent with the procedures set forth in this chapter, adapted as necessary to the source or sources of interest. A standard set of default meteorological, air quality and dispersion conditions are assumed that, for the most part, are consistent with the IWAQM (1998) and FLAG (2000) recommendations. For many sources in the CENRAP region, the screening approach may be sufficient to show whether it is a contributor to visibility problems in a particular Class I area. To support screening applications of CALPUFF, model-ready meteorological data sets have been developed for three CENRAP sub-regional domains (Figures 5-1 through 5-4). These data sets, described in Chapter 5, expedite the screening analysis and provide for consistency of application across the CENRAP region.

The CALPUFF screening methodology possesses a higher degree of conservatism (i.e., systematic tendency to over-predict visibility impacts) compared with the source-specific methodology in Chapter 7. For large sources that will clearly exceed the screening thresholds, the screening step may be skipped as the analysis proceeds directly to source-specific modeling.

6.1 Methodology

The screening methodology recommended for sources in the CENRAP region uses the CALPUFF model with three years of meteorological data and the standard compliment of model algorithms invoked. To ensure that no sources pass the screening test when they should fail, the simple approach, by its nature, must be the most conservative of all the conditions likely to be examined for the source in question. For example, many factors influence the contribution of a source to the Class I area other than distance. The frequency of winds transporting the pollutants toward the Class I area may often be important to include for a reliable screening analysis. Also, a more distant Class I area downwind in the predominant wind direction from a source may receive a higher visibility impact than a closer Class I area that is infrequently downwind of the source. Further, correlations between winds from certain directions and meteorological conditions may be conducive for higher visibility impacts. Such effects and relationships are addressed in the screening approach. It is designed to ensure conservatism by comparing the maximum visibility impact with the 0.5 dv threshold in making a determination of no contribution to visibility impairment and also by using conservative model settings.

The impact of the source or sources is calculated from the daily visibility values for each receptor by determining the change in deciviews compared against natural visibility conditions. EPA's "Guidance for Estimating Natural Visibility Conditions Under the Regional Haze Rule," EPA-454/B-

03-005 (September 2003) lists recommended natural visibility conditions. To determine whether a source may reasonably be anticipated to cause or contribute to visibility impairment at Class I area, the impacts predicted by CALPUFF are compared against the pertinent natural visibility background and the threshold that has been selected. The steps in the screening approach are outline below. It is described diagrammatically in Figure 1-1 in the introductory chapter.

6.2 Protocol Development and Negotiation

The first step is the development and negotiation of a modeling protocol with the state and FLM. An outline of a typical protocol is presented in Table 6-1, containing the basic elements of such a document. Portions of these CENRAP BART Modeling Guidelines may be adopted or referenced directly in a specific screening protocol as appropriate.

6.3 CALMET Model Configuration and Application

As discussed in Chapter 5, the model configurations used to generate the common CALMET meteorological files for visibility screening of BART eligible sources followed the IWAQM recommendations (EPA, 1998, Appendix A), except as noted. For CALPUFF screening assessments, there is no need to compile CALMET inputs, run the model or process the outputs. As discussed in Chapter 7, for source-specific modeling, these activities with CALMET may indeed be appropriate.

6.4 CALPUFF Model Configuration and Application

6.4.1 Model Codes

For screening applications, the latest ‘beta’ versions of the CALMET/CALPUFF modeling system should be used as given in Table 6-2. Note that these are *not* the EPA guideline codes but rather updated versions containing recent (as of this writing) science improvements and bug fixes. (The current guideline CALPUFF code is version 5.7, level 030402). This substitution results from EPA phasing out the use of the legacy Pasquill-Gifford (P-G) dispersion parameters with the introduction of AERMOD as a new guideline model. CALPUFF employs the AERMOD turbulence-based dispersion coefficients and probability density function (pdf) dispersion methods scheme instead of P-G.

The appropriate model codes may be downloaded from www.src.com or purchased with the latest graphical user interface (GUI) from the model developer. The sequence of model processors listed in Table 6-2 corresponds to the order in which the programs are typically run.

6.4.2 Domain Definition

Three sub-regional modeling domains and associated CALMET meteorological data bases have been developed for CENRAP and are available to the states and source operators for performing CALPUFF screening analyses for any Class I areas within the domain. The modeling data sets cover three contiguous years (2001, 2002, and 2003) and are resolved to a 6 km horizontal resolution grid. Details of the modeling domains and the meteorological data bases for 2001, 2002, and 2003 were discussed in Chapter 5.

Receptor Network and Class I Receptors. Experience with the CALPUFF modeling system has shown that sizeable emissions sources can have discernible impacts beyond 300 km. Given CALPUFF's propensity towards overprediction, one could easily expect CALPUFF to predict that a source causes or contributes to visibility impairment at Class I areas greater than 300 km. As discussed in Chapter 8, recent model inter comparisons between CALPUFF and full science models such as CAMx and CMAQ (Morris et al., 2003) amply demonstrate that CALPUFF substantially over predicts concentrations of visibility-reducing fine particulates under various real-world conditions at the larger downwind distances when compared to one-atmosphere models. Thus, a dilemma arises in that experience with CALPUFF indicates a tendency to overpredict at great downwind distances yet sources having a modeled effect beyond, say, 300km should not necessarily be neglected because there may be some validity to a particular CALPUFF model simulation of far downwind impacts.

There are a significant number of BART eligible sources in the CENRAP region with no Class I areas within 300 km. Additionally, numerous BART sources are located no closer than 500-600 km to their nearest Class I area. The science-based approach to this dilemma is to use a regional model to address far downwind impacts. However, for most screening analyses, even out to 500-600km, States and source operators will likely find it necessary to employ CALPUFF notwithstanding the uncertainties associated with its bias at large transport scales. If CALPUFF is viewed to be a suitable model for use over such distances (say 300 – 600 km) States may wish to consider the use of puff splitting despite the lack of quantitative measurements demonstrating that puff splitting actually reduces CALPUFF model overprediction at large scales. Implementation of puff splitting, coupled with fine grid resolution (~ 12 km or less) might be considered as an approach for distant Class I receptors, but this strategy will likely lead to computer run times approaching and even exceeding those of one-atmosphere models.

In sum, discrete receptor coordinate data for all Class I federal areas within 600 km of the source should be developed, preferably using the National Park Service (NPS) Convert Class I Areas (NCC) computer program. Whether all Class I receptors need to be modeled is an issue to be resolved in the modeling protocol process in cooperation with the regulatory agencies and land managers. Receptor elevations provided by the NPS conversion program should be used. All receptors should be included in a single CALPUFF simulation. (http://www2.nature.nps.gov/air/Maps/Receptors/index.cfm).

6.4.3 Model Set-Up

Following the procedures set forth in the protocol, the agreed to version of CALPUFF is set up on one or more of the three CENRAP domains. The screening analysis should use a CALPUFF computational domain that includes all Class I areas within 300 km of a source. These Class I areas are specified in the CALPUFF control file for analysis. States could decide to require a different value for the maximum distance threshold for the CALPUFF domain, depending on the locations of the Class I areas in their states and other factors such as meteorological conditions and the magnitudes of the emissions from BART-eligible sources. The regional CALMET domain will be unchanged by these adjustments.

At the election of the state or source operator, the screening approach may be designed to significantly reduce the CALPUFF simulation time by restricting the computational domain size to include only areas where significant impacts are feasible rather than the entire regional domain. CALPUFF allows its computational domain to be specified as a subset of the CALMET meteorological domain by settings within the CALPUFF input file. The advantage of selecting a smaller CALPUFF computational domain is that the model run time is proportional to the number and residence time of the puffs on the domain (and other factors such as the number of receptors and the internal time step computed by the model). This technique, if used, must be fully described in the modeling protocol beforehand.

6.4.4 Emissions Input Development

Stack Parameters. Stack parameters required for modeling BART-eligible units include: height of the stack opening from ground, inside diameter, flow-rate, exit gas temperature, ground elevation of the stack base, and location coordinates of the stack. Because the BART modeling focuses on mesoscale transport to Class I areas, other source term parameters (needed to calculate localized impacts) such as building heights and widths for calculating downwash may not be needed.

Emission Rates. Emission rates for CALPUFF screening analyses follow EPA's BART guidance and recent staff recommendations. Source terms in the modeling should be based on emissions during periods of high capacity utilization during normal operating conditions. Specifically, the 24-hour average actual emission rate with normal operations from the highest emitting day of the year should be modeled. Excluded from consideration are days where start-up, shutdown or malfunctions occurred unless these activities are regular, frequently occurring components of the source's operation cycle. (Note that while potential emissions are used to determine if a source is BART-eligible, 24-hour average maximum emissions are used for CALPUFF screening modeling purposes). Pollutants considered include SO_2, H_2SO_4, NO_x and PM_{10}. Excluded from the modeling are pollutants with emissions less than *de minimis* levels (40 tons per year for SO_2 and NO_x and 15 tons per year for PM_{10}).

Identification of the maximum 24-hr actual emissions rates should be made for the most recent 3 or 5 years, according to the following prioritization:

- Continuous Emissions Monitoring (CEM) data;
- Facility emissions tests;
- Emissions factors;
- Permit limits; or lastly,
- Potential to emit.

In cases where a unit is permitted to burn more than one fuel, the fuel resulting in the highest 24-hr emission rates should be used for the modeling. Caution is urged when estimating emissions rates in cases where abnormal and infrequent fuel usage overstate the potential for visibility improvement. Typically BART controls are expected to include the utilization of cleaner fuels (such as those burned by a facility in the more recent years). Thus emissions rates should solely be based upon data from the most recent years, in order to accurately characterize potential visibility improvements from BART controls.

Emissions Speciation. Definition of the PM speciation profile for the highest 24-hour average actual emissions may prove particularly challenging but reliable estimates are necessary given the widely varying effects of different types of particulate matter on visibility. For example, the extinction coefficient ranges in value from 0.3 to 0.6 m^2/g for coarse particles, to 1.0 to 1.25 m^2/g for fine inorganic particulate matter, to 1.5 to 4.0 m^2/g for sulfate and nitrate precursors, to 1.8 to 4.7 m^2/g for organic aerosols, and up to 8-12 m^2/g for elemental carbon (Tombach and McDonald, 2003). Thus, generalized, conservative, or arbitrary assignments of particulate emissions to different pollutant categories can have a considerable influence on modeled visibility impacts attributable to a single facility. Currently, data are quite limited on appropriate speciation of organic/inorganic and filterable/condensable emissions by source category. While speciation profiles are available for gas- and oil-fired combustion turbines and coal combustion processes, detailed profiles for the full range of BART-eligible sources is lacking.

In practice, except in cases where facilities operate continuous emission monitors on all affected equipment, there is likely to be limited information of regarding actual emissions on the requisite time resolution (24-hour average), much less speciation profiles for PM species. Thus it is particularly important for state/local agencies to work with BART-eligible sources to collect this information. Where available, facility-specific particulate matter speciation measurements may be used to assign PM_{10} to its components (e.g., assume primary sulfate is a fraction of SO_2 emissions, primary sulfate is a fraction of PM_{10} emissions, all PM_{10} emissions are $PM_{2.5}$). Absent this information, default speciation profiles may be used as agreed upon in the protocol.

Condensable Emissions. Condensable emissions are considered primary fine particulate matter. For screening assessments all condensable mass should be assigned to the < 0.625 μm category unless the source operator has evidence of a different value based on emissions testing or other reliable information. This maintains conservatism in the analysis where there may be uncertainty regarding the exact size of condensable PM mass. If actual source emissions data are not available, the modeling should be based on permit limits. If source-specific size categories are not available, then AP-42 factors may be used for sources where AP-42 factors are available. For sources where AP-42 factors are not available, assumptions for partitioning should be resolved with the reviewing agencies during the protocol development process.

Size Classification of Primary PM Emissions. PM emissions should be segregated by size category. NPS has developed PM_{10} emissions speciation for certain source groups and this information can be used where appropriate. Modelers using information from AP-42 or other ‘reference’ documents must remember that the PM size classification should be applied only to the “filterable” PM mass. Furthermore, when modeling PM size classes, an appropriate “mass mean diameter” must be used that is within the specified particle size range. Use of a mass mean diameter equal to the top of the range is inappropriate since it will overestimate PM deposition and possibly underestimate PM concentrations and visibility impacts.

6.4.5 CALPUFF Model Configuration

This section discusses the procedures and input assumptions that States or source operators should follow in applying the CALPUFF model in a screening mode to assess whether a particular source is subject to BART (i.e., BART exemption modeling).

CALPUFF Model Options. The model options, parameter settings, and ‘switches’ for exercising CALPUFF in the BART screening mode are discussed below. Appendix B contains tables that list the recommended screening configurations for CENRAP BART modeling. The tables also identify the default recommendations from the IWAQM Phase 2 Report (EPA, 1998).

Visibility Modeling Domain. The CALPUFF domain should be configured to include the source and all Class I areas within 300 km. An additional 50 km buffer zone should be established in each cardinal direction from the source. For screening applications, CENRAP recommends CALPUFF for all source-receptor distances unless otherwise negotiated in the modeling protocol.

Dispersion

Building Downwash. In the unlikely case where a source is immediately upwind of a Class I area (say, within 20 km), the IWAQM-recommended algorithms for sources subject to downwash should be used. For consistency across all CENRAP regional modeling studies, the CALPUFF building downwash algorithms should be used for all source-receptor distances if building data are available.

Puff Dispersion. The EPA (1998) guidance for plume dispersion modeling should be followed, including the use of the Pasquill-Gifford curves. The use of turbulence-based dispersion coefficients and probability density function dispersion methods have not been extensively evaluated for use in long range transport evaluations. Until such an evaluation has been completed and documented, the use of turbulence-based coefficients is outside the current CENRAP guidance and will require a case-by-case determination by the appropriate regulatory reviewing authorities.

Puff Representation. Use the default integrated puff sampling methodology in CALPUFF.

Puff Splitting. There is no quantitative evidence that the horizontal and vertical puff-splitting algorithms in CALPUFF yield improved accuracy and precision in model estimates of inert or linearly reactive pollutants although conceptually the methods have appeal in that they attempt to mimic lateral and vertical wind speed and direction shears. Since there is no direct evidence confirming the correctness of the puff-splitting algorithms, the decision whether to invoke the algorithms should be addressed in the modeling protocol. For screening applications, an added degree of conservatism at large down wind distances (> 200 km) *may* result if puff splitting is not be invoked. For source-specific applications (Chapter 7), puff splitting may be used as set forth in the protocol subject to concurrence by the cognizant reviewing agency. In sum, until verified with atmospheric data, the puff splitting remains an *ad hoc* procedure whose real impact on model reliability is unknown. In some cases, it may be prudent to use full-science regional models to circumvent this limitation of Lagrangian models.

Chemistry

Chemical Mechanism. The MESOPUFF II module should be used for all screening (and source-specific) BART applications. For the aqueous phase conversion of SO_2 to sulfate (important when the plume interacts with clouds and fog), the IWAQM defaults are recommended, i.e., nighttime SO_2 loss rate (RNITE1) is assumed to be 0.2 percent per hour. The nighttime NOx loss rate (RNITE2) and HNO_3 formation rate (RNITE3) are both set to 2.0 percent per hour.

Species Modeled. Species to be modeled in the screening assessment include SO_2, SO_4, NO_x, HNO_3, NO_3 and particulate matter. Absent detailed speciation and size distribution data from the source, PM should be modeled in two (2) size categories, fine (0.0-2.5 µm) and coarse (2.5-10.0 µm), consistent with the IMPROVE reconstructed mass equation. Particulate matter emissions by size category should be combined wherever possible into the appropriate species for the visibility analysis. These species include (a) elemental carbon (EC), (b) fine PM or “soil” (< 2.5 µm in diameter), (c) coarse PM (between 2.5-10 µm in diameter) and (d) organics, referred to as secondary organic aerosols in the CALPOST postprocessor. If source-specific emissions factors are not available, AP-42 factors can be used to estimate the PM speciation for those source sectors for which AP-42 emissions factors have been developed. Otherwise assumptions will need to be proposed by the source operator and approved by the state, EPA and FLM.

Background Ozone Concentrations. Ozone concentration data for 2001-2003 from ambient AIRS/AQS monitors located within the particular domain being modeled should be used to develop background estimates. Only non-urban ozone stations should be used in the OZONE.DAT file. Monthly average ozone background values should be computed from daytime average ozone concentrations (6 am to 6 pm average).

Background Ammonia Concentrations. In CALPUFF screening applications, the background ammonia concentration is assumed to be temporally and spatially invariant. Background ammonia estimates should be developed from CENRAP's most recent CMAQ or CAMx simulation for the 2002 base year. Because CMAQ/CAMx modeled and observed monthly averaged ammonia concentrations exhibit wide spatial variability, we recommend obtaining separate monthly-averaged ammonia concentrations from CMAQ or CAMx for the CENRAP north, central and south modeling domains, respectively. These would then be used as input to CALPUFF. The CENRAP 2002 monthly domain average ammonia for each CENRAP subdomain should also be used for the corresponding months in 2001 and 2003.

6.4.6 Post Processing

POSTUTIL Parameters. User-selected options, parameter settings, and 'switches' for exercising POSTUTIL in a screening mode are presented in Appendix C. This appendix contains tables that list the recommended screening and default configurations for CENRAP BART modeling. The ammonia-limiting method (ALM) in CALPUFF (Escoffier-Czaja and Scire, 2002, 2005) repartitions nitric acid and nitrate on a receptor-by-receptor and hour-by-hour basis to account for the models systematic over-prediction due to overlapping puffs. For screening applications, the user should set the parameter MNIRATE=1 in POSTUTIL to implement this approximate correction in its simplest form. The background ammonia concentration obtained from CAMx or CMAQ regional simulations on the three CENRAP subdomains should be used for consistency.

CALPOST Parameters. Appendix D contains summarizes the CALPOST post-processor options, parameters, and switches. Tables are presented containing recommended and default configurations for CENRAP BART modeling. While all receptors should be included in a single CALPUFF simulation, one may calculate the visibility impacts in CALPOST for each Class I area separately using the NDRECP parameter. It specifies the receptor range to be processed in CALPOST. Given the importance of the CALPOST processor to the entire BART visibility estimation, process, we focus specifically on the parameter settings and input assumptions for CALPOST in the following section.

6.5 Visibility Assessment

The recommended procedure for quantifying visibility impacts was described in Chapter 3. The key point is that the light extinction coefficient (b_{ext}) can be calculated from the IMPROVE Equation as:

$$b_{ext} = 3\ f(RH)\ [(NH_4)_2SO_4] + 3\ f(RH)\ [NH_4NO_3] + 4[OC] + 1[Soil] + \qquad (6\text{-}1)$$

$$+ 0.6[\text{Coarse Mass}] + 10[\text{EC}] + b_{Ray}$$

The monthly site-specific f(RH) values are obtained for each mandatory Federal Class I Area from Table A-3 in the EPA (2003) guidance document. Then, the haze index (HI), in deciviews, is calculated in terms of the extinction coefficient via:

$$HI = 10 \ln (b_{ext}/10) \quad (6\text{-}2)$$

The change in visibility (measured in terms of 'delta-deciviews') is then compared against background conditions. The delta-deciview, Δdv, value is calculated from the source's contribution to extinction, b_{source}, and background extinction, $b_{background}$, as follows:

$$\Delta dv = 10 \ln (\{b_{background} + b_{source}\}/ b_{background}) \quad (6\text{-}3)$$

If the Δdv value is greater than the 0.5 dv threshold, the source is said to contribute to visibility impairment and is thus 'subject to BART' controls. If not, it is BART-exempt.

6.5.1 Visibility Impacts from BART-Eligible Sources

Class I Receptors. Within the CENRAP domain, there are twenty three (23) Federally mandated Class I areas. These areas are listed in Table 6-4. For each area, the National Park Service has developed a receptor file containing specific coordinates and elevation data. (http://www2.nature.nps.gov/air/Maps/Receptors/index.cfm).

Visibility Impact Method. In the screening approach, CALPOST should be run using Method 6 (MVISBK=6) for calculating extinction. That is, monthly f(RH) adjustment factors are applied directly to the background and modeled sulfate and nitrate concentrations, as recommended in the BART guidelines. Note that the RHMAX parameter (the maximum relative humidity factor used in the particle growth equation) is not used when Method 6 is selected. Similarly, the relative humidity adjustment factor (f(RH)) curves in CALPOST (e.g., IWAQM growth curve and the 1996 IMPROVE curve) are not used when MVISBK is equal to 6.

Monthly average Class I area-specific relative humidity values should be employed in the extinction analysis (EPA, 2003, Table A-3). Species to be considered include SO_4, NO_3, EC, SOA (i.e., condensable organic emissions), soil, and coarse PM. With Method 6, background extinction coefficients are computed from EPA (2003) monthly estimates of concentrations of ammonium sulfate (BKSO4), ammonium nitrate (BKNO3), coarse particulates (BKPMC), organic carbon (BKOC), soil (BKSOIL), and elemental carbon (BKEC). Values for these coefficients are listed in Table 6-3 and Appendix B. In screening analyses, the extinction due to Rayleigh scattering (i.e., the scattering of light by natural particles much smaller than the wavelength of the light) should be set to 10 Mm^{-1} (BEXTRAY = 10.0) for all Class I areas.

Natural Background Light Extinction. EPA's BART guidance recommends that visibility impacts should evaluated against 'natural' background conditions. EPA (2003) describes the calculation of the annual average background extinction (in 1/Mm) for a Class I area using the area's annual f(RH) and average natural concentrations based on the area's geographic location. Annual average background extinction values (in 1/Mm) are converted to annual average Haze Index (HI) values (in deciview or dv). Then, the average HI value for the 20% best visibility days (Best Days (dv)) is estimated from 10th percentile of the annual average HI value for a Class I area assuming a normal distribution. Thus, no average natural concentrations are provided for determining extinction for the 20% best visibility days. EPA maintains that the above definition of natural visibility baseline as the 20% best visibility days is likely to be reasonably conservative and consistent with the Regional Haze Rule goal of natural conditions.

There are major technical issues with this approach: (a) the same concentrations assumed at all Class I areas in the East or West, (b) the same concentrations assumed to occur every month of the year, and (c) fine sea salt and associated water is not included. Also, in the calculation of 20% best visibility days, the same frequency distribution is assumed for every Class I area in the East or in the West. In other words, 'one size fits all' (Tombach, 2004). But this really is not the case.

The background extinction computation with Method 6 in CALPOST involves user-supplied monthly concentrations of SO_4, NO_3, PM coarse, organic carbon, soil, and elemental carbon species. In practice, concentrations for only 2 species, SO_4 ([BKSO4]) and soil ([BKSOIL]), are supplied in the CALPOST input file to represent hygroscopic and non-hygroscopic portions of background extinction, respectively. Furthermore, the species concentrations are held constant over the annual cycle (i.e., no daily, monthly, or seasonal variation). Finally, the EPA natural background default values are defined separately for the eastern and western U.S. result in natural background extinction values that vary spatially and temporally only in response to the spatial distribution and monthly variation of climatologically-representative relative humidity values (EPA, 2003, Table A-3). Thus, the default definition of natural conditions does not take into account meteorologically caused visibility impairment.

For CALPUFF screening analyses, these EPA (2003) default procedures for calculation of light extinction should be used for current and natural background conditions. Table 6-3 provides the species concentrations representing natural background conditions for the western and eastern Class I areas. As shown in Figure 6-1, EPA's east-west division cuts through the middle of the CENRAP domain. Accordingly, in the modeling protocols, the states and source operators will need to determine whether receptors in a particular Class I area fall within the East or West domains as this determines the appropriate default background light extinction values to use from Table 6-3.

Impact Threshold. The EPA BART guidance recommends that the threshold value for defining whether a source "contributes" to visibility impairment is 0.5 dv change from natural conditions. States may set a lower threshold. BART determinations are based upon the 98th percentile of the predicted 24 hour averaged deciview impact deduced from the CALPOST postprocessor. More specifically, to determine if a source may be exempted from BART, the highest modeled delta-deciview value for each modeling day for each modeled receptor should be determined. Depending on the yearly distribution of the results, the most conservative (i.e., highest) 98 % impact may come from the maximum 8th highest value for each of the three years or the 22nd highest value for all years combined (if three years of data and 365 values for each year are calculated). States and source operators should use both methods in order to identify the higher value. The peak impact is then compared to the 0.5 dv contribution threshold value. If the maximum 8th highest value for each of the three years (or the 22nd highest value for all years combined) exceeds the "contribution" threshold of 0.5 deciviews the source is declared 'subject to BART', potentially triggering a source-specific CALPUFF modeling analysis (Chapter 7). Otherwise, the source is BART-excluded. In a cooperative agreement with EPA Regions VI and VII and federal land managers, CENRAP guidance deviates from use of the 98^{th} percentile. The CALMET datasets as described in this protocol were processed with the 'NO-OBs' options, (i.e., surface observations were not used in the CALMET wind field interpolation). Aware that exercising CALMET with 'NO-OBs' may lead, in some applications, to potentially less conservatism in the CALPUFF visibility results compared with the use of CALMET with observations, CENRAP has agreed to EPA's recommendation that the maximum visibility impact rather than the 98^{th} percentile value should be used for screening analyses using the CENRAP developed CALMET datasets.

To conserve computational and analysis resources, the CALPUFF screening modeling may be performed sequentially for calendar years 2001, 2002, and 2003. If a BART source is found to be subject to BART following the first or second annual evaluation, the additional year(s) need not be processed. Evaluation of all three years will be required to exclude a BART eligible source from the BART determination process.

Since the current regulatory version of CALPOST does not generate 98 percentile results, states or source operators may wish to use a modified version of CALPOST that generates a file with a full distribution of daily delta-deciview values for each receptor. The Colorado Department of Public Health and Environment (CDPHE, 2005) has developed a FORTRAN processor to generate 98^{th} percentile results and it is available upon request.

6.5.2 Change in Visibility Due to BART Controls

According to the BART guidelines, a single source responsible for a 1.0 dv change or more should be considered to "cause" visibility impairment and a source that causes less than a 1.0 dv change may still *contribute* to visibility impairment and thus be subject to BART. For sources determined to be subject to BART, additional modeling is needed to assist in identifying various control options and selecting the "best" alternative. The BART guidelines identify five factors to be considered when determining what BART should be for a specific source. These include: (a) any pollution control equipment in use at the source (which affects the availability of options and their impacts), (b) the costs of compliance with control options, (c) the remaining useful life of the facility, (d) the energy and non air-quality environmental impacts of compliance, and (e) the degree of improvement in visibility that may reasonably be anticipated to result from the use of such technology.

For the visibility analysis (the fifth factor in determining what BART should be), it is up to the state to determine how to weigh the impacts. The 1.0 Δdv threshold might be one of the parameters that is used although it is not required. The 98% value at this step in the analysis is also not required. For example, visibility improvement of 1.0 Δdv may be predicted on 4 days out of the year, and the state may determine that is significant rather than judging it to be insignificant because it does not occur on 8 or more days.

6.6 Presentation of Modeling Results

The CALPOST processor computes the daily maximum change in deciviews. As noted above, the maximum 8^{th} highest value for each of the three years or the 22^{nd} highest value for all years must be compared to the 0.5 deciviews threshold. At a minimum, tabular presentation of the following results should be provided:

- > Number of receptors within each Class I area with impacts > 0.5 dv;

- > Number of days at all receptors within each Class I area with impacts > 0.5 dv;
- > Number of Class I areas with impacts > 0.5 dv; and
- > At each receptor, the magnitude of the change in extinction.

A variety of other tabular and graphical summaries may be desirable as well.

6.7 Reporting of CALPUFF Screening Assessment Modeling Results

The report accompanying the screening CALPUFF modeling should provide a clear description of the modeling procedures followed and the results of the analysis. Any departures from the approved modeling protocol should be discussed and justified. The report should also include a discussion of the uncertainty in the modeling results and the likelihood that the screening process was effective in its determination. Any needs for source-specific or alternative modeling should be identified. Accompanying the modeling report should be an electronic archive (CDs, DVDs, or removable USB2/IEEE 1394 hard drives as appropriate) that includes the full set of CALPUFF inputs and model output fields and well as any pre- or post-processor codes used to generate the results. The CENRAP 6 km regional CALPUFF-ready meteorological fields do not need to be included in the archive. The modeling data archive should be sufficiently complete as to allow an independent modeler to fully corroborate the CALPUFF screening results.

Table 6-1. Contents of a Typical Screening BART Modeling Protocol.

- **1.0 INTRODUCTION**
  - **1.1 Objectives**
  - **1.2 Location of Source and Relevant Class I Areas**
  - **1.3 Source Impact Evaluation Criteria**
  - **1.4 Modeling Study Participants**
  - **1.5 Protocol Review Process**
  - **1.6 Schedule**
- **2.0 SOURCE DESCRIPTION**
  - **2.1 Unit-specific Source Data**
  - **2.2 Nearby Sources Affecting Same Class I Areas**
- **3.0 MODEL INPUT DATA**
  - **3.1 Modeling Domain**
  - **3.2 Terrain and Land Use**
  - **3.3 Emissions Data Base**
    - **3.3.1 Stack Parameters**
    - **3.3.2 Emissions Rates**
    - **3.3.3 Condensable Emissions**
    - **3.3.4 Speciation and Size Distributions**
  - **3.4 Meteorological Data Base**
    - **3.4.1 CENRAP CALMET Data Sets**
    - **3.4.2 Observational Data**
  - **3.5 Air Quality Data Base**
    - **3.5.1 Ozone Concentrations**
    - **3.5.2 Ammonia Concentrations**
    - **3.5.3 Concentrations of Other Pollutants**
    - **3.5.5 CENRAP Regional Modeling Data Sets**
  - **3.6 Natural Conditions at Class I Areas**
- **4.0 CALPUFF MODELING METHODOLOGY**
  - **4.1 Model Selection**
  - **4.2 Domain Configuration and Receptors**
  - **4.3 CALPUFF Configuration**
  - **4.4 Light Extinction and Haze Impact Calculations**
  - **4.5 Modeling Results**
  - **4.6 Uncertainty Analysis**
- **5.0 EXEMPTION MODELING**
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APPENDIX A: CALMET Inputs
APPENDIX B: CALPUFF Inputs
APPENDIX C: POSTUTIL Inputs
APPENDIX D: CALPOST Inputs

Table 6-2. CALMET/CALPUFF Model Codes for Screening Applications.

PROCESSOR	VERSION	LEVEL
TERREL	3.311	030709
CTGCOMP	2.42	030709
CTGPROC	2.42	030709
MAKEGEO	2.22	030709
CALMM5[a]	2.4	050413
CALMET	5.53a	040716
CALPUFF	5.711a	040716
POSTUTIL	1.4	040818
CALPOST	5.51	030709

a: The versions of CALMM5 (version 2.4, level 050413) and of CALMET (version 5.53a, level 040716) are not compatible as published. Alpine Geophysics developed software modifications to reconcile the two. The code is available at: www.alpinegeophysics.com.

Table 6-3. Default Natural Background Concentrations (μg/m$_3$) for Eastern and Western U.S. Class I areas. (Source: EPA, 2003, Table 2-1)

	Average Natural Concentration West (μg/m^3)	Average Natural Concentration East (μg/m^3)	Error Factor	Dry Extinction Efficiency (m^2/g)
Ammonium sulfate[b]	0.12	0.23	2	3
Ammonium nitrate	0.10	0.10	2	3
Organic carbon mass[c]	0.47	1.40	2	4
Elemental carbon	0.02	0.02	2-3	10
Soil	0.50	0.50	1½ - 2	1
Coarse Mass	3.0	3.0	1½ - 2	0.6

a: After Trijonis (1990)
b: Values adjusted to represent chemical species in current IMPROVE light extinction algorithm; Trijonis estimates were 0.1 μg/m^3 and 0.2 μg/m^3 of ammonium bisulfate.
c: Values adjusted to represent chemical species in current IMPROVE light extinction algorithm; Trijonis estimates were 0.5 μg/m^3 and 1.5 μg/m^3 of organic compounds.

Table 6-4. Federal Class I Areas in the CENRAP Domain.

Federal Class I Areas in the CENRAP Domain		
Class I Area	ST	Name
Big Bend National Park	TX	BIBE
Boundary Waters Canoe Area	MN	BOWA1
Breton	LA	BRET1
Caney Creek	AR	CACR1
Guadalupe Mountains Nat'l Park	TX	GUMO1
Hercules Glades	MO	HEGL1
Mingo	MO	MING1
Upper Buffalo Wilderness	AR	UPBU1
Voyageurs National Park	MN	VOYA2
Wichita Mountains	OK	WIMO1

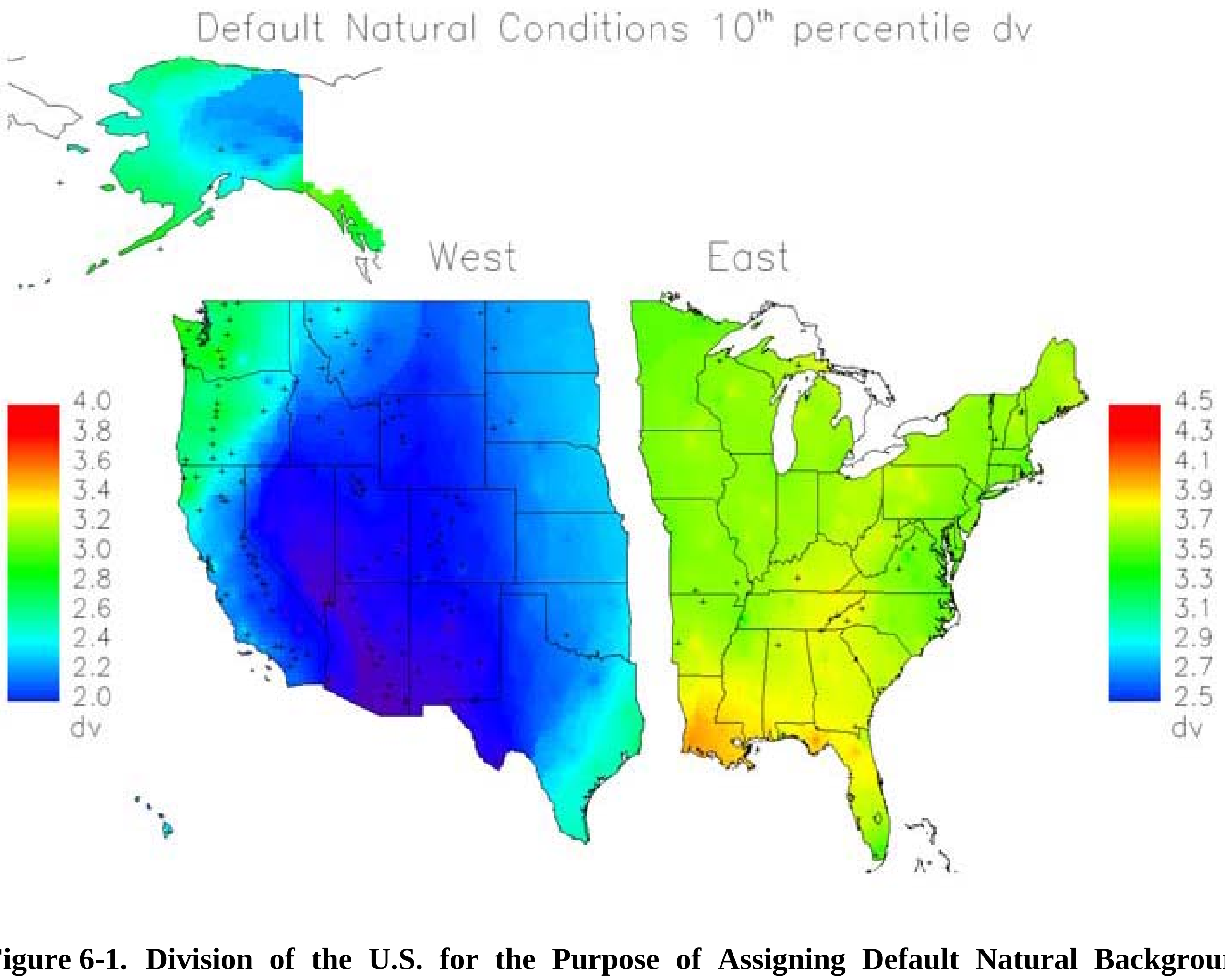

Figure 6-1. Division of the U.S. for the Purpose of Assigning Default Natural Background Concentrations (µg/m_3) for Eastern and Western U.S. Class I areas. Depicted are the Estimates of the Default 10% Natural Haze Index Values (in dv). (Source: EPA, 2003).

7.0 CALPUFF SOURCE-SPECIFIC APPLICATIONS

The BART process provides an option for source-specific modeling to be performed. There are a number of reasons why a more detailed approach than that discussed previously may be desired. For example, sources very close to Class I areas may elect to use finer grid resolution than the 6 km gridded fields provided by CENRAP. Also, it may be desirable to reduce the uncertainties in assumed background ammonia, hydrogen peroxide, and ozone concentrations. These and other refinements in model inputs may help to clarify whether a source should be excluded from BART and/or to quantify the expected visibility impacts of alternative BART controls on an affected source.

7.1 Methodology

Source-specific CALPUFF modeling may be helpful in demonstrating more convincingly that a source does not cause or contribute to visibility impairment in any Class I areas, and thus can be exempted from BART controls. If the initial modeling does not pass the screening threshold for visibility impacts, the next step is to conduct source-specific modeling, perhaps using a finer grid resolution for the meteorological fields, improved treatment of terrain effects and land use variability, and the inclusion of more refined model parameterizations such as consideration of time and space-varying ammonia and ozone concentration fields. As with the screening method, in the source-specific modeling, the visibility threshold is based on the BART guidance of the 98^{th} percentile change in deciview value.

The BART guidance indicates that the emissions rates to be used for exemption modeling is the highest 24-hr rate during the modeling period. Depending on the availability of source data, the following *24-hr maximum emissions rate information* (listed in order of priority) should be used with CALPUFF for BART exclusion modeling:

- Emissions for the period 2001-2003 (CEM data);
- Emissions for 2002 (CEM data);
- Actual 2002 emissions rates in state CERR inventory;
- Emissions factors from AP-42 source profiles;
- Permit allowable emissions, if available; or finally
- Potential to emit.

A source-specific modeling analysis will likely be required for all sources located within 50 km of a Class I area. EPA's BART guidance recommends that expert modeling judgment be used, "giving consideration to both CALPUFF and other methods." While the PLUVUE-II plume visibility model is mentioned as a possible alternative approach to consider in addition to CALPUFF within 50 km of a source, the CALPUFF model appears to offer greater realism, provided sufficiently small grid resolution ($\leq$ 4 km) is used. As discussed in Chapter 3, there are no fundamental reasons why CALPUFF cannot be used for much shorter transport distances than 50 km, as long as the scale of the plume is larger than the scale of the output grid. This requirement must be met in order that the maximum concentrations and the width of the plume are adequately represented (and the sub-grid details of plume structure can be ignored when estimating effects on light extinction). Use of a 1 km CALPUFF modeling grid for Class I area receptors should be sufficient for source-receptor distances in the 25-50 km range; a finer grid may be needed for transport distances much smaller than 25-30 km.

If source-specific modeling shows that a particular source causes or contributes to visibility impairment at a Class I area, the CALPUFF modeling system can then be used to quantify the visibility benefits from various BART control options. This is accomplished by running CALPUFF with the baseline emissions rates and with emissions after BART controls. It is important that emission reductions be evaluated in the post-processing step rather than by using “negative” emission rates in the CALPUFF model. The chemical scheme requires that emission rates always be positive.

7.2 Source-Specific Considerations

7.2.1 Protocol Development and Negotiation.

For any source-specific application, a modeling protocol that defines source properties and the specific model configuration and application approach is required. An example of typical elements of a source-specific protocol is given in Table 7-1. This protocol should be reviewed with the state, EPA, and FLM.

7.2.2 Domain Definition.

While source-specific modeling can be carried out on one or more of the three CENRAP domains (Figures 5-1 through 5-3) with the 6 km MM5/CALMET fields for 2001-2003, it may be more appropriate to develop a specialized modeling domain and with finer resolution meteorological fields. Because CENRAP has not developed fine-scale CALMET files, the state or source operator will have to do this. Particularly in rough terrain or in coastal areas, finer horizontal grid spacing may be useful in source-specific simulations to better characterize the flow fields and land use changes. A typical source-specific CALMET meteorological domain might consist of a 300 x 300 array of 1-2 km grid cells covering the domain of interest. This produces a reasonable number of grid points that can easily be accommodated on personal computers. Domains with up to 600^+ x 600^+ grid cells are sometimes necessary (for long transport distances), while domains with fewer than 100 x 100 cells generally are not used in a source-specific analyses because they cover insufficient territory.

For source-receptor distances < 50km, even finer grid resolution than 1 km may be needed, particularly if complex terrain or coastal meteorological effects are likely to be important. This determination should be made on a case-by-case basis. There is no single distance at which a particular grid size is appropriate. It depends on factors such as the complexity of the terrain, the source-receptor distances involved, the location of the source relative to the terrain features, the physical stack parameters (e.g., a tall stack in complex terrain may be unaffected by the terrain-forced flow), proximity of the source and Class I area to a coastline, and other factors including availability of representative observational data.

7.3 CALMET Configuration for Source-Specific Assessments

The CALMET processor accepts observational data in the form of hourly surface observations of winds, temperature, pressure and cloud data, hourly precipitation observations, and twice-daily upper air sounding data of winds, pressure and temperature. In addition, CALMET allows the use of three-dimensional gridded fields of data from prognostic models such as MM5. CALMET can be run in a mode using observations only (Obs-mode), prognostic data only (No-Obs mode) or both sets of data (hybrid mode). For example, one possible approach is to consider using the CALMET “hybrid” mode which incorporates surface observations with prognostic data, but does not include the use of upper air data (option NOOBS = 1).

In preparing the regional MM5/CALMET fields for the CALPUFF *screening* applications (Chapter 6), CALMET was exercised on a regional 6 km resolution domain (Figure 5-1) in No-Observations mode using the highest resolution MM5 data available for each year modeled. For *source-specific* modeling of Class I areas located in complex terrain or coastal regions, it may be desirable to develop meteorological fields over finer resolution grids (i.e.,. 1-4 km scale). In these cases there may be reasons to invoke the hybrid mode of CALMET option. In determining which method to use, the State or source operator should evaluate the following factors in the specific context of the source and the affected Class I area.

Time and space resolution of observational data. Upper air observational data are available at roughly 12-hourly intervals and the spacing between sounding locations is typically several hundred kilometers. Because CALMET performs a time interpolation of wind data between the sounding intervals, this linear time-interpolated wind data will not be able to retrieve important patterns of wind variation at scales less than 12 hours.

Time and space resolution of 3-D prognostic data. The MM5 output fields provide hourly "soundings" over a 36 km or 12 km grid at hourly intervals. This hourly time resolution of the prognostic model fields is likely to better characterize the time variation of wind flows across the domain. However, on scales smaller than the MM5 grid nest (say below 12 km) the MM5 fields may miss potentially important local flow features that might be reflected in local surface measurement networks.

Representativeness of observational data. A key question, then is whether one has confidence that the spatial and temporal representativeness of the local measurement stations is sufficient to favor measurements over prognostic modeled fields at the local scale. While use of measurements is attractive in many situations, too great a reliance measurements introduces the possibility of spurious wind or thermodynamic variable variations because the CALMET data interpolation methods does not obey the combined laws of momentum and energy conservation. This is particularly an issue where there are measurement sites of questionable representativeness or data quality. Therefore, careful inspection of the actual surface measurement sites to be used in the Obs-mode is needed before the method is used.

Discrepancies between prognostic winds and observations. The CALMET diagnostic wind field module attempts to reduce discrepancies between the prognostic model-derived initial guess fields and the observations by giving greater weight to the observations in the "vicinity' of the observations and greater weight to the prognostic wind fields in portions of the domain away from the observations. Although the prognostic model simulation reflects observational data through the use of four-dimensional data assimilation, there will sometimes be discrepancies between the observations (which may reflect a very localized flow) and the 36 km or 12 km resolved MM5 winds. Sometimes the differences are due to poor time resolution of the observational data; at other times they may result from poor instrument placement or faulty observations. In such cases, blending of the MM5 data with the observations (i.e., the hybrid mode) can lead to wind structures which may not be realistic.

Model biases. The MM5 model predictions of winds and temperatures may contain biases relative to the real atmosphere. In particular, MM5 sometimes underestimates the frequency of light wind and calm wind conditions and possibly underestimates the strength of the nocturnal surface temperature inversion. These biases may be most important for near surface sources when relative coarse grid resolution is used. If the adequacy of the MM5 fields becomes a concern, the state or source operator may wish to examine the detailed MM5 model evaluation reports prepared by the original modelers (see Chapter 5).

Level of effort vs. benefit. The preparation of observational datasets for CALMET on large regional domains involves a considerable effort due to the large number of surface, precipitation and upper air stations involved. The question is whether the effort associated with the preparation of this dataset is worthwhile given that the regional winds over the three CENRAP sub-domains (Figure 5-1) may be better characterized by the three-dimensional MM5 model dataset than time- and space-interpolated of observational data, especially above the surface where sounding data is fairly sparse spatially and poorly-resolved in time. For source-specific modeling, the decision whether to exercise CALMET in the hybrid mode is left to the state or source operator who are in the best position to assess the relative strengths and drawbacks of the two modes of operation *in the specific context of the source they are modeling*. Given the orography of the CENRAP domain, the regional wind patterns are likely to be adequately characterized at the 6 km scale via the use of MM5/CALMET with No-obs. However, at the finer grid scales that may be considered in source specific modeling (1-4 km), introduction of particularly well sited monitors – especially in key impact areas – may be appropriate.

Care must be taken to ensure that the introduction of the local observations into the CALMET processing does not extend the influence of the observational data beyond its true representativeness and result in internally inconsistent flow features. On smaller domains with higher CALMET grid resolution, more control over the region of influence of the meteorological observations can be achieved and it may be easier for the diagnostic model to allow the local flow observations to have appropriate influence in the vicinity of the observation, yet still allow terrain-adjusted flow to dominate away from the observations. Given that the sub-regional domains will be used especially in complex flow situations (complex terrain and coastal regions), the relatively coarse-scale MM5 simulations are less likely to be adequate, and the introduction observational data may indeed yield improvements in the resulting meteorological fields.

The decision on how the MM5/CALMET processing should be performed for source-specific modeling requires consultation with the State, regional EPA office and the FLM overseeing the Class I area of concern. A decision to allow ingestion of meteorological observations into the CALMET processing at the finer grid scales (i.e., below 6 km) should be contingent upon commitment to a thorough analysis of the instrument location, quality assurance record, and spatial/temporal representativeness of the each monitoring station to be used in the CALMET interpolation. For the reasons discussed above, absent this assessment of the measurement data representativeness, ingestion of observational data may in fact degrade the integrity of the resultant CALMET meteorological fields and the modeler/decision-maker may not be aware of it.

7.4 CALPUFF Configuration for Source-Specific Assessments

Domain-specific CALPUFF input parameters must be defined for each source-specific modeling analysis. In addition to finer grid spacing in the CALMET and CALPUFF models and the possible introduction of observational data in the CALMET simulations, several other modeling enhancements can serve to increase the realism of the source-specific modeling. These include use of higher resolution terrain digital elevation model data (~3 arcsec USGS data) in defining the gridded terrain fields, and the use of time-varying ammonia and ozone concentrations rather than constant values.

7.4.1 Background Conditions

Background Ozone Concentrations. Ozone concentrations required as input to source-specific CALPUFF should be derived from regional model simulations obtained from CENRAP or the other RPOs in preference to the use of AIRS/AQS ozone measurements at discrete monitors (see discussion in section 7.4.3 below).

Background Ammonia Concentrations. NH_3 concentrations required as input to source-specific CALPUFF modeling should be derived from regional model simulations obtained from CENRAP/s CAMx or CMAQ modeling or the modeling by other RPOs in preference to the use of CASTNet or other network ammonia measurements at discrete monitors (see discussion in section 7.4.3 below). In addition to representing a better-science approach, this has the advantage of making the BART analyses more consistent with the CENRAP's reasonable progress modeling for regional haze.

7.4.2 Ammonia Limiting Method (ALM)

CALPUFF calculates linear oxidation of sulfur dioxide (SO_2) to sulfate (SO_4) and nitric oxides (NO_x) to nitric acid (HNO_3) and nitrate (NO_3). The equilibrium between nitric acid and nitrate that is a nonlinear function of temperature and relative humidity and the equilibrium constant can vary substantially over a typical diurnal cycle, as the temperature and relative humidity change. In addition, the availability of ammonia (to form ammonium nitrate) affects ambient concentrations of nitrate. Because sulfate preferentially scavenges ammonia, the amount of ammonia remaining for the formation of nitrate may be limited. Thus, ammonia-limiting effects can be important under certain conditions in assessing the impacts of nitrate aerosols on visibility (Blanchard and Hidy; 2003; Escoffier-Czaja and Scire, 2002).

In the screening approach (Chapter 6), the ALM was recommended using a constant background ammonia concentration relevant to the dominant land use in the Class I area being modeled was assumed (i.e., 0.5 ppb for forest, 1.0 ppb for arid lands, 10 ppb for grasslands.) For *source-specific analyses*, time-varying, user-supplied NH_3 concentrations may be imposed as boundary conditions to each modeled puff, while cumulative ammonia consumption is modeled in the POSTUTIL processor for conditions at the final endpoint of the puff (i.e., the Class 1 receptor). In addition, the boundary concentration module within CALPUFF can be invoked to allow for time- and space-varying background concentrations. Use of the ALM method in conjunction with background source boundary conditions may improve the modeled NO_3 predictions somewhat in source-specific analyses.

In CALPUFF, a nominal background ammonia concentration is used in conjunction with the HNO_3/NO_3 equilibrium relationship to estimate the amount of nitrate formed. However, the model's Lagrangian puff formulation causes an overestimation of the amount of ammonia available to form nitrate because the competition for ambient ammonia by individual puffs and by background sources is neglected. ALM was developed to treat this limitation. The post-processing method repartitions nitric acid and nitrate on a receptor-by-receptor and hour-by-hour basis and approximates the influence of other background sources of sulfate and nitrate in computation of incremental nitrate formation. Details of the ALM, incorporated into POSTUTIL are described by Escoffier-Czaja and Scire (2005).

Here we provide a summary of their description of the method as it might be used in CENRAP source-specific modeling.

With the ALM procedure, the contribution of an individual source or facility to nitrate formation is determined via a four-step procedure:

Step 1. The total background ammonia (ambient free ammonia + ammonia associated with sulfate/nitrate aerosols) is estimated either through (a) use of observational data at existing monitoring networks such as CASTNet, (b) from the output of one-atmosphere models such as CMAQ or CAMx. For example, assume weekly average sulfate, nitrate and nitric acid concentrations at CASTNet stations can be used to estimate the ammonia in the domain. An iterative scheme is used split total nitrate ($TNO_3 = HNO_3 + NO_3$) into HNO_3 and NO_3, leading to the following relationship,

$$[NH_3]_{total} = [NO_3] + 2\,[SO_4] + NH_3(g)$$

where $[NO_3]$ is the observed nitrate concentration (ppb), $[SO_4]$ is the observed sulfate concentration (ppb), and $NH_3(g)$ is the estimated free ammonia concentration (ppb) derived by applying the chemical equilibrium relationship. Using a 5-year monthly average of NO_3 and TNO_3 ($= NO_3 + HNO_3$) and the hourly temperature and relative humidity measured at a CASTnet site, an iterative scheme is used to estimate the free component of the NH_3 and the estimation of background sulfate and nitrate.

Step 2. The project sources are modeled in the normal way by CALPUFF to predict TNO_3 from those sources.

Step 3. The ‘boundary condition’ CALPUFF model is used to simulate pollutant concentrations (SO_2, SO_4, NO_x, HNO_3 and NO_3) from distant sources (outside the modeling domain) at the receptors of interest. The background sulfate concentrations are used with the monthly averaged total NH_3 in Step 1 to compute available ammonia (i.e., after consumption by sulfate). The available ammonia will vary hourly and spatially even though the total ammonia may be constant, because the sulfate concentrations are varying.

Step 4. POSTUTIL is then used to develop the total concentrations of sulfate, nitrate and nitric acid from all sources (project source, boundary conditions and background in-domain sources if any), and to re-partition the nitrate to reflect the total concentrations of ammonia-scavenging pollutants from all sources. In this step, the ammonia consumed by background sources of sulfate and nitrate as well as due to puff overlap from modeled sources is all accounted for in the re-application of the equilibrium relationship.

In a separate run of POSTUTIL, the contribution of any individual source or group of sources to the total nitrate can be determined. The flow chart diagram in Figure 7-1 shows the POSTUTIL process to attribute a fraction of total NO_3 to any individual source (Step 3 in Figure 7-1). Once the total nitrate from all sources is determined with ammonia limiting effects evaluated (i.e., Steps 1 and 2 in Figure 7-1), a separate POSTUTIL run computes the TNO_3 from the project source alone, and attributes the nitrate formed from that particular source as a fraction of the total NO_3 formed based on that source’s contribution to total TNO_3.

The distribution of CASTNet and IMPROVE monitoring sites in the central United States is shown in Figure 5-5. Most Class I areas in this region include either a CASTNet and/or an IMPROVE monitoring site and many others are in the vicinity. CALPUFF's ALM procedure described above uses the CASTNet monitoring network to produce boundary conditions of sulfate, nitrate and precursors and to derive empirical estimates of ammonia concentrations. However, CASTNet measurements have inherent errors and biases that tend to overestimate HNO_3 and underestimate NO_3 (some NO_3 will volatilize to HNO_3 within the sample after collection and before laboratory analysis). Thus, applying CASTNet data to estimate background NH_3 would tend to underestimate the ambient NH_3 and would therefore underestimate visibility impacts.

One-atmosphere regional modeling results are an alternative to the use of CASTNet or other monitoring network observations. CENRAP's gridded, hourly CAMx or CMAQ data bases for 2002 may be used in the CALPUFF ALM methodology in two ways:

- **Boundary Conditions and Background Ammonia**. Regional model concentrations of SO_2, SO_4, NO_3, HNO_3 and NO_x can be used to define the boundary conditions for the CALPUFF boundary module run. Regional model ammonia concentration fields over the Class I receptors of interest can also be used directly as input to the ALM method in CALPUFF. Monthly averaged, BCs and NH_3 concentrations can easily be derived from CENRAP's 2002 annual CMAQ or CAMx modeling files.

- **Sulfate, Nitrate and Ammonia at Class I Receptors**. One may extract SO_4, NO_3 and NH_3 concentrations at the Class I receptors from regional model simulations on an hourly or longer time-average at the Class I receptors as direct input into the CALPUFF ALM procedure. Here, the CALPUFF boundary condition module is replaced by the direct use of CMAQ-predicted concentrations.

The value in using CMAQ or CAMx modeling results include the availability of hourly concentrations of all relevant gas phase and fine particulate aerosol species from all sources in the U.S. The models have been evaluated against virtually all of the individual monitoring stations identified in Figure 5-5 and these results are easily obtained from the UCR/CENRAP website:

(http://pah.cert.ucr.edu/aqm/cenrap/index.shtml).

Considering the various sources of uncertainty (e.g., inadequate aerosol chemistry in CALPUFF, uncertainties in regional ammonia emissions inventories; inconsistency in measurement protocols among the monitoring networks in Figure 5-5, and uncertainties in regional models), use of CMAQ or CAMx modeling data bases is an attractive option over reliance on one or more CASTNet sites for some source-specific analyses.

For source-specific modeling, we recommend using regional model ozone, nitrate, sulfate, and ammonia concentration fields available over the central U.S. for 2001, 2002, 2003 from the CENRAP, VISTAS, and MRPO modeling studies instead of ammonia concentrations based on CASTNet, IMPROVE, and STN measurements and ozone measurements based on the AIRS/AQS data. Straightforward processing of the modeled CMAQ or CAMx nitrate and sulfate fields can be used to generate the inputs needed for CALPUFF boundary conditions. Gridded model output fields should be used to generate daily average ozone and NH_3 concentrations (averaged for each calendar month) along the trajectory path from source to Class I area. This approach offers an improved characterization of the atmospheric environment through which BART plumes traverse compared to point measurements that likely do not coincide with the plume path and certainly do not characterize the full chemical history of the plume. Gridded CMAQ or CAMx output files are available from CENRAP and the other RPOs.

7.4.3 Computing Light Extinction

The methodology for calculating light extinction outlined in the BART guidance constitutes the default approach presently, but ongoing research suggests that improved methods are or soon will be available and recommended for use by the IMPROVE committee, EPA, and other knowledgeable groups. Thus, any changes to the default method (e.g., deviation from the use of the EPA monthly *f*(RH) CALPOST Method 6) will have to be justified in the source-specific modeling protocol and evaluated on a case-by-case basis.

Currently, the IMPROVE Steering Committee, EPA, the Electric Power Research Institute, the Federal Land Managers, the Regional Planning Organizations and other scientists are discussing whether refinements are warranted to the method recommended in EPA's guidance for calculating light extinction (i.e., the IMPROVE equation). Among the topics being considered are:

> Increase OC to OC Mass multiplier from 1.4 to 2;
> Use formula to provide for varying sulfate and nitrate extinction efficiencies depending on concentration;
> Accounting for anthropogenic transboundary pollution'
> Corrections to the statistical assumptions used to estimate 20% best and 20% worst days; and
> Use actual IMPROVE derived relative humidity data rather than EPA's "climatological" values

Other refinements under consideration, which also apply to the CALPOST extinction formula (Equation 3-1), include the following:

> Adding a sea salt term to the formula, which would include a growth factor due to relative humidity;

> Increasing the factor used to calculate the mass of particulate organic matter from organic carbon measurements;

> Slightly modifying the relative humidity growth formula, f(RH), for sulfates and nitrates; and

> Revising some of the extinction efficiencies (the numerical constants in Equation 3-1), including making those for sulfates, nitrates, and organic carbon vary with concentration

Presumably any changes that are made by the IMPROVE Steering Committee would also be reflected in the EPA's approach. If this is the case, then CENRAP source-specific modeling protocol**s** should adopt the emergent recommendations unless the source can justify, and the state approves, a different approach. Thus, for example, in the source-specific modeling, consideration of sea salt in the natural background, elevation effects on Rayleigh scattering (see below) and natural weather effects such as fog, rain and snow might be appropriate. Specific configuration settings for these and other model features should be proposed in the source-specific modeling protocol and negotiated with the state, regional EPA office and the FLM.

7.4.4 Estimating Rayleigh Scattering.

The Rayleigh scattering coefficient for clear air has a default value 10 Mm^{-1} (see Equation 3-1). This default value is appropriate for an elevation of 1600 m (about 5000 ft). Since the correct value at sea level is about 12 Mm^{-1}, the default value could never be attained at low altitude sites and therefore the relative impact (in dv) of a source on haze would be overstated by using the default Rayleigh value. Publicly available codes are available for making the elevation-dependent adjustments to the high elevation default value of 10 Mm^{-1}. For the source-specific analyses, an effort should be made to be consistent with the approach taken by the CENRAP and the other RPOs in defining the Rayleigh scattering coefficient for their regional analyses.

7.4.5 Natural Baseline Conditions.

The visibility impacts of BART-eligible sources must be evaluated against natural conditions. Default values of natural conditions have been specified in EPA guidance documents. These values are held as constant throughout the East, which result in natural background extinction that varies spatially and temporally only in response to the spatial distribution and monthly variation of climatologically-representative relative humidity values. (This default definition of natural conditions does not take into account meteorologically caused visibility impairment such as fog and rain.)

The EPA allows refinements to the default natural conditions values, with adequate scientific justification. Three changes seem to have wide support: (a) increasing the multiplier of the measured organic carbon concentration from 1.4 to a larger value, probably in the range of 1.8 to 2.1; (b) changing the estimates of natural conditions extinction on the 20% clearest and haziest days to better reflect the statistical distribution of extinction; and (c) including sea salt in the IMPROVE/EPA formula, as discussed in the preceding section. The organic carbon multiplier adjustment applies to all BART-related calculations. Since most of the extinction under natural conditions is attributed to organic carbon, the first change will substantially increase the natural background level of extinction from the default level. This, in turn, will reduce the modeled percentage or deciview impacts of most sources, which may affect their BART status.

The statistical adjustment applies for the calculation of conditions on the 20% clearest and haziest days. The clearest days adjustment is relevant if the baseline for evaluating source impacts in the BART exclusion modeling is based on the 20% clearest days. It would increase the deciview impact of a source’s emissions. The haziest days adjustment is of relevance for the assessment of the benefits of the application of BART, for which the 20% haziest days are the baseline. It slightly increases the default haziness on those days and therefore reduces the absolute deciview impact of a source’s emissions. Finally, the sea salt adjustment applies to the description of natural conditions, and has effect mainly near the seacoast.

Other refinements to natural conditions estimates may be appropriate at specific locations or at specific times of the year. Also, any refinements to the light extinction estimation formula of Equation 3-1 would be reflected in natural conditions extinction estimates.

7.4.6 Visibility Impact Assessment.

As recommended in the final BART guidance, the test for evaluating whether a source is contributing to visibility impairment is based on the 98th percentile modeled value (rather than the highest predicted value used for the screening evaluation). States or sources can accomplish this in one of two ways. First, a coding change can be made to the CALPOST postprocessor to allow the 98th percentile change in extinction to be computed. This may be accomplished by using a specific program that post-processes the CALPOST output (CDPHE, 2005). Alternatively, because the CALPOST processor produces visibility impacts in deciviews, these impacts can be externally processed in a spreadsheet to calculate the changes in deciviews. Table 7-2 shows a hypothetical example of the ranked visibility impacts (change in dv) for each of three years at six different Class I areas. The 98th percentile (8th highest value) in the sorted table would be compared to the contribution threshold (e.g., 0.5 dv). In the example shown in Table 7-2, the source passes the refined analysis because the highest 98th percentile visibility impact is below the contribution threshold of 0.5 dv. The actual procedure selected by the State or source should be set forth clearly in the protocol. Any CALPUFF code changes should be documented and copies of the source code and input/output files provided to the reviewing agency for corroboration.

7.5 Assessment of Modeling Results

The report accompanying the source-specific CALPUFF modeling should provide a clear description of the modeling procedures followed and the results of the analysis. Any departures from the approved modeling protocol should be specifically discussed and justified. The report should also include a discussion of uncertainty in the modeling results. There are many sources of uncertainty in modeling due to factors such as errors and approximations used in the calculation of emission rates, speciation of the emissions, particle size distributions, meteorological data inputs including the MM5 data sets used for determining the wind fields, the representativeness of meteorological observations used in the analysis, uncertainties in the meteorological and dispersion model itself due to its parameterizations of transport, dispersion and chemical transformation, and in the methods used to compute light extinction from particulate matter concentrations predictions. In addition, the use of monthly average relative humidity in the hygroscopic aerosol growth equations results in error. Furthermore, grid resolution affects the ability of the model to resolve terrain features and for wind and other meteorological fields to respond to geophysical features such as terrain, land-sea boundaries, surface characteristics such as roughness, albedo and other parameters.

As appropriate, the main sources of uncertainty in the BART modeling should be addressed in the final report. Good discussions of uncertainty in air quality modeling are readily available, e.g., Russell and Dennis (2000) and the citations in the reference section of this document. The uncertainty analysis is not intended to be exhaustive but rather shed light on important areas of model uncertainty and the likely range of applicability of the CALPUFF (or alternative model) results.

Accompanying the modeling report should be an electronic archive (CDs, DVDs, or removable USB/IEEE 1394 hard drives as appropriate) that includes the full set of CALPUFF inputs and model output fields and well as any pre- or post-processor codes used to generate the results. While it is not necessary to archive the MM5 data files used to generate the CALMET fields, the CALPUFF-ready meteorological fields should be included in the archive. The modeling data archive should be sufficiently complete as to allow an independent group to corroborate the modeling results developed in the source-specific analysis.

Table 7-1. Contents of a Typical Source-Specific BART Modeling Protocol.

1.0 INTRODUCTION
- **1.1 Objectives**
- **1.2 Location of Source and Relevant Class I Areas**
- **1.3 Source Impact Evaluation Criteria**
- **1.4 Modeling Study Participants**
- **1.5 Protocol Review Process**
- **1.6 Schedule**

2.0 SOURCE DESCRIPTION
- **2.1 Unit-specific Source Data**
- **2.2 Nearby Sources Affecting Same Class I Areas**

3.0 MODEL INPUT DATA
- **3.1 Modeling Domain**
- **3.2 Terrain and Land Use**
- **3.3 Emissions Data Base**
  - **3.3.1 Stack Parameters**
  - **3.3.2 Emissions Rates**
  - **3.3.3 Condensable Emissions**
  - **3.3.4 Speciation and Size Distributions**

- **3.4 Refined Meteorological Modeling Base**
  - **3.4.1 MM5 Simulations**
  - **3.4.2 CALMET Data Sets**
  - **3.4.2 Observational Data**

- **3.5 Air Quality Data Base**
  - **3.5.1 Ozone Concentrations**
  - **3.5.2 Ammonia Concentrations**
  - **3.5.3 Concentrations of Other Pollutants**
  - **3.5.5 CENRAP Regional Modeling Data Sets**

- **3.6 Natural Conditions at Class I Areas**

4.0 CALMET MODELING METHODOLOGY
- **4.1 Domain Configuration**
- **4.2 MM5 Extraction Procedures**
- **4.3 CALMET Configuration**
  - **4.3.1 Terrain**
  - **4.3.2 Land Use**
  - **4.3.3 Vertical Layer Structure**
  - **4.3.4 Diagnostic Model Settings**
  - **4.3.5 BIAS, RMIN2, IXTERP settings**
  - **4.3.6 R1, R2, RMAX1, RMAX2, RMAX3 settings**
  - **4.3.7 Surface Stations**
  - **4.3.8 Upper Air Stations**

Table 7-2. Example of Hypothetical Visibility Impact Rankings at Five CENRAP Class I Areas.

Class I Area	2001	2002	2003
	Delta-Deciview Ranks 1-8	Delta-Deciview Ranks 1-8	Delta-Deciview Ranks 1-8
Caney Creek	0.99	0.95	1.20
	0.88	0.63	0.90
	0.62	0.51	0.73
	0.59	0.50	0.72
	0.55	0.46	0.59
	0.52	0.42	0.47
	0.48	0.37	0.45
	0.47	0.36	0.42
Upper Buffalo	0.67	0.81	0.76
	0.45	0.69	0.47
	0.43	0.65	0.37
	0.33	0.50	0.35
	0.29	0.45	0.31
	0.27	0.33	0.30
	0.25	0.31	0.28
	0.23	0.29	0.28
Boundary Waters	0.66	0.73	0.75
	0.43	0.69	0.45
	0.41	0.63	0.36
	0.35	0.52	0.34
	0.26	0.46	0.28
	0.24	0.34	0.27
	0.23	0.29	0.26
	0.22	0.26	0.25
Voyageurs	0.26	0.54	0.61
	0.23	0.47	0.42
	0.22	0.43	0.30
	0.21	0.37	0.29
	0.20	0.37	0.28
	0.19	0.31	0.28
	0.18	0.31	0.25
	0.16	0.30	0.25
Hercules Glade	0.34	0.52	0.27
	0.33	0.43	0.24
	0.31	0.32	0.23
	0.26	0.31	0.20
	0.24	0.30	0.14
	0.20	0.28	0.13
	0.18	0.24	0.11
	0.17	0.24	0.10

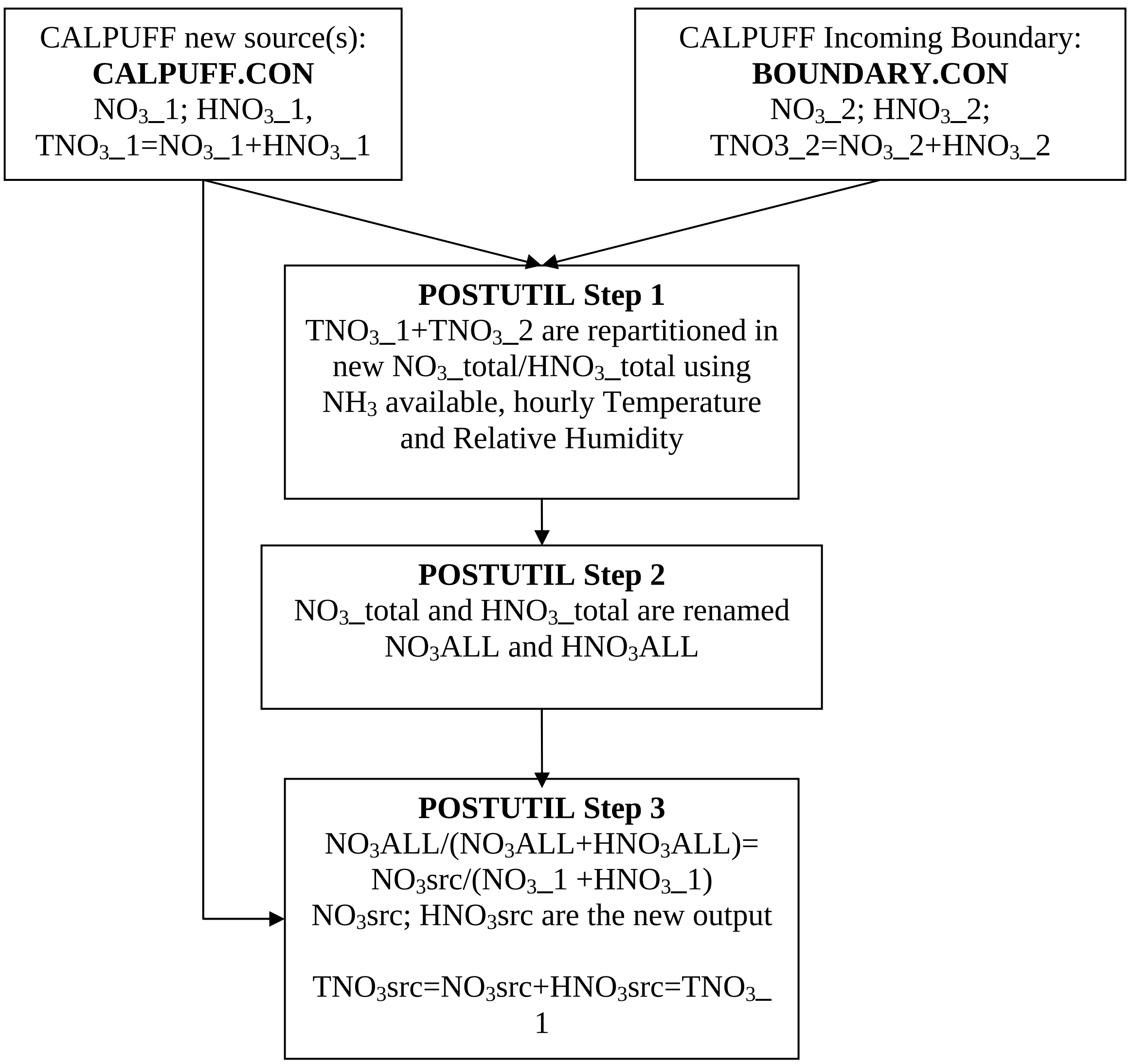

Figure 7-1. POSTUTIL Processing of the Ammonia Limiting Method (ALM), NO_3/HNO_3 Repartitioning for an Individual Source, and Estimating Ammonia Consumption from Modeled Sources and Boundary Conditions. (Source: Escoffier-Czaja and Scire. 2005.)

8.0 ALTERNATIVE MODEL APPLICATIONS

Recent model inter-comparisons between CALPUFF and full science models such as CAMx and CMAQ (Morris et al., 2003) amply demonstrate that CALPUFF substantially overpredicts concentrations of visibility-reducing fine particulates under various real-world at the larger downwind distances when compared to one-atmosphere models. Perhaps only a few BART eligible sources in the CENRAP region will consider seriously the use of alternative models to EPA's CALPUFF model. But for those sources whose anticipated control costs are substantial, the application of comprehensive, full-science regional visibility assessment tools will yield more realistic BART control requirements than those generated by a puff model. In this chapter, the steps required to select and apply a state-of-science regional model and attendant data bases are presented. While there are other alternatives to CALPUFF (i.e., PLUVUE-II, SCICHEM), only full-science models have the requisite chemistry and physics formulations to surmount the many limitations associated with CALPUFF (discussed in Chapter 3). In addition, we briefly summarize the scope and availability of the emissions, meteorological, and air quality modeling data bases for the CENRAP region that can be used to support alternative BART modeling.

8.1 Use of One-Atmosphere Models in Refined Assessments

States or source operators interested in conducting truly refined visibility modeling of BART-eligible sources have several options for using one-atmosphere models supported by current RPO data bases. Options available include:

> Modeling Systems: CMAQ4.5 or CAMx4.2

> Sub-Grid-Plume Treatment: CMAQ-PinG, CMAQ-APT-PM, CMAQ-MADRID-APT, CAMx PM IRON PiG, and CAMx multi-scale flexi-nesting;

> Modeling Years: 2001 (MRPO), 2002 (CENRAP, MRPO, VISTAS, WRAP), 2003 (MRPO)

> Modeling Resolutions: 12 km (VISTAS, WRAP, MPRO), 36 km (CENRAP, MPRO, VISTAS, CENRAP, WRAP)

Figures 8-1 thorough 8-6 present the various grid domains used by the RPOs and the Five States Study[1] (Tesche et al., 2005b). Clearly, each CENRAP state is covered by all of the 36 km domains and by many of the higher resolution 12 km domains as well. Depending on the source's location and the Class I area(s) of concern, there are likely to be several model/data base configurations available. All of the modeling performed on these domains has been rigorously evaluated and publicly disseminated.

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[1] The Five States Study is an integrated 8-hr ozone and annual $PM_{2.5}$ modeling study in the Upper Midwest aimed at identifying effective SO_2, NOx, and VOC controls to address the residual nonattainment beyond imposition of CAIR controls. Using augmented versions of the MRPO 2002 regional haze data sets, a suite of nested 36/12/4 km ozone and 36/12 km annual $PM_{2.5}$ simulations are being carried out for 2002 and 2009 to address emissions controls needed for attainment of the 8-hr ozone and annual $PM_{2.5}$ NAAQS. These data sets will be publicly available.

8.1.1 Regional Haze Modeling Data Bases

The readiness of one-atmosphere regional models for visibility impact assessment has been substantially strengthened in the past three years as the result of the RPO efforts to address the Regional Haze Rule. CENRAP and the other four RPOs have developed and evaluated comprehensive data sets for regional haze model applications (Morris et al., 2004, 2005a,b,d; Baker, 2005a-c; Brewer and Adlhoch, 2005; Boylan and Russell, 2005; Tesche et al., 2005). Over the CENRAP domain, annual fine particulate and visibility modeling data bases now exist for calendar years 2001, 2003, and 2003 (Baker, 2005c). Availability of these public data bases significantly reduces the resource burden on that subset of states or source operators who may elect to carry out alternative BART modeling.

Emission Inventories. Comprehensive modeling inventories for 2002 have been developed by all of the RPOs using common national data sets (2002 NEI) together with local and state-specific emissions information. Generally, all of these inventories are consistent with on another although there are naturally some differences stemming from availability of local information. The elements of the CENRAP modeling inventory well-characterize the work performed by all the RPOs.

As part of the CENRAP regional haze modeling program, a gridded, hourly emissions inventory for 2002 of criteria air pollutants (CAPs) and ammonia (NH_3) emissions inventories for point, area, and nonroad sources has been developed (Pechan and CEP, 2005; UCR, 2005). The original Base_A 2002 inventory files completed during February 2005 were updated to incorporate comments provided by the CENRAP State, Local, and Tribal (S/L/T) agencies and the Emissions Inventory (EI) and Modeling Workgroups. As a result of the updates, the updated Base_B inventory was developed and is now being used in CENRAP's 2002 and 2018 regional haze modeling. The CENRAP modeling inventories and supporting data prepared include the following:

- Comprehensive, county-level, mass emissions and modeling inventories for point, area, and nonroad sources of 2002 emissions for the CAPs and NH_3 for the state, local, and tribal agencies included in the CENRAP region;

- Modeling inventory files containing 2018 projection year emissions for EGUs; and

- A modeling inventory for Ontario fires during 2002.

The mass emissions inventory files were prepared in the National Emissions Inventory (NEI) Input Format Version 3.0 (NIF 3.0) and then converted to the SMOKE/IDA format. These point, area, mobile and nonroad inventories were temporally allocated (hourly), chemically speciated (for the CB4 mechanism) and spatially distributed (on a 36/12 km grid) over the CENRAP domain for the full calendar year 2002. The inventories include emissions rates for sulfur dioxide (SO_2), oxides of nitrogen (NO_x), volatile organic compounds (VOC), carbon monoxide (CO), NH_3, and particles with an aerodynamic diameter less than or equal to a nominal 10 and 2.5 micrometers (i.e., primary PM_{10} and $PM_{2.5}$). The inventories included summer day, winter day, and average day emissions. The temporal profiles developed by Pechan and CEP (2005) were used by the CENRAP modeling team to generate gridded, speciated, hourly emissions of photochemical, particulate, and regional haze precursors.

Meteorological Data Bases The MM5 model has been used exclusively by the RPOs in support of the regional haze modeling and the modeling files used in the CENRAP and MRPO haze modeling are the same ones that have been processed to yield the CALMET fields discussed in Chapter 5. In particular, the following annual MM5 simulations have been used to construct CAMx and CAMQ modeling data bases over the U.S.

> 2001 MM5 data set at 36/12 km resolution developed for EPA by Alpine Geophysics (McNally and Tesche, 2002; McNally 2003);

> 2002 MM5 data set ad 36/12 km resolution developed for VISTAS by Baron Advanced Meteorological Services (Olerud and Sims, 2004);

> 2002 MM5 data set at 36 km resolution developed for CENRAP by Iowa DNR (Johnson, 2003a,b);

> 2003 MM5 data set at 36 km resolution developed for the Midwest RPO (Baker, 2005; Baker et al., 2004; Kembell-Cook et al., 2005); and

> 2004 MM5 data set at 36 km resolution developed for the Midwest RPO (Baker, 2005).

Each of these studies included a performance evaluation of the MM5 against surface meteorological observations and the results of these evaluations are contained in the reports or presentations cited above.

Regional Haze Modeling Data Bases Regional modeling data bases using the emissions and MM5 fields have been developed and evaluated by VISTAS (CAMx/CMAQ for 2002 at 36/12 km); MRPO (CAMx for 2001, 2002, 2003 at 36 km [and some 12 km]); CENRAP (CMAQ/CAMx for 2002 at 36 km [and some 12 km]). Details of these date base development activities and associated model performance evaluations are thoroughly described in the literature references.

8.1.2 Obtaining Regional Modeling Data Bases

As discussed in Chapter 4, the aggregate file sizes of the regional haze modeling data sets are substantial, requiring several 300-500 Gbyte external disk drives to store the information. In addition to the CENRAP CMAQ and CAMx modeling data bases, the MRPO and VISTAS have indicated a willingness to provide their data sets to CENRAP for use by CENRAP states or source operators. It is anticipated that CENRAP will serve as the central repository, collecting one complete distribution of the pertinent MRPO and/or VISTAS data bases on a set of high-capacity disk drives and then making them available to the states or source operators on an as requested basis for advanced modeling. Parallel sources of these data sets are the modeling contractors performing the regional haze modeling for CENRAP, VISTAS, and WRAP.

8.1.3 Protocol Development

EPA’s BART guidance clearly indicates the need for a detailed modeling protocol to support any application of alternative models for BART analyses. An example of the content of such a one-atmosphere modeling protocol would be the CMAQ/CAMx modeling protocols developed for CENRAP (Morris et al., 2004c) and VISTAS (Morris et al, 2004a). In addition, certain components of the screening and source-specific protocols developed with CALPUFF (Tables 6-1 and 7-2) would be appropriate. The alternative modeling protocol should be submitted to the state, regional EPA office and FLM for review and negotiation. Note that EPA's role in the development of the protocol is only advisory as the "states better understand the BART-eligible source configurations" and factors affecting their particular Class I areas (70 FR 39126).

8.2 Model Applications

Assessment of BART sources with regional models is a straightforward, albeit computationally intensive exercise. Two types of regional model simulations are required.

8.2.1 Regional Base Case Simulation

The first step is to re-run one of the existing regional simulations for the 2002 annual basecase to establish comparability with the base case run reported by the RPO from whom the CMAQ or CAMx modeling files were obtained. The purpose of this annual simulation is two-fold. First, it establishes proper operation of the modeling system on the host computer via comparison with the RPO model output files. Second, it provides the gridded 24-hourly estimates of $(NH_4)_2SO_4$, NH_4NO_3, OC, EC, soil, and coarse mass needed to calculate daily extinction coefficients from the IMPROVE extinction equation for every grid cell in the domain, including the Class I areas. (Further discussion of natural visibility conditions is given in the following section). On a modern Linux cluster of 4-6 nodes, a 36 km simulation would require approximately two weeks to complete execution.

An important question to be addressed in the modeling protocol is whether one annual simulation of 2002 would be sufficient to provide the necessary assessment of a BART source's visibility impact. Recent annual CAMx simulations of 2001, 2002, and 2003 by the MRPO (Baker, 2005c) indicated that for these three years:

> CAMx model performance by specie was very consistent from one year to the next;

> Sulfate predictions exhibited the greatest year to year variability, likely due to the interannual variability of atmospheric water content;

> CAMx performance was best for sulfate and elemental carbon; and

> Organic carbon predictions during the summer months were the poorest of the secondary particulate species; and

> Nitrate performance, a challenge in all regional modeling studies, needs additional improvement.

The performance levels achieved in the MRPO CAMx modeling are generally consistent with that of the other RPOs. These results are included in Figure 4-9, presented previously. Because the regional models include all of the important known gas-phase, aerosol, and aqueous-phase chemistry producing visibility-impairing particulates, a strong case can be made that only one year of modeling would be needed instead of the three years of CALPUFF modeling. However, if the reviewing agencies require a full three years of modeling data, a valid approach remains nonetheless with the 2001-2003 CAMx data sets developed by the MPRO.

8.2.2 BART Source Simulation with SGS Technology

Once the base case is established, the CMAQ or CAMx simulation is repeated with the emissions from the BART source are included in the point source emissions file. For this application, depending upon the host model chosen, one of several plume-in-grid or nested grid options should be used to provide near source resolution of the SO_2, NOx, NH_3, and VOC emissions of the BART source. For most single point BART simulations conducted with a full-science photochemical grid model, the plume-in-grid technique is generally recommended over the use of multi-scale grid nesting although the latter may still be appropriate in addition to the plume-in-grid approach for other reasons, including replication of meteorology and transport phenomena. Prescription of how the sub-grid-scale (SGS) technology is used within the regional model is a key point to be addressed in the modeling protocol. The use of SGS will allow the simulation of BART plume impacts down to very small scales (on the order of 1 km or less) depending upon the need.

8.2.3 Assessing Modeled BART Source Impacts

The direct impacts of the BART sources on 24-hr visibility is quantified by subtracting the 2002 Base Case simulation from the BART source simulation and plotting the residual aerosol species concentrations and HI values in daily tile plots. Figure 8-7 provides an example of such an incremental 24-hr average concentration tile plot. From the CAMx PM PinG modeling by Yarwood et al, (2005) using the 2002 MPRO data base, incremental 24-hr average SO_2, sulfate, nitrate, and NH_4 concentration fields on 14 June 2002 are shown. This plume reveals the individual plume signatures downwind from their origin. Similar plots of delta-deciviews can be determined using the IMPROVE extinction equation with the modeled aerosol fields from both model simulations. Tabular summaries of the visibility impacts in all grid cells, but especially the Class I areas are easily produced.

8.3 Estimation of Natural Visibility Conditions

8.3.1 Flexibility Suggested by EPA

Under the Regional Haze Rule, by 2008, the states must develop a strategy for reducing regional haze in Class I areas during the following decade. The rate of improvement of visibility is intended to be at a rate sufficient to reach "natural conditions" in 2064, and thus depends on quantifying what the visibility would be under those conditions. The initial, "default" estimate of natural conditions recommended by EPA (2003) – based on pre-1990 research (Trijonis, 1990) does not take into account spatial and temporal variability and local geographic and meteorological conditions. Consequently, the default natural visibility conditions are out-of-date and do not reflect the very substantial theoretical, observational, and modeling data bases now available for estimating natural background concentrations (Tombach and Brewer, 2005). Recognizing that the "default" concentrations (see Table 6-3) are not appropriate for every Class I area, EPA allows states the option to develop "refined" estimates of natural conditions that reflects local conditions.

States might wish to adopt a refined approach to estimating natural visibility conditions for several reasons, including:

> The default estimates are shown, through more recent Class I area-specific observations and/or modeling analyses to be out-dated and/or incorrect;

> If the default estimates of the natural background conditions are close to the current

visibility conditions, small uncertainties can have significant impacts on states' ability to meet SIP goals;

> In some regions, natural sources are known to exhibit predictable seasonal influences on visibility; therefore, states might wish to use refined estimates of natural visibility conditions to account for these influences;

> States which receive significant visibility impacts from biomass smoke might wish to distinguish more explicitly between man-made and natural sources.

EPA identifies several possible refined approaches which can be adopted for developing ore realistic estimates of natural visibility conditions and states may identify others that are more appropriate for their own situations. Approaches suggested by EPA include: (a) develop refined estimates of the constant values of one or more natural species, (b) estimate natural visibility using species concentrations that vary (e.g., seasonally, monthly, or climatologically), or (c) adjust the estimated constant species to account for infrequent natural events, such as forest fires or wind-blown dust, as major influences on visibility. This latter approach would require estimating the frequency and magnitude of the natural contribution to particle concentrations during the events. EPA encourages flexibility in these approaches so that default and refined annual average, seasonal, monthly, and event-specific species concentrations provide the best estimates of natural visibility for each of the mandatory Federal Class I areas. States wishing to employ a refined approach should supply demonstrations that the refined approach is technically sound and provides regionally representative estimates of natural visibility conditions.

8.3.2 Refined Procedures for One-Atmosphere Modeling

The whole purpose of estimating natural visibility conditions is to develop a reasonable background against which a human observer might be able to discern the added presence of a BART source plume. With Lagrangian models such as CALPUFF, this necessity arises because puff models cannot calculate the three-dimensional, hourly varying gas phase and particulate concentration fields that contain the various visibility-limiting pollutant species. Consequently, some independent estimate of natural visibility conditions is required. Historical measurements of pristine conditions measured in the 1980s have been used to fill this void.

One-atmosphere models, by design, eliminate the need to estimate natural background conditions against which individual plume contributions are assessed. This is done directly via the simulation of the hour-by-hour, day-by-day emissions (including sea salt), meteorology (rain, snow, fog), transport, chemical transformation and removal of gaseous and particulate emissions from all sources (natural and manmade) in the region of interest for one or more calendar years. Today, the CENRAP, WRAP, MRPO, and VISTAS regional haze programs have all developed base year 2002 fine particulate and visibility estimates for the entire U.S. at grid scales of 36 km and 12 km using the CMAQ and/or CAMx models (depending upon RPO). Importantly, the MRPO has even extended the CAMx visibility modeling to include the same three year period (2001-2003) being use in the screening and source-specific CALPUFF modeling. The 24-hour averaged modeled ground level concentration predictions of $(NH_4)_2SO_4$, NH_4NO_3, OC, EC, soil, and coarse mass (i.e., all components in the IMPROVE extinction equation) from any of these regional simulations provide a direct quantification on a day-to-day basis of current background visibility conditions in not only the Class I areas, but in every 12 km or 36 km grid cell in the U.S. By simply re-running one or more of these regional one-atmosphere model simulations *with the BART source emissions included*, and then subtracting the outputs of the two simulations, a direct, gridded estimate is produced of the change in visibility (measured in terms of 'delta-deciviews') compared against realistic, current background conditions. As with the screening CALPUFF modeling, if the Δdv value is greater than the 0.5 dv threshold, the source is said to contribute to visibility impairment and is thus 'subject to BART' controls.

This approach to calculating a realistic natural visibility background condition departs from EPA's suggestions in two respects. First, it is far more rigorous, and thus is more resource intensive to carry out. Second, the natural visibility background conditions over the Class I areas simulated by the CAMx/CMAQ models in the 2002 base cases will in all likelihood be less 'pristine' then those estimated by Trijonis and others in the late 1980s. But, we maintain, they will be more representative of the actual current conditions in the Class I areas against which the BART plume impacts should realistically be compared.

Clearly, the acceptability of this refined one-atmosphere modeling procedure for calculating natural visibility background conditions in the Class I areas will need to be discussed with state, EPA, and FLM staff in order to reach consensus on the merits and acceptability of the approach. The fallback is to use the default (EPA, 2003) numbers.

8.4 Cumulative Impact Assessments

While the use of regional models incorporating plume-in-grid or multi-scale nesting allow for rigorous assessment of 24-hr average point source annual visibility impacts over one or more years, where one-atmosphere models are most useful is in cumulative impact assessments. The example shown in Figure 8-7 is one such application. The modeling performed by Yarwood et al., (2005) treated several dozen point sources with plume-in-grid technology allowing for the opportunity to assess the cumulative impact of all of these sources in the context of all anthropogenic and biogenic sources in the central U.S.

As noted in Chapter 1, each CENRAP state is required to carry out four types of visibility modeling under the Regional Haze Rule: (a) single-source modeling to determine which BART-eligible sources are 'subject to BART', (b) single-source modeling to determine the degree of visibility improvement attributable to proposed BART controls for each source subject to BART, (c) cumulative modeling to determine the combined effect of proposed BART controls for sources subject to BART in each CENRAP state; and (d) regional-scale modeling to determine if the combined effect of proposed BART controls for all CENRAP states ultimately satisfy the RHR visibility improvement goals. The third responsibility, cumulative impact assessment of all state sources subject to BART, is best addressed through the use of regional models.

8.5 Concluding Remarks

Only a few states and/or BART eligible sources are expected to seriously examine the merits of using full-science models as an alternative CALPUFF. But for those who do, the review of one-atmosphere modeling capabilities (Chapter 4) and the procedures one would follow in their application to BART sources (this chapter) will hopefully provide useful information to inform decision-making. Fortuitously, the recent work by the various RPOs and model developers has produced a suite of state-of-science models and associated data bases that are ideally suited to rigorous BART visibility impact modeling. While the resource requirements of an alternative modeling study – using existing models and data bases-- exceed those of a typical CALPUFF analysis, the potential to develop more reasonable control limits on certain BART sources may easily eclipse the additional costs of full-science modeling.

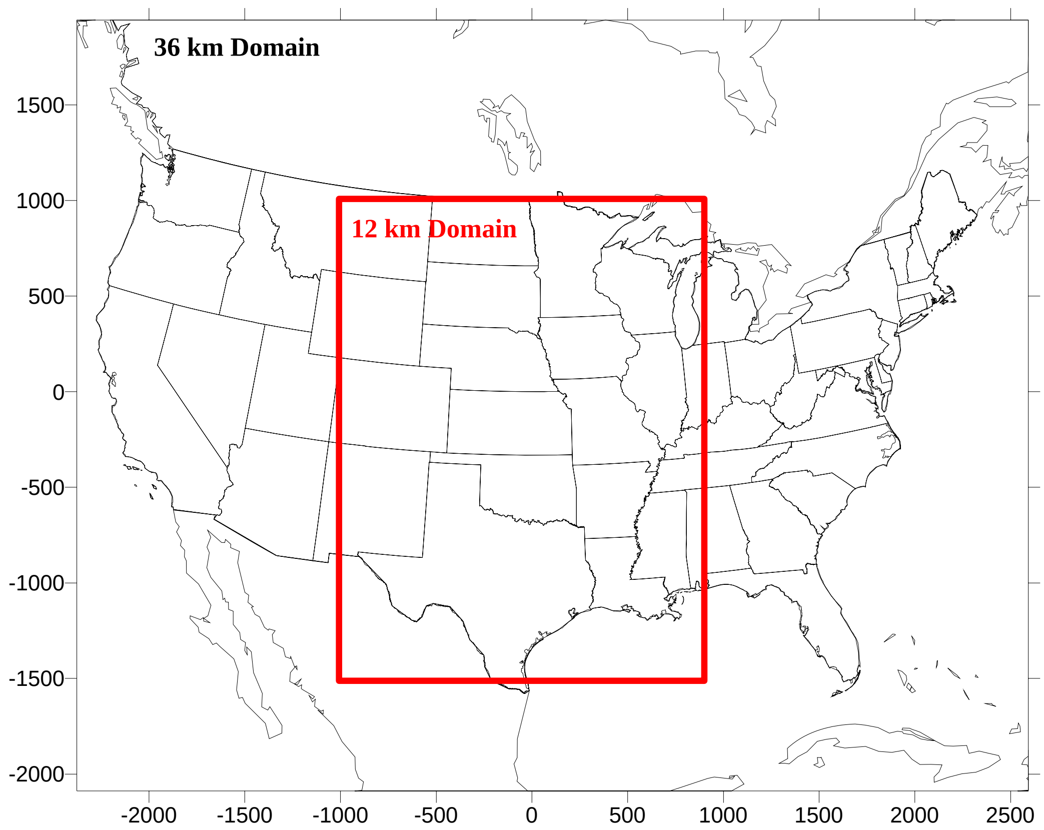

Figure 8-1. CENRAP 36/12 km CMAQ/CAMx Domain Used for 2002 Annual One-Atmosphere Regional Haze Simulations. 36 km domain is outer grid; 12 km domain is colored red. (Note: Model Simulations on 12 km domain may not be performed for full annual cycle). (Source: Morris et al., 2005d).

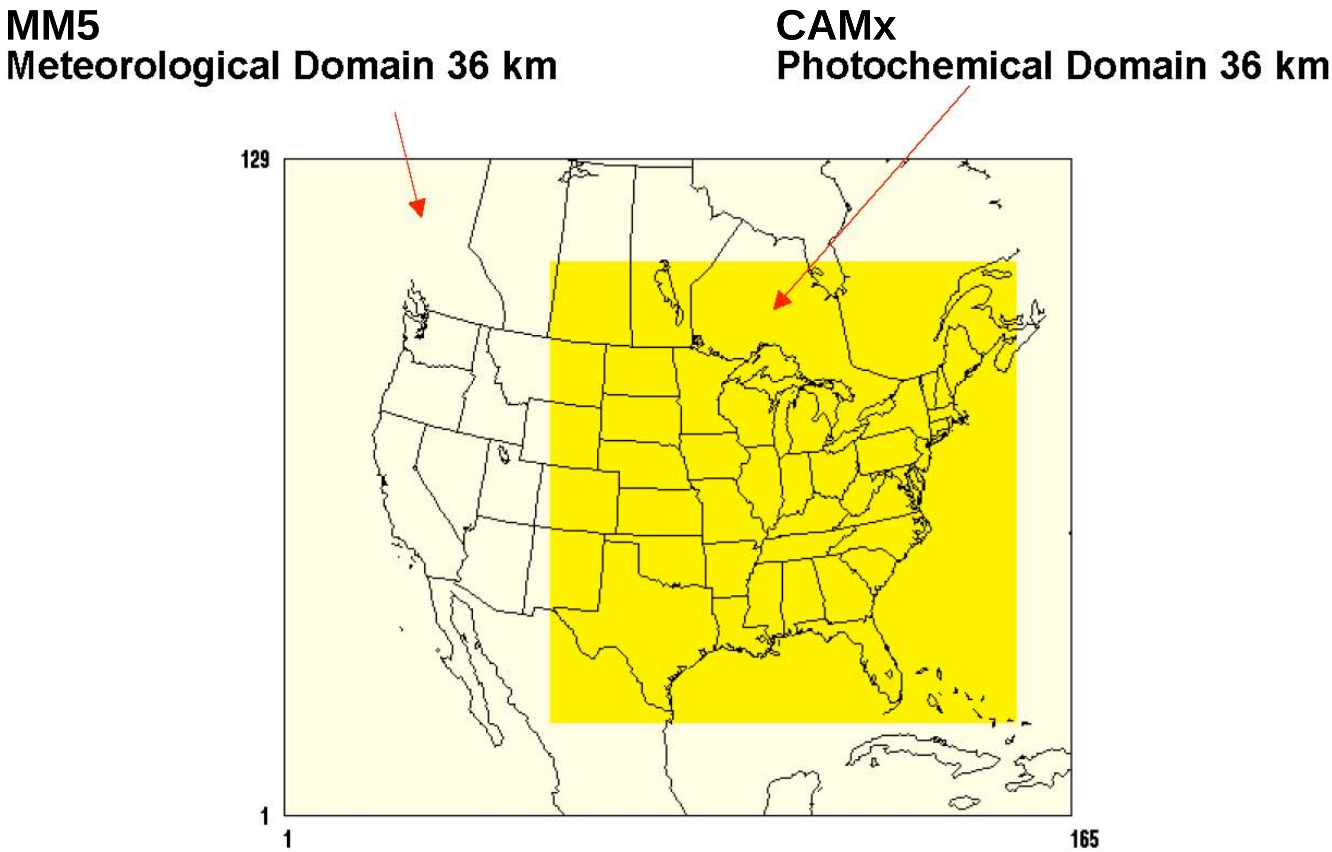

Figure 8-2. MRPO 36 km CAMx Domain Used for 2001, 2002, 2003 Annual One-Atmosphere Regional Haze Simulations (Source: Baker, 2005c).

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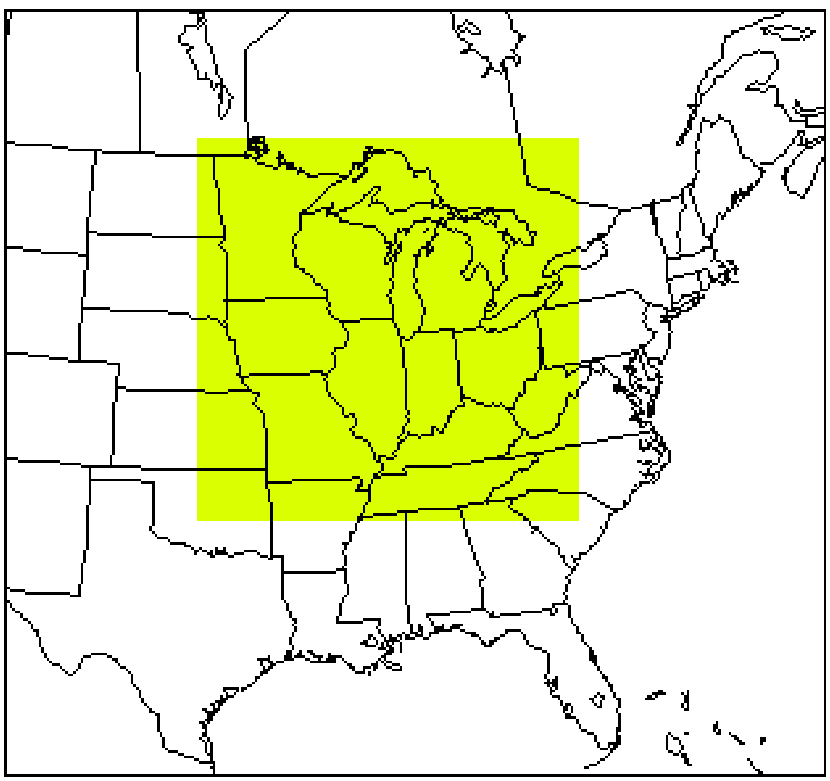

Figure 8-3. MRPO 36/12 km CAMx Domain Used for 2002 Annual One-Atmosphere Regional Haze Simulations. 36 km domain is outer grid; 12 km domain is colored green (Source: Koerber, 2005).

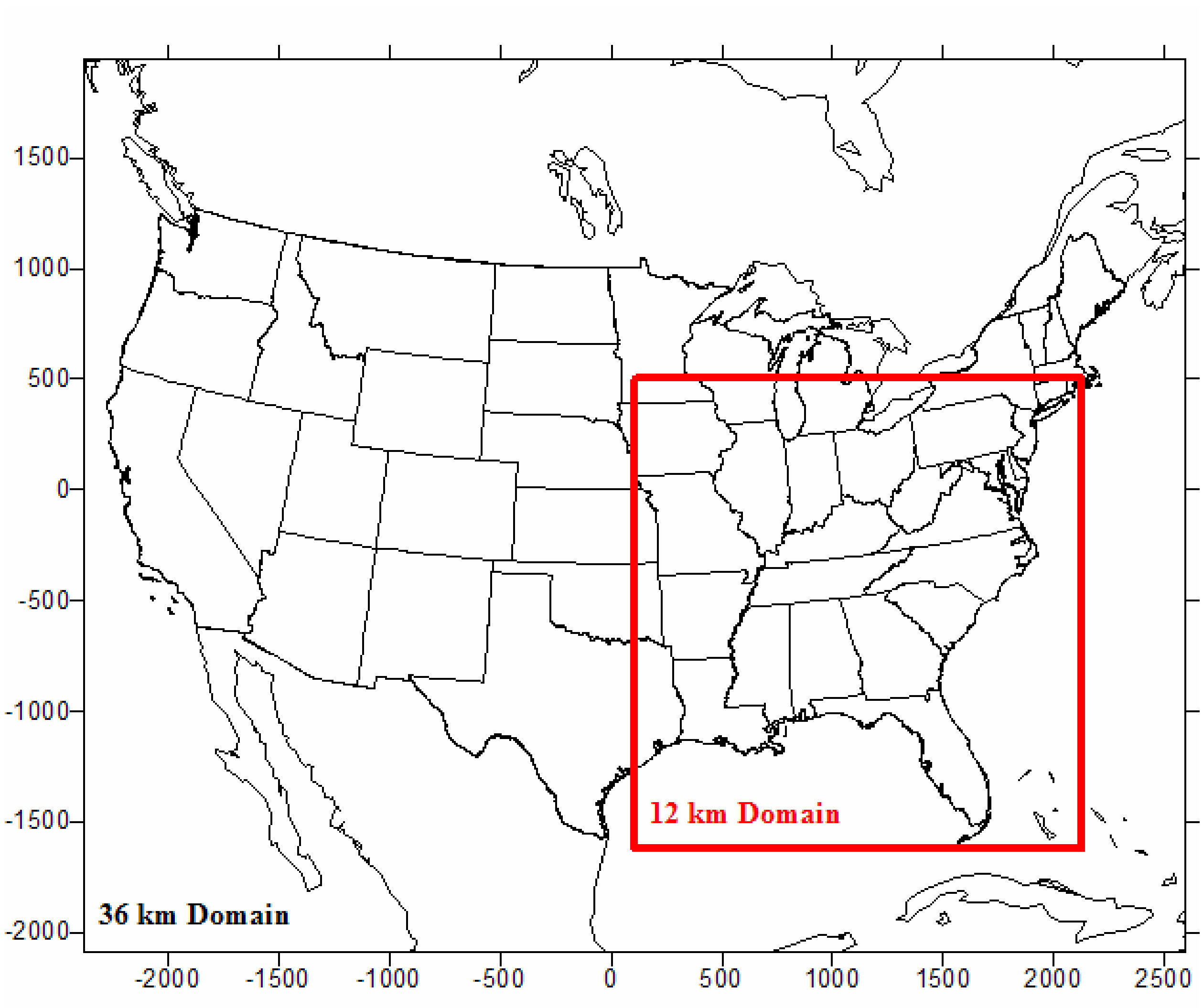

Figure 8-4. VISTAS 36/12 km CMAQ/CAMx Domain Used for 2002 Annual One-Atmosphere Regional Haze Simulations. 36 km domain is outer grid; 12 km domain is colored green (Source: Tesche et al., 2005).

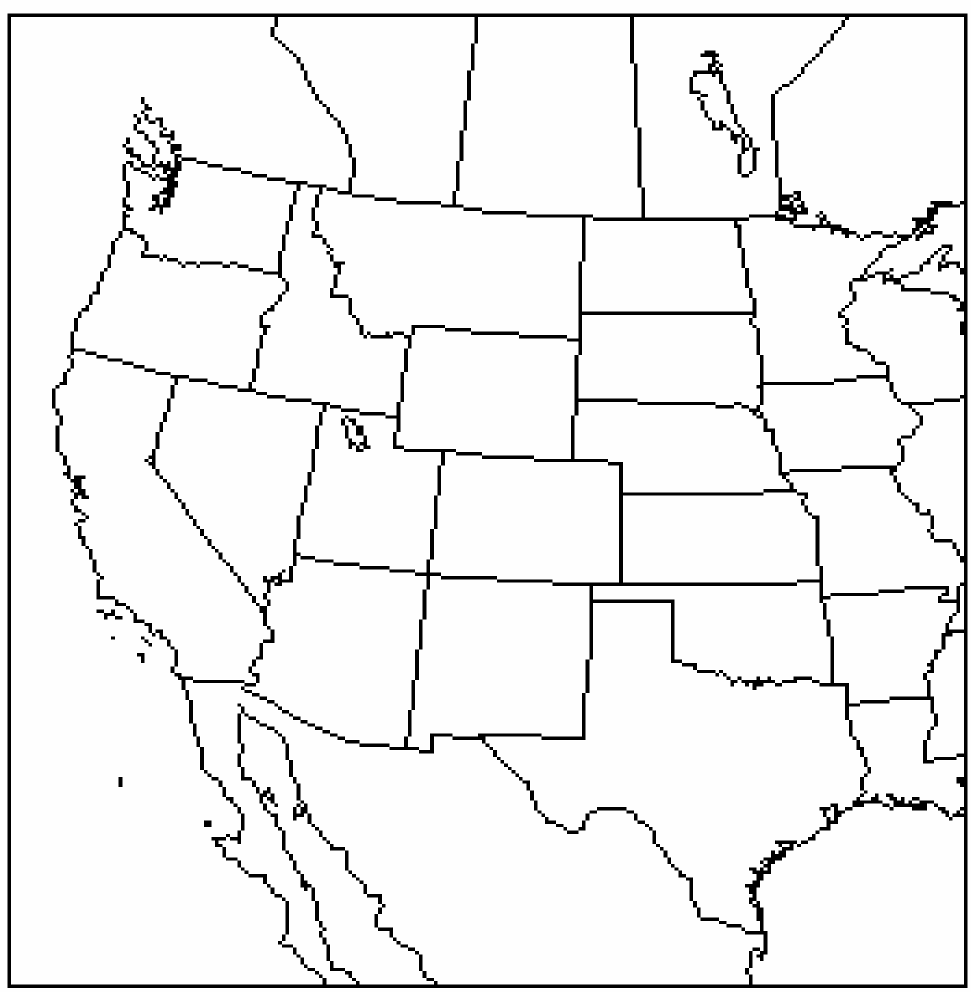

Figure 8-5. WRAP 36 km CMAQ/CAMx Domain Used for 2002 Annual One-Atmosphere Regional Haze Simulations. (Source: Morris et al., 2004b).

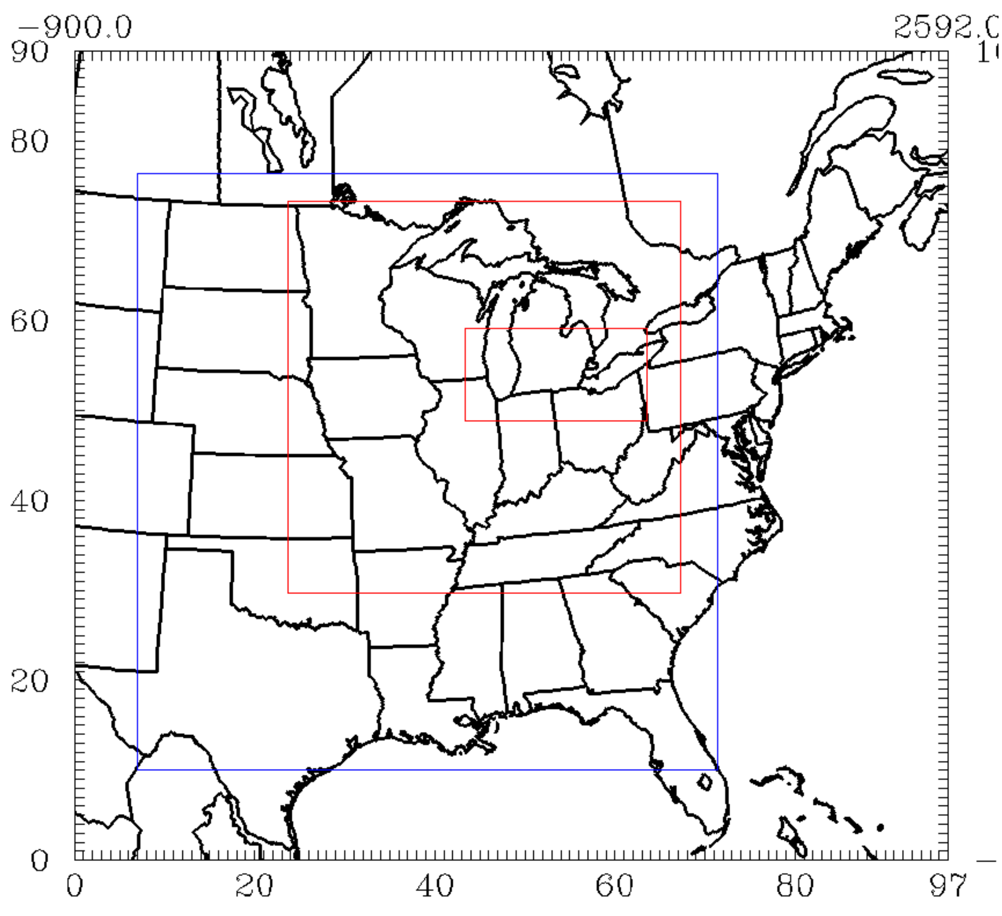

Figure 8-6. Five States Study 36/12/4 km PM2.5/8-hr Ozone Study Using CAMx for the 2002 Annual Period. (Source: Tesche, et al., 2005b).

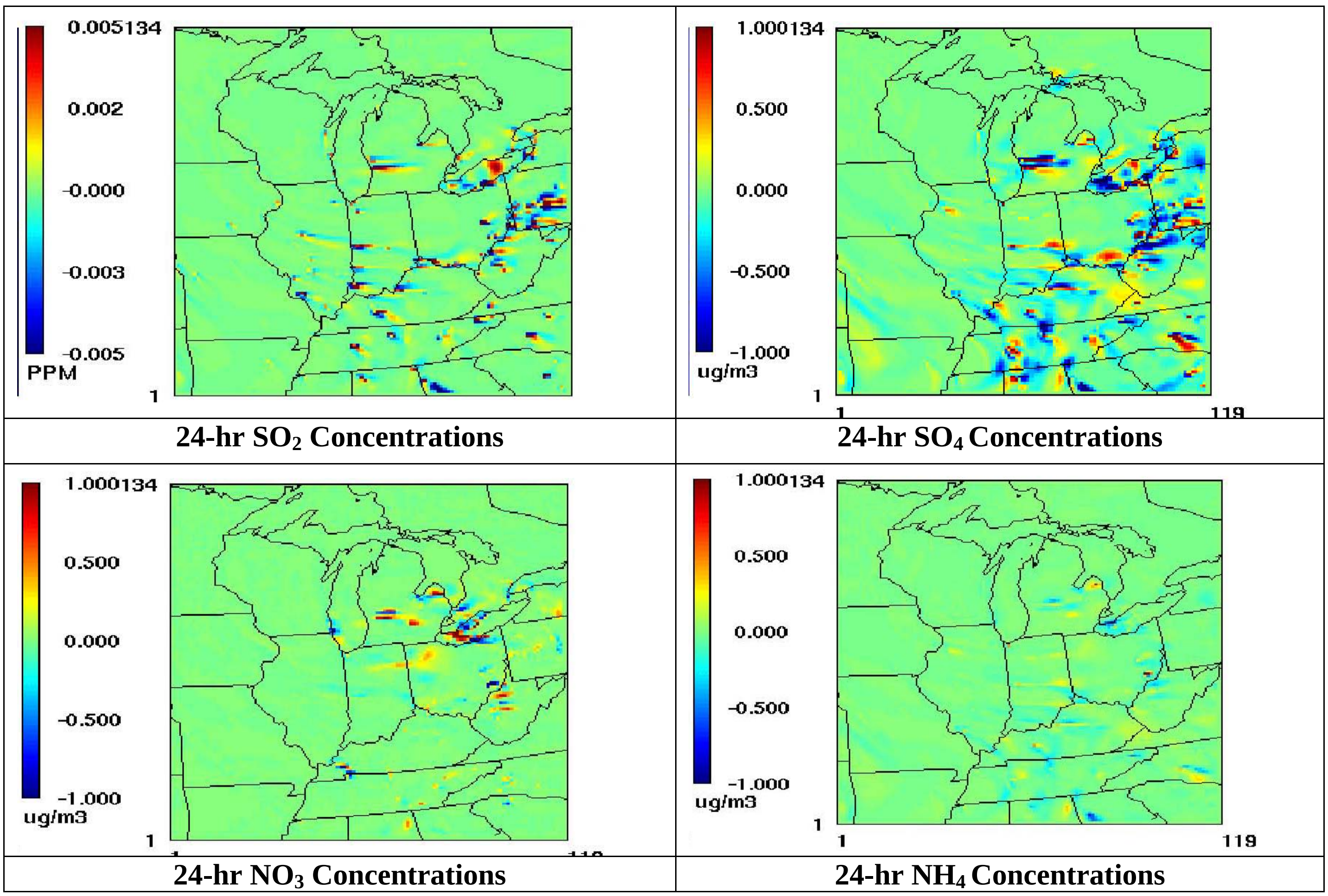

Figure 8-7. Incremental 24-hr Average SO_2, Sulfate, Nitrate, and NH_4 Concentrations Fields on 14 June 2002 from the CAMx PM PiG Simulation Over the Upper Midwest. Apparent in this figure are the individual plume footprints downwind from their origin. The modeled plumes result from full chemistry interaction between the background regional atmosphere and the chemical and physical dynamics of the individual plumes. (Adapted from Yarwood et al., 2005).

9.0 QUALITY ASSURANCE

9.1 Objective of the QA Program

A quality assurance (QA) program is needed to ensure that products produced in the BART exemption or BART control applications satisfy the regulatory objectives of the program. The scope of the QA program for a particular application should be defined in the protocol. Common elements include the configuration, data base development, setup and execution of the CALPUFF air quality model and processing of modeling results to determine compliance with visibility thresholds. In most if not all screening cases (see Chapter 6), states or source operators will use the CALMET datasets provided by CENRAP. Applications involving source-specific or alternative modeling that use different datasets, modeling options or tools will need to ensure that an appropriate QA program is defined in their protocols. More extensive quality assurance will be required in these latter applications. It is the responsibility of the state ensure that an adequate QA program, defined in the protocol, is implemented faithfully.

The CALPUFF modeling system contains features to facilitate quality assurance. These include the automatic production of "QA" files for various datasets, including geophysical fields, sources and receptors, and imbedded tracking of model options and switches within the output files from the major modules. The CALPUFF Graphical User Interface system (GUI) allows these QA files to be displayed graphically. In addition, a software management system is available to track version and level numbers associated each program and utility. This information reproduced in all of the output files, creating an audit trail of software versions and major model options.

The BART modeling process involves multiple organizations. As mentioned earlier, the states have overall responsibility for the process and may also execute some or all of the modeling. CENRAP is contributing general guidance via these guidelines and has funded the development of meteorological fields for use in screening applications. BART-eligible source operators will need to provide process information and emissions data for use in the analyses. Furthermore, 'subject to BART' sources will need to be actively involved in control technology decisions and assessments. Finally, some or all of the modeling steps may be carried out by contractors on behalf of a state or a source operator.

Each of these organizations has a responsibility to ensure that it is providing correct information to others and to evaluate the quality of any analyses it is performing, whether with data of its own or from others. This chapter provides general guidance and information on those aspects of quality assurance that are specific to the CALPUFF modeling effort, regardless of which organization is carrying out the effort. The focus is on the CALPUFF screening analyses described in Chapter 6. More comprehensive QA is needed for the unique aspects of the CALPUFF source-specific or the use of alternative models described in Chapters 7 and 8, respectively.

9.2 Quality Assurance Procedures

Chapter 6 recommends procedures for conducting CALPUFF screening modeling to determine the whether a particular source or group of sources is subject to BART controls. For initial applications, the regional 6 km resolution CALMET data files developed for CENRAP are available to modelers for the screening assessments. The development of these CALMET datasets was subject to a QA program. Thus, the amount of effort for modelers performing QA of these pre-defined meteorological fields is less than that required when developing source-specific meteorological fields at finer scale and/or over tailored domains.

9.2.1 Input Data

The input data required by the model depends on the application. At a minimum, source data is required by CALPUFF (see Section 6.3.4) along with specification of the model configuration (choices of options and switches). Most of the modeling option choices are specified or recommended by regulatory guidance and default values (see Appendix A through Appendix D). If an application uses CENRAP's CALMET files and the CALPUFF screening configuration recommended in Chapter 6, the quality assurance of input data will be straightforward. More detailed steps are needed for the setup of modeling files for CALPUFF source-specific applications using domains and meteorological fields that are not already developed.

The basic procedures that will apply to all CALPUFF model applications include a confirmation of the source data, including units, verification of the correct source and receptor locations, including datum and projection, confirmation of the switch selections relative to modeling guidance, checks of the program switches and file names for the various processing steps, and confirmation of the use of the proper version and level of each model program. An independent modeler should review the CALPUFF input files to confirm the switches and data entry in the model input files are correct. The independent reviewer should also exercise the CALPUFF modeling system for one or a few corroboration simulations (e.g., run of the worst case event) as a confirmation check.

The protocol should stipulate that a set of DVDs be created that contain all of the data and program files needed to reproduce the results presented in the final report. The model list files from each step should be included on the project DVD. This information allows independent checking and confirmation of the modeling process and facilitates archival of the study results.

9.2.2 MM5 and CALMET Applications

The CALMET meteorological data sets are available on external USB2 or IEEE 1394 (Firewire) hard drives in a format ready for use with CALPUFF. The QA steps used in the development of the CENRAP common datasets are described in the documentation attending the distribution to CENRAP. While these QA steps need not be repeated, some testing should be performed to show that the data are indeed suitable for the application for which it is being used. This is discussed in more detail below.

Appendix A contains a list of recommended CALMET switch settings for screening and source-specific modeling. Except as modified in a source-specific protocol, these configurations should be used in setting up the CALMET simulations. The CALMET model obtains the switch settings from an ASCII control file with a default name of CALMET.INP. Whether the model is run using a GUI or from the control line in DOS or Linux, it is essential that the control file be reviewed as part of the CALMET QA analysis. The CALMET GUI retains all of the input descriptive information that is part of the standard CALPUFF.INP file structure. This includes the default value for each variable, a text description of the variable, the meaning of each variable option, the units of the variable and inter-relationships among variables indicating if/when the variable is used. If CALMET is set up and run from the command line or if other user interfaces are employed, this QA step may become somewhat more difficult. It is essential nonetheless.

Part of the CALPUFF modeling system's built-in QA capability is a variable tracking system that retains the control file inputs for CALMET and CALPUFF in the output files create by the models. This information includes the Version and Level numbers of the processor codes and main model codes used in the simulations as well as the control files from the main models (CALMET and CALPUFF). The information from the preprocessing steps and the CALMET and CALPUFF model simulations is all carried forward and saved in the CALPUFF/postprocessor output files so that the final concentration/flux files contain a history of the model options and switch settings. This allows a user or reviewing agency to confirm the switch settings provided in a control file with that actually used in the model simulations. An optional switch in the CALPOST processor creates a complete listing of the QA data. This step requires access to the output CALPUFF concentration and/or flux files, which are normally practical to store on CDs or DVDs and to provide a part of the project CD/DVD set.

9.2.3 CALPUFF Applications

The minimum source data required by CALPUFF includes:

- Number of sources
- Locations (e.g., UTM coordinates, UTM zone and datum)
- Stack heights above the ground
- Stack diameters
- Exit velocities
- Exit temperatures
- Emission rates (SO_2, H_2SO_4, NO_x and PM_{10}).

There are additional requirements for building dimension information (building width, length, height and corner locations) for short stacks that are less than Good Engineering Practice (GEP) height. This information is used in providing effective structure dimensions for building downwash calculations. The requirement to conduct building downwash modeling may be waived by individual States where the pertinent transport distance to the nearest Class I area is large.

The source coordinates must be expressed in the coordinate system used to define the CALMET and CALPUFF modeling domains. For CENRAP screening applications, a Lambert Conformal Conic (LCC) coordinate system is used. The required parameters include two matching parallels, latitude/longitude of the projection origin, coordinate datum, and false Easting and Northing (if used) of the projection origin. For source-specific CALMET/CALPUFF domains, either an LCC or UTM projection may be used. The CALPUFF user interface includes software (e.g., COORDS) to compute to/from latitude/longitude, LCC and UTM coordinates for a large number of datum. In addition, the CALVIEW graphics feature allows the use of georeferenced satellite or aerial photographs to be used as base maps to confirm source locations. Links to sources of suitable base maps can be found on the CALPUFF data site (www.src.com) in the section on "Aerial Photos". The CALPUFF QA files provide the source coordinates used by the model in a CALVIEW-ready format for plotting. Many errors are found in source coordinates and related projection/datum parameters, so confirmation of the source location is an important part of the model QA.

The PM_{10} emissions should be broken into filterable and condensable components. The filterable PM_{10} emissions should be speciated into elemental carbon (EC), fine particulate matter (PMF) less than 2.5 µm diameter and coarse particulate matter (PMC) between 2.5 to 10 µm diameter. The condensable emissions should be divided into a primary H_2SO_4 component and organic and non-

H_2SO_4 inorganic components. (The sources of this information, such as source-specific data and AP-42 tables, are not addressed in this protocol.) The speciation of the PM_{10} emissions is important because the light extinction efficiency varies by more than a factor of 16 for different species, from 0.6 for coarse particulate matter to 10.0 for elemental carbon. Plus, hygroscopic aerosols are subject to a humidity growth factor (f(RH)), which can increase the light scattering from dry conditions by more than an order of magnitude in highly humid conditions. Thus, careful QA of the source and emissions data is an important component of the modeling.

The locations of the Class I area receptors may be obtained from the National Park Service (NPS) receptor dataset. Although the latitude and longitude of each receptor point is provided, it is necessary to ensure that the proper UTM or LCC coordinates have been computed for computational domain selected. In particular, the datum of the NPS conversion software is not specified, so it is recommended that coordinates be checked using the CALPUFF GUI's COORDS software or another comparable coordinate translation software package that recognizes various datums.

Most of the CALPUFF input variables contain default values. Appendix B contains a list of recommended CALPUFF switch settings for CENRAP screening applications. CALPUFF is configured using the ASCII "control file", CALPUFF.INP file. As with CALMET, whether CALPUFF is exercised GUI or from the command line in a DOS, Linux, or Unix window, it is essential that the control file be reviewed manually as part of the QA analysis. The CALPUFF GUI retains all of the input descriptive information that is part of the standard CALPUFF.INP file structure. This includes the default value for each variable, a text description of the variable, the meaning of each variable option, the units of the variable and inter-relationships among variables indicating if/when the variable is used.

9.2.4 Application of CALPOST and POSTUTIL

CALPOST is run separately for each Class I area in order to obtain the necessary visibility statistics for evaluating compliance with the BART screening and refined modeling thresholds. The inputs to CALPOST involve selection of the visibility method (Method 6), entry of Class I area-specific data for computing background extinction and monthly relative humidity factors for hygroscopic aerosols. CALPOST contains a receptor screening that allow subsets of a receptor network modeling in CALPUFF to be selected for processing in a given CALPOST run. This is how receptors within a single Class I area are selected for processing from a CALPUFF output file that may contain receptors from several Class I areas. CALPOST contains options for creating plot files that will help in the confirmation that the proper receptor subset is extracted.

The CALPOST output file contains a listing of the highest visibility impact each day of the model simulation over all receptors included in CALPOST analysis. Receptors will normally be selected in each CALPOST run so that each CALPOST run represents the impacts at a single Class I area. For a screening assessment, the peak value of the change in extinction is presented near the end of the CALPOST output file. For a source-specific studies where the 98^{th} percentile value (8^{th} highest day) is used for comparison against the BART threshold of 0.5 deciviews, the standard CALPOST output must be additionally processed. One may either obtain special-purpose processing software (see, for example CDPHE, 2005) or perform the processing manually. That is, one may import the results of the CALPOST table into a sorting program such as a spreadsheet to rank the daily change in extinction values in order to identify the 98^{th} percentile or 8^{th} highest day visibility increment.

CALPOST inputs that require particular QA review include:

> Visibility technique (Method 6);

> Monthly Class I-specific relative humidity factors for Method 6;

> Background light extinction values;

> Inclusion of all appropriate species from modeled sources (e.g., sulfate, nitrate, organics, (as SOA), coarse and fine particulate matter and elemental carbon;

> Appropriate species names for coarse PM used;

> Extinction efficiencies for each species;

> Appropriate Rayleigh scattering term (10 Mm^{-1} for screening modeling but Class I area specific value for source-specific modeling); and

> Screen to select appropriate Class I receptors for each CALPOST simulation.

The CALPOST program produces plot files compatible with CALVIEW that allow confirmation of receptor locations that is useful in evaluating the receptor screening step.

POSTUTIL allows the user to sum the contributions of sources from different CALPUFF simulations into a total concentration file. In addition, it contains options to scale the concentrations from different modeled species (e.g., different particle sizes) into species- dependent size distributions for the particulate matter. For example, PM is often simulated with unit emission rates for each particle size category and, in the POSTUTIL stage, the contributions of each size category based on the species being considered (e.g., elemental carbon, coarse particulate matter, etc) is combined to form the species concentrations for input into CALPOST. This process, although simple, requires a careful review of the weighting factors for each source.

POSTUTIL also allows a repartitioning of nitric acid and nitrate to account for the effects of ammonia limiting conditions. The four-step procedure for applying the ALM method is summarized in Chapter 7 and described in detail in Appendix A of the VISTAS protocol[1]. If source-specific modeling is performed using different sources of ammonia data or different techniques, the protocol should provide justification for all assumptions and a QA plan specific for the application and the data bases used.

9.2.5 QA Issues for Alternative Source-Specific or Alternative Modeling

The level of QA required for application of source-specific or alternative modeling protocols will be substantially higher than for the use of datasets that has already been subject to a QA procedure. For example, source-specific CALPUFF protocols may include the use of on-site meteorological datasets, the use of higher resolution prognostic meteorological (e.g., MM5) datasets, alternative visibility calculations, different extinction coefficients, or other changes to the screening

[1] "Comments on the Computation of Nitrate Using the Ammonia Limiting Method in CALPUFF", (Scire et al., 2005)

approach. Source-specific must therefore include the development of a QA plan to properly evaluate the data used in the modeling.

The critical CALMET input parameters depend on the mode in which the model is run (observations mode, hybrid mode or no-observations mode), and the location and spatial representativeness of any observational data. In a source specific protocol involving the development of a meteorological dataset, the elements of the QA process include preparation of wind rose (using observed, MM5 and CALMET-derived data), including examination of the data as a function of season and time of day (e.g., 4am, 10am, 4pm wind roses), time series analyses, and presentation of 2-D vector plots illustrating terrain effects/sea breeze circulation or other features of the flow expected to occur within the domain. For example, 2-D vector plots produced during light wind speed stable conditions (e.g., early morning such as 4am) are good for assessing the performance of the CALMET model configuration and switches in reproducing terrain effects because these conditions are likely to maximize the terrain impacts in the model. Seasonal wind roses at 4am, 10am and 4pm would be expected to show the development of seas breeze circulations that may be important for certain applications. Customization of the QA process for the individual source-specific domain based on the availability of data and the physical processes expected to be important at that location should be conducted as part of the source-specific QA plan development.

If source-specific CALPUFF simulations involving the ALM are conducted, the procedure summarized in Chapter 7 should be used. This includes an evaluation of the performance of the model in reproducing observed CASTNet or IMPROVE sulfate and nitrate concentrations at measurements sites within the source-specific modeling domain. The use of alternative ammonia concentration data (e.g., one-atmosphere model output rather than derived ammonia based on aerosol measurements) will require a review of the CMAQ or CAMx model performance results developed for CENRAP by the regional modeling contractor (Morris et al., 2005d)

9.3 Quality Assessment Summary

Each BART application requires a modeling report that includes a discussion of the datasets, modeling assumptions and a general discussion of limitations and uncertainties of the modeling exercise. Where CALPUFF screening analyses are performed followed by source-specific modeling, it will be possible to assess the relative conservatism of the screening approach. This may be helpful in assessing the impact of uncertainties in screening sources from BART controls. The reliability of source-specific CALPUFF modeling is expected to be somewhat better in predicting changes in visibility impacts due to BART controls than in predicting absolute visibility values. This is because errors and uncertainties in defining meteorological conditions, real-world atmospheric chemistry, and plume transport and dispersion rates may be diminished somewhat since the errors are included in both the base and sensitivity simulation cases.

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APPENDIX A -- CALMET SCREENING CONFIGURATION

The tables below identify the CALMET configurations used in developing the processed 6 km meteorological fields over the three CENRAP BART modeling domains shown in Figures 5-1 through 5-4. Also included in the tables below are the default CALMET options and parameter settings recommended in the IWAQM Phase 2 Report (EPA, 1998).

Table A-1. Input Groups in the CALMET Control File.

Input Group	Description	Applicable to CENRAP BART
0	Input and output file names	Yes
1	General run control parameters	Yes
2	Map Projection and Grid Control Parameters	Yes
3	Output Options	Yes
4	Meteorological Data Options	Yes
5	Windfield Options and Parameters	Yes
6	Mixing Height, Temperature and Precipitation Parameters	Yes
7	Surface Meteorological Station Parameters	Yes
8	Upper Air Meteorological Station Parameters	Yes
9	Precipitation Station Parameters	Yes

Table A-2. CALMET Model Input Group 0: Input and Output File Names.

Parameter	Default	CENRAP	Comments
Input	GEO.DAT	GEO.DAT	
Input	SURF.DAT	SURF.DAT	
Input	CLOUD.DAT	CLOUD.DAT	
Input	PRECIP.DAT	PRECIP.DAT	
Input	MM4.DAT	MM4.DAT	
Input	WT.DAT	WT.DAT	
Output	CALMET.LST	CALMET.LST	
Output	CALMET.DAT	CALMET.DAT	
Output	PACOUT.DAT	PACOUT.DAT	
NUSTA	--	0	Number of upper air stations
NOWSTA	--	0	Number of over water met stations
Input	UP1.DAT	UP1.DAT	
Input	UP2.DAT	UP2.DAT	
Input	UP3.DAT	UP3.DAT	

Input	SEA1.DAT	SEA1.DAT	
Input	DIAG.DAT	DIAG.DAT	
Input	PROG.DAT	PROG.DAT	
Output	TEST.PRT	TEST.PRT	
Output	TEST.OUT	TEST.OUT	
Output	TEST.KIN	TEST.KIN	
Output	TEST.FRD	TEST.FRD	
Output	TEST.SLP	TEST.SLP	

Table A-3. CALMET Model Input Group 1: General Run Control Parameters.

Parameter	Default	CENRAP	Comments
IBYR	-	2001	Starting year
IBMO	-	1	Starting month
IBDY	-	1	Starting day
IBHR	-	1	Starting hour
IBTZ	-	6	Base time zone
IRLG	-	8736	Length of run
IRTYPE	1	1	Run type (must = 1 to run CALPUFF)
LCALGRD	T	F	Compute CALGRID data fields
ITEST	2	2	Stop run after SETUP to do input QA

Table A-4. CALMET Model Input Group 2: Map Projection and Grid Control Parameters.

Parameter	Default	CENRAP	Comments
PMAP	UTM	LCC	Map Projection
RLATO	--	40N	Latitude (dec. degrees) of projection origin
RLONO	--	97W	Longitude (dec. degrees) of projection origin
XLAT1	--	33N	Matching parallel(s) of latitude for projection
XLAT2	--	45N	Matching parallel(s) of latitude for projection
DATUM	WGS-G	WGS-G	
NX	--	300	Number of X grid cells in meteorological grid
NY	--	192	Number of Y grid cells in meteorological grid
DGRIDKM	--	6.0	Grid spacing, km
XORIGKM	--	-1008.	Ref. Coordinate of SW corner of grid cell (1,1)
YORIGKM	--	0.0	Ref. Coordinate of SW corner of grid cell (1,1)
NZ	--	10	No. of vertical layers
ZFACE	--	0, 20 40,	Cell face heights in arbitrary vertical grid, m

		80, 160, 320, 640, 1200, 2000, 3000, 4000	

Table A-5. CALMET Model Input Group 3: Output Options.

Parameter	Default	CENRAP	Comments
LSAVE	T	T	Disk output option
IFORMO	1	1	Type of unformatted output file
LPRINT	F	F	Print met fields
IPRINF	1	1	Print intervals
IUVOUT(NZ)	NZ*0	NZ*0	Specify layers of u,v wind components to print
IWOUT(NZ)	NZ*0	NZ*0	Specify layers of w wind component to print
ITOUT(NZ)	NZ*0	NZ*0	Specify levels of 3-D temperature field to print
LDB	F	F	Print input met data and variables
NN1	1	1	First time step for debug data to be printed
NN2	1	1	Last time step for debug data to be printed
IOUTD	0	0	Control variable for writing test/debug wind fields
NZPRN2	1	0	Number of levels starting at surface to print
IPR0	0	0	Print interpolated wind components
IPR1	0	0	Print terrain adjusted surface wind components
IPR2	0	0	Print initial divergence fields
IPR3	0	0	Print final wind speed and direction
IPR4	0	0	Print final divergence fields
IPR5	0	0	Print winds after kinematic effects
IPR6	0	0	Print winds after Froude number adjustment
IPR7	0	0	Print winds after slope flows are added

IPR8	0	0	Print final wind field components

Table A-6. CALMET Model Input Group 4: Meteorological Data Options.

Parameter	Default	CENRAP	Comments
NOOBS	0	2	2 = No surface, overwater, or upper air observations; use MM5 for surface, overwater, and upper air data
NSSTA	--	0	Number of meteorological surface stations
NPSTA	--	0	Number of precipitation stations
ICLOUD	--	3	Gridded cloud fields
IFORMS	2	2	Formatted surface meteorological data file
IFORMP	2	2	Formatted surface precipitation data file
IFORMC	2	2	Formatted cloud data file

Table A-7. CALMET Model Input Group 5: Windfield Options and Parameters.

Parameter	Default	CENRAP	Comments
IWFCOD	1	1	Model selection variable
IFRADJ	1	1	Compute Froude number adjustment effects?
IKINE	0	0	Compute kinematic effects?
IOBR	0	0	Use O'Brien (1970) vertical velocity adjustment?
ISLSOPE	1	1	Compute slope flow effects?
IEXTRP	-4	-1	Extrapolate surface wind obs to upper levels?
ICALM	0	0	Extrapolate surface winds even if calm?
BIAS	NZ*0	0, 0, 0, 0, 0, 0, 0, 0, 0, 0	Layer-dependent biases weighting aloft measurements
RMIN2	4.	-1.0	Minimum vertical extrapolation distance
IPROG	0	14	14 = Yes, use winds from MM5.DAT file as initial guess field [IWFCOD = 1
ISTEPPG	1	1	MM5 output timestep
LVARY	F	T	Use varying radius of influence
RMAX1	--	30.	Maximum radius of influence over land in sfc layer
RMAX2	--	30.	Maximum radius of influence over land aloft

RMAX3	--	50.	Maximum radius of influence over water
RMIN	0.1	0.1	Minimum radius of influence used anywhere
TERRAD	--	12.	Terrain features radius of influence
R1	--	1.	Weighting of first guess surface field
R2	--	1.	Weighting of first guess aloft field
RPROG	--	0.	MM5 windfield weighting parameter
DIVLIM	5.E-6	5.E-6	Minimum divergence criterion
NITER	50	50	Number of divergence minimization iterations
NSMMTH	2, 4, 4, 4, 4, 4, 4	2, 4, 4, 4, 4, 4, 4	Number of passes through smoothing filter in each layer of CALMET
NITR2	99.	5, 5, 5, 5, 5, 5, 5, 5, 5, 5	Maximum number of stations used in each layer for the interpolation of data to a grid point
CRITFN	1.0	1.0	Critical Froude number
ALPHA	0.1	0.1	Kinematic effects parameter
FEXTR2	NZ*0.0	NZ*0.0	Scaling factor for extrapolating sfc winds aloft
NBAR	0	0	Number of terrain barriers
IDIOTP1	0	0	Surface temperature computation switch
ISURFT	--	4	Number of sfc met stations to use for temp calcs
IDIOPT2	0	0	Domain-averaged lapse rate switch
IUPT	0	2	Upper air stations to use for lapse rate calculation
ZUPT	200.	200.	Depth through which lapse rate is calculated
IDIOPT3	0	0	Domain-averaged wind component switch
IUPWND	-1	-1	Number of aloft stations to use for wind calc
ZUPWND	1., 1000.	1., 1000.	Bottom and top of layer through which the domain-scale winds are computed
IDIOPT4	0	0	Observed surface wind component switch
IDIOPT5	0	0	Observed aloft wind component switch
LLBREZE	F	F	Use Lake Breeze Module
NBOX	0	0	Number of lake breeze regions
NLB	--	0	Number of stations in the region
METBXID(NLB)	--	0	Station ID's in the region

Table A-8. CALMET Model Input Group 6: Mixing Height, Temperature and Precipitation.

Parameter	Default	CENRAP	Comments

CONSTB	1.41	1.41	Neutral stability mixing height coefficient
CONSTE	0.15	0.15	Convective stability mixing height coefficient
CONSTN	2400.	2400.	Stable stability maxing height coefficient
CONSTW	0.16	0.16	Overwater mixing height coefficient
FCORIOL	1.E-4	1.E-4	Absolute value of Coriolis parameter
IAVEZI	1	1	Conduct spatial averaging? Yes = 1
MNMDAV	1	10	Maximum search radius in averaging process
HAFANG	30.	30.	Half-angle of upwind looking cone for averaging
ILEVZI	1	1	Layers of wind use in upwind averaging
DPTMIN	0.001	0.001	Minimum potential temperature lapse rate in the stable layer above the current convective mixing ht
DZZI	200.	200.	Depth of layer above current conv. mixing height through which lapse rate is computed
ZIMIN	50.	50.	Minimum overland mixing height
ZIMAX	3000.	3000.	Maximum overland mixing height
ZIMINW	50.	50.	Minimum overwater mixing height
ZIMAXW	3000.	3000.	Maximum overwater mixing height
ITPROG	0	2	3D temperature from observations or from MM5?
IRAD	1	1	Type of interpolation; 1 = 1/R
TRADKM	500.	36.	Temperature interpolation radius of influence
NUMTS	5	5	Max number of stations for temp interpolation
IAVET	1	1	Spatially average temperatures? 1 = yes
TGDEFB	-.0098	-.0098	Temp gradient below mixing height over water
TGDEFA	-.0045	-.0045	Temp gradient above mixing height over water
JWAT1	--	55	Beginning land use categories over water
JWAT2	--	55	Ending land use categories for water
NFLAGP	2	2	Precipitation interpolation flag; 2 = 1/R-squared
SIGMAP	100.	50.	Radius of influence for precipitation interpolation
CUTP	0.01	0.01	Minimum precipitation rate cutoff (mm/hr)

APPENDIX B -- CALPUFF SCREENING CONFIGURATION

The tables below identify the recommended CALPUFF screening configurations for CENRAP BART modeling. Also identified are the default recommendations from the IWAQM Phase 2 Report (EPA, 1998).

Table B-1. Input Groups in the CALPUFF Control File.

Input Group	Description	Applicable to CENRAP BART
0	Input and output file names	Yes
1	General run control parameters	Yes
2	Technical options	Yes
3	Species list	Yes
4	Grid control parameters	Yes
5	Output options	Yes
6	Sub grid scale complex terrain inputs	Yes
7	Dry deposition parameters for gases	Yes
8	Dry deposition parameters for particles	Yes
9	Miscellaneous dry deposition for parameters	Yes
10	Wet deposition parameters	Yes
11	Chemistry parameters	Yes
12	Diffusion and computational parameters	Yes
13	Point source parameters	Ye
14	Area source parameters	Yes
15	Line source parameters	Yes
16	Volume source parameters	Yes
17	Discrete receptor information	Yes

Table B-2. CALPUFF Model Input Group 1: General Run Control Parameters.

Parameter	Default	CENRAP	Comments
METRUN	0	0	All model periods in met file(s) will be run
IBYR	-	2001	Starting year
IBMO	-	1	Starting month
IBDY	-	1	Starting day
IBHR	-	1	Starting hour
XBTZ	-	6	Base time zone (6 = CST)
IRLG	-	8760	Length of run
NSPEC	5	10	Number of MESOPUFF II chemical species
NSE	3	8	Number of chemical species to be emitted
ITEST	2	2	Program is executed after SETUP phase
MRESTART	0	0	Do not read or write a restart file during run
NRESPD	0	0	File written only at last period
METFM	1	1	CALMET binary file (CALMET.MET)
AVET	60	60	Averaging time in minutes
PGTIME	60	60	PG Averaging time in minutes

Table B-3. CALPUFF Model Input Group 2: Technical Options

Parameter	Default	CENRAP	Comments
MGAUSS	1	1	Gaussian distribution used in near field
MCTADJ	3	3	Partial plume path terrain adjustment
MCTSG	0	0	Sub-grid-scale complex terrain not modeled
MSLUG	0	0	Near-field puffs not modeled as elongated
MTRANS	1	1	Transitional plume rise modeled
MTIP	1	1	Stack tip downwash used
MSHEAR	0	0	(0, 1) Vertical wind shear (not modeled, modeled)
MSPLIT	0	0	Puffs are not split
MCHEM	1	1	MESOPUFF II chemical parameterization scheme
MAQCHEM	0	0	Aqueous phase transformation not modeled
MWET	1	1	Wet removal modeled
MDRY	1	1	Dry deposition modeled
MDISP	3	3	PG dispersion coefficients

MTURBVW	3	3	Use both σ_v and σ_w from PROFILE.DAT to compute σ_y and σ_z (n/a)
MDISP2	3	3	PG dispersion coefficients
MROUGH	0	0	PG σ_y and σ_z not adjusted for roughness
MPARTL	1	1	No partial plume penetration of elevated inversion
MTINV	0	0	Strength of temperature inversion computed from default gradients
MPDF	0	0	PDF not used for dispersion under convective conditions
MSGTIBL	0	0	Sub-grid TIBL module not used for shoreline
MBCON	0	0	Boundary concentration conditions not modeled
MFOG	0	0	Do not configure for FOG model output
MREG	1	1	Technical options must conform to USEPA Long Range Transport (LRT) guidance

Table B-4. CALPUFF Model Input Group 3: Species List-Chemistry Options.

CSPEC	Modeled[1]	Emitted[2]	Dry Deposition[3]	Output Group Number
SO_2	1	1	1	0
SO_4^{-2}	1	0	2	0
NOx	1	1	1	0
HNO_3	1	0	1	0
NO_3^-	1	0	2	0
NH_3	1	1	1	0
PMC	1	1	2	0
PMF	1	1	2	0
EC	1	1	2	0
SOA	1	1	2	0

Notes:
1 0=no, 1=yes
2 0=no, 1=yes (depends on speciation breakdown available)
3 0=none; 1=computed-gas; 2=computed-particle; 3=user-specified

Table B-5. CALPUFF Model Input Group 4: Map Projection and Grid Control Parameters.

Parameter	Default	CENRAP	Comments
PMAP	UTM	UTM	Map Projection
NX	-	66	Number of X grid cells in meteorological grid
NY	-	66	Number of Y grid cells in meteorological grid
NZ	-	10	Number of vertical layers in meteorological grid
DGRIDKM	-	6	Grid spacing (km)
ZFACE	-	0, 20 40, 80, 160, 320, 640, 1200, 2000, 3000, 4000	Cell face heights in meteorological grid (m)
XORIGKM	-	5.	Reference X coordinate for SW corner of grid cell (1,1) of meteorological grid (km)
YORIGKM	-	3327.	Reference Y coordinate for SW corner of grid cell (1,1) of meteorological grid (km)
IUTMZN	-	12	UTM zone of coordinates (NAD83)
IBCOMP	-	1	X index of lower left corner of the computational grid
JBCOMP	-	1	Y index of lower left corner of the computational grids
IECOMP	-	66	X index of the upper right corner of the computational grid
JECOMP	-	66	Y index of the upper right corner of the computational grid
LSAMP	T	F	Sampling grid is not used
IBSAMP	-	1	X index of lower left corner of the sampling grid
JBSAMP	-	1	Y index of lower left corner of the sampling grid
IESAMP	-	66	X index of upper right corner of the sampling grid
JESAMP	-	66	Y index of upper right corner of the sampling grid
MESHDN	1	1	Nesting factor of the sampling grid

Table B-6. CALPUFF Model Input Group 5: Output Options.

Parameter	Default	CENRAP	Comments
ICON	1	1	Output file CONC.DAT containing concentrations is created
IDRY	1	1	Output file DFLX.DAT containing dry fluxes is created
IWET	1	1	Output file WFLX.DAT containing wet fluxes is created
IVIS	1	1	Output file containing relative humidity data is created
LCOMPRS	T	T	Perform data compression in output file
IMFLX	0	0	Do not calculate mass fluxes across specific boundaries
IMBAL	0	0	Mass balances for each species not reported hourly
ICPRT	0	1	Print concentration fields to the output list file
IDPRT	0	0	Do not print dry flux fields to the output list file
IWPRT	0	0	Do not print wet flux fields to the output list file
ICFRQ	1	1	Concentration fields are printed to output list file every hr
IDFRQ	1	1	Dry flux fields are printed to output list file every 1 hour
IWFRQ	1	1	Wet flux fields are printed to output list file every 1 hour
IPRTU	1	3	Units for line printer output are in g/m3 for concentration and $g/m^2/s$ for deposition
IMESG	2	2	Messages tracking the progress of run written to screen
LDEBUG	F	F	Logical value for debug output
IPFDEB	1	1	First puff to track
NPFDEB	1	1	Number of puffs to track
NN1	1	1	Meteorological period to start output
NN2	10	10	Meteorological period to end output

Table B-7. CALPUFF Model Input Group 6: Sub-Grid Scale Complex Terrain Inputs.

Parameter	Default	CENRAP	Comments
NHILL	0	0	Number of terrain features
NCTREC	0	0	Number of special complex terrain receptors
MHILL	-	2	Input terrain and receptor data for CTSG hills input in CTDM format
XHILL2M	1	1	Conversion factor for changing horizontal dimensions to meters
ZHILL2M	1	1	Conversion factor for changing vertical dimensions to meters
XCTDMKM	-	0.0 E+00	X origin of CTDM system relative to CALPUFF coordinate system (km)
YCTDMKM	-	0.0 E+00	Y origin of CTDM system relative to CALPUFF coordinate system (km)

Table B-8. CALPUFF Model Input Group 7: Dry Deposition Parameters for Gases.

Species	Default	CENRAP	Comments
SO_2	0.1509	0.1509	Diffusivity
	1000.	1000.	Alpha star
	8.0	8.0	Reactivity
	0.0	0.0	Mesophyll resistance
	0.04	0.04	Henry's Law coefficient
NO_x	0.1656	0.1656	Diffusivity
	1.0	1.0	Alpha star
	8.0	8.0	Reactivity
	5.0	5.0	Mesophyll resistance
	3.5	3.5	Henry's Law coefficient
HNO_3	0.1628	0.1628	Diffusivity
	1.0	1.0	Alpha star
	18.0	18.0	Reactivity
	0.0	0.0	Mesophyll resistance
	8.0E-8	8.0E-8	Henry's Law coefficient
	0.000359	0.000359	Henry's Law coefficient

Table B-9. CALPUFF Model Input Group 8: Dry Deposition Parameters for Particles.

Species	Default	CENRAP	Comments
SO_4^{-2}	0.48	0.48	Geometric mass mean diameter of $SO4^{-2}$ [µm]
NO_3^-	2.0	0.48	Geometric mass mean diameter of $NO3^-$ [µm]
PMC	2.0	6.0	Geometric mass mean diameter of PMC [µm]
PMF	2.0	0.48	Geometric mass mean diameter of PMF [µm]
EC	2.0	0.48	Geometric mass mean diameter of EC [µm]
SOA	0.48	0.48	Geometric mass mean diameter of SOA [µm]

(Geometric Standard Deviation for all species assumed to be 2.0 µm).

Table B-10. CALPUFF Model Input Group 9: Miscellaneous Dry Deposition Parameters.

Parameter	Default	CENRAP	Comments
RCUTR	30	30	Reference cuticle resistance (s/cm)
RGR	10	10	Reference ground resistance (s/cm)
REACTR	8	8	Reference pollutant reactivity
NINT	9	9	Number of particle size intervals for effective particle deposition velocity
IVEG	1	1	Vegetation in non-irrigated areas is active and unstressed

Table B-11. CALPUFF Model Input Group 10: Wet Deposition Parameters.

Species	Default	CENRAP	Comments
SO_2	3.21E-05	3.21E-05	Scavenging coefficient for liquid precipitation [s^{-1}]
	0.0	0.0	Scavenging coefficient for frozen precipitation [s^{-1}]
SO_4^{-2}	1.0E-04	1.0E-04	Scavenging coefficient for liquid precipitation [s^{-1}]
	3.0E-05	3.0E-05	Scavenging coefficient for frozen precipitation [s^{-1}]
HNO_3	6.0E-05	6.0E-05	Scavenging coefficient for liquid precipitation [s^{-1}]
	0.0	0.0	Scavenging coefficient for frozen precipitation [s^{-1}]
NO_3^-	1.0E-04	1.0E-04	Scavenging coefficient for liquid precipitation [s^{-1}]
	3.0E-05	3.0E-05	Scavenging coefficient for frozen precipitation [s^{-1}]
NH_3	8.0E-05	8.0E-05	Scavenging coefficient for liquid precipitation [s^{-1}]
	0.0	0.0	Scavenging coefficient for frozen precipitation [s^{-1}]
PMC	1.0E-04	1.0E-04	Scavenging coefficient for liquid precipitation [$^{s-1}$]
	3.0E-05	3.0E-05	Scavenging coefficient for frozen precipitation [s^{-1}]

PMF	1.0E-04	1.0E-04	Scavenging coefficient for liquid precipitation [$^{s-1}$]
	3.0E-05	3.0E-05	Scavenging coefficient for frozen precipitation [s^{-1}]
EC	1.0E-04	1.0E-04	Scavenging coefficient for liquid precipitation [$^{s-1}$]
	3.0E-05	3.0E-05	Scavenging coefficient for frozen precipitation [s^{-1}]
OC	1.0E-04	1.0E-04	Scavenging coefficient for liquid precipitation [$^{s-1}$]
	3.0E-05	3.0E-05	Scavenging coefficient for frozen precipitation [s^{-1}]

Table B-12. CALPUFF Model Input Group 11: Chemistry Parameters.

Parameter	Default	CENRAP	Comments
MOZ	1	1	Read ozone background concentrations from ozone.dat file (measured values).
BCKO3	12*80	12*40	Background ozone concentration (ppb)
BCKNH3	12*10	12*3	Background ammonia concentration (ppb)
RNITE1	0.2	0.2	Nighttime NO_2 loss rate in percent/hour
RNITE2	2	2	Nighttime NOX loss rate in percent/hour
RNITE3	2	2	Nighttime HNO_3 loss rate in percent/hour
MH202	1	1	Background H_2O_2 concentrations (Aqueous phase transformations not modeled)
BCKH202	1	1	Background monthly H_2O_2 concentrations (Aqueous phase transformations not modeled)
BCKPMF	1.	1.	Fine particulate concentration for SOA Option (micrograms per cubic meter)
OFRAC	.2	.2	Organic fraction of fine particulate for SOA Option
VCNX	50.	50.	VOC/NOx ratio for SOA Option

Table B-13. CALPUFF Model Input Group 12: Dispersion/Computational Parameters.

Parameter	Default	CENRAP	Comments
SYDEP	550	550	Horizontal size of a puff in meters beyond which the time dependant dispersion equation of Heffter (1965) is used
MHFTSZ	0	0	Do not use Heffter formulas for sigma z
JSUP	5	5	Stability class used to determine dispersion rates for puffs above boundary layer
CONK1	0.01	0.01	Vertical dispersion constant for stable conditions
CONK2	0.1	0.1	Vertical dispersion constant for neutral/stable conditions
TBD	0.5	0.5	Use ISC transition point for determining the transition point between the Schulman-Scire to Huber-Snyder Building Downwash scheme
IURB1	10	10	Lower range of land use categories for which urban dispersion is assumed
IURB2	19	19	Upper range of land use categories for which urban dispersion is assumed
ILANDUIN	20	*	Land use category for modeling domain
XLAIIN	3.0	*	Leaf area index for modeling domain
ZOIN	-0.25	*	Roughness length in meters for modeling domain
ELEVIN	0.0	*	Elevation above sea level
XLATIN	-999	-	North latitude of station in degrees
XLONIN	-999	-	South latitude of station in degrees
ANEMHT	10	10	Anemometer height in meters
ISIGMAV	1	1	Sigma-v is read for lateral turbulence data
IMIXCTDM	0	0	Predicted mixing heights are used
XMXLEN	1	1	Maximum length of emitted slug in meteorological grid units
XSAMLEN	1	10	Maximum travel distance of slug or puff in meteorological grid units during one

			sampling unit
MXNEW	99	60	Maximum number of puffs or slugs released from one source during one time step
MXSAM	99	60	Maximum number of sampling steps during one time step for a puff or slug
NCOUNT	2	2	Number of iterations used when computing the transport wind for a sampling step that includes transitional plume rise
SYMIN	1	1	Minimum sigma y in meters for a new puff or slug
SZMIN	1	1	Minimum sigma z in meters for a new puff or slug
SVMIN	.50	.50	Minimum lateral turbulence velocities (m/s)
SWMIN	0.20, 0.12, 0.08, 0.06, 0.03, 0.016	0.20, 0.12, 0.08, 0.06, 0.03, 0.016	Minimum vertical turbulence velocities (m/s)
WSCALM	0.5	0.5	Minimum non-calm wind speeds (m/s)
XMAXZI	3000.	3000.	Maximum mixing height (m)
XMINZI	50.	20.	Minimum mixing height (m)
SL2PF	10.	10.	Maximum Sy/puff length
PLXO	0.07, 0.07, 0.10, 0.15, 0.35, 0.55	0.07, 0.07, 0.10, 0.15, 0.35, 0.55	Wind speed power-law exponents
WSCAT	1.54, 3.09, 5.14, 8.23, 10.80	1.54, 3.09, 5.14, 8.23, 10.80	Upper bounds of 1st 5 wind speed classes
PGGO	0.020, 0.035	0.020, 0.035	Potential temp gradients PG E & F (deg/km)
CDIV	0.01	0.01	Divergence criterion for dw/dz (1/s)
PPC	0.5, 0.5, 0.5, 0.5, 0.35, 0.35	0.5, 0.5, 0.5, 0.5, 0.35, 0.35	Plume path coefficients (only if MCTADJ=3)
NSPLIT	3	3	Number of puffs when puffs split
IRESPLIT	-	1900	Hour(s) when puff is eligible to split

ZISPLIT	100	100	Previous hour's minimum mixing height, m
ROLDMAX	0.25	0.25	Previous Max mixing height/current mixing height ratio, must be less than this value to allow puff to split
NSPLITH	5	5	Number of puffs resulting from a split
SYSPLITH	1.0	1.0	Minimum sigma-y of puff before it may split
SHSPLITH	2.0	2.0	Minimum puff elongation rate from wind shear before puff may split
CNSPLITH	1.0E-07	1.0E-07	Minimum species concentration before a puff may split
EPSSLUG	1.0E-04	1.0E-04	Criterion for SLUG sampling
EPSAREA	1.0E-06	1.0E-06	Criterion for area source integration
DSRISE	1.0	1.0	Trajectory step length for numerical rise algorithm
Note: Values indicated by an asterisk (*) were allowed to vary spatially across the domain and were obtained from CALMET			

Table B-14. CALPUFF Model Input Group 13: Point Source Parameters.

Parameter	Default	CENRAP	Comments
NPT1	-	Varies by scenario	Number of point sources with constant stack parameters or variable emission rate scale factors
IPTU	1	1	Units for point source emission rates are g/s
NSPT1	0	-	Number of source-species combinations with variable emissions scaling factors
NPT2	-	-	Number of point sources with variable emission parameters provided in external file
MISC	-	-	Other point source inputs include stack height (H), stack diameter (d), exit temperature (T), exit velocity (v), downwash flag, and emissions by species.

Table B-15. CALPUFF Model Input Group 14: Area Source Parameters.

Parameter	Default	CENRAP	Comments
NAR1		Varies by scenario	Number of polygon area sources
IARU	1	1	Units for area source emission rates are $g/m^2/s$
NSAR1	0	-	Number of source species combinations with variable emissions scaling factors
NAR2	-	-	Number of buoyant polygon area sources with variable location and emission parameters

Table B-16. CALPUFF Model Input Group 15: Line Source Parameters.

Parameter	Default	CENRAP	Comments
NLN2	-	-	Number of buoyant line sources with variable location and emission parameters
NLINES	-	-	Number of buoyant line sources
ILNU	1	-	Units for line source emission rates is g/s
NSLN1	0	-	Number of source-species combinations with variable emissions scaling factors
MXNSEG	7	-	Maximum number of segments used to model each line
NLRISE	6	-	Number of distance at which transitional rise is computed
XL	-	-	Average line source length (m)
HBL	-	-	Average height of line source height (m)
WBL	-	-	Average building width (m)
WML	-	-	Average line source width (m)
DXL	-	-	Average separation between buildings (m)
FPRIMEL	-	-	Average buoyancy parameter (m4/s3)

Table B-17. CALPUFF Model Input Group 16: Volume Source Parameters.

Parameter	Default	CENRAP	Comments
NVL1	-	-	Number of volume sources
IVLU	1	-	Units for volume source emission rates is grams per second
NSVL1	0	-	Number of source-species combinations with variable emissions scaling factors
IGRDVL	-	-	Gridded volume source data is not used
VEFFHT	-	-	Effective height of emissions (m)
VSIGYI	-	-	Initial sigma y value (m)
VSIGZI	-	-	Initial sigma z value (m)

Table B-18. CALPUFF Model Input Group 17: Discrete Receptor Information.

Parameter	Default	CENRAP	Comments
NREC	-	5630	Number of non-gridded receptors

APPENDIX C – POSTUTIL SCREENING CONFIGURATION

The tables below identify the recommended POSTUTIL processor screening configurations for CENRAP BART modeling.

Table C-1. Input Groups in the POSTUTIL Processor Control File.

Sub Group	Description	Applicable to CENRAP BART
0a	Input and output file names	Yes
1	NMET – Number of CALMET data files (365)	Yes
2	NFILES – Number of CALPUFF data files	Yes

Table C-2. POSTUTIL Processor Input Group 1: General Run Control Parameters.

Parameter	DEFAULT	CENRAP	Comments
ISYR	--	2001	Starting year
ISMO	--	1	Starting month
ISDY	--	1	Starting day
ISHR	--	0	Starting hour
NPER	--	8760	Number of periods to process
NSPECINP	--	6	Number of CALPUFF species to process
NSPECOUT	--	6	Number of species to output
NSPECCMP	--	0	Number of species to derive
MDUPLCT	--	1	Stop run if duplicate name
NSCALED	--	0	Number of CALPUFF files to 'scale'
MNITRATE	--	1	Recompute the HNO_3/NO_3 partition for CALPUFF modeled concentrations? 1 = yes for all sources combined
BCKNH3	10.	3.	Default NH_3 concentration (ppb) for HNO_3/NO_3 partitioning

Table C-3. POSTUTIL Processor Input Group 2: Species Processing Information.

Parameter	DEFAULT	CENRAP	Comments
ASPECI	--	SO_2, SO_4, NO_x, HNO_3, NO_3, PM_{10}	Species to post-process
ASPECO	--	SO_2, SO_4, NO_x, HNO_3, NO_3, PM_{10}	Species to output
CSPECCMP	--	CSPECCMP = N SO_2 = 0.0 SO_4 = 0.291667 NO = 0.466667 NO_2 = 0.304348 HNO_3 = 0.222222 NO_3 = 0.451613 PM_{10} = 0.0	Nitrogen species to be computed by scaling and summing one or more of the processed input species using the scaling factors for each of the NSPECINP input species
CSPECCMP	--	CSPECCMP = S SO_2 = 0.50 SO_4 = 0.333333 NO = 0.0 NO_2 = 0.0 HNO_3 = 0.0 NO_3 = 0.0 PM_{10} = 0.0	Sulfur species to be computed by scaling and summing one or more of the processed input species using the scaling factors for each of the NSPECINP input species
MODDAT	--	A (Default=1.0) SO_2 = 1.1 SO_4 = 1.5 HNO3 = 0.8 NO_3 = 0.1 B (Default=0.0) SO_2 = 0.0 SO_4 = 0.0 HNO_3 = 0.0 NO_3 = 0.0	Each species in NSCALED CALPUFF data files may be scaled before processing (e.g., to change the emission rate for all sources modeled in the run that produced a data file). For each scaled species the scaling factors are A and B where x' = Ax + B.

APPENDIX D – CALPOST SCREENING CONFIGURATION

The tables below identify the recommended CALPOST processor screening configurations for CENRAP BART modeling.

Table D-1. Input Groups in the CALPOST Processor Control File.

Group	Description	Applicable to CENRAP BART
0	Input and output file names	Yes
1	General Run Control Parameters	Yes
2	Visibility Parameters	Yes
3	Output Options	Yes

Table D-2. CALPOST Processor Input Group 1: General Run Control Parameters.

Parameter	DEFAULT	CENRAP	Comments
ISYR	--	2001	Starting year
ISMO	--	1	Starting month
ISDY	--	1	Starting day
ISHR	--	0	Starting hour
NPER	--	8760	Number of periods to process
NREP	1	1	Process every hour of data? Yes = 1
ASPEC	--	VISIB	Process species for visibility
ILAYER	1	1	Layer/deposition code; 1 for CALPUFF concentrations
A	0.0	0.0	Scaling factor, slope
B	0.0	0.0	Scaling factor, intercept
LBACK	F	F	Add hourly background concentrations or fluxes?
LG	F	F	Process gridded receptors?
LD	F	T	Process discrete receptors?
LCT	F	F	Process complex terrain receptors?
LDRING	F	F	Report receptor ring results?
NDRECP	-1	-1	Select all discrete receptors
IBGRID	-1	-1	X index of LL corner of receptor grid
JBGRID	-1	-1	Y index of LL corner of receptor grid
IEGRID	-1	-1	X index of UR corner of receptor grid

JEGRID	-1	-1	X index of UR corner of receptor grid
NGONOFF	0	0	Number of gridded receptor rows
NGXRECP	1	0	Exclude specific gridded receptors, Yes = 0

Table D-3. CALPOST Processor Input Group 2: Species Processing Information.

Parameter	DEFAULT	CENRAP	Comments
RHMAX	98	95	Maximum RH (%) used in particle growth curve
LVSO4	T	T	Compute light extinction for sulfate?
LVNO3	T	T	Compute light extinction for nitrate?
LVOC	T	T	Compute light extinction for organic carbon?
LVMPC	T	T	Compute light extinction for coarse particles?
LVMPF	T	T	Compute light extinction for fine particles?
LVEC	T	T	Compute light extinction for elemental carbon?
LVBK	T	T	Include background in extinction calculation?
SPECPMC	PMC	PMC	Coarse particulate species
SPECPMF	PMF	PM10	Fine particulate species
EEPMC	0.6	0.6	Extinction efficiency for coarse particulates
EEPMF	1.0	1.0	Extinction efficiency for fine particulates
EEPMCBK	0.6	0.6	Extinction efficiency for coarse part. background
EESO4	3.0	3.0	Extinction efficiency for ammonium sulfate
EENO3	3.0	3.0	Extinction efficiency for ammonium nitrate
EEOC	4.0	4.0	Extinction efficiency for organic carbon
EESOIL	1.0	1.0	Extinction efficiency for soil
EEEC	10.0	10.0	Extinction efficiency for elemental carbon
MVISBK	2	6	Method 6 for background light extinction: Compute extinction from speciated PM measurements. FLAG RH adjustment factor applied to observed & modeled sulfate and nitrate
BEXTBTBK	--	12	Background extinction for MVISBK=1 (1/Mm)
RHFRAC	--	10	Percentage of particles affected by RH
RHFAC	12*value	Depends on Class I Area	Extinction coefficients for modeled and background hygroscopic species computed using EPA (2003) monthly RH adjustment factors
BKSO4	0.12	0.12	Background sulfate extinction coeff – west
BKNO3	0.10	0.10	Background nitrate extinction coeff – west
BKPMC	3.00	3.00	Background coarse part. extinction coeff – west
BKSOC	0.47	0.47	Background organic carbon extinct. coeff – west

BKSSOIL	0.50	0.50	Background soil extinction coeff – west
BKSEC	0.02	0.02	Background elem. carbon extinct. coeff – east
BKSO4	0.23	0.23	Background sulfate extinction coeff – east
BKNO3	0.10	0.10	Background nitrate extinction coeff – east
BKPMC	3.00	3.00	Background coarse part. extinction coeff – east
BKSOC	1.40	1.40	Background organic carbon extinct. coeff – east
BKSSOIL	0.50	0.50	Background soil extinction coeff – east
BKSEC	0.02	0.02	Background elem. carbon extinct. coeff – east
BEXTRAY	10.0	10.0	Extinction due to Rayleigh scattering (1/Mm)

Table D-4. CALPOST Processor Input Group 3: Output Options.

Parameter	DEFAULT	CENRAP	Comments
LDOC	F	F	Print documentation image?
IPRTU	1	3	Print output units ($\mu g/m^3$) for concentrations and ($\mu g/m^2/sec$) for deposition
L1HR	T	F	Report 1 hr averaging times
L3HR	T	F	Report 3 hr averaging times
L24HR	T	T	Report 24 hr averaging times
LRUNL	T	F	Report run-length (annual) averaging times
LT50	T	F	Top 50 table
LTOPN	F	F	Top 'N' table
NTOP	4	4	Number of 'Top-N' values at each receptor
ITOP	1,2,3,4	1,2,3,4	Ranks of 'Top-N' values at each receptor
LEXCD	F	F	Threshold exceedances counts
THRESH1	-1.0	-1.0	Averaging time threshold for 1 hr averages
THRESH3	-1.0	-1.0	Averaging time threshold for 3 hr averages
THRESH24	-1.0	-1.0	Averaging time threshold for 24 hr averages
THRESHN	-1.0	-1.0	Averaging time threshold for NAVG-hr averages
NDAY	0	0	Accumulation period, days
NCOUNT	1	1	Number of exceedances allowed
LECHO	F	F	Echo option
LTIME	F	F	Time series option
LPLT	F	F	Plot file option
LGRD	F	F	Use grid format instead of DATA format
LDEBUG	F	F	Output information for debugging?