

# Protocol for the Application of Preferred or Alternative Models for Analyses of Best Available Retrofit Technology (BART)

(Revised Draft)

September 20, 2005

Visibility Improvement State and Tribal Association  
of the Southeast (VISTAS)

**Comment:** General Comments:  
Protocol spends too much time describing/repeating the words from rules, guidelines, user manuals, preambles and describing the features and capabilities of the CALPUFF modeling system.

The protocol should contain an example analysis, with supporting figures and tables, of one facility located near a Class I area. The appendix should contain the CALPUFF/CALPOST input/output files so the modeler would know what options should be selected.

URS has commented extensively on the subject concerning the need to do line-of-sight (LOS) modeling for CALPUFF regional haze modeling. The technical merits for this modeling approach are provided in the attached slide presentation prepared for the EPA 's 8<sup>th</sup> Conference on Air Quality Modeling held in RTP in Sept of 2005 and are supported by Pitchford and Malm (1992) and Richards (1999). An approximate 1.0 deciview change was defined by Pitchford and Malm (1992) as a "just noticeable change" to the observer when the background visual range equals the line of sight. According to L. Willard Richards in "Use of the Deciview Haze Index as an Indicator for Regional Haze" if a shorter line of sight distance than the background visual range (natural conditions) is used in performing the calculations then a higher extinction value, or deciview, is needed to cause a "just noticeable change". In other words, when the line of sight is less than the background visual range, then it would require a higher deciview value in order to be a "just noticeable change".

Where this protocol briefly touches on the LOS issue additional comments have been provided.

Many places in the protocol the word visibility is used as a surrogate for regional haze. It should be noted that visibility is a short-term concern or an acute issue. BART modeling addresses longer averaging periods and is more chronic in nature.

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# TABLE OF CONTENTS

	Page	
<b>PREFACE</b>	iv	Deleted: 111
<b>1. INTRODUCTION AND PROTOCOL OBJECTIVES</b>	<b>1</b>	Inserted: 11
<b>2. REVIEW OF EPA'S GUIDANCE FOR BART MODELING</b>	<b>3</b>	Deleted: 4443
2.1 Overview of the Regional Haze BART Process	4	Inserted: 44
2.2 Model Recommendations for the BART Analysis	6	Inserted: 4
2.3 Performance of a Cap and Trade Program	7	Deleted: 6665
<b>3. OVERVIEW OF THE <u>PREFERRED</u> CALPUFF MODELING SYSTEM</b>	<b>8</b>	Inserted: 66
3.1 Capabilities and features of CALPUFF	8	Inserted: 6
3.1.1 Major Features of CALMET	10	Deleted: 7776
3.1.2 Major Features of CALPUFF	12	Inserted: 77
3.1.3 Major Features of Postprocessors (CALPOST and POSTUTIL)	17	Deleted: 8887
3.2 Discussion of CALPUFF Applicability and Limitations	17	Inserted: 88
3.2.1 Transport and Diffusion	17	Inserted: 8
3.2.2 Aerosol Constituents	20	Deleted: 8887
3.2.3 Regional Haze	27	Inserted: 88
<b><u>3.A OVERVIEW OF ALTERNATIVE MODELS (PLUVUEII &amp; SCIPUFF)</u></b>		Inserted: 8
<u>3.1a Capabilities and Features of PLUVUE-II</u>		Deleted: 1010109
<u>3.2a Discussion of PLUVUE-II Applicability and Limitations</u>		Inserted: 1010
<u>3.3a Capabilities and Features of SCIPUFF</u>		Inserted: 10
<u>3.4a Discussion of SCIPUFF Applicability and Limitations</u>		Deleted: 12121211
<b>4. VISTAS' COMMON MODELING PROTOCOL</b>	<b>31</b>	Inserted: 1212
4.1 Overview of Common Modeling Approach	31	Inserted: 12
4.1.1 BART Exemption Analysis	31	Deleted: 17171716
4.1.2 BART Control Evaluation	33	Inserted: 1717
4.1.3 VISTAS Treatment of VOC and NH3	34	Inserted: 17
4.2 Optional Source-Specific Modeling	34	Deleted: 17171716
4.3 Screening Procedure for BART Exemption	35	Inserted: 1717
4.3.1 Overview of Screening Approach	35	Inserted: 17
4.3.2 Discussion of Regional Screening Approach	35	Deleted: 17171716
4.3.3 Model Configuration and Settings for Screening Analysis	39	Inserted: 1717
4.4 Refined Modeling Procedures	42	Deleted: 20202019
4.4.1 Rationale for and Overview of Refined Modeling Approach	42	Inserted: 2020
4.4.2 Model Configuration and Settings for Refined Modeling	44	Inserted: 20
4.5 Presentation of Modeling Results	45	Deleted: 27272726
4.5.1 Sample Summary Tables of Visibility Results	45	Inserted: 2727



## **PREFACE**

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This protocol describes common procedures for carrying out air quality modeling to support BART determinations that are consistent with guidelines of the U.S. Environmental Protection Agency. It is intended to serve as the basis for a common understanding among the organizations that will be performing BART analyses or reviewing the BART modeling results in the VISTAS region. This document was prepared jointly by VISTAS, its contractor Earth Tech, Inc., and VISTAS' Technical Advisor. It is an outgrowth of an earlier draft protocol dated 22 March 2005.

# 1. INTRODUCTION AND PROTOCOL OBJECTIVES

Under the regional haze regulations, the Environmental Protection Agency (EPA) has issued final guidelines dated July 6, 2005 for Best Available Retrofit Technology (BART) determinations (70 FR, 39104-39172). The regional haze rule includes a requirement for a BART evaluation for certain large stationary sources. Sources are BART-eligible if they meet three criteria including emissions of at least 250 tons per year of a visibility-impairing pollutant, began operation on or after August 7, 1962 and were in existence on August 7, 1977, and fall within one of the 26 listed source categories in the guidance. A BART evaluation and possibly air emission 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 cause or contribute to visibility impairment in a Class I area.

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Throughout this document the term “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 facility has several emission units, only those that meet the BART-eligible criteria are included in the definition “BART-eligible source”.

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As of September 20, 2005, VISTAS States had identified a total of 275 BART-eligible sources that fall into 20 of the 26 BART source categories. Of the 275 sources with BART-eligible units, 86 sources are electric generating units (EGUs) and 189 are non-EGU industrial sources.

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The objective of this VISTAS’ BART Modeling Protocol is to describe common procedures for performing air quality modeling to support BART exemption modeling analyses and BART evaluation modeling analyses that are consistent with the EPA guidelines. This protocol will serve as the basis for establishing a common understanding among those who will be performing the BART analyses or those reviewing the BART modeling results, including VISTAS State and Local air regulatory agencies, EPA, Federal Land Managers (FLMs), source operators, and contractors for the sources. This revised draft protocol incorporates EPA final guidance and comments that were received on VISTAS’ draft protocol<sup>1</sup> and provides additional description of modeling procedures. VISTAS intends to finalize the protocol in November 2005, after incorporating comments received on this revised draft protocol.

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The VISTAS States have accepted EPA’s guidance to use the CALPUFF modeling system or other acceptable models in order to meet the BART modeling requirements of the regional haze rule. If a BART-eligible source elects to perform their own dispersion modeling, they are encouraged to submit a site-specific modeling protocol to the State for review and approval prior to performing the BART modeling. States will consult with Federal Land Managers and

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<sup>1</sup> Draft BART Modeling Protocol for VISTAS, March 22, 2005

Environmental Protection Agency in evaluating the site-specific BART protocols. The site-specific protocol should include the source-specific data on source location, stack parameters, and emissions rates. The methods of the VISTAS common modeling protocol will be followed in the site-specific protocol unless the source proposes to the State, and the State approves, alternative models or methods or assumptions.

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Each VISTAS State or Local agency retains responsibility for the specific procedures and processes it will follow in working with the BART sources under its jurisdiction, the FLMs, EPA, and the public. Each VISTAS State or Local agency also retains full responsibility for the review of any BART control evaluations performed by the source and will make the final decision regarding any air emission controls. Nothing in the VISTAS process replaces States' responsibility to determine BART controls. No BART sources are located on Tribal lands.

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The remainder of this document describes the Preferred CALPUFF modeling system and the application of CALPUFF or another alternative models to two situations:

- Air quality modeling to determine whether a BART-eligible source is “subject to BART”, and, if required,
- 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.

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Chapter 2 of this document reviews EPA's guidance for regional haze BART analysis modeling, as outlined in the 6 July 2005 Federal Register notice. The CALPUFF model is the preferred model recommended by the EPA for BART modeling analyses and its characteristics and limitations are discussed in Chapter 3. The modeling guidance does allow for the use of appropriate alternative models, however, this protocol will focus primarily on guidance for the application of the preferred CALPUFF modeling approach. It is understood that there could be instances where more accurate modeling results may occur by using the CALPUFF model in conjunction with another alternative model or by applying CALPUFF with modeling methodologies that remove some of the conservatism incorporated into current CALPUFF regional haze modeling procedures. However, these modeling issues are best discussed in site specific modeling protocols and not in this common protocol. Other alternative models maybe needed for modeling facilities very near Class I areas or for other specialized long-range transport situations. Chapter 3a briefly discusses other models such as PLUVUE-II and SCIPUFF and provides a brief overview of how these models could be applied in a BART analysis.

The specific steps to determine whether a BART-eligible source is subject to BART and to evaluate BART controls are described in Chapter 4. The procedures include screening BART-eligible sources using regional meteorological datasets and CALPUFF run in a conservative mode. For sources determined to be subject to BART based on these first screening analyses, further refined CALPUFF analyses would be performed. The model configuration for the common modeling protocol is described in Chapter 4. Details of the source-specific protocol are

described in Chapter 5. A quality assurance plan is outlined in Chapter 6. A set of three appendices provides more details on major issues concerning the proposed model configuration and technical approach. *[In the final protocol these appendices should be moved into the appropriate sections. An Appendix will be added that summarizes an evaluation of CALPUFF predictions for secondary pollutants, light extinction, and sulfur and nitrogen deposition in a Class I area in Wyoming.]*

This protocol does not address a preferred modeling approach to demonstrate the effectiveness of an optional emissions cap and trade program. Such a cap and trade program is not required, but can be implemented in lieu of BART if desired by the VISTAS States. VISTAS States are deferring discussion of options for a regional trading alternative until the recently-proposed EPA trading guidance (70 FR 44154-44175) is finalized later in 2005.

## 2. REVIEW OF EPA'S GUIDANCE FOR BART MODELING

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The final guidance for regional haze BART determinations was published in the Federal Register on 6 July 2005 (70 FR 39104 to 39172). It provides guidance for modeling approaches that are to be used for various stages of the BART analysis process.

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### 2.1 Overview of the Regional Haze BART Process

The process of establishing BART emission limitations consists of four steps:

1) 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 begun operation on or after August 7, 1962 and must have been in existence on August 7, 1977 in order to be BART-eligible. Finally, 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<sub>10</sub>) and gaseous precursors to secondary fine particulate matter such as SO<sub>2</sub> and NO<sub>x</sub>. Whether ammonia and Volatile Organic Compounds (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<sub>2.5</sub> emissions and not VOCs for BART purposes.

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2) Determine whether a BART-eligible source can be excluded from a BART evaluation by demonstrating that the source cannot be reasonably expected to cause or contribute to visibility impairment in a Class I area. The preferred approach is an assessment with an air quality model such as CALPUFF or other appropriate models followed by comparison of the estimated 24-hr visibility impacts against a threshold above estimated natural conditions to be determined by the States or as defined by the Source with State approval.<sup>2</sup> The threshold to determine whether a single source "causes" visibility impairment is set at a 1.0 deciview change from natural conditions (background visual range) over a 24-hour averaging period in the final BART rule (70 FR 39118). An approximate 1.0 deciview change was defined by Pitchford and Malm (1992) as a "just noticeable change" to the observer when the background visual range equals the line of sight. According to L. Willard Richards in "Use of the Deciview Haze Index as an Indicator for Regional Haze" if a shorter line of sight distance than the background visual range (natural conditions) is used in performing the calculations then a higher extinction value, or deciview, is needed to cause a "just noticeable change". In other words, when the line of sight is less than the background visual range, then it would require a higher deciview value in order to be a "just noticeable change".

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<sup>2</sup> The level of the natural conditions baseline that is to be used needs to be clarified. It is described differently in the BART guideline and in the preamble to the BART rule. The BART guideline text says "natural conditions" at 70 FR 39162, col. 3, while the preamble says "natural visibility baseline for the 20% best visibility days" at 70 FR 39125, col. 1.

However, this protocol uses a conservative modeling approach by comparing the extinction changes from a single source at Class I area receptors only (not along the line of sight) to the background visual range (natural conditions) in order to compare to the 1.0 deciview change threshold.

If the 98<sup>th</sup> percentile value on a receptor by receptor basis exceeds this threshold, a BART review would be required.<sup>3</sup> 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. The recommendation in the EPA guidance is to compare the 98<sup>th</sup> percentile value from the modeling with the contribution threshold of 0.5 deciviews (or a lower level set by a State) to determine if a source does not contribute to visibility impairment and therefore is not subject to BART. Over an annual period, this implies the 8<sup>th</sup> highest day at a particular receptor is compared to the contribution threshold (if assume complete record with samples every 3rd day.) Over a 3-year modeling period, the 98<sup>th</sup> percentile value may be interpreted as the highest of the three annual 98<sup>th</sup> percentile values at a particular receptor.

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Alternatively, States have the option of considering that all BART-eligible sources within the State are subject to BART and skipping the initial impact analysis. In rare cases, a State might be able to do exactly the opposite, and use regional modeling to conclude that all BART-eligible sources in the State do not cumulatively contribute to “measurable” visibility impairment in any Class I areas. Also, the States have an option to exempt individual sources based on modeling results with “model plants” that share specific characteristics with actual sources such as emission amounts, stack parameters and distance to a Class I area.

3) Determine BART controls 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.

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<sup>3</sup> The guideline itself is ambiguous about what modeling value is to be compared with the causality threshold. The interpretation given here is based on personal communication with Todd Hawes of the U.S. EPA; further clarification is being sought.

4) Incorporate the BART determination into the State Implementation Plan for Regional Haze, which is due by 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 that is designed to achieve regional haze improvements that are greater than the visibility improvements that could be expected from BART.<sup>4</sup> 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, air quality modeling comparing the expected improvements in visibility from the trading program and from BART would be required. (See the proposed BART Alternative rule, at 70 FR 44160.) EPA suggests that regional modeling using a photochemical grid model may be more appropriate than CALPUFF for this purpose.

## 2.2 Model Recommendations for the BART Analysis

To evaluate the regional haze 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 as “the best regulatory modeling application currently available for predicting a single source’s contribution to visibility impairment” (70 FR 39162). The use of another “appropriate model” is allowed although the EPA prefers the use of CALPUFF.

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For modeling the impact of a source closer than 50 km to a Class I area, EPA’s BART guidance recommends that expert modeling judgment be used “giving consideration to both CALPUFF and other methods.” The PLUVUE-II model is mentioned as a possible model to consider in addition to CALPUFF within 50 km of a source.

Comment: Preamble: “states may run CALPUFF or another appropriate dispersion model”. Last sentence says that both CALPUFF and an alternative model is needed.

The EPA guidance notes that “regional scale photochemical grid models may have merit, but such models have been designed to assess cumulative impacts, not impacts from individual sources” and they are “very resource intensive and time consuming relative to CALPUFF”, but States may consider their use for SIP development in the future as they may be adapted and “demonstrated to be appropriate for single source applications” (70 FR 39123). Photochemical grid models may be more appropriate 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 (70 FR 39163).

According to the BART guidance, a modeling protocol should be submitted by the source to the State 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

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<sup>4</sup> The EPA’s BART rule points out that the Clean Air Interstate Rule (CAIR) would satisfy the BART requirements for affected electric generating units (EGUs), which could affect the modeling efforts a State would need to undertake (70 FR 39138-39139).

understand the BART-eligible source configurations” and factors affecting their particular Class I areas (70 FR 39126). States will make the final approval of the protocols.

In the BART modeling analyses 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 State use the highest 24-hour average actual emission rate for the meteorological period modeled, (excluding periods with start-up, shutdown and malfunctions) (70 FR 39129).

**Comment:** BART Guideline states, “24-hour average actual emission rate from the highest emitting day of the meteorological period modeled.” This would be for the period 2001-2003.

If a source is found to be subject to BART, CALPUFF or another appropriate model should be used to evaluate the improvement in regional haze resulting from the application of BART controls. Regional haze improvements may be evaluated on a pollutant-specific basis in the BART determination (70 FR 39129).

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For evaluating the improvement in regional haze resulting from the application of BART, the EPA guidelines state that 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” (70 FR 39129).

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### 2.3 Performance of a Cap and Trade Program

If a State or States elect to pursue an optional cap and trade program, they are required to demonstrate greater “reasonable progress” in reducing haze than would result if BART were applied to the same sources. In some cases, a State may simply be able to demonstrate that a trading program that achieves greater progress at reducing emissions will also achieve greater progress at reducing haze. Such would be the case if the likely geographic distribution of emissions under the trading program would not be greatly different from the distribution if BART was in place.

If the expected distribution of emissions is different under the two approaches, then “dispersion modeling” of all sources must be used to determine the difference in visibility at each impacted Class I area, in order to establish that the optional trading program will result in regional haze improvements aggregated over all Class I areas that are “better than BART” (70 FR 39137-39138). The BART guidance does not specify the method to be used for this modeling. From a technical perspective, either applying CALPUFF to every source or using a regional photochemical model would satisfy the need.

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A rulemaking procedure is currently underway to establish final guidance for such alternatives to BART (70 FR 44154-44175). The rule is expected to be finalized late in 2005.

### 3. OVERVIEW OF THE CALPUFF MODELING SYSTEM

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#### 3.1 Capabilities and features of CALPUFF

The CALPUFF modeling system (Scire et al., 2000a, b) is recommended as the preferred model for use in the BART analyses. CALPUFF and its meteorological model CALMET, are designed to handle the complexities posed by the complex terrain, the large source-receptor distances, chemical transformation and deposition, and other issues related to Class I regional haze impacts. 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 (68 FR 18440-18482). CALPUFF is recommended for Class I impact assessments by the Federal Land Managers Workgroup (FLAG 2000) and the Interagency Workgroup on Air Quality Modeling (IWAQM) (EPA 1998). The final BART guidance recommends CALPUFF as “the best modeling application available for predicting a single source’s contribution to visibility impairment” (70 FR 39122). As a result of these recommendations, the VISTAS modeling protocol is primarily focused on the use of CALPUFF for its BART determinations.

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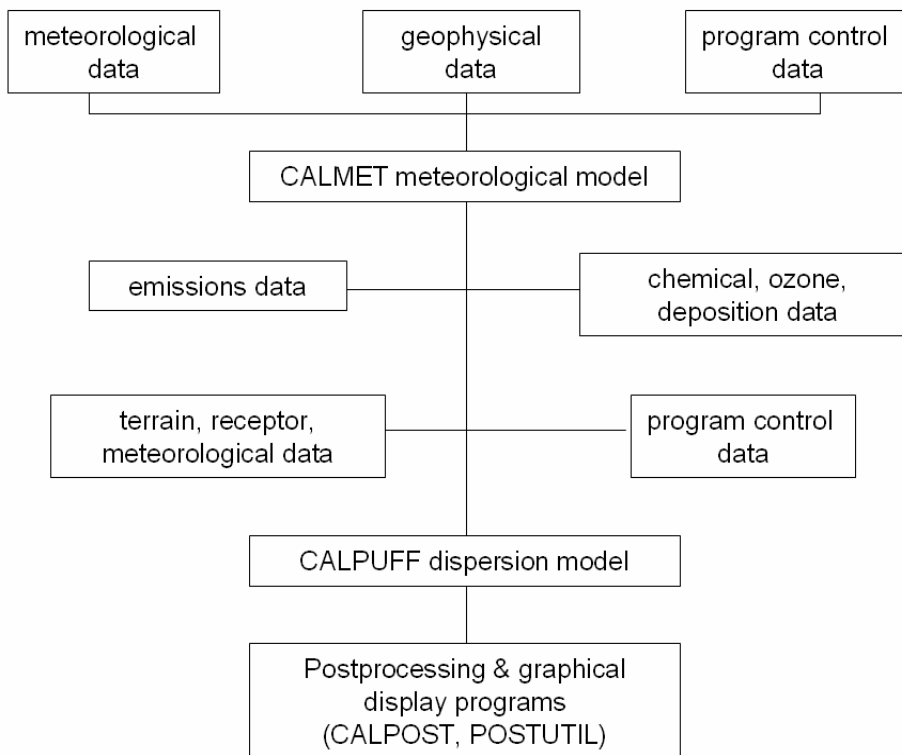
The main components of the CALPUFF modeling system are shown in Figure 3-1. CALMET is a diagnostic meteorological model that is used to drive the CALPUFF dispersion model. It produces three-dimensional wind and temperature fields and two-dimensional fields of mixing heights and other meteorological fields. It contains slope flow effects, terrain channeling, and kinematic effects of terrain. CALMET includes special algorithms for treating the overwater boundary layer and coastal interaction effects. CALMET can use meteorological observational data and/or three-dimensional output from prognostic numerical meteorological models such as MM5 (Grell et al., 1995) or RUC (Benjamin et al., 2004) in the developments of its fine-scale meteorological fields.

CALPUFF is a non-steady-state Lagrangian puff transport and dispersion model that advects Gaussian puffs of multiple pollutants from modeled sources. CALPUFF’s algorithms have been designed to be applicable on spatial scales from a few tens of meters to hundreds of kilometers from a source. It includes algorithms for near-field effects such as building downwash, stack tip downwash and transitional plume rise as well as processes important in the far-field such as chemical transformation, wet deposition, and dry deposition. CALPUFF contains an option to allow puff splitting in the horizontal and vertical directions, which extends the distance range of the model. The primary outputs from CALPUFF are hourly concentrations and hourly deposition fluxes evaluated at user-specified receptor locations.

A set of postprocessing programs associated with CALPUFF computes visibility effects and allows cumulative source impacts to be assessed, including potential non-linear effects of ammonia limitation on nitrate formation. The CALPOST postprocessor contains several options for computing change in extinction and deciviews for visibility assessments. The POSTUTIL postprocessor includes options for summing contributions of individual sources or groups of sources to assess cumulative impacts. POSTUTIL also contains CALPUFF’s nitric acid-nitrate

chemical equilibrium module, which allows the cumulative effects of ammonia consumption by background sources to be assessed in the postprocessor. In addition, the combination of CALPUFF and POSTUTIL allows the effects of source emissions of ammonia to be incrementally added to background ammonia levels in determining nitrate formation.

The rest of this chapter summarizes the capabilities and features of the CALPUFF modeling components in more detail.



**Figure 3-1. CALPUFF modeling system components.**

### 3.1.1 Major Features of CALMET

The CALMET meteorological model consists of a diagnostic wind field module and micrometeorological modules for overwater and overland boundary layers. When modeling a large geographical area, as would be necessary for the regional VISTAS 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.

**Table 3-1. Major Features of the CALMET Meteorological Model**

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- **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

#### *CALMET Boundary Layer Models*

The CALMET model contains two boundary layer models for application to overland and overwater grid cells.

*Overland Boundary Layer Model:* 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 model also determines gridded fields of PGT stability class and hourly precipitation rates.

*Overwater Boundary Layer Model:* The aerodynamic and thermal properties of water surfaces suggest that a different method is best suited for calculating the 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.

### ***Diagnostic Wind Field Module***

The diagnostic wind field module uses a two-step approach to the computation of the wind fields (Douglas and Kessler, 1988). In the first step, an initial-guess wind field is adjusted for kinematic effects of terrain, slope flows, and terrain blocking effects to produce a Step 1 wind field. Gridded MM5 can be used to define the initial guess field. The second step consists of an objective analysis procedure to introduce observational data into the Step 1 wind field to produce a final wind field.

***Step 1 Wind Field.*** Development of the Step 1 wind field begins with the initial guess field defined by the MM5 prognostic meteorological model. Normally, the CALMET computational domain is specified to be at finer grid resolution than the MM5 dataset used to initialize the initial guess field. For example, 36-km MM5 data available for VISTAS modeling may be used to develop the initial guess field on a 12-km or even a 1-km CALMET grid. The Step 1 algorithms in CALMET described below apply terrain adjustments to the initial guess field on the fine-scale CALMET grid. Thus, the CALMET winds are adjusted to respond to fine-scale terrain features not necessarily seen by the coarser scale MM5 model.

*Kinematic Effects of Terrain:* The approach of Liu and Yocke (1980) is used to evaluate the effects 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 in CALMET 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.

**Step 2 Wind Field.** The wind field resulting from the above adjustments of the initial-guess wind is the Step 1 wind field. The second step of the procedure involves the introduction of observational data into the Step 1 wind field through an objective analysis procedure. An inverse-distance squared interpolation scheme is used which weighs observational data heavily in the vicinity of the observational station, while the Step 1 wind field dominates the interpolated wind field in regions with no observational data. The resulting wind field is subject to smoothing, an optional adjustment of vertical velocities based on the O'Brien (1970) method, and divergence minimization to produce a final Step 2 wind field. The introduction of observational data in the Step 2 calculation 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. In No-Obs mode, observational data is not used in the Step 2 calculations.

### 3.1.2 Major Features of CALPUFF

By its puff-based formulation and through the use of three-dimensional meteorological data developed by the CALMET meteorological model, CALPUFF can simulate the effects of time- and space-varying meteorological conditions on pollutant transport from sources in complex terrain. The major features and options of the CALPUFF model are summarized in Table 3-2. Some of the technical algorithms are briefly described below.

*Complex Terrain:* The 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 in CALPUFF, 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.

*Puff Sampling Functions:* A set of accurate and computationally efficient puff sampling routines are included in CALPUFF which solve many of the 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.

*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:* Several options are provided in CALPUFF for the computation of dispersion coefficients, including the use of turbulence measurements ( $\sigma_v$  and  $\sigma_w$ ), the use of similarity theory to estimate  $\sigma_v$  and  $\sigma_w$  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.

*Overwater and Coastal Interaction Effects:* Because the CALMET meteorological model contains both overwater and overland boundary layer algorithms, the effects of water bodies on plume transport, dispersion, and deposition can be simulated with CALPUFF. The puff formulation of CALPUFF is designed to handle spatial changes in meteorological and dispersion conditions, including the abrupt changes, which occur at the coastline of a major body of water.

*Dry Deposition:* A resistance model is provided in CALPUFF 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  $\mu\text{m}$  diameter) from coarse particulate matter (2.5-10  $\mu\text{m}$  diameter).

*Wind Shear Effects:* CALPUFF contains an optional puff splitting algorithm that allows vertical wind shear effects across individual puffs to be simulated. Differential rates of dispersion and transport among the “new” puffs generated from the original, well-mixed puff can substantially increase the effective rate of horizontal spread of the material. 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.

*Wet Deposition:* An empirical scavenging coefficient approach is used in CALPUFF 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).

*Chemical Transformation:* CALPUFF includes options for parameterizing chemical transformation effects using the five species scheme ( $\text{SO}_2$ ,  $\text{SO}_4^-$ ,  $\text{NO}_x$ ,  $\text{HNO}_3$ , and  $\text{NO}_3^-$ ) employed in the MESOPUFF II model or a set of user-specified, diurnally-varying transformation rates. The MESOPUFF II scheme is recommended by IWAQM. It produces secondary fine particulate matter (sulfate and nitrate) from emissions of  $\text{SO}_2$  and  $\text{NO}_x$  that allows analyses of visibility impacts. Ambient ozone concentrations are used in the parameterized chemical transformation module as a surrogate for OH radicals during daylight hours. Ambient ammonia concentrations are used together with a temperature and relative humidity-dependent equilibrium relationship to partition nitric acid and nitrate on an hour-by-hour and receptor-by-receptor basis.

**Table 3-2. Major Features of the CALPUFF Dispersion Model**

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- **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 ( $\sigma_y$ ,  $\sigma_z$ ) options**
  - Direct measurements of  $\sigma_y$  and  $\sigma_w$
  - Estimated values of  $\sigma_y$  and  $\sigma_w$  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
  
- **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)

**Table 3-2. Major Features of the CALPUFF Dispersion Model (Cont'd)**

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- **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

### 3.1.3 Major Features of Postprocessors (CALPOST and POSTUTIL)

The two main postprocessor of interest for BART applications are the CALPOST and POSTUTIL programs. 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 POSTUTIL processor is a program that 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), and contains a chemistry module to evaluate the equilibrium relationship between nitric acid and nitrate aerosols. This capability allows the potential non-linear effects ammonia scavenging by background sulfate and nitrate sources to be evaluated in the formation of nitrate from an individual source. See Appendix A for more information on ammonia limiting effects.

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..

The POSTUTIL process will also compute the impacts of individual sources or groups of sources on sulfur and nitrogen deposition into aquatic, forest and coastal ecosystems. The postprocessor allow the changes in deposition fluxes resulting from changes in emissions to be quantified. For example the output of POSTUTIL and CALPOST can be used as input into an Acid Neutralizing Capacity (ANC) analysis, or for comparison to Deposition Analysis Thresholds (DATs).

## 3.2 Discussion of CALPUFF Applicability and Limitations

### 3.2.1 Transport and Diffusion

According to the IWAQM Phase 2 report (page 18), “CALPUFF is recommended for transport distances of 200 km or less. Use of CALPUFF for characterizing transport beyond 200 to 300 km should be done cautiously with an awareness of the likely problems involved.”<sup>5</sup>

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<sup>5</sup> The IWAQM presentation at EPA’s 6<sup>th</sup> Modeling Conference provides the background for this recommendation: “The IWAQM concludes that CALPUFF be recommended as providing unbiased estimates of concentration impacts for transport distances of order 200 km and less, and for transport times of order 12 hours or less. For larger transport times and distances, our experience thus far is that CALPUFF tends to underestimate the horizontal extent of the dispersion and hence tends to overestimate the surface-level concentration maxima. This does not preclude the use of CALPUFF for transport beyond 300 km, but it does suggest that results in such instances be used cautiously and with some understanding.” (From page D-12 of the IWAQM Phase 2 report.)

IWAQM's 200-km limitation derives from the observation that, when compared to the data of the Cross Appalachian Tracer Experiment (CAPTEX), the basic configuration of CALPUFF overestimated inert tracer concentrations by factors of 3 to 4 at receptors that were 300 to 1000 km from the source. The apparent reason was insufficient horizontal dispersion of the simulated plume, presumably because an actual large plume does not remain coherent in the presence of vertical wind shears that typically occur, especially during the night, and of horizontal wind shears over the large puffs that arise over long transport distances.

To better represent such situations, an optional puff splitting algorithm has since been added to CALPUFF to simulate wind shear effects across a well-mixed individual puff by dividing the puff horizontally and vertically into two or more pieces. Differential rates of transport among the new puffs thus generated can increase the horizontal spread of the material in the plume due to vertical wind speed shear and wind direction shear. The horizontal puff splitting algorithm is designed to allow large puffs that may grow to be several grid cells or more in size to split into smaller puffs that can then more accurately respond to variations in the local wind field across the original large puff. This will also tend to increase horizontal dispersion of the plume. Since the creation of additional puffs via puff splitting will increase the computational requirements of the model, possibly substantially, puff splitting is not enabled by default, but can be turned on at the option of the user. Puff splitting may be appropriate for transport distances over 200 to 300 km, or possibly over shorter distances in complex terrain.

Turning to the shorter distance end of the transport range, the CALPUFF section of Appendix A of the *Guideline on Air Quality Models* (40 CFR 51, Appendix W) states, "CALPUFF is intended for use on scales from tens of meters from a source to hundreds of kilometers." This is supported by the IWAQM Phase 2 report, which indicates that the diffusion algorithms in CALPUFF were designed to be suitable for both short and long distances. In this regard, CALPUFF does contain algorithms for such near-field effects as plume rise, building downwash, and terrain impingement and includes routines that deal with the computational difficulties encountered when applying a puff model in the field near to a source.

The recommendations for regulatory use in Appendix A of the *Guideline on Air Quality Models* state, "CALPUFF is appropriate for long range transport (source-receptor distance of 50 to several hundred kilometers)", but provisions for using CALPUFF in the near-field in "complex flow" situations are also included in the regulatory guidance. Complex flow situations may include complex terrain, coastal areas, situations where plume fumigation is likely, and areas where stagnation, flow reversals, recirculation or spatial variability in wind fields (e.g., as due to changes in valley orientation) are important.

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. In this light, the BART guidance strongly recommends using CALPUFF for

source-receptor distances greater than 50 km but also presents CALPUFF as an option that can be considered for shorter transport distances.

**Comment:** This paragraph indicates that CALPUFF should only be used when plumes are diffused over time and space. The light extinction calculations included in CALPUFF/CALPOST are best applied for long averaging periods (>24 hrs.) if modeling a single source. URS has demonstrated that in most high impact cases for sources located > 50 km from a Class I area a distinct plume can be plotted.

In fact, if screening level modeling indicates > a 1 deciview impact is occurring in the Class I area then this is a clear indication of a potentially visible plume requiring a sight (light) path analysis.

There do not appear to be any scientific reasons why CALPUFF cannot be used for even shorter transport distances than 30 km, though, 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. (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.)

**Comment:** This statement is not supported with any reference or analysis.

As an additional consideration, if the plume width is small compared to the visual range, the atmospheric extinction along a typical sight path of tens of kilometers through the plume will be inhomogeneous and the simple CALPOST point estimate of regional light extinction at a receptor point will not be correct. However, the effect of averaging light extinction estimates for 24 hours, during which the plume location shifts over various receptor points, is likely to mitigate this problem in most cases and suggests that using CALPUFF at distances well under 30 km will often be appropriate.

**Comment:** A LOS modeling approach was discussed by VISTAS technical consultant in the initial draft of the VISTAS Modeling Protocol dated 31 January 2005 under section 4.1.4 (Additional Technical Considerations) for CALPUFF modeling of sources located less than 50 kilometers from a Class I Area. These paragraphs have been extracted from the Initial Draft VISTA Modeling Protocol and clearly indicate the technical consultant understands the concept of LOS modeling when using CALPUFF; Statement 1 from Initial VISTAS Draft Protocol:

"A more difficult issue to address is that CALPOST calculates the extinction coefficient at each receptor point. That value represents extinction in the vicinity of that point, but does not necessarily represent the impact of the source on extinction over any sight path, particularly over the longer sight paths that are likely under natural conditions. The human perception of visibility takes place over sight paths, not at points. For example, consider a 40-km sight path that represents the visual range and includes 10 CALPUFF receptor points on a 4 km grid. If there is a 10% change in extinction (a 1 dv change) at two receptors and no change at the others, the actual change in haziness over the ... [1]

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, additional studies of model performance have been performed at shorter distances, including at a power plant in New York state in complex terrain (at source-receptor distances of 2 - 8.5 km) and a second 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). Other CALPUFF evaluation studies over short-distances include ones by Chang et al. (2001) and Morrison et al. (2003). These studies demonstrate good model performance over source-receptor distances from a few hundred meters to 50 km.

**Comment:** CALPUFF model validation studies are largely based on how well the model predicts concentrations impacts not how good the model predicts regional haze impacts from isolated point sources.

An example of the CALPUFF model's ability to predict secondary pollutant concentrations such as sulfate and nitrate, light extinction, and sulfur and nitrogen deposition at a Class I areas over a range of source-receptor distances is reported in Scire et al. (2001). In that study, in which a large number of sources were modeled simultaneously, sulfate and nitrate predictions at the IMPROVE 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. [A summary of the results of this study will be presented in Appendix D.]

**Comment:** This validation applies to a CALPUFF analysis for multiple regional emission sources. This study may support using CALPUFF in large scale regional emission studies but provides limited insight on how good CALPUFF is for modeling an individual source.

### 3.2.2 Aerosol Constituents

#### **Primary PM<sub>2.5</sub>**

Appendix A of the *Guideline on Air Quality Models* (40 CFR 51, Appendix W) states that CALPUFF can treat primary pollutants such as PM<sub>10</sub>. In actuality, CALPUFF can simulate PM<sub>10</sub> or PM<sub>2.5</sub> or some other size range, because the assumed size distribution of the particles is a user input. The smaller the particles, the more they disperse like an inert gas. In most cases, the dispersion of inert PM<sub>2.5</sub> particles will be only minutely different from that of an inert gas, but the behavior of larger particles will differ.

A particularly important contributor to PM concentrations is the rate of deposition to the surface. PM<sub>2.5</sub> 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<sub>10</sub> particles larger than PM<sub>2.5</sub>) 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<sub>10</sub>, is accounted for in the calculation of the deposition velocity. Effects of inertial impaction (important for the upper part of the PM<sub>10</sub> 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.

A primary PM<sub>2.5</sub> emission from coal-fired electric generating units (EGUs) that is of relevance to visibility calculations is that of primary sulfate. Although primary sulfate emissions account for only a small fraction of the total sulfur emissions from such sources, it may be important to simulate their effect with CALPUFF, especially at shorter distances before significant formation of secondary sulfate conversion from SO<sub>2</sub> has taken place.

#### **Sulfur Dioxide and Secondary Particulate Sulfate**

The MESOPUFF-II chemistry algorithm used in CALPUFF<sup>6</sup> simulates the gas phase oxidation of sulfur dioxide to sulfate by a linear transformation rate that was developed using regression

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<sup>6</sup> CALPUFF offers two options for parameterizing chemical transformations: the 5 species (SO<sub>2</sub>, SO<sub>4</sub><sup>2-</sup>, NO<sub>x</sub>, HNO<sub>3</sub>, and NO<sub>3</sub><sup>-</sup>) MESOPUFF-II system and the 6 species RIVAD system (which treats NO and NO<sub>2</sub> separately). IWAQM recommends using the MESOPUFF-II system with CALPUFF. The RIVAD system is believed to be

relationships derived from the analysis of chemical conversion rates produced by a complex photochemical box model (see Scire et al., 1984, for a description of the development of the chemical module). As in all empirically-derived models, the relationships are based on easily-computed or observed parameters used as surrogates for the factors that control SO<sub>2</sub> oxidation.

The surrogate factors included in the parameterized chemistry during the daytime hours include solar radiation intensity, ambient ozone concentration, and atmospheric stability class. For example, gas phase SO<sub>2</sub> oxidation is a function of OH radical concentrations. Ozone concentrations are correlated with OH radical concentrations during daytime hours, and their use in the daytime SO<sub>2</sub> conversion rate in CALPUFF is based on this correlation relationship. The philosophy is that OH radical measurements are not available and cannot easily be computed within a model like CALPUFF, but ozone is commonly measured throughout the country, so the use of the well-known surrogate variable (ozone) is more useful in the empirical relationship than factors that are unknown or have a high degree of uncertainty. The same logic applies to the other variables in the relationship. They are surrogates for factors than the regression analysis has shown to be important in SO<sub>2</sub> oxidation rates. At night, the SO<sub>2</sub> conversion is set to a constant low value (default is 0.2%/hr). Aqueous phase oxidation of SO<sub>2</sub> is represented by an additive term that varies with relative humidity and peaks at 3%/hr at 100% relative humidity. CALPUFF represents the chemical conversion as a linear process because it requires linear independence between puffs, although as explained below, non-linear behavior in nitrate formation can be modeled.

The IWAQM Phase 2 report concludes that this chemistry algorithm is adequate for representing the gas phase sulfate formation but that it does not adequately account for the aqueous phase oxidation of SO<sub>2</sub>. Actual aqueous phase oxidation in clouds or fog can proceed at rates much greater than 3% per hour, leading IWAQM to suggest that sulfate might be underestimated in such situations. However, aqueous phase oxidation depends on liquid water content, not relative humidity. In reality, liquid water does not exist in the atmosphere at relative humidity much below 100%, while the CALPUFF aqueous reaction term produces sulfate at lower relative humidity. This can lead CALPUFF to overestimate sulfate concentrations when the humidity is high but the cloud water that enables aqueous conversion is not present. Therefore, the direction of the bias in the aqueous chemistry simulation of sulfate formation can vary.

Other potential sources of error in the sulfate formation mechanism of CALPUFF include (1) overestimation of sulfate formation when NO<sub>x</sub> concentrations in the plume are high and in actuality they deplete the local availability of ozone and hydrogen peroxide for oxidizing the SO<sub>2</sub>; and (2) lack of direct consideration of the effect of temperature on the conversion rates, which may cause the model to overstate sulfate formation on cold days (below 10C or 50°F). However, in CALPUFF, the effects of temperature are accounted for indirectly by the use of the solar

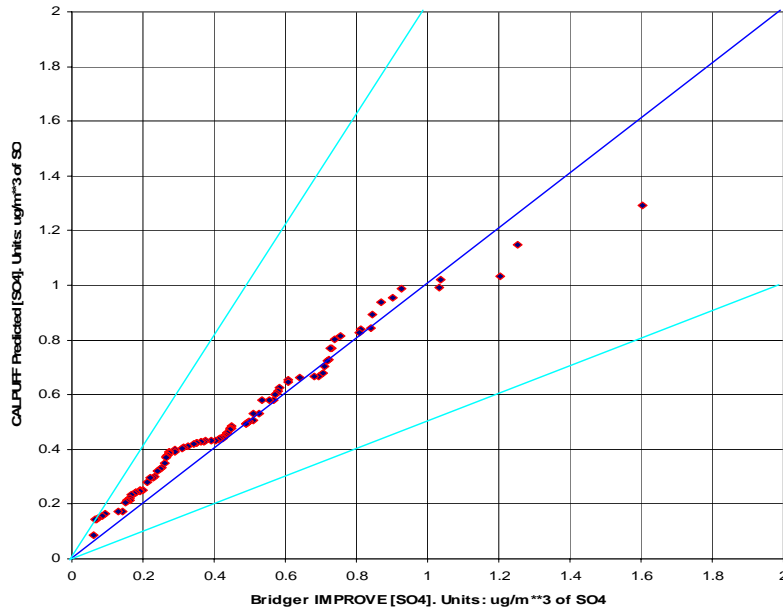
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more appropriate for clean environments, however, and therefore was used in the Southwest Wyoming Regional CALPUFF Air Quality Modeling Study in 2001. For the VISTAS region, the IWAQM- and FLM-recommended MESOPUFF-II chemistry is most appropriate.

radiation surrogate variable in the empirical conversion equations. Figure 3-2 shows a comparison of predicted and observed 24-hour sulfate concentrations at the Pinedale IMPROVE site in Wyoming for the 1995 period (Scire et al., 2001). Overall, in this case there was very little bias in the sulfate predictions.

CALPUFF does not identify the chemical form of the sulfate compound that results from its reactions, which will generally be some form of ammoniated sulfate whose degree of neutralization will depend on the availability of ammonia in the atmosphere. This consideration, which has been found to be relevant for calculating light extinction in the VISTAS region, is not addressed by CALPUFF or CALPOST.

In most applications, the ozone concentrations required for the sulfate formation calculations are derived from ambient measurements, although concentrations simulated by regional models can be used.



**Figure 3-2. Observed vs. CALPUFF-predicted 24-hour sulfate concentrations at the IMPROVE monitoring site in Pinedale, Wyoming for 1995.**

### *NO<sub>x</sub> and Secondary Ammonium Nitrate*

The MESOPUFF-II chemistry algorithm used in CALPUFF simulates the oxidation of NO<sub>x</sub> to nitric acid and organic nitrates (both gases) by transformation rates that depend on NO<sub>x</sub> concentration, ambient ozone concentration, and atmospheric stability class during the day. The conversion rate at night is set at to a constant value (default is 2.0 %/hr). The temperature- and humidity-dependent equilibrium between nitric acid gas and ammonium nitrate particles is taken into account when estimating the ammonium nitrate particle concentration, an equilibrium that depends on the ambient concentration of ammonia. The user supplies the value of the ambient concentration of ammonia. CALPUFF assumes that the sulfate reacts preferentially with that ammonia to form ammonium sulfate and the left over ammonia is available to form ammonium nitrate.

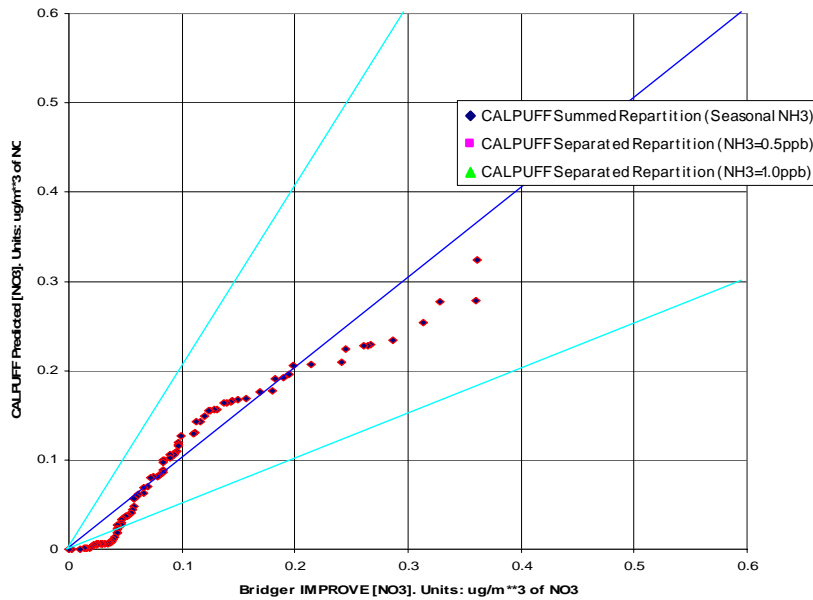
The IWAQM Phase 2 report considers that this mechanism is adequate for representing nitrate chemistry. Potential situations where this assumption may not be correct, however, include (1) plumes with high concentrations of NO<sub>x</sub> that deplete the ambient ozone and thus limit the transformation of NO<sub>x</sub> to nitric acid in the plume; and (2) when ambient temperature is below 10 C, and thus the transformation rate is much slower and the nitrate concentration may be lower than that simulated by CALPUFF. In both cases, CALPUFF may overestimate the amount of nitrate that is produced. In particular, the impact of ammonium nitrate concentrations on visibility at Class I areas in the VISTAS region is greatest in the winter, when temperatures are lowest, the nitrate concentrations are the greatest, and the sulfate concentrations tend to be the least. CALPUFF is likely to overstate the impacts of NO<sub>x</sub> emissions at those times, especially in the colder northern states. This expected trend toward overprediction of nitrate was not evident in the nitrate evaluation with actual observational data in the Wyoming study (Scire et al., 2001) (see Figure 3-3a), however.

Another factor in the calculation of nitrate is that CALPUFF makes the full amount of the background concentration of ammonia available to each puff, and that amount is scavenged by the sulfate in the puff. If puffs overlap, then that approach could overstate the amount of ammonium nitrate that is formed in total if, in reality, the combined scavenging by the overlapping puffs at a location would deplete the available ammonia enough that the combined nitrate formation was limited by the availability of ammonia. This effect of such ammonia limiting can be large in summer; for a source 75 km west of Mammoth Cave National Park, one modeling analysis found the maximum light extinction impact of the source to be 7.4% (roughly 0.74 deciviews) at the park when CALPUFF was used without consideration of ammonia limiting and about 30% less, between 5.5 and 5.8% (roughly 0.55 to 0.58 dv), when the effect of ammonia limiting was considered (Escoffier-Czaja and Scire, 2002).

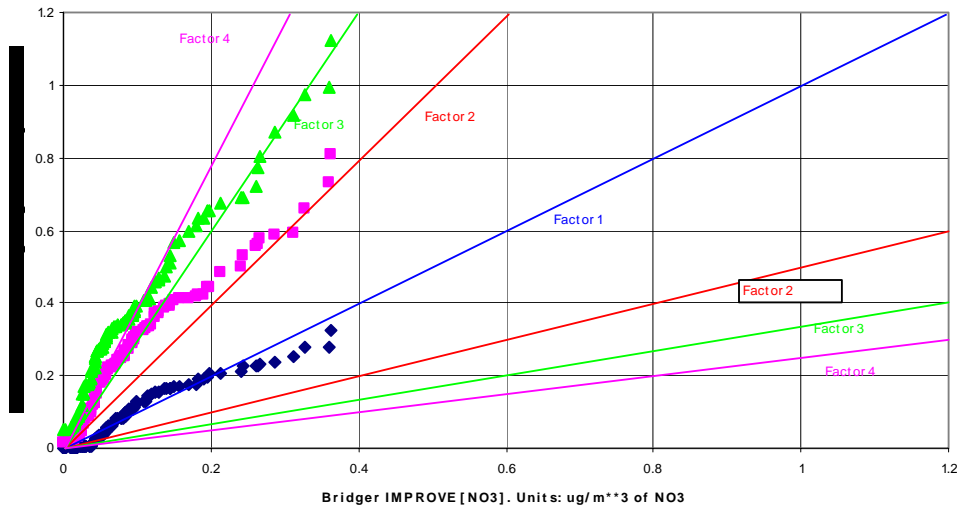
To address the issue, since 1999 (i.e., after the IWAQM Phase 2 report) the CALPUFF system has included the optional POSTUTIL postprocessing program, which repartitions the ammonia and nitric acid concentrations estimated by CALPUFF to reflect potential ammonia-limiting effects on the development of nitrate (see Appendix A). It computes the total sulfate concentrations from all sources (modeled sources plus inflow boundary conditions) and estimates

the amount of ammonia available for total nitrate formation after the preferential scavenging of ammonia by sulfate. This allows non-linearity associated with ammonia limiting effects to be included in the CALPUFF model estimates.

Reliable estimates of the ambient concentrations of ammonia, especially with the temporal and spatial resolution that would be optimal for use with CALPUFF, are needed to take full advantage of the increased accuracy provided by POSTUTIL. Current ammonia inventories are still quite uncertain and typically represent averages over a long period of time (e.g., a month) and a large area (e.g., a county). Nevertheless, benefit is obtained by considering seasonal trends of ammonia and using POSTUTIL to determine the diurnal variability in available ammonia due to the daily cycle of nitrate formation associated with temperature and relative humidity effects. For example, results of the Wyoming study (see Figure 3-3a) show that POSTUTIL adjustments produced daily average nitrate concentrations well within the factor of two lines and with very little mean bias. On the other hand, the use of constant ammonia of 0.5 ppb or 1.0 ppb produced consistent overpredictions of nitrate by factors of 2-3 and 3-4, respectively (see Figure 3-3b).



**Figure 3-3a. Observed vs. CALPUFF-predicted 24-hour nitrate concentrations at the IMPROVE monitoring site in Pinedale, Wyoming for 1995 using the ammonia limiting method.**



**Figure 3-3b. Observed vs. CALPUFF-predicted 24-hour nitrate concentrations at the IMPROVE monitoring site in Pinedale, Wyoming for 1995 using the ammonia limiting method (blue), constant ammonia at 0.5 ppb (pink) and constant ammonia at 1.0 ppb (green).**

### *Secondary Organic Aerosol*

Ongoing research studies at several Class I areas throughout the country (Fallon and Bench, 2004) and at SEARCH sites in the Southeast (Edgerton et al., 2004) are finding that, typically, 90 to 95% of the rural organic carbon fine particle concentration consists of modern carbon (e.g., that from the burning of vegetation and deriving from VOC emissions from vegetation) and only 5 to 10% is attributable to man’s burning of fossil fuels. In addition, a field study at Great Smoky Mountains National Park in August 2002 (Tanner, et al., 2005) found that an average of 83% of the fine carbon was modern carbon

According to IMPROVE measurements, organics account for roughly 10% of the particle-caused light extinction in Class I areas in the Southeast. We can thus conclude that, in general, secondary organic carbon particles derived from anthropogenic fossil fuel burning emissions are unlikely to have a large impact (around 1%) on current visibility. (Man-caused burning of vegetation can have significant localized, short-term impacts, however.)

Current organic fine particle concentrations in the Southeast are typically within a factor of 2 of the  $1.4 \mu\text{g}/\text{m}^3$  concentration assumed for natural conditions by the EPA, which means that current fossil fuel burning would contribute less than 2% to visibility in an atmosphere that represents

natural conditions. Thus, it is unlikely that VOC and organic particle contributions from BART sources will cause a large impact to visibility at Class I areas, but a 5% (0.5 dv) localized impact from a particularly large VOC source cannot be dismissed out of hand.

CALPUFF has only rudimentary capabilities for addressing formation of visibility-impairing organic particles from some forms of volatile organic carbon (VOC). The capabilities that do exist include the following.

First, PM<sub>10</sub> emissions (such as from power plants) are often divided into filterable and condensable components, with the condensable mass being 100-200% of the filterable mass. For purposes of visibility analyses with CALPUFF, a fraction of the condensable part is typically treated as organic particles, i.e., it is assumed that a fraction of the condensable components in the PM<sub>10</sub> emissions condense into organic PM<sub>2.5</sub> particles. The size of this organic fraction varies with process and process equipment, and can range from 20 to 100% of the condensable mass. These fine organic particles can be readily modeled by CALPUFF. (The remaining condensable material may be sulfuric, hydrochloric, or hydrofluoric acid.)

Second, a module that treats the formation of secondary organic particles from organic emissions was recently developed and is now part of the CALPUFF system. (Scire et al., 2001). This simplified secondary organic aerosol (SOA) module is a linear, parameterized representation that is currently considered best suited for biogenic organics. It relies on the conventional wisdom that only hydrocarbons with more than six carbon atoms can form significant SOA (Grosjean and Seinfeld, 1989). For example, according to this rule, isoprene (C<sub>5</sub>H<sub>8</sub>) does not make SOA but terpenes do, making pine trees more important biogenic contributors to SOA than oak trees.<sup>7</sup>

Limited evaluation of the performance of CALPUFF at simulating SOA with its biogenic SOA module at one IMPROVE site in a regional modeling study in Wyoming found that 95% of 101 estimated 24-hr SOA concentrations were within 2% of the measured values (Earth Tech, Inc., 2002). This performance seems promising, although the developers view the SOA module as needing more testing and evaluation.

Thus, CALPUFF includes approaches for dealing with condensable VOC emissions that are characterized as condensable PM<sub>10</sub> and with biogenic VOCs, although the soundness of concentration estimates by these approaches when modeling a plume from a single source is largely untested.<sup>8</sup> The CALPUFF simulation of VOC emissions from sources whose VOC emissions are predominantly anthropogenic is problematic, however. Perhaps the approach used for the simplified biogenic SOA module may be extended to anthropogenic VOCs when speciated VOC emissions information is available. If only those VOCs with more than six carbon atoms are presumed to be of importance, this eliminates many anthropogenic sources of VOC

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<sup>7</sup> Recent research suggests that isoprene may be a SOA precursor, however.

<sup>8</sup> Note that neither of these VOC-related simulation approaches is described in the current (Version 5) CALPUFF User's Guide dated January 2001. See the Wyoming report referenced above for a description of this module.

emissions. For example, the fugitive emissions of butane and ethane during petroleum processing are not important, while aromatic emissions (such as of toluene and xylene) are considered by the SOA module's mechanism. Development, testing, and evaluation would be needed before one could rely on such a module for estimating SOA from anthropogenic SOA emissions, though.

Therefore, to demonstrate the visibility impacts of VOC emissions from BART-eligible sources, means other than CALPUFF will be needed. A technical approach using a regional photochemical model to evaluate visibility impacts of VOC emissions is presented in Section 4.1.3. CALPUFF can be used to estimate the contribution from the primary condensable fraction of PM<sub>10</sub> emissions, though.

### 3.2.3 Regional Haze

Calculation of the impact of the simulated plume particulate matter component concentrations on light extinction is carried out in the CALPOST postprocessor. The formula used is the usual IMPROVE/EPA formula, which is applied to determine a change in light extinction due to changes in component concentrations. Using the notation of CALPOST, the formula is the following:

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

The concentrations, in square brackets, are in  $\mu\text{g}/\text{m}^3$  and  $b_{ext}$  is in units of  $\text{Mm}^{-1}$ . The Rayleigh scattering term ( $b_{Ray}$ ) has a default value of  $10 \text{ Mm}^{-1}$ , as recommended in EPA guidance for tracking reasonable progress (EPA, 2003a).

There are a few important differences in detail and in notation between the CALPOST formula for estimating light extinction (i.e., Equation 3-1) and that of IMPROVE. First, the *OC* in the formula above represents organic carbonaceous matter (OMC in IMPROVE's notation), which is 1.4 times the *OC* (i.e., organic carbon alone) in the IMPROVE formula. The *EC* above is synonymous with *LAC* in the IMPROVE formula. CALPOST still uses the old IMPROVE  $f(RH)$  curve, whose values are documented in the December 2000 FLAG report. That curve differs slightly from the  $f(RH)$  now used by IMPROVE and EPA (as documented in EPA's regional haze guidance documents), 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%.

The haze index (HI) is calculated from the extinction coefficient via the following formula:

$$HI = 10 \ln (b_{ext}/10) \quad (3-2)$$

where *HI* is in units of deciviews (dv) and  $b_{ext}$  is in  $\text{Mm}^{-1}$ . The impact of a source is determined by comparing HI for estimated natural background conditions with the impact of the source and without the impact of the source.

## ***CALPOST Methods***

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 (called Methods 1-7). 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). A brief summary of the techniques is provided below. See Appendix B for a more detailed discussion of the main methods most commonly used for Class I analyses. Method 2 is the current default, recommended by both IWAQM (EPA, 1998) and FLAG (2000) for refined analyses. Method 6 is recommended by EPA's BART guidance (70 FR 39162).

Methods 4 and 5 use optically measured hourly background extinctions, which represent current actual levels of extinction and thus are not consistent with the "natural conditions" the BART proposal says should be used as a baseline. Methods 1 through 3 and 6 and 7 allow for user inputs of estimated (e.g., natural conditions) background extinction or component concentrations, and thus are consistent with the BART proposal.

Method 1 allows the user to specify a single value of a "dry" background extinction coefficient for each receptor, specify that a certain fraction of that coefficient is due to hygroscopic species, and use relative humidity measurements to vary the extinction hourly via a 1993 IWAQM  $f(RH)$  curve or, optionally, the EPA regional haze  $f(RH)$  curve (EPA, 2003b). The  $RH$  is capped at 98% or a user-selected value (95% for the EPA curve). The same  $f(RH)$  is applied to both the modeled sulfate and nitrate.

For an example of the use of Method 1, one could use the dry particle extinction coefficient of  $9.09 \text{ Mm}^{-1}$  that results from EPA's default natural conditions concentrations, together with an assumption that for natural conditions, say,  $0.9 \text{ Mm}^{-1}$  (or 10%) of this amount results from hygroscopic ammonium sulfate and ammonium nitrate, and then apply  $f(RH)$  to this 10%.

In Method 2, user-specified, speciated monthly concentration values are used to describe the background during. 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 (a different one

than that in Method 1) or, optionally, the EPA regional haze f(RH) curve.<sup>9</sup> Again the RH is capped at either 98% (default) or a user-selected value (most commonly at 95%).

Method 3 is the same as Method 2, except that any hour in which the RH exceeds 98% (or the selected maximum) is dropped from the analysis. When 24-hr extinction is computed, no fewer than 6 valid hours are accepted at each receptor; otherwise the value for the day is tabulated as “missing”.

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.

Method 7 is a new variant of Method 2 that was developed as a result of a ruling by the Assistant Secretary of the Interior for Fish and Wildlife and Parks, in response to a New Source Review case in Montana, that “natural conditions” should reflect the visibility impairment caused by significant meteorological events such as fog, precipitation, or naturally occurring haze (DOI, 2003).<sup>10</sup> Under Method 7, during hours when visibility is obscured by meteorological conditions, the actual measured visibility is used to represent natural conditions instead of the value that is calculated from EPA’s default natural conditions concentrations under Method 2. A recent modification developed in response to FLM comments on Method 7, in which the daily average natural extinction is calculated somewhat differently, is called Method 7’, i.e., “7 prime”. See Appendix B for more details on Method 7 and Method 7’.

### ***Refined Estimates of Extinction and Natural Background Visibility***

Separate from the BART discussions, EPA, IMPROVE, and the Regional Planning Organizations are evaluating whether refinements are warranted to the methods recommended in EPA’s guidance to calculate extinction and the default estimate of natural background visibility. If

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<sup>9</sup> 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.

<sup>10</sup> The Secretary’s guidance applies only to Federal Land Managers. EPA’s position on this interpretation of natural conditions is unknown.

#### [3.a Overview of ALTERNATIVE MODELS \(PLUVUEII & SCIPUFF\)](#)

[VISTAS should give some expert advise to states on how to use other alternative models such as PLUVUE-II, SCIPUFF or other applicable models for a BART analysis.](#)

changes to these methods are recommended by VISTAS for the purposes of calculating current, future, and natural background visibility at VISTAS Class I areas as part of the reasonable progress analyses, then these changes would need to be incorporated into CALPOST as well. These issues are discussed in Appendix B.

## 4. VISTAS' COMMON MODELING PROTOCOL

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### 4.1 Overview of Common Modeling Approach

In this section, guidance is provided on the use of the CALPUFF modeling system for three purposes:

- 1) Evaluating whether a BART-eligible source is exempt from a BART evaluation because it is not reasonably expected to cause or contribute to impairment of visibility in Class I areas;
- 2) Quantifying the visibility benefits of BART control options; and
- 3) Demonstrating the effectiveness of an optional cap and trade program.

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For purpose 1), States must determine whether a source emits any air pollutant (SO<sub>2</sub>, NO<sub>x</sub>, PM, VOC) that “may reasonably be anticipated to cause or contribute to any impairment of visibility” in a Class I area. The States have 3 options to accomplish this:

- A) Conclude that all BART-eligible sources in State are subject to BART;
- B) Demonstrate that all BART-eligible sources in the State together do not cause or contribute to any visibility impairment; or
- C) Determine if the 98<sup>th</sup> percentile 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.

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VISTAS States intend to follow Option C (determine if the visibility impact from individual sources exceeds a contribution threshold) for SO<sub>2</sub>, NO<sub>x</sub>, and PM emissions. The methods for Option C are described in Section 4.1.1. Option B (demonstrate that all BART eligible sources in a State do not impact visibility) is being pursued for VOC and NH<sub>3</sub> emissions. Methods for Option B are described in Section 4.1.3.

#### 4.1.1 BART Exemption Analysis

As illustrated in Figure 4-1, two steps will evaluate whether a BART-eligible source of SO<sub>2</sub>, NO<sub>x</sub>, or PM is subject to BART:

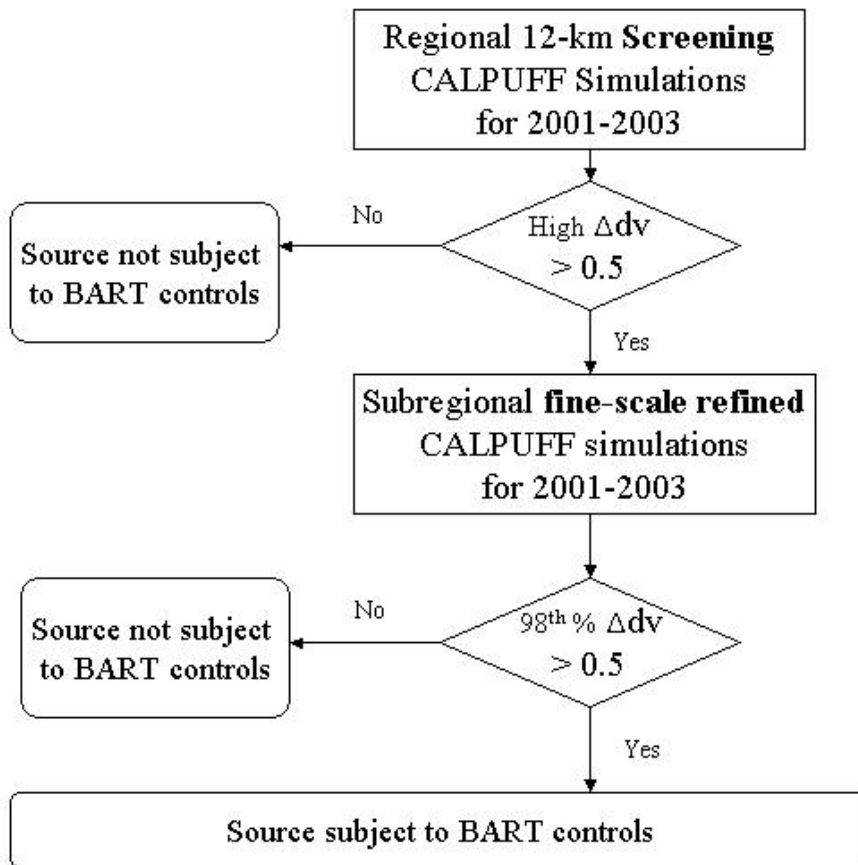


Figure 4-1. [DRAFT] Flow chart showing the components of the VISTAS common protocol.

1) An optional screening assessment using the CALPUFF model with the coarse scale 12-km regional VISTAS domain can be used to answer questions whether (a) a particular source should be subject to a refined CALPUFF analysis and if so, (b) what Class I areas should be included in the refined analysis. Assumptions for the screening assessment are conservative so that a source that contributes to regional haze impairment is not exempted in error. If a source is shown not to contribute to regional haze impairment using the screening assessment, the State may choose to exempt the source from BART or to require refined CALPUFF modeling to confirm it is not subject to BART. If a source is shown to contribute to regional haze impairment using the screening assessment, the source has the option to undertake refined CALPUFF modeling to evaluate further whether it is subject to BART.

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2) A refined CALPUFF modeling analysis using a subregional CALMET domain with fine scale grid resolution. This will be the definitive test as to whether a source is subject to BART.

#### 4.1.2 BART Control Evaluation

For sources that are determined to be subject to BART evaluations, part of the BART review process involves evaluating the regional haze benefits of different BART control measures. These benefits will be determined by performing additional CALPUFF simulations using the same CALMET and CALPUFF configuration as those used in the refined analysis of Step 2. The only exception is that the source and emissions data used in the CALPUFF control evaluation simulations will reflect the BART control measures being evaluated. Using the same model configuration will produce an “apples-to-apples” comparison, where differences in impacts are due to the effectiveness of the controls rather than model configuration differences. For example, a control scenario evaluation that uses more conservative assumptions than the base case simulation may produce results showing no or little improvement in regional haze impacts. That control scenario run with the same model configuration as the base case may show significant regional haze improvement. Therefore, in order to not obscure the response to predicted regional haze improvements by differences in the modeling approach, the same model configuration should be used in the BART control evaluation simulation as in the base case simulation.

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The base case to which the effectiveness of BART controls is compared is the “current emissions” scenario for which the refined Step 2 modeling was performed. The postprocessing steps and procedures are the same as in the BART eligibility simulation. Side-by-side comparison of the regional haze impacts will be tabulated to quantify the effectiveness of each control scenario relative to the base case.

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### 4.1.3 VISTAS Treatment of VOC and NH<sub>3</sub>

#### *Volatile Organic Compounds*

CALPUFF is currently not recommended for addressing visibility impacts from VOC because its capability to simulate secondary organic aerosol formation from VOC emissions is not adequately tested, especially for anthropogenic emissions. (Separately, condensable organic carbon can be calculated from PM<sub>10</sub>.)

VISTAS is currently performing a weight of evidence analysis to demonstrate, using the CMAQ regional air quality model, that all VOC emissions from all point sources (BART-eligible and non-BART) in each State do not contribute to ~~regional haze~~ impairment. Emissions sensitivity simulations run for VISTAS by Georgia Institute of Technology using VISTAS' 12 x 12 km grid and CMAQ v 4.3 for episodes in July 2001 and January 2002 demonstrated very low to no response of organic carbon levels and light extinction at Class I areas to changing VOC emissions from all anthropogenic sources in the VISTAS 12-km modeling domain (eastern US). Georgia Tech is currently repeating the sensitivity analyses for VISTAS using the VISTAS 12-km domain and CMAQ v 4.4 with refined SOA module for a summer (Jun 1-Jul 10) and winter (Nov 19-Dec 19) period in 2002. VOC emissions from all anthropogenic point sources in each VISTAS State are being reduced. If the 98<sup>th</sup> percentile impact of eliminating all VOC emissions from all point sources in a State is less than 0.5 dv, then the impact of any one BART-eligible source would be less than 0.5 dv. If the current analyses confirm the existing results, the VISTAS States would recommend that VOC emissions not be subject to BART.

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#### *Ammonia*

EPA has given states the option to address ammonia (NH<sub>3</sub>) emissions from BART-eligible sources. VISTAS has also contracted with Georgia Tech to perform emissions sensitivities using CMAQ v 4.4 with refined SOA module and the Jun-Jul and Nov-Dec periods in 2002. All NH<sub>3</sub> emissions from point sources (BART-eligible and not-BART) in each State will be reduced. If the sensitivity evaluation shows that the collective impact of all point NH<sub>3</sub> emissions is less than 0.5 dv, then the impact of a single BART eligible source would be less than 0.5 dv. In that case, the VISTAS States would recommend that NH<sub>3</sub> emissions not be subject to BART.

## 4.2 Optional Source-Specific Modeling

In some circumstances, a source may want to apply techniques designed to evaluate the impacts in a more detailed way than the standard VISTAS common protocol. A source may propose source-specific modeling procedures to address special issues to the State for State review. For example, sources very close to Class I areas may be better treated by a finer grid resolution than the generic Step 2 "fine" grid resolution meteorological fields provided by VISTAS. In some situations, higher resolution MM5 or other prognostic meteorological datasets may be available than the standard 12-km or 36-km MM5 datasets provided by VISTAS. Because it is not possible to anticipate all of the situations where there would be a benefit to conducting more detailed

source-specific analyses, the option to pursue this option is left as an open issue, to be resolved and justified based on specific factors relevant for the source in question.

If source-specific modeling is to be performed, a detailed modeling protocol explaining the data sources, model configuration and rationale for changes in the model approach from the common protocol must be provided and approved by the State. Discussion of approaches to source-specific modeling and an outline of the typical contents of the source-specific protocol are presented in Chapter 5. Discussions with the State should be conducted prior to development of a source-specific protocol to ensure all of the relevant issues are included in the protocol.

## 4.3 Screening Procedure for BART Exemption

### 4.3.1 Overview of Screening Approach

The first step in the common protocol, the screening assessment in Figure 4-1, is a simple procedure to evaluate whether a source can be exempted from a BART evaluation using a consistent set of meteorological and dispersion options. A pre-computed set of meteorological files and a pre-defined CALPUFF input option configuration, based on guidance in the final BART rule (70 FR 39104-39172) and other EPA and FLAG model guidance, will allow relatively simple screening simulations. The regional screening domain is designed to allow any Class I areas within the VISTAS area to be evaluated with a single meteorological database and consistent CALPUFF modeling options. The second important question that this first screening step will answer is, if screening indicates a source may impact visibility significantly, what Class I areas should be included in a refined analysis? Due to the multitude of factors affecting the contribution of a source to visibility in a Class I area, simple screens or rules of thumb alone (such as that the closest Class I area will produce the controlling visibility impacts) are not likely to be universally reliable.

The screening methodology uses three-dimensional meteorological fields and the full CALPUFF model, and thus can be considered to be a reasonable indicator of the outcome from a refined CALPUFF analysis (and therefore a useful screen), yet with a high probability of moderate conservatism. Screening procedures that are so conservative that few sources will pass the screen are in practice not very useful. Likewise, screening procedures that allow sources to pass the screen that would have failed the refined analysis are not successful screens. For large sources that will clearly exceed the screening thresholds, this step can be skipped and the analysis may proceed directly to the refined modeling analysis, which is described in detail in Section 4.4.

### 4.3.2 Discussion of Regional Screening Approach

#### *Meteorological Fields*

**Comment:** URS has developed a 5-year NWS CALMET data base. One year includes MM4 data. The location of the met stations are shown in the URS slide presentation for the EPA's 8<sup>th</sup> Conference on Air Quality Models. As stated earlier, this presentation is being submitted to VISTAS as part of our comments on this protocol. The Guideline on Air Quality Models states "For LRT situations (subsection 7.2.3) and for complex wind situations (paragraph 8.2.8(a)), if only NWS or comparable standard meteorological observations are employed, five-years of meteorological (within and near the modeling domain) should be used. Consecutive years from the most recent, readily available 5-year period are **preferred**. We would prefer to use this dataset since it's currently available and it would be less time consuming/expensive to use it for both screening level and refined BART modeling. More guidance is needed from VISTAS on whether this modeling methodology would be acceptable. The draft protocol implies that MM data is better than observational data. From our understanding of regulatory guidance this isn't always the case.

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A regional screening domain and a set of pre-computed regional CALMET meteorological files will be prepared for VISTAS, to allow any Class I areas within the VISTAS area to be evaluated with a consistent meteorological database and consistent CALPUFF modeling options.

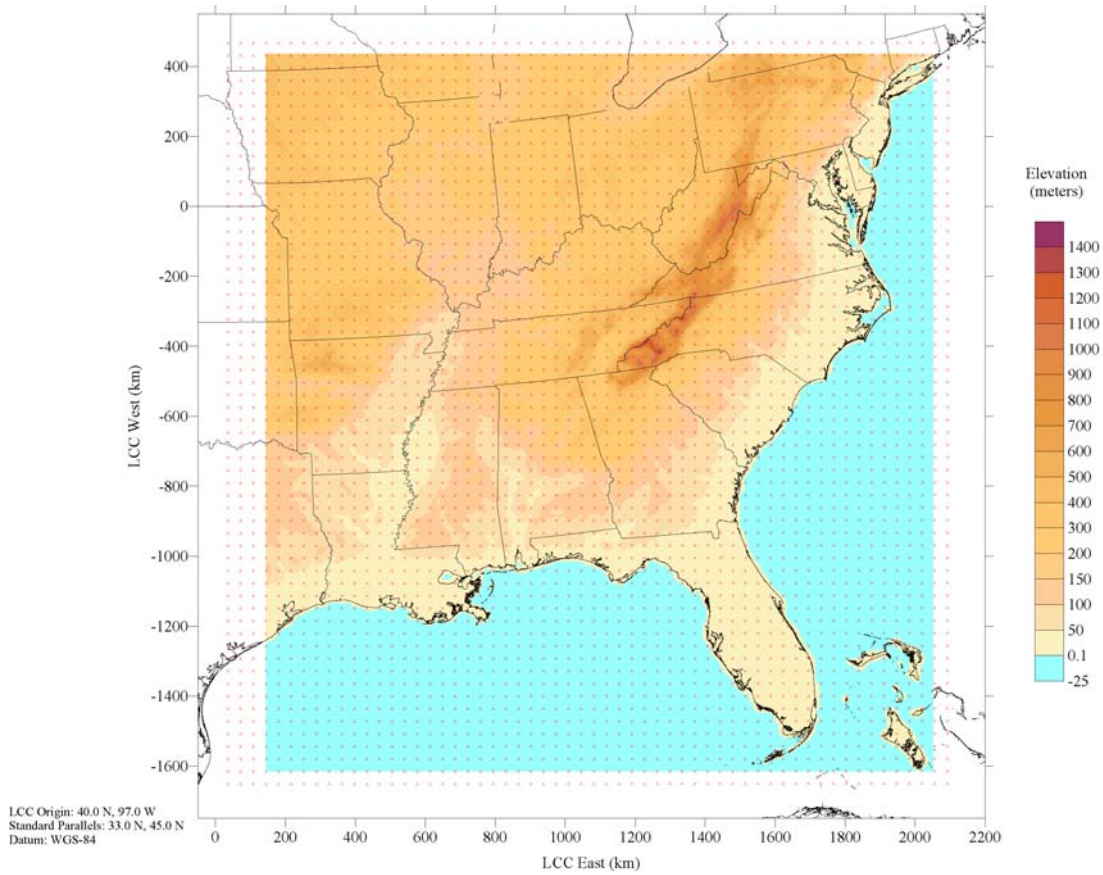
VISTAS has conducted Eulerian modeling with the Community Model for Air Quality (CMAQ) on a domain covering the VISTAS region. To support that modeling, the following three years of MM5 meteorological data has been assembled by VISTAS and that data can be used for the regional CALPUFF modeling effort:

- 2001 MM5 dataset at 12 km and 36 km grid (developed for EPA)
- 2002 MM5 dataset at 12 km and 36 km grid (developed by VISTAS)
- 2003 MM5 dataset at 36 km grid (developed by the Midwest Regional Planning Organization).

These data sets will be provided to Earth Tech by VISTAS, and from them Earth Tech will produce annual CALMET meteorological files at a 12km grid resolution for the domain shown in Figure 4-2. The CALMET modeling output files in the form of CALPUFF-ready three-dimensional meteorological files will be available on external hard drives to the States and other parties through VISTAS.

The screening procedure to determine if a BART-eligible source is subject to BART uses the pre-computed CALMET meteorological fields for the years 2001-2003 on the 12-km CALMET domain in Figure 4-2 and simulates with CALPUFF any BART-eligible source to be screened. The CALMET simulations will be developed using the highest resolution MM5 data available for each year (i.e., 36-km MM5 data for 2003, 12-km MM5 data for 2001 and 2002).

The development of the regional CALMET meteorological fields from MM5 data will be conducted in No-Observations (“No-Obs”) mode. (Appendix C explains the rationale for using CALMET in No-Observations mode for the regional run.) For 2003, the 36-km MM5 data will be used as CALMET’s initial guess field and then the CALMET diagnostic terrain adjustments (see Section 3.1.1) will be applied to reflect terrain on the scale of the CALMET grid (i.e., 12-km). When the 12-km MM5 (2001 and 2002) data are used, the diagnostic CALMET terrain adjustments will be turned off since the grid resolution of the MM5 data is the same as the CALMET grid and the terrain adjustments appropriate on the 12-km grid scale will be reflected in the MM5 dataset. In this case, the MM5 winds will be interpolated by CALMET to the CALMET layers and CALMET’s boundary layer modules will compute mixing heights, turbulence parameters and other meteorological parameters that are required by CALPUFF.



**Figure 4-2. VISTAS regional 12-km resolution CALMET modeling domain (color area with terrain contours). The locations of the 36-km resolution MM5 grid points are shown on the plot.**

### ***Impact Threshold***

The final BART guidance recommends that the threshold value to define whether a source “contributes” to visibility impairment is 0.5 dv change from natural conditions (although states may set a lower threshold). The 98<sup>th</sup> percentile at each receptor (8<sup>th</sup> highest annual) predicted value using CALPOST Method 6 (monthly average relative humidity values) or Method 7 if approved by the State is to be compared to this contribution threshold value. Method 7 accounts for periods of precipitation and fog. According to clarification of the BART guidance received from EPA, for a three-year simulation the modeling value to be compared is the highest of the three annual 8<sup>th</sup> highest values over all receptors within a given Class I area. *[Need to verify this interpretation.]*

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As indicated in the EPA BART guidance, the maximum 98<sup>th</sup> percentile deciview change at each receptor over the three-year period is compared to the contribution threshold.

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### ***Credibility and Conservatism of Results***

The final BART rule states that “alternatives should not be used to exempt a source from BART review without more rigorous evaluations and sensitivity tests showing that the results are at least as conservative as the CALPUFF model” (70 FR 39126). In response, the screening methodology described here uses the CALPUFF model with full three-dimensional meteorological data, chemistry, and deposition processes included, and preserves the spatial relationships between sources and individual Class I areas.

In order to ensure the screen passes no sources when they should fail, simple approaches, by their nature, must use the most conservative cases from the empirical analysis used to derive them. This may involve a high degree of conservatism, or it may neglect important factors that influence visibility impacts. For example, there are many factors that influence the contribution of a source beyond just the distance to the Class I area. 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. Also, there may be correlations between winds from certain directions and meteorological conditions conducive for higher visibility impacts. Such effects and relationships are accounted for in the CALPUFF-based screening analysis.

Secondary particulate matter formation by chemical conversion of precursor emissions of SO<sub>2</sub> and NO<sub>x</sub> is the principal source of visibility impacts for many sources. There is a tradeoff between more sulfate and nitrate production with larger transport distances versus the greater dilution of the plume due to dispersion that makes the drop of visibility impacts less than one would expect based on distance considerations alone. In fact the contribution of a source can potentially increase with distance in certain cases if the production of sulfate and nitrate exceeds

dilution effects. To properly deal with such phenomena, the screening procedure uses the full capabilities of CALMET and CALPUFF, including three-dimensional winds derived from the MM5 datasets.

### ***4.3.3 Model Configuration and Settings for Screening Analysis***

The screening analysis uses 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.

Also, the screening approach is designed to significantly reduce the CALPUFF simulation time by restricting the CALPUFF 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 in the regional CALPUFF simulations is that CALPUFF 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). A CALPUFF domain covering an area 300 km from a source in all directions would involve only 50 x 50 12-km grid cells, which will require modest computational resources.

Because the format used in the MM5 data files provided by VISTAS does not contain the sea surface temperature of each water cell, it is necessary to include buoy data in the regional CALMET simulations, making it more accurately a “partial No-Obs” simulation. Otherwise, the stability of the overwater boundary layer will not be properly characterized. The details of the CALMET regional mode configuration are discussed below.

CALMET output files for the VISTAS regional domain shown in Figure 4-2 will be provided to VISTAS by Earth Tech. These files will be in CALPUFF-ready format, and as such, no CALMET user inputs will be required. The basic characteristics of the CALMET, CALPUFF and CALPOST configurations for the screening analyses are listed below.

#### ***CALMET Modeling Configuration (Regional screening runs)***

The CALMET model configuration for the regional CALMET simulations will be defined by Earth Tech in collaboration with the VISTAS States. The basic model configuration will follow the recommended IWAQM guidance (EPA, 1998, Pages A-1 through A-6), except as noted below.

The basic features of the modeling simulation are the following:

**Deleted:** The screening approach is designed to ensure conservatism by considering the highest visibility impact value over a three-year simulation period rather than the 98<sup>th</sup> percentile value in making a determination of no contribution to visibility impairment and also by using conservative model settings. Note that there is a built-in evaluation capability in the VISTAS common methodology in that, for sources that don't pass the screen and will be run in refined mode, information on the relative conservatism of the screening approach will be readily available by comparing the screening and refined results. ¶

- Modeling period: 3 years (2001-2003)
- Meteorological inputs: MM5 data provide initial guess fields in CALMET
- CALMET grid resolution: 12-km (same Lambert Conformal coordinate system and grid cells as the 12-km 2001/2002 MM5 simulations)
- CALMET vertical layers: 10 layers. Cell face heights (meters): 0, 20, 40, 80, 160, 320, 640, 1200, 2000, 3000, 4000.
- CALMET mode: No-Observations mode except SEA.DAT files with buoy data provided.
- Diagnostic options: IWAQM default values, except as follows: diagnostic terrain blocking and slope flow algorithms used for 2003 simulations (using 36-km MM5 data), but no diagnostic terrain adjustments in 2001 and 2002 simulation (using 12-km MM5 data)
- CALMET options dealing with radius of influence parameters (R1, R2, RMAX1, RMAX2, RMAX3), BIAS, ICALM parameters are not used in No-Observations mode.
- TERRAD (terrain scale) is required for runs with diagnostic terrain adjustments (i.e., the 2003 simulations). Values of ~10-20 km will be 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 Atlantic Ocean and the Great lakes to be properly characterized by buoy observations.
- Mixing height averaging parameter (MNMDAV) will be determined by Earth Tech for the regional simulations based on 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.
- Geophysical data for regional runs: SRTM-GTOPO30 30-arcsec terrain data, Composite Theme Grid (CTG) USGS 200m land use dataset. References for these and other CALMET datasets can be found on the CALPUFF data page of the official CALPUFF site ([www.src.com](http://www.src.com)).

***CALPUFF Modeling Configuration (Regional screening runs)***

The CALPUFF model configuration for the regional CALPUFF screening simulations will follow the recommended IWAQM guidance (EPA, 1998, Pages B-1 through B-8), except as noted below:

- CALPUFF domain configured to include source and all Class I areas within 300km of the source plus 50km buffer zone in each direction. CALPUFF is recommended for all source-receptor distances to be considered in the BART analyses.

- Chemical mechanism: MESOPUFF II module

- Species modeled: SO<sub>2</sub>, SO<sub>4</sub>, NO<sub>x</sub>, HNO<sub>3</sub>, NO<sub>3</sub> and particulate matter in size categories of <0.625 μm, 0.625-1.0 μm, 1.0-1.25 μm, 2.5-6.0 μm, 6-10 μm aerodynamic diameters. As noted below, the particulate matter emissions by size category will be combined into the appropriate species for the visibility analysis (i.e., elemental carbon (EC), fine PM or “soil” (< 2.5 μm in diameter), coarse PM (between 2.5-10 μm in diameter) and organics (called secondary organic aerosols (SOA) in the CALPOST postprocessor).

- Emission rates for modeling based on EPA BART guidance, i.e., 24-hour average actual emission rate with normal operations from the highest emitting day of the meteorological period modeled (excluding days where start-up, shutdown or malfunctions occurred.) Note that potential emissions are used to determine if a source is BART-eligible, but 24-hour average maximum emissions are used for modeling purposes (70 FR 39162). Pollutants considered include SO<sub>2</sub>, H<sub>2</sub>SO<sub>4</sub>, NO<sub>x</sub> and PM<sub>10</sub>.

Condensable emissions are considered as primary fine particulate matter and allocated equally to the two submicron particle size classes. 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 will be investigated by VISTAS based on review of available source categories. *[For purposes of the screening analyses, VISTAS is seeking comment on using simplifying assumptions to assign PM10 to its components (e.g. assume primary sulfate is a fraction of SO2 emissions, assume primary sulfate is a fraction of PM10 emissions, assume all PM10 emissions are PM2.5.)]*

Exclude from the modeling are pollutants with emissions less than *de minimis* levels (40 tons per year for SO<sub>2</sub> and NO<sub>x</sub> and 15 tons per year for PM<sub>10</sub>).

- Pollutant speciation: Break down, as appropriate, filterable and condensable particulate matter into the following species categories: elemental carbon (soot), “soil” (fine PM <2.5 μm diameter), coarse particulate matter (2.5-10 μm diameter) and organics. 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 and reviewed, and approved by the state.

- Class I receptors: Use FLM Class I receptor list with receptor elevations provided (available from the NPS).

- CALPUFF model options: Use EPA (1998) guidance, except use turbulence-based dispersion coefficients and probability density function (pdf) dispersion.

- Ozone dataset – use observed ozone data for 2001-2003 from CASTNet and AIRS stations. Only non-urban ozone stations should be used in the OZONE.DAT file. Monthly average ozone (backup) background values are to be computed based on daytime average ozone concentrations from the OZONE.DAT file (6am-6pm average ozone concentrations computed by month).

- Background ammonia concentration: VISTAS is seeking comment whether a constant background ammonia concentration based on guidance in IWAQM using the dominant land use in the Class I area being modeled (0.5 ppb for forest, 1ppb for arid lands, 10 ppb for grasslands) or spatially and temporally varying ammonia based on VISTAS' 2002 CMAQ run should be used. (Note that POSTUTIL can be used to adjust this value for each Class I area.)

- Puff representation: integrated puff sampling methodology.

- Building downwash: Use IWAQM-recommended algorithms for all sources subject to downwash (all source-receptor distances), if building data are available.

#### ***CALPOST Configuration (Regional screening runs)***

- Visibility Method 6 (for screening) using EPA (2003) Class I area-specific (centroid) monthly relative humidity values or Method 7 to periods of fog and precipitation, if approved by the State.

- Species considered in visibility analysis: SO<sub>4</sub>, NO<sub>3</sub>, EC, SOA (i.e., condensable organic emissions), soil, Coarse PM

- Natural background light extinction: EPA (2003) values **[Resolve whether annual average or 20% best days?]**

- Rayleigh scattering value: 10 Mm<sup>-1</sup> (all Class I areas)

- Light extinction efficiencies: default EPA (2003) values

The screening results will be based on the 98<sup>th</sup> percentile change in light extinction (deciviews) at each receptor from natural conditions over the three-year modeling period for each Class I area considered. Predicted changes exceeding the “contribution” threshold (0.5 deciviews unless defined to be lower by the States) will trigger a refined CALPUFF modeling analysis.

Deleted: highest

## **4.4 Refined Modeling Procedures**

### ***4.4.1 Rationale for and Overview of Refined Modeling Approach***

There are three potential applications for refined CALPUFF modeling:

**BART Exemption Modeling.** Refined CALPUFF modeling to demonstrate that a source does not cause or contribute to visibility impairment in any Class I areas, and thus can be excluded from a BART evaluation. As shown in Figure 4-1, if the initial regional screening modeling does not pass the screening threshold for visibility impacts, the next step is to conduct more refined modeling using a finer grid resolution for the meteorological fields and in the treatment of terrain effects and land use variability, and to include improved model parameterizations such as consideration of time and space-varying ammonia concentrations on nitrate formation (e.g., ammonia limiting effects). In the refined modeling the visibility threshold is based on the BART guidance of the 98<sup>th</sup> percentile change in deciviews.

Deleted: Exclusion

Deleted: controls

Deleted: value rather than the more conservative threshold used in the screening analysis.

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

- 24 hr maximum value emissions for the period 2001-2003 (Continuous Emission Monitor, CEM data)
- 24 hr maximum value for 2002 (CEM data)
- actual 2002 emissions in state CERR inventory
- emissions factors from AP-42 source profiles
- permit allowable emissions, if available
- potential to emit

Comment: Unclear why 2002 emission data recommended when BART covers a longer period.

**Quantify Benefits of BART.** The second application of refined modeling is to quantify the visibility benefits from the 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 postprocessing step rather than by using “negative” emission rates in the CALPUFF model. The chemical scheme requires that emission rates always be positive.

Comment: No discussion on how to do benefit analysis for alternative model.

**Assess Performance of an Emissions Trading Program.** The third application involves modeling to assess the performance of a cap and trade program (see Section 4.6.)

For any of these applications, a supplementary modeling protocol that defines source properties and the specific model configuration is required. The supplementary protocol can refer to this document for those aspects that follow this common protocol.

#### 4.4.2 Model Configuration and Settings for Refined Modeling

Grid resolution substantially better than 12-km is needed for a refined CALPUFF assessment of visibility impacts in most cases involving Class I areas in complex terrain or coastal areas. Thus, the CALMET fine grid resolution in the subregional modeling domains used for refined modeling will depend on the terrain, land use (especially coastal boundaries), location of the source, distance of the source from Class I areas, and total size of the subregional modeling domain. As part of the initial demonstration of CALMET and CALPUFF for VISTAS, recommendations will be developed for appropriate sizes of fine scale grids and subregional modeling domains.

VISTAS may provide pre-computed fine-scale CALMET files for one or more sub-regional domains, depending on available funding. In complex terrain or in coastal areas, fine resolution is required in a refined simulation to properly characterize the flow fields and land use changes that affect dispersion. It is difficult to provide a single rule of thumb for determining the appropriate grid size, because it depends on many as outlined above, but as a general rule, most CALMET applications are done using with 200-300 by 200-300 grid cells over the domain. This produces a reasonable number of grid points that is quite practical to execute with modest computational requirements on current-generation PCs. Domains with 600<sup>+</sup> x 600<sup>+</sup> grid cells are sometimes necessary, but they are used somewhat rarely, while domains with fewer than 100 x 100 cells generally are not used in refined analyses.

**Comment:** This is a big unknown factor for making cost estimates for conducting refined modeling.

An application for source-receptor distances within about 50km may require a grid resolution less than 1km, if complex terrain effects are likely to be important. This determination should be made on a case-by-case basis. There is not a 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.

Earth Tech will develop CALPUFF-ready meteorological fields as requested by VISTAS. The goal is to provide pre-computed CALMET fields for the years 2001-2003 for refined BART analyses at one or more subregional domains, depending on funding levels available.

**Comment:** VISTAS needs to provide a list of Class I areas where this work maybe performed. Otherwise industry will need to do the work to meet schedule deadlines.

As discussed in Appendix C, it is recommended that the fine-scale refined CALMET simulations be run in hybrid mode, using both MM5 data to define the initial guess fields and observational data in the Step 2 calculations. Overwater (buoy) data would be provided in addition to the hourly surface observations, precipitation observations and twice-daily upper air sounding data.

**Comment:** VISTAS needs to provide a listing of all upper air and surface stations that are currently available in a CALMET ready format for 2001-2003. Upper air met processing for a refined analysis is a very time consuming and expensive task to perform.

A domain-specific set of modeling parameters will be defined for each subregional domain. The proper selection of the CALMET diagnostic wind field parameters that are used to blend observations with the Step 1 wind field depends on factors such as the location of the meteorological stations relative to terrain and coastal features (which affects the representativeness of the observational data), the terrain length scale, and the quality (resolution)

of the MM5 data used to define the initial guess field and its ability to properly resolve wind flows on the fine-scale CALMET domain. The definition of the proper CALMET parameters is done as part of sensitivity testing where model performance is evaluated against available observations and expected terrain effects, such as channeling of flows within a valley. A generic set of CALMET wind field parameters usable for all areas is not appropriate because issues such as the representativeness of surface or upper air meteorological wind observations can vary dramatically depending upon the area being modeled.

In addition to the better grid resolution and the introduction of observational data in the refined simulations, several other modeling refinements can enhance the accuracy of the refined modeling. These include the use of the higher resolution terrain DEM data (~3 arcsec USGS data) in defining the gridded terrain fields, and the use of time-varying ammonia concentrations rather than constant ammonia (see Appendix A). An open question is whether to use CMAQ-derived ammonia predictions instead of ammonia concentrations based on CASTNet measurements. Further testing and comparison of the CMAQ ammonia concentrations to CASTNet, SEARCH, and Midwestern monitoring data will be performed, and a decision will be based on results of these planned analyses. Additional refinements, such as changes to the IMPROVE equation for calculating light extinction including use of elevation-dependent Rayleigh scattering and consideration of sea salt in the natural background and considering natural weather effects such as fog, rain and snow (see Appendix B) are beyond the scope of refined modeling under the common VISTAS protocol.

**Comment:** The line-of-sight modeling approach is also a refinement. Would this be outside the scope of the common protocol? Is this and the other refinements given in this paragraph an issue best made by the states?

As recommended in the final BART guidance, for the refined BART exclusion analysis the test for evaluating whether a source is contributing to visibility impairment is based on the 98<sup>th</sup> percentile modeled value (rather than the highest predicted value used for the screening evaluation). A coding change is required in the CALPOST postprocessor in order to allow the 98<sup>th</sup> percentile change in extinction to be computed. Otherwise, the source configuration, emissions, pollutant speciation, Class I receptors, ozone datasets and CALPUFF model options will be the same as in the screening runs.

**Comment:** If CALPOST is modified the ability to printout more than 50 receptors would be beneficial.

The CALPOST processor produces visibility impacts in deciviews, which can be further processed in a spreadsheet to calculate the changes in deciviews. Alternatively, a change to the CALPOST code could be made to allow the visibility changes to be evaluated automatically from two CALPUFF simulations.

## 4.5 Presentation of Modeling Results

### 4.5.1 Sample Summary Tables of Visibility Results

The CALPOST processing computes the daily maximum change in deciviews. A sample of the summary table produced by CALPOST is shown in Table 4-1. For evaluating compliance with the VISTAS screening threshold, the highest 98<sup>th</sup> percentile change in extinction value at each receptor, located at the bottom of the CALPOST list file is compared to the threshold value (e.g., 0.5 dv). For example, in the sample shown in Table 4-1, the summary at the bottom shows that

the highest visibility impact is 1.219 dv, with 9 days over the year showing values greater than 0.5 dv. [Example should be modified] Therefore this source would not pass the screening analysis, and refined modeling would be required. The table contains the highest change in deciview value on each day over all the receptors in a particular Class I area. Also shown are the coordinates of the receptor, receptor type (D indicates discrete receptors), the total haze level (background + source, in dv), the background haze in deciviews, and the change in haziness (delta dv). Also shown in the table is the humidity term applied to hygroscopic aerosols (F(rh)) and the contribution of each species to light extinction (in percent of the total source contribution) for SO<sub>4</sub>, NO<sub>3</sub>, organics, elemental carbon, coarse and fine particulate matter.

**Comment:** Technically, unless a line-of-sight (LOS) analysis is performed for this receptor location the true delta deciview value isn't known. (see URS slide presentation).

This receptor value only defines where additional modeling is needed, in the form of plume plots, to help define an appropriate LOS to model.

For the refined analysis, the data in the table is imported into a spreadsheet and sorted on the delta dv column. Table 4-2 shows an example of the ranked visibility impacts (change in dv) for each of three years at six different Class I areas. The 98<sup>th</sup> percentile (8<sup>th</sup> highest value) in the sorted table would be compared to the contribution threshold (e.g., 0.5 dv). In the example shown in Table 4-2, the source passes the refined analysis because the highest 98<sup>th</sup> percentile visibility impact is below the contribution threshold of 0.5 dv.

#### 4.5.2 Identification of Sources of Uncertainty and Estimation of Uncertainty

The modeling results should 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. *[Specific expectations still to be resolved after discussions with States.]*

**Comment:** This may be the biggest and most important area of uncertainty.

**Table 4-1. Example of CALPOST Output, Showing Maximum Daily Impacts of Source and Locations of Those Impacts.**

YEAR	DAY	HR	RECEPTOR	COORDINATES (km)		TYPE	DV(Total)	DV(BKG)	DELTA DV	F(RH)	%_SO4	%_NO3	%_OC	%_EC	%_PMC	%_PMF
2001	2	0	3	20.540	79.782	D	5.397	5.358	0.039	4.314	44.33	47.22	3.07	1.07	0.00	4.30
2001	3	0	9	31.680	79.822	D	4.566	4.421	0.145	1.767	40.75	33.89	9.19	3.24	0.00	12.94
2001	4	0	1	24.723	77.951	D	4.540	4.540	0.000	2.076	0.00	0.00	0.00	0.00	0.00	0.00
2001	5	0	77	30.228	94.571	D	4.950	4.939	0.011	3.144	43.13	44.74	4.64	1.45	0.00	6.05
2001	6	0	1	24.723	77.951	D	5.181	5.166	0.015	3.772	38.58	56.05	1.90	0.70	0.00	2.76
2001	7	0	3	20.540	79.782	D	6.366	5.745	0.620	5.439	44.98	44.99	3.69	1.26	0.00	5.08
.																
.																
.																
2001	363	0	113	27.414	103.782	D	5.725	5.652	0.073	5.164	53.49	35.51	4.03	1.39	0.00	5.58
2001	364	0	113	27.414	103.782	D	6.554	6.521	0.033	7.826	48.12	47.09	1.67	0.64	0.00	2.48
2001	365	0	1	24.723	77.951	D	6.499	6.499	0.000	7.757	0.00	0.00	0.00	0.00	0.00	0.00
--- Number of days with Delta-Deciview =>							0.50:	9								
--- Number of days with Delta-Deciview =>							1.00:	2								
---							Largest Delta-Deciview =	1.219								

**Table 4-3. Example of Visibility Impact Rankings at Six Class I Areas**

Class I Area	2001	2002	2003
	Delta- Deciview Ranks 1-8	Delta- Deciview Ranks 1-8	Delta- Deciview Ranks 1-8
Great Smoky NP	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
Linville Gorge	0.47	0.36	0.42
	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
Shining Rock	0.25	0.31	0.28
	0.23	0.29	0.28
	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
Cohutta	0.24	0.34	0.27
	0.23	0.29	0.26
	0.22	0.26	0.25
	0.26	0.54	0.61
	0.23	0.47	0.42
	0.22	0.43	0.30
	0.21	0.37	0.29
Joyce Kilmer-Slickrock	0.20	0.37	0.28
	0.19	0.31	0.28
	0.18	0.31	0.25
	0.16	0.30	0.25
	0.34	0.52	0.27
	0.33	0.43	0.24
	0.31	0.32	0.23
Mammoth Cave NP	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
	0.56	0.57	0.50
	0.44	0.56	0.37
Mammoth Cave NP	0.38	0.53	0.36
	0.29	0.35	0.35
	0.25	0.33	0.31
	0.24	0.33	0.24
	0.22	0.30	0.21
	0.21	0.29	0.19

#### 4.6 Assess the Performance of a Cap and Trade Program

EPA guidance allows states to demonstrate that a cap and trade program could be more effective than source-by-source BART controls. Specific guidance has been proposed under a rulemaking process that is currently under way.

In order to determine the efficacy of the cap and trade program, assumptions would need to be made how emissions under a cap and trade scenario would differ from source-by-source BART control implementation. If the expected geographic distribution of emissions is different under the two approaches, then “dispersion modeling” of all sources must be used in order to establish that the optional trading program will result in visibility improvements at all Class I areas that are, overall, “better than BART”. From a technical perspective, either CALPUFF applied to every source or a regional air quality model could then be used to determine the difference in visibility at each impacted Class I area due to the two alternative assumptions.

VISTAS is using CMAQ to evaluate visibility improvement in 2018 from potential control strategies for regional haze. One control strategy being evaluated is the benefit of the Clean Air Interstate Rule, CAIR, which targets SO<sub>2</sub> and NO<sub>x</sub> emissions from Electric Generating Units (EGUs) in the eastern US. A second planned control strategy is implementation of assumed BART control measures for all EGU and non-EGU BART sources in the VISTAS states. Because BART controls will not be finalized by the States at this point, these second analyses will be indicative of potential benefits but may not represent final BART control determination.

Because the DC Circuit Court overruled the methods used by the WRAP states to demonstrate that a regional SO<sub>2</sub> trading program is better than BART, an acceptable modeling methodology for assessing the effectiveness of a cap and trade program, remains unclear. Prior to deciding if and how to demonstrate the benefits of a regional cap and trade program, VISTAS intends to review results of the evaluations of the planned regional haze control strategies discussed above, to monitor EPA’s development of guidance for a trading program, and to evaluate progress by EPA and WRAP to define appropriate methods for assessing a trading program

## 5. OPTIONAL SOURCE-SPECIFIC MODELING APPROACHES

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### 5.1 Overview of Source-Specific Modeling

The BART analysis process provides an option for source-specific modeling to be performed. There are a number of reasons why a more detailed approach than that provided for in the standard VISTAS protocol may be desired. For example, sources very close to Class I areas require finer grid resolution than the generic “fine” grid resolution meteorological fields provided by VISTAS for refined modeling under the common protocol. If a source-specific modeling that differs from the common approach is to be used in an analysis, a detailed modeling protocol explaining the data sources, model configuration and rationale for changes in the model approach from the common protocol must be provided and approved by the State. An outline of the typical contents of the site-specific protocol is provided in Table 5-1. Discussions with the regulatory authorities should be conducted prior to development of a protocol to ensure all of the relevant issues are included in the protocol.

### 5.2 Options for Site-Specific Analyses

#### 5.2.1 Alternative Methods for Sources within 50km to Class I Areas

For modeling the impact of a source 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.” For example, 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.

As discussed in Section 3.2, there are no scientific 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 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; a finer grid will be needed for transport distances that are smaller than that.

**Comment:** The need for a CALPUFF LOS modeling approach cannot be overstated in this modeling situation and should be encouraged by VISTAS. Also, the need to use PLUVUE-II modeling for distinct plumes >50 km should also not be ruled out. The user guide for PLUVUE-II states that the model could be used for distances > 50 km and this may be a conservative approach.

**Table 5-1. Sample Table of Contents of a Source-Specific Fine-Scale Modeling Protocol.**

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1. INTRODUCTION
    - 1.1 Objectives
    - 1.2 Location of Source vs. Relevant Class I Areas
    - 1.3 Source Impact Evaluation Criteria
  2. SOURCE DESCRIPTION
    - 2.1 Unit-specific Source Data
    - 2.2 Boundary Conditions
  3. GEOPHYSICAL AND METEOROLOGICAL DATA
    - 3.1 Modeling Domain and Terrain
    - 3.2 Land Use
    - 3.3 Meteorological Data Base
      - 3.3.1 MM5 Simulations
      - 3.3.2 Measurements and Observations
    - 3.4 Air Quality Data Base
      - 3.4.1 Ozone Concentrations – Measured or Modeled
      - 3.4.2 Ammonia Concentrations – Measured or Modeled
      - 3.4.3 Concentrations of Other Pollutants – Measured or Modeled
    - 3.5 Natural Conditions at Class I Areas
  4. AIR QUALITY MODELING METHODOLOGY
    - 4.1 Plume Model Selection
      - 4.1.1 Major Relevant Features of CALMET
      - 4.2.2 Major Relevant Features of CALPUFF
    - 4.2 (Optional) Selection of Regional Model for VOC
    - 4.3 Modeling Domain Configuration
    - 4.4 CALMET Meteorological Modeling
    - 4.5 CALPUFF Computational Domain and Receptors
    - 4.6 CALPUFF Modeling Option Selections
    - 4.7 (Optional) Regional Modeling of VOC
    - 4.8 Light Extinction and Haze Impact Calculations
    - 4.9 Modeling Products
  5. REVIEW PROCESS
    - 6.1 CALMET Fields
    - 6.2 CALPUFF, CALPOST, and POSTUTIL Results
  6. REFERENCES
- APPENDICES
- A.1 VISTAS BART MODELING PROTOCOL
  - A.2 ... other appendices as needed

### 5.2.2 Alternative Methods for Computing Light Extinction

EPA, IMPROVE, and the Regional Planning Organizations are evaluating whether refinements are warranted to the methods recommended in EPA's guidance to calculate light extinction. VISTAS will make a recommendation how to address these issues in the fall of 2005. The CALPUFF modeling protocol should follow the VISTAS recommendations unless the source can justify, and the State approves, a different approach.

The refinements under consideration would also apply to the CALPOST extinction formula, Equation 3-1. Refinements under consideration 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 (OC in Eq. 3-1) from organic carbon measurements
- Slightly modifying the relative humidity growth formula,  $f(RH)$ , for sulfates and nitrates
- 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
- Performing light of sight calculations to determine the average change in deciview along the sight path equivalent to the background visual range. This basis for this refined calculation is contained in the Pitchford and Malm paper (1992) which defines 1.0 deciview as a "just noticeable change" when the background visual range (natural conditions) equals the line of sight distance.

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The IMPROVE Steering Committee has commissioned a panel, with participation by National Park Service, EPA, industry, and academia, to review its light extinction formula in light of current knowledge. A report is expected in the fall of 2005. Presumably any changes that are made by IMPROVE will also ultimately be reflected in the EPA's approach.

### 5.2.3 Alternative Definitions of Natural Conditions Baseline

EPA's BART proposal requires that the visibility impacts of BART-eligible sources be evaluated against natural conditions. Default values of natural conditions have been specified in EPA guidance documents. These values are 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. CALPOST Method 7 offers one way to take such impairment into account. This issue is discussed in more detail in Appendix B.) Method 7 should be used. Method 7' is a total revision to how the model has calculated light extinction for the past 10 or more years

**Comment:** This issue is a very important concern of industry and we cannot perform CALPUFF modeling without addressing this issue.

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The EPA allows refinements to the default natural conditions values, with adequate scientific justification. Although a discussion of natural conditions refinements is beyond the scope of this document, three changes seem to have wide support – (1) 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; (2) Changing the estimates of natural conditions extinction on the 20% clearest and haziest days to better reflect the statistical distribution of extinction; and (3) 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. *[This needs to be resolved.]* 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.

The sea salt adjustment applies to the description of natural conditions, and has effect mainly near the seacoast. It is discussed further in Appendix B.

One other adjustment is included in the common protocol and is particularly appropriate for source-specific analyses. The Rayleigh scattering coefficient for clear air has a default value  $10 \text{ Mm}^{-1}$  in 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  $12 \text{ Mm}^{-1}$ , 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.<sup>11</sup>

**Comment:** It is unclear to us why this fact needs to be debated. VISTAS should just include it as an option.

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#### 5.2.4. Calculation of a Source's Impact on Visibility

<sup>11</sup> Air Resource Specialists, Inc., of Ft. Collins, CO has available a small computer program that calculates the Rayleigh scattering coefficient for any ambient atmospheric condition.

The modeling described above uses CALPOST to calculate the change in extinction at each receptor point. That value represents extinction in the vicinity of that point, but does not necessarily represent the impact of the source on extinction over any sight path, particularly over the longer sight paths that are likely under natural conditions. The human perception of visibility takes place over sight paths, not at points.

**Comment:** Text is from initial draft VISTAS BART modeling Protocol dated January 31, 2005.

For example, consider a 40-km sight path that represents the visual range and includes 10 CALPUFF receptor points on a 4 km grid. If there is a 10% change in extinction (a 1 dv change) at two receptors and no change at the others, the actual change in haziness over the sight path is 2% (or 0.2 dv). If, as the EPA asserts in its BART proposal, a 0.5 dv change is barely perceptible, then this change in haziness would be wholly imperceptible even though two receptor points exceed the 0.5 dv threshold!

Thus, if the scale of the plume is small compared to the visual range under natural conditions, which is likely to be the case at all but the longest transport distances (and will be especially true for the small plumes very close to the source), the change in extinction at any receptor point is not representative of the effect of the source on the ability to see through the haze. Rather, in such cases, a sight path must be selected and the average change in extinction over that sight path calculated.

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.

## 6. QUALITY ASSURANCE

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### 6.1 Scope and Purpose of the QA program

The purpose of the quality assurance (QA) program is to describe the procedures for ensuring that products produced by the application of the modeling techniques for BART studies satisfy the regulatory objectives of the BART program. The regional haze rule includes a requirement for BART for certain large stationary sources. Air quality modeling covered under this protocol is an important tool for use in determining whether a BART-eligible source can be reasonably expected to cause or contribute to visibility impairment in a Class I area, and therefore whether this source should be subject to BART controls, and if so, to determine the relative benefits of various BART controls.

The scope of the QA program affects different users differently. Common features of most applications will be the setup and execution of the CALPUFF air quality model and processing of modeling results to determine compliance with visibility thresholds. In many cases, users will be provided meteorological datasets that have been developed with VISTAS funding under a suitable QA program for use in the BART modeling. Other users will be involved in site-specific or source-specific analyses that will use different datasets and different modeling options and/or tools. More extensive quality assurance will be required in these latter types of applications. It is the responsibility of the modeler to ensure that an adequate QA protocol is in place for a particular application.

**Comment:** Industry agrees completely on this issue. We understand that additional time will be needed should we need to do site-specific modeling.

The CALPUFF modeling system contains built-in features to facilitate quality assurance of the modeling results. 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 modeling units of the modeling system. The Graphical User Interface system (GUI) provided as part of the latest CALPUFF modeling system allows these QA files to be displayed graphically.

In addition, a detailed software management system is in place to track version and level numbers associated each program and utility within the CALPUFF modeling system. This information is carried forward in all of the output files to create an audit trail of software versions and major model options used that can be retrieved and displayed from the model output files.

Because the required QA procedures will depend heavily on the exact application, there will be differences among different users and different applications.

In addition, the BART modeling process involves multiple organizations. The States have overall responsibility for the process and may also execute some or all of the modeling. VISTAS is contributing general guidance via this protocol and is preparing meteorological fields and performing modeling under the guidance of the States. The sources that are BART-eligible need to provide process information and emissions data for use in the analyses. In addition, those sources that are involved in BART assessments will need to be actively involved in control

technology decisions and assessments. Finally, some of the modeling steps may be carried out by contractors on behalf of VISTAS, a State, or a source.

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, irrespective of which organization is carrying out the effort. The focus is on the common protocol efforts described in Chapter 4. As described in Section 6.3, more comprehensive QA may be needed for the unique aspects of the source-specific modeling described in Chapter 5.

## 6.2 QA Procedures for Common Protocol Modeling

The VISTAS common protocol (Section 4) describes the methods and procedures for use in conducting regional scale screening modeling to determine whether a particular source or group of sources is subject to BART controls. In the initial application, the regional CALPUFF-ready meteorological data files will be provided by VISTAS for modelers to perform screening analyses. The amount of effort for end-users performing QA of these pre-defined meteorological fields will be reduced from what is required in developing source-specific meteorological fields, as described below. Also, VISTAS is planning to provide one or more subregional CALMET meteorological datasets in a CALPUFF-ready format. The development of these CALMET datasets will be subject to a QA program as part of their development, so the necessary quality assurance activity of end-users is again reduced from what would be required in the development of the dataset. It is not expected that the quality assurance steps in the development will be repeated in each application. The pre-defined CALMET regional and any VISTA-funded subregional meteorological fields will include a test case simulation for demonstrating expected modeling results are obtained on the user's computer platform. This test should be repeated by every user.

**Comment:** Please provide a listing of these sub regional grids so industry can make proper cost estimates.

Although the CALPUFF modeling system is recommended by the U.S. Environmental Protection Agency for application to BART analyses, a considerable amount of expertise and modeling judgment is needed at certain stages of the analysis. The modeling is not a “cookbook” exercise, which was recognized by the U.S. EPA in describing the expertise needed for CALMET modeling (p. 9-10, EPA, 1998). Current methods for performing refined chemistry calculation also require an understanding of the chemical and meteorological processing affecting ammonium nitrate formation. VISTAS has committed to provide appropriate CALPUFF training to assist States in obtaining the necessary expertise with the latest CALPUFF modeling tools and techniques. An appropriate level of knowledge of the model formulation, technical approach and assumptions is essential for successful BART modeling.

### 6.2.1 Quality Control of Input Data

The input data required by the model depends on the application. At a minimum, source data is required by CALPUFF (see Section 6.2.3) along with a list of choices made about model options

and switches. Most of the modeling option choices are specified or recommended by regulatory guidance and default values (see references in Section 4.3.3). If the Ammonia Limited Method (ALM) is applied to a VISTAS-provided subregional refined modeling domain, the multi-step postprocessing procedure described in Appendix A is required. However, remodeling of the boundary conditions is not required for VISTAS-provided refined domains so the expertise level is not as high as it would be for development of the boundary conditions files from scratch.

To the extent that modeling applications are using pre-defined CALMET files and CALPUFF templates, the quality assurance will be straightforward. More detailed steps are needed for the setup of modeling files for source-specific applications of subregional domains that are not already developed.

The basic procedures that will apply to all CALPUFF model applications will 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. It is a common and recommended procedure for an independent modeler not involved in the setup of the modeling files to independently confirm the model switches and data entry in the actual model input files and to conduct an independent run of the worst case event as a confirmation check.

In addition, common practice requires that a model project CD (or DVD or set of DVDs) be created that contains all of the data and program files needed to reproduce the model results presented in a report. The model list files from each step are included on the project CD. This information allows independent checking and confirmation of the modeling process.

### ***6.2.2 Quality Control of Application of CALMET***

For users of the VISTAS CALPUFF-ready CALMET meteorological files, a number of large datafiles will be provide by VISTAS on external USB2 or Firewire hard drives in a format ready for use with the CALPUFF model. The QA steps associated with the development of the VISTAS common datasets will be provided separately as part of the modeling documentation. It is not expected that the QA steps conducted in the development of the meteorological datasets will be repeated in each application, although tests to confirm that the dataset is suitable for the application for which it is being used should be performed as part of the QA. This is discussed in more detail below.

The regional screening CALMET grid is defined in Chapter 4 on a 12-km Lambert Conformal Conic (LCC) grid system. The subregional and source-specific domains may be defined in either LCC or Universal Transverse Mercator (UTM) coordinates. In the case of the LCC projection, two matching parallels, latitude/longitude of the projection origin, coordinate datum, and false Easting and Northing (if used) of the projection origin must also be defined. For any domains in UTM coordinates, the UTM zone (see Appendix D of the CALMET User's Guide) and datum

must be defined. The appropriate projection and map factors are provided as part of the definition of the VISTAS regional grid system. For a source-specific domain, the grid parameters will be provided as part of the source-specific protocol.

The Appendix A of the IWAQM report contains a list of recommended CALMET switch settings. Except as modified in Chapter 4 of this protocol or in a source-specific protocol, the IWAQM guidance 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 a DOS, Linux, or Unix window, 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. Some third-party commercial GUIs strip out this descriptive information, which makes the QA step more difficult, although it is essential for perform nonetheless using the variable names as references for the variables in the file.

Part of the CALPUFF modeling system’s built-in QA capabilities 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.

### ***6.2.3 Quality Control of Application of CALPUFF***

At a minimum, source data is required by CALPUFF including the following parameters:

- Location (e.g., UTM coordinates, UTM zone and datum)
- Stack height above the ground
- Stack diameter
- Exit velocity
- Exit temperature

- Emission rates (SO<sub>2</sub>, H<sub>2</sub>SO<sub>4</sub>, NO<sub>x</sub> and PM<sub>10</sub>).

There are also some 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 for long-range transport distances.

The source coordinates must be expressed in the coordinate system used to define the CALMET and CALPUFF modeling domains. For the regional screening simulations, a Lambert Conformal Conic (LCC) coordinate system will be used. The required parameters to define an LCC coordinate include two matching parallels, latitude/longitude of the projection origin, coordinate datum, and false Easting and Northing (if used) of the projection origin. Subregional and source-specific domains may be using either an LCC or UTM projection. The Earth Tech GUI system provides software (called COORDS) to compute to/from latitude/longitude, LCC and UTM coordinates for a large number of datums. 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](http://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<sub>10</sub> emissions should be broken into filterable and condensable components. The filterable PM<sub>10</sub> 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 will be divided into a primary H<sub>2</sub>SO<sub>4</sub> component and organic and non-H<sub>2</sub>SO<sub>4</sub> inorganic components. The sources of this information, such as source-specific data and AP-42 tables, are dealt with separate from this protocol. The speciation of the PM<sub>10</sub> 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. The quality assurance of the source and emissions data is a major component of the CALPUFF modeling.

The locations of the Class I area receptors are another important CALPUFF input. The use of pre-defined receptors as provided by the National Park Service (NPS) receptor dataset is recommended in the VISTAS common protocol. However, 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 of the IWAQM report contains a list of recommended CALPUFF switch settings. Except as modified in Chapter 4 of this protocol or in a source-specific protocol, the IWAQM guidance should be used in setting up the CALPUFF simulations. The CALPUFF model obtains the switch settings from an ASCII “control file” with a default name called the CALPUFF.INP file. As is the case with the comparable CALMET file, whether the model is run using a GUI or from the control line in a DOS, Linux, or Unix window, it is essential that the control file be reviewed manually as part of the CALPUFF 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. Some third-party commercial GUIs strip out this descriptive information, which makes the QA step more difficult, although it is essential for perform nonetheless using the variable names as references for the variables in the file.

#### ***6.2.4 Quality Control of 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 in the standard EPA BART guidance), 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. The table includes the data shown in the example in Table 4-1. For a screening assessment, the peak value of the change in extinction is shown at the bottom of the visibility table (see Table 4-1). For a refined simulation, the 98<sup>th</sup> percentile value (8<sup>th</sup> highest day) is used for comparison against the BART threshold of 0.5 deciviews. It is necessary to import the results of the CALPOST table into a sorting program such as a spreadsheet to rank the daily change in extinction values such as is presented in Table 4-2.

The CALPOST inputs that need to be carefully checked as part of the CALPOST quality assurance are:

- Visibility technique (Method 6 in the common VISTAS protocol)
- 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 ( $10 \text{ Mm}^{-1}$  for screening modeling but Class I area specific value for refined modeling)
- 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 described in Appendix A. An example of the type of evaluation of the model inputs in applying ALM is illustrated for an example in the Great Smoky Mountains National Park in Figure 7 of the Appendix A. For the VISTAS-sponsored regional modeling simulation, it is not necessary to repeat Steps 1 of 3 of the ALM procedure, nor the evaluation of the effectiveness of the boundary condition run. However, Steps 2 and 4 of the procedure must be repeated for each refined BART application using the ALM.

If source-specific modeling is performed using different sources of ammonia data or different techniques, the source-specific modeling protocol should provide justification for deviations from the VISTAS common protocol, and a QA plan specific for the application provided to address the quality assurance of the data used.

### **6.3 Additional QA Issues for Alternative Source-Specific Modeling**

The level of QA required for application of source-specific protocols will be substantially higher than for the use of datasets that has already been subject to a QA procedure. For example, source-specific 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 common protocol. In addition to providing a source-specific modeling protocol describing and justifying the changes to the modeling approach from the VISTAS common protocol, the site-specific applications should include the development of a QA plan to properly evaluate the data used in the site-specific 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 site 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. Season 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 site-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 site-specific QA plan development.

If site-specific CALPUFF simulations involving the ALM are conducted, the procedure described in Appendix A should be conducted. 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 site-specific modeling domain. The use of alternative ammonia concentration data (e.g., CMAQ output rather than derived ammonia based on aerosol measurements) will require an evaluation of the model performance relative to the techniques in the VISTAS common protocol.

In any site-specific protocol a site-specific QA plan should be prepared.

## **6.4 Assessment of Uncertainty in Modeling Results**

*[The need for a formal uncertainty analysis for each BART application will be determined based on discussions with the States and Stakeholders.]*

## **6.5 Quality Assessment**

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. To the extent that screening analyses will be performed followed by fine-scale refined

analyses, data will be developed on the relative conservatism of the screening approach. This will be helpful in assessing the impact of uncertainties in screening our sources from BART controls. To the extent that the performance of the screening approach can be documented by comparison with refined simulations, the States may decide to adjust the screening threshold. It is recommended that the States or EPA collect and summarize the modeling results from BART applications applying to develop a dataset of the performance of the screening approach in predicting refined modeling results.

It is expected that the performance of the model will be better in predicting changes in visibility impacts due to BART controls than in predicting absolute visibility values. This is because uncertainties in meteorological conditions transport and dispersion is expected to be less important in evaluating a change in impact since the same effect will be included in both the base and sensitivity simulation. A detailed sensitivity and uncertainty analysis may be useful in confirming and quantifying this expected results. (See comments in Section 6.4 regarding whether a formal sensitivity/uncertainty analysis will be required for individual BART applications.)

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A LOS modeling approach was discussed by VISTAS technical consultant in the initial draft of the VISTAS Modeling Protocol dated 31 January 2005 under section 4.1.4 (Additional Technical Considerations) for CALPUFF modeling of sources located less than 50 kilometers from a Class I Area. These paragraphs have been extracted from the Initial Draft VISTA Modeling Protocol and clearly indicate the technical consultant understands the concept of LOS modeling when using CALPUFF;

Statement 1 from Initial VISTAS Draft Protocol:

“A more difficult issue to address is that CALPOST calculates the extinction coefficient at each receptor point. That value represents extinction in the vicinity of that point, but does not necessarily represent the impact of the source on extinction over any sight path, particularly over the longer sight paths that are likely under natural conditions. The human perception of visibility takes place over sight paths, not at points. For example, consider a 40-km sight path that represents the visual range and includes 10 CALPUFF receptor points on a 4 km grid. If there is a 10% change in extinction (a 1 dv change) at two receptors and no change at the others, the actual change in haziness over the sight path is 2% (or 0.2 dv). If, as the EPA asserts in its BART proposal, a 0.5 dv change is barely perceptible, then this change in haziness would be wholly imperceptible even though two receptor points exceed the 0.5 dv threshold!

Thus, if the scale of the plume is small compared to the visual range under natural conditions, which is likely to be the case at all but the longest transport distances (and will be especially true for the small plumes very close to the source), the change in extinction at any receptor point is not representative of the effect of the source on the ability to see through the haze. Rather, in such cases, a sight path must be selected and the average change in extinction over that sight path calculated.”

Statement 2 from Initial VISTAS Draft Protocol:

“... Also, when the plume is narrow, the aerosol concentrations across it may vary considerably from one CALPUFF receptor to the next, and the concentration field is unlikely to be uniform over the distance one can see (the visual range), especially if the background is assumed to be at default natural conditions. Therefore the light extinction impact of the source will vary depending on the sight path. In such situations, this variability of the aerosol from one CALPUFF receptor to the next should be taken into account by averaging the CALPOST-calculated light extinction over all receptors along each of the sight paths of interest within a Class I area.”

Statement 3 from Initial VISTAS Draft Protocol:

“Thus, if the scale of the plume is small compared to the visual range under natural conditions, which is likely to be the case at all but the longest transport distances (and will be especially true for the small plumes very close to the source), the change in extinction at any receptor point is not representative of the effect of the source on the ability to see through the haze. Rather, in such cases, a sight path must be selected and the average change in extinction over that sight path calculated.<sup>1</sup>

Our consultant believes when conducting an hourly plume visibility analysis for sources located less than 50 kilometers from a Class I area the LOS modeling approach should automatically be triggered.

For a source greater than 50 kilometers from a Class I area a source should have the option of making a demonstration that a LOS modeling approach is applicable by providing plots that show the plume distribution within the modeling domain. If a highly concentrated plume is shown over the 24-hour period then a LOS analysis can and should be conducted. Example of these kind of plots are contained in a slide presentation discussed under general comments.