## DRAFT

## BART Modeling Protocol for VISTAS

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## 1 Objective

This document has been prepared by VISTAS to present methods for carrying out air quality modeling in connection with Best Available Retrofit Technology (BART) determinations for managing regional haze. Its objective is to describe consistent approaches that can be used in all of the VISTAS States, both by the States themselves and by operators of BART-eligible sources.

The protocol presented here applies to three situations in which modeling of regional haze impacts is to be addressed under the guidance for regional haze BART determinations in Appendix Y of 40 CFR 51 (as proposed by the U.S. EPA on 5 May 2004), namely:

- Air quality modeling or use of screening methods to determine whether a BARTeligible source is "subject to BART" and therefore the BART analysis process must be applied to its operations.
- Air quality modeling of emissions from sources that have been found to be subject to BART, to evaluate regional haze benefits of alternative control options and to document the benefits of the preferred option.
- Regional air quality modeling to demonstrate the effectiveness of an optional 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.

The next section (Section 2) of this document reviews EPA's guidance for regional haze BART analysis modeling, as expressed in the proposed version of the BART guidance. Since the CALPUFF model is strongly preferred by the EPA, its characteristics, appropriate applications, and limitations are addressed in Section 3, and some alternatives are presented for special situations. Recommended modeling approaches for the three situations listed above are then described in Section 4, which also includes recommendations for circumstances that are not specifically addressed in the regional haze BART guidance. This document concludes in Section 5 with a review of practical considerations involved in the application of CALPUFF and other models for BART purposes.

The information presented here strives to follow the spirit of EPA's proposed guidance, "fills in the blanks" where the guidance is incomplete, and provides recommendations when the draft guidance is inconsistent or unclear. Effort has been made to harmonize this draft protocol with perspectives expressed by relevant EPA staff members since the draft guidance was proposed. It should be recognized, though, that since EPA's regional haze BART guidance is only in proposed form, this protocol may be revised once EPA's final guidance is released.

## 2 Review of EPA's Proposed Guidance for BART Modeling

The proposed guidance for regional haze BART determinations, to be in Appendix Y of 40 CFR 51, was published in the Federal register on 5 May 2004 (69 FR 25184 to 25232) It prescribes the modeling approaches that are to be used for various stages of the BART analysis process. Once the guidance is finalized in 2005, EPA intends that the States will be "required to follow it in all BART determinations" (69 FR 25214).

### 2.1 Overview Of The Regional Haze BART Process

The proposed regional haze BART process for a "major stationary source" involves a State taking the following four steps (with the option of asking the source owner to carry out some of the required analyses):<sup>1</sup>

- (1) Identifying 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. Qualifying pollutants also include the following gaseous precursors to visibility-impairing particulate matter: SO<sub>2</sub>, NO<sub>x</sub>, and VOC.
- (2) Determining whether a BART-eligible source is "subject to BART" (for any visibility-impairing pollutant, regardless of the amount emitted), based on air quality modeling of the source's impact on visibility. The preferred approach is an assessment with an air quality model (although simpler screening approaches are being considered, according to EPA's proposal), followed by comparison of the estimated 24-hr visibility impacts against a proposed metric of an increase in haziness of 0.5 deciviews above estimated natural conditions.

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.

(3) Determining BART for the source by considering various control options and selecting the "best" alternative, taking into consideration:

<sup>&</sup>lt;sup>1</sup> Note that steps 2 and 4 in this list differ slightly from those that apply for the BART process under EPA's 1980 visibility regulations that is concerned with the mitigation of "reasonably attributable" visibility impairment due to emissions from a source or small group of sources. This protocol does not address modeling for such "reasonably attributable" BART determinations.

- The costs of compliance,
- The energy and non air-quality environmental impacts of compliance,
- Any existing pollution control technology in use at the source,
- The remaining useful life of the source, and
- The degree of improvement in visibility that may reasonably be anticipated to result from the use of such technology.
- (4) Incorporating the BART determination into the State Implementation Plan for Regional Haze, which is due no later than three years from January 2005.

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>2</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, regional air quality modeling comparing the expected improvements in visibility from the trading program and from BART would be required.

## 2.2 Which Models Does the Proposed BART Rule Specify?

#### 2.2.1 To Assess Whether a Source is Subject to BART

To evaluate the visibility impacts of a BART-eligible source that is more than 50 km distant from a Class I area, "an air quality model able to estimate a single source's contribution to visibility impairment," should be used, according to the preamble to EPA's BART proposal (69 FR 25189). The preferred model is CALPUFF (69 FR 25194). The proposed BART Guideline (Appendix Y) specifically labels modeling for this purpose as "CALPUFF modeling" (69 FR 25218).

According to the proposed BART Guideline, it appears that submitting a modeling protocol to the EPA is expected in all cases (69 FR 25218), although it is not clear whether EPA approval of protocols prepared by States is required. If the modeling is being performed by a source owner, "they should prepare a modeling protocol that is acceptable" to the State and to the EPA (69 FR 25218). Also, application of CALPUFF for distances greater than 200 km requires development of a written modeling protocol that is approved by the "appropriate reviewing authority" (69 FR 25194).

For modeling the impact of a source closer than 50 km to a Class I area, EPA's BART proposal recommends that States used their discretion, "giving consideration to both

 $<sup>^{2}</sup>$  The EPA's BART proposal points out that it is likely that the Clean Air Interstate Rule, as currently proposed, would satisfy the BART requirements for affected electric generating units (EGUs), which could affect the modeling efforts a State would need to undertake.

CALPUFF and other EPA-approved methods." The plume visibility model, PLUVUEII, is presented as an acceptable example (69 FR 25194).<sup>3</sup>

Using CALPUFF to determine whether every BART-eligible source in a State is subject to BART could be very burdensome. Recognizing this, the BART proposal states that EPA is "also considering alternative approaches that would be credible" and would be simpler to implement (69 FR 25195). Four such "screening" approaches, one of which involves using CALPUFF in a screening mode, were presented in the BART proposal for public comment.

Modeling of source impacts with CALPUFF or another plume model may be supplemented with source apportionment data or source apportionment modeling that is acceptable to the State and the EPA regional office (69 FR 25218), presumably in a weight-of-evidence type of analysis.

#### 2.2.2 To Evaluate Potential Visibility Improvement from Applying BART

If a source is found to be subject to BART and therefore a BART assessment is carried out, the BART proposal's preamble states that CALPUFF or another EPA-approved model should be used to evaluate the improvement resulting from the application of BART (69 FR 25203). The proposed Appendix Y states specifically that CALPUFF is to be used for assessment of the degree of improvement when the source-receptor distance is 50 km or more (69 FR 25227).<sup>4</sup>

For sources that are less than 50 km from a Class I area, the method to be used for evaluating the benefits of BART is at the discretion of the State, which is expected to consider both CALPUFF and other EPA-approved methods such as PLUVUEII (69 FR 25203).

Evaluating visibility benefits with CALPUFF or another plume model may be supplemented with source apportionment data or source apportionment modeling that is acceptable to the State and the EPA regional office (69 FR 25228).

<sup>&</sup>lt;sup>3</sup> Apparently "EPA-approved" is not limited to the Preferred/Recommended ("Guideline") models listed in Appendix W to 40 CFR 51. For example, PLUVUEII is listed as an "Alternative" model by EPA's Support Center for Regulatory Air Models

<sup>(</sup>http://www.epa.gov/scarm001/tt25.htm). However, it is not clear whether case-by-case approval of specific models that are not on current EPA lists would be feasible or acceptable.

<sup>&</sup>lt;sup>4</sup> Possible use of a simpler screening version of CALPUFF to do this analysis is laid out for public comment in the BART proposal (69 FR 25203).

#### 2.2.3 To Determine the 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 visibility improvements at all Class I areas that are, overall, "better than BART" (FR 25231). The proposed 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.

### 2.3 How Should the Models Be Applied?

EPA's BART proposal does not give a great deal of guidance concerning the details of applying air quality models for BART purposes. The main recommendation is that the Phase 2 recommendations of the Interagency Workgroup on Air Quality Modeling<sup>5</sup> (IWAQM) be followed for CALPUFF modeling for both the initial assessment (69 FR 25218) and the BART evaluation (69 FR 25227).

IWAQM was formed in the early part of the 1990s by the EPA and the Federal agencies that manage Class I areas (the U.S. Forest Service, the National Park Service, and the U.S. Fish and Wildlife Service). Its purpose was to provide a focus for developing technically sound recommendations regarding air quality modeling for assessment of air pollutant source impacts on Class I areas. The Phase 2 recommendations, published in 1998 as an EPA report, recommended that CALPUFF be used for characterizing long range transport and dispersion in connection with estimating impacts associated with Prevention of Significant Deterioration (PSD) and National Ambient Air Quality Standards (NAAQS). The IWAQM recommendations were adopted by FLAG (Federal Land Managers' AQRVs Workgroup) for review of new sources by Federal Land managers.<sup>6</sup>

<sup>&</sup>lt;sup>5</sup> Interagency Workgroup on Air Quality Modeling (IWAQM) Phase 2 Summary Report and Recommendations for Modeling Long Range Transport Impacts. EPA-454/R-98-019. December 1998.

<sup>&</sup>lt;sup>6</sup> Federal Land Managers' Air Quality Related Values Workgroup (FLAG) Phase I Report. December 2000.

EPA's description of CALPUFF in its *Guideline on Air Quality Models* (40 CFR 51, Appendix A to Appendix W, Section A.3) further specifies that, "For regulatory applications ... the regulatory default option should be used." It also notes that, "Inevitably, some of the model control options will have to be set specific for the applications using expert judgment and in consultation with the relevant reviewing authorities."

One of IWAQM's recommendations is that there be five years of hourly modeling if NWS meteorological data are used, with use of a shorter period an option on a case-bycase basis if meteorological data are provided by a prognostic meteorological model (e.g., MM5) with four-dimensional data assimilation (FDDA) or if on-site meteorological measurements are available at the source location in addition to regional NWS data.

EPA's *Guideline on Air Quality Models* (40 CFR 51, Appendix W, Section 9.3.1.2.d) provides similar recommendations, with the additional specification that at least three, not-necessarily-consecutive, years of data are acceptable for long-range transport modeling if outputs from a prognostic meteorological model are available. For EPA, FDDA is desirable but not mandatory. Also, in EPA's modeling guidance, use of on site plus NWS data does not provide grounds for modeling less than five years.

As another consideration, an interesting situation can occur if a portion of a Class I area is less than 50 km from a source and another portion of the same Class I area is more than 50 km from the source. If EPA's proposed guidance is followed it is possible that two different modeling approaches could be used for the same Class I area and source, depending on the State's chosen methods (69 FR 25218 and 25227). How to reconcile possible discrepancies between the two models' estimates at the 50-km mark is not addressed in EPA's proposed guidance (VISTAS is recommending using CALPUFF for modeling cases both <50 km and >50 km from the nearest Class I area boundary).

According to EPA's proposal, VOC is one of the pollutants that would make a source BART-eligible if emitted at greater than 250 tpy (69 FR 25192). (VOC impacts should be assessed for a BART-eligible source even if it emits less than 250 tpy of VOC.) However, EPA's preferred CALPUFF model approach does not simulate the formation of carbonaceous particles from VOC<sup>7</sup> and therefore is unable to assess the visibility impact of anthropogenic VOC emissions or the visibility benefit of VOC controls. Therefore, if VOC emissions from BART-eligible sources are expected to account for a major fraction of observed carbonaceous particle concentrations at Class I areas, alternative means of estimating VOC impacts are needed. This topic will be discussed further in Sections 3 and 4 of this document.

<sup>&</sup>lt;sup>7</sup> Except that a new module simulates the effects of biogenic emissions, as will be described in Section 3.3.

## **3 Overview of the CALPUFF Model**

This section provides a brief description of the CALPUFF model, discusses the appropriate application of CALPUFF for BART modeling in the VISTAS region, and addresses situations where using CALPUFF would not be appropriate.

### 3.1 Summary Description of the Model

CALPUFF is an air quality model that simulates the time- and space-varying transport, diffusion, deposition, and (for  $SO_2$ ,  $NO_x$ , and, to a very limited extent, VOC) chemical transformation of gaseous and particulate air pollutant emissions from point, line, and area sources. The model simulates transport and diffusion by representing the emitted material as diffusing puffs that are transported with the wind and within which certain chemical reactions take place. It simulates deposition of particles and gases. It simulates the formation of sulfate and nitrate particles from  $SO_2$  and  $NO_x$  emissions, and has very limited capability of simulating the formation of secondary organic aerosol from biogenic VOC emissions.

The model has been adopted by the U.S. EPA in its *Guideline on Air Quality Models* (Appendix W to 40 CFR 51) as the preferred model for assessing long-range (>50 km) transport of pollutants and their impacts on Federal Class I areas and, on a case-by-case basis, for certain near-field applications involving complex meteorological conditions.

The CALPUFF label actually represents a modeling system that consists of three main components plus preprocessing and postprocessing programs, as diagrammed in Figure 3-1..The three major components of the modeling system are CALMET (a diagnostic 3-dimensional meteorological model), CALPUFF (an air quality dispersion model), and CALPOST (a postprocessing package). Specifically, as described in the user's guide for the CALPUFF model:<sup>8</sup>

• CALMET is a diagnostic meteorological model that accepts prognostic and/or observational meteorological data and develops hourly wind and temperature fields on a gridded 3-dimensional modeling domain, using meteorological observation data or output from a prognostic meteorological model as input. Associated two-dimensional fields such as mixing height, surface characteristics, and dispersion properties are also included in the file produced by CALMET. Geophysical pre-processors incorporate data on land use types, terrain elevations, and surface parameters.

<sup>&</sup>lt;sup>8</sup> A User's Guide for the CALPUFF Dispersion Model (Version 5). J.S. Scire, D.G. Strimaitis, and R.J. Yamartino, Earth Tech, Inc. January 2000. Downloaded on 2 December 2004 from http://earthtec.wwh.net/cdownload/calpuff.pdf

- CALPUFF is a non-steady-state Lagrangian transport and dispersion model that advects Gaussian puffs of material emitted from modeled sources, simulating dispersion and transformation processes along the way, using the fields generated by CALMET. The primary output fields from CALPUFF contain either hourly concentrations or hourly deposition fluxes evaluated at selected receptor locations.
- CALPOST is used to process the CALPUFF outputs, producing tabulations that summarize the results of the simulations, identifying the highest and second-highest hourly-average concentrations at each receptor, for example. When performing visibility-related modeling, CALPOST uses concentrations from CALPUFF to compute extinction coefficients and relate measures of visibility, reporting these for selected averaging times and locations.

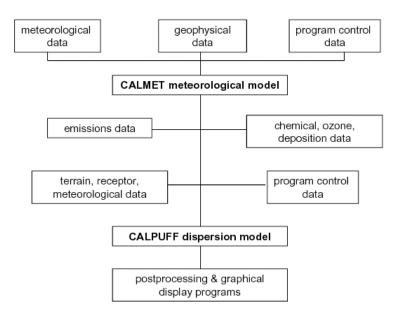


Figure 3-1. The CALPUFF Modeling System<sup>9</sup>

Detailed flow diagrams for each of the three modules can be found in Section 1 of the CALPUFF Users' Guide.

The principal scientific features of the CALMET and CALPUFF modules are summarized in Tables 3-1 and 3-2.<sup>10</sup> Some of these features that are relevant to the BART application are discussed in detail later in this section.

<sup>&</sup>lt;sup>9</sup> Courtesy of Joseph Scire, Earth Tech, Inc.

<sup>&</sup>lt;sup>10</sup> Tables 3-1 and 3-2 are adapted from tables in the CALMET and CALPUFF user's guides and from similar tables in other reports prepared by Earth Tech, Inc. staff.

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

#### Boundary Layer Modules

- 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

- 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

#### Table 3-2. Major Features and Options of the CALPUFF Dispersion Model

#### Source types simulated

- 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 inputs

- 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
- Dispersion coefficient ( $\sigma_y$ ,  $\sigma_z$ ) options
  - Direct measurements of  $\sigma_{v}$  and  $\sigma_{w}$
  - Estimated values of  $\sigma_{v}$  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 options

- Huber-Snyder method
- Schulman-Scire method
- Complex terrain
  - Steering effects in CALMET wind field
  - Optional puff height adjustment

#### Table 3-2. Major Features and Options of the CALPUFF Model (Continued)

#### • Subgrid scale complex terrain (CTSG option)

- Dividing streamline, H<sub>d</sub>,:
  - Above  $H_{\text{d}},$  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<sub>2</sub>, SO<sub>4</sub><sup>=</sup>, NO<sub>x</sub>, HNO<sub>3</sub>, and NO<sub>3</sub><sup>-</sup> (MESOPUFF II method)
- Pseudo-first-order chemical mechanism for SO<sub>2</sub>, SO<sub>4</sub><sup>=</sup>, NO, NO<sub>2</sub>, HNO<sub>3</sub>, and NO<sub>3</sub><sup>-</sup> (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

## 3.2 Applicability of CALPUFF – 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>11</sup> (Hence the EPA's BART proposal's requirement for an approved modeling protocol for distances greater than 200 km.)

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, CALPUFF contains an optional puff splitting algorithm that simulates wind shear effects across a well-mixed individual puff by dividing the puff horizontally or vertically into two or more pieces. Differential rates of dispersion and transport among the new puffs thus generated can increase the horizontal spread of the material in the plume. Since the creation of additional plumes via puff splitting will increase the computer capabilities required by the model, often substantially, puff splitting is not enabled by default, but can be turned on at the option of the user.<sup>12</sup> Vertical puff splitting may be appropriate when transport occurs overnight, while horizontal 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

<sup>&</sup>lt;sup>11</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 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.)

<sup>&</sup>lt;sup>12</sup> High computing demands can be mitigated by reducing the number of sources simulated in each CALPUFF run, which means performing additional runs to account for all sources.

with the computational difficulties encountered when applying a puff model in the field near to a source.

However, 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)...." Indeed 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.

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 proposed BART guidance strongly recommends using CALPUFF for source-receptor distances greater than 50 km but presents CALPUFF as an option that can be considered for shorter transport distances.

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.)

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. Rather, the effect of the plume on visibility should be calculated by integrating the extinction over all the cells along each sight path of interest. 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.<sup>13</sup>

Note that these recommendations of transport distances for CALPUFF applicability, especially at the longer distance end, are based largely on model evaluations against measurements from field studies with inert tracers and SO<sub>2</sub>. There do not appear to be

<sup>&</sup>lt;sup>13</sup> For assessment of control strategies, the guidance in the reproposal advocates averaging over the 20% haziest days, in which case this spatial averaging of light extinction will be even more extensive and the concern with sight path effects will be even less.

any comparable evaluations of CALPUFF performance at simulating the formation of sulfate and nitrate particles over the full range of distances of interest here.

## 3.3 Applicability of CALPUFF – Aerosol Constituents

#### 3.3.1 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  $PM_{10}$ . In actuality, CALPUFF can simulate  $PM_{10}$  or  $PM_{2.5}$  or some other size range, because the assumed size distribution of the particles is a user input. The smaller the particles, the more they behave like an inert gas. In most cases, the dispersion of inert  $PM_{2.5}$  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.  $PM_{2.5}$  particles, which have a mass median diameter around 0.5 µm, have an average net deposition velocity of about 1 cm/min (or about 14 m/day) and thus the deposition of fine particles is not usually significant except for ground-level emissions. On the other hand, coarse particles (those  $PM_{10}$  particles larger than  $PM_{2.5}$ ) have an average deposition velocity of more than 1 m/min (or 1440 m/day), which is significant, even for emissions from elevated stacks.

CALPUFF includes parametric representations of both particle and gas deposition in terms of atmospheric, deposition layer, and vegetation layer "resistances" and, for particles, the gravitational settling speed. Gravitational settling, which is of particular importance for the coarse fraction of  $PM_{10}$ , is accounted for in the calculation of ground-level concentrations by adjusting downward the puff centerline height at each receptor ("tilted plume approach") by the amount of gravitational settling during the period of transport. Effects of inertial impaction, and wet scavenging are also addressed.

However, use of the deposition module is computationally demanding and requires additional inputs of physical and chemical properties of pollutants and of land use. Thus a switch is provided in the model to bypass all the dry deposition calculations, which will provide for faster model execution. Generally, bypassing the dry deposition calculations will result in overestimates of concentrations in the plume and therefore will overestimate ground level concentrations except in the zone where the tilted plume approach might result in high concentrations closer to the source. Thus screening calculations could switch off the deposition calculations.

A primary  $PM_{2.5}$  emission from coal-fired EGUs that is of relevance to visibility calculations is that of primary sulfate. Although primary sulfate emissions account for only a minute 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.

#### 3.3.2 Sulfur Dioxide and Secondary Particulate Sulfate.

The MESOPUFF-II chemistry algorithm used in CALPUFF<sup>14</sup> simulates the gas phase oxidation of sulfur dioxide to sulfate by a linear transformation rate that depends on solar radiation intensity, ambient ozone concentration, and atmospheric stability class during the day and is set at a constant 0.2%/hr at night. (CALPUFF can only represent chemical conversion as a linear process because it requires linear independence between puffs.) 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% RH.

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 %/hr, 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 humidities much below 100%, while CALPUFF's aqueous reaction term produces sulfate at much lower relative humidities. 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 consideration of the effect of temperature on the conversion rates, which causes the model to overstate sulfate formation on cold days (below 10C or 50°F).<sup>15</sup>

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.

<sup>&</sup>lt;sup>14</sup> CALPUFF offers two options for parameterizing chemical transformations: the 5 species (SO<sub>2</sub>,  $SO_4^{=}$ ,  $NO_x$ ,  $HNO_3$ , and  $NO_3$ -) 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 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-recommended MESOPUFF-II chemistry seems appropriate.

<sup>&</sup>lt;sup>15</sup> Evaluation of the Sulfate and Nitrate Formation Mechanism in the CALPUFF Modeling System. R. Morris, C. Tana, and G. Yarwood. Proceedings of the A&WMA Specialty Conference -- Guideline on Air Quality Models: The Path Forward. Mystic, CT. 22-24 October 2003.

In most applications, the ozone concentrations required for the sulfate formation calculations are derived from ambient measurements, although concentrations simulated by regional models are sometimes used. Since the BART analyses determine source impact relative to natural conditions, there is some support for the position that natural background concentrations of ozone should be used instead. There is scientific information for making such estimates, although natural background ozone concentration estimates are unfamiliar to air pollution scientists.

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

The MESOPUFF-II chemistry algorithm used in CALPUFF simulates the oxidation of  $NO_x$  to nitric acid and organic nitrates (both gases) by transformation rates that depend on  $NO_x$  concentration, ambient ozone concentration, and atmospheric stability class during the day. The conversion rate at night is set at a constant 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 plume 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 temperatures are below 10 C, and thus the transformation rate is much slower and the nitrate concentration lower than that simulated by CALPUFF.<sup>10</sup> In both cases, CALPUFF will 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.

There is also third source of error. 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 was to 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.<sup>16</sup>

To address this potential error, 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.<sup>17</sup> 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. Of course, 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 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). In such a setting, the benefit of the refinement provided by POSTUTIL is uncertain because of the nonlinear instantaneous relationship between ammonia concentrations and the formation of nitrate particles.

As with sulfate, the issue arises whether to use current or natural background concentrations of ozone for the nitrate modeling. The same question also applies to ammonia. Present-day natural conditions (which is the definition of "natural conditions") ammonia emissions can be "backed out" of current ammonia emissions inventories by deleting anthropogenic sources. Natural background concentrations of ammonia could then be estimated using a regional air pollution model. The credibility of such concentration estimates is unknown.

#### 3.3.4 Secondary Organic Aerosol

Ongoing research studies at several Class I areas throughout the country<sup>18</sup> and at SEARCH sites in the Southeast<sup>19</sup> are finding that, typically, 90 to 95% of the rural

<sup>&</sup>lt;sup>16</sup> The Effects of Ammonia Limitation on Nitrate Aerosol Formation and Visibility Impacts in Class I Areas. C. Escoffier-Czaja and J. Scire. Paper J5.13, 12<sup>th</sup> AMS/A&WMA Conference on the Applications of Air Pollution Meteorology, Norfolk, VA. 2024 May 2002.

<sup>&</sup>lt;sup>17</sup> POSTUTIL is not described in the current (Version 5) User's Guide, but the inputs are described in the control file (POSTUTIL.INP). A new User's Guide is expected to be available in the first half of 2005.

<sup>&</sup>lt;sup>18</sup> *IMPROVE Special Study: Hi-Vol Sampling for Carbon-14 Analysis of PM 2.5 Aerosols.* S. Fallon and G. Bench, Draft Report, Lawrence Livermore National Laboratory, 24 September 2004. This summer 2004 study found, for example, that 90% of the carbon sampled at Great Smoky Mountains was modern carbon.

<sup>&</sup>lt;sup>19</sup> *Natural Sources of PM*<sub>2.5</sub> *and PM*<sub>coarse</sub> *Observed in the SEARCH Network*. E. Edgerton, B. Hartsell, and J. Jansen. Paper #68, Proceedings (CD-ROM) of the A&WMA Specialty Conference on Regional and Global Perspectives on Haze: Causes, Consequences, and Controversies. Asheville, NC 26-29 October 2004.

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

Current organic fine particle concentrations in the Southeast are typically within a factor of 2 of the 1.4  $\mu$ g/m<sup>3</sup> 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) impact from a particularly large VOC source cannot be dismissed out of hand.

CALPUFF has only rudimentary capabilities for addressing formation of visibilityimpairing 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 condensible components, with the condensible mass being 100-200% of the filterable mass. For purposes of visibility analyses with CALPUFF, a fraction of the condensible part is typically treated as organic particles, i.e., it is assumed that a fraction of the condensible 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 condensible mass. These fine organic particles can be readily modeled by CALPUFF. (The remaining condensible 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.<sup>20</sup> 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.<sup>21</sup> 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>22</sup>

<sup>&</sup>lt;sup>20</sup> *The Southwest Wyoming Regional CALPUFF Air Quality Modeling Study.* Report prepared for the Wyoming DEQ by Earth Tech, Inc. February 2002.

<sup>&</sup>lt;sup>21</sup> Parameterization of the Formation Potential of Secondary Organic Aerosols. D. Grosjean and J. Seinfeld. Atmospheric Environment, Vol. 23, pp 1733-1747. 1989.

<sup>&</sup>lt;sup>22</sup> Recent research suggests that isoprene may be a SOA precursor, however.

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.<sup>15</sup> This performance seems promising, although the developers view the SOA module as needing more testing and evaluation.

Thus, CALPUFF includes approaches for dealing with condensible VOC emissions that are characterized as condensible 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>23</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 sources of VOC 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, if significant BART-eligible sources of VOCs exist, means other than CALPUFF will be needed to estimate their impacts on organic carbon particle concentrations. A technical approach for doing so using a regional photochemical model is presented in Section 4.1.3. For consistency, that regional modeling approach could also be used for estimating organics from the condensible fraction of PM<sub>10</sub>, thereby relieving CALPUFF of any organics simulations.

## 3.4 Applicability of CALPUFF – 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 here to determine a change in light extinction due to changes in component concentrations. Using the notation of CALPOST, the formula is the following:

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

The concentrations, in square brackets, are in  $\mu g/m^3$  and  $b_{ext}$  is in units of Mm<sup>-1</sup>.

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,

<sup>&</sup>lt;sup>23</sup> Note that neither of these VOC-related simulation approaches is addressed in the current (Version 5) CALPUFF User's Guide.

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:

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

where HI is in units of deciviews (dv) and  $b_{ext}$  is in Mm<sup>-1</sup>. 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.

#### 3.4.1 The 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, five methods are documented in the CALPUFF User's Guide (Version 5), and information about a sixth method (Method 6) appears in the CALPOST chapter (Section 5) of that user's guide. There is also a Method 7 (as well as a variant, Method 7'), which is described below but is not yet documented in the CALPUFF User's Guide. Method 6 is the current default.

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) 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.<sup>24</sup> 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.

<sup>&</sup>lt;sup>24</sup> Guidance for Estimating Natural Visibility Conditions Under the Regional Haze Rule, Appendix A. EPA-454/B-03-005. Sept. 2003,

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>25</sup> Again the *RH* is capped at either 98% (default) or a user-selected value.
- 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".
- The relatively new Method 6 is the same as 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, but with extinction based on a monthly-average relative humidity, are compared against the monthly-constant background extinction to evaluate relative impact.
- 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, on January 10, 2003, that "natural conditions" should reflect the visibility impairment caused by significant meteorological events such as fog, precipitation, or naturally occurring haze.<sup>26</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.<sup>27</sup> (A recent

 $<sup>^{25}</sup>$  Note that the hourly-varying natural background extinction here is not consistent with that prescribed by the EPA's natural conditions guidance (footnote 23), for which a "climatologically-representative" f(RH) that only varies monthly is to be used.) Method 6 addresses these monthly average humidity values.

<sup>&</sup>lt;sup>26</sup> Letter from the Assistant Secretary of the Interior to the Director of the Montana Department of Environmental Quality. The Secretary's guidance applies only to Federal Land Managers. EPA's position on this interpretation of natural conditions is unknown.

<sup>&</sup>lt;sup>27</sup> An explanation of Method 7 appears in Appendix E of the report, *Application of CALMET and CALPUFF to Assess the Impacts of the Proposed Prairie State Generating Station at the Mingo* 

modification, in which the daily average natural extinction is calculated somewhat differently, is called Method 7', i.e., "7 prime".)

Note that EPA's decision to use monthly "climatologically representative" relative humidity in Method 6 when calculating light extinction impacts of the source and the background natural conditions creates an artificial situation where the daily estimates of source impact may be quite different from those that would occur if real-world relative humidities had been used. Because hygroscopic sulfates and nitrates are only a minor component of the total default natural conditions aerosol in the East, the background extinction will be only weakly sensitive to the choice of RH. On the other hand, sulfate-or nitrate-rich plumes will be quite sensitive to the RH. Since the effect of the long term averaging of f(RH) is to suppress the extreme (peak or minimum) f((RH) values that occur on some days, the overall effect of Method 6 over Method 2 will be to decrease peak 24-hr impacts relative to natural conditions on humid days, and conversely, to increase peak 24-hr impacts on dry days. Whether that will increase or decrease the likelihood of an impact of 0.5 dv or greater will depend on local conditions at the time. The consequences for evaluations of alternative control strategies are likely to be minor.

#### 3.4.2 Improved 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 estimates of natural background visibility. If changes to these methods are recommended by VISTAS for the purposes of calculating current, future, and natural background visibility at VISTAS Class I areas, then these changes would need to be incorporated into CALPOST as well. These issues are discussed in further detail in Appendix A.

*Wilderness Area,* which was prepared by Earth Tech, Inc. and submitted to the Illinois Environmental Protection Agency in July 2003.

## **4 Recommended Modeling Approaches**

This VISTAS draft protocol is intended to provide practical guidance and consistency for BART modeling analyses across the VISTAS states.

This section describes VISTAS recommendations for air quality modeling for three situations – (1) to assess whether a source is subject to BART; (2) to evaluate the visibility benefits of alternative control options; and (3) to demonstrate the effectiveness of an optional cap and trade program. The modeling methodology suitable for the first two situations is virtually identical, with a plume model the preferred approach – although, as we show below, a regional air quality model could also play a role. Because the DC Circuit Court overruled the methods used by the WRAP states to demonstrate that a regional SO2 trading program is better than BART, an acceptable modeling methodology for the third situation, assessing the effectiveness of a cap and trade program, is currently unclear.

In line with this grouping of methodologies, Section 4.1 below presents a recommended approach for the assessment of whether a source should be subject to BART. Unresolved technical considerations and alternative modeling approaches that are not addressed in EPA's proposed guidance are discussed. Section 4.2 then describes the approach for evaluating visibility benefits from potential BART controls (little different than that described in Section 4.1). Section 4.3 discusses options for assessing the effectiveness of a cap and trade program.

## 4.1 Assess Whether a Source is Subject to BART

#### 4.1.1 Background

EPA's proposed BART guidance recommends that CALPUFF or an alternative EPAapproved model be used for assessing whether a BART-eligible source is subject to BART. EPA also recommends that the CALPUFF model, whether used in a screening mode or as a complete modeling system, be operated in accordance with guidance in the Phase 2 IWAQM report. Although VISTAS accepts this concept in general, it is important to recognize that the IWAQM guidance was established for purposes of evaluating the potential incremental impact of a single proposed new source, not for evaluating benefits of emissions control measures for many existing sources. Thus, as described below, VISTAS is recommending adjustments to the IWAQM-recommended procedures where schedule and budget make impractical the application of new source review guidance to BART control determinations.

#### 4.1.2 Recommendations

1. VISTAS will hire a contractor to assist in BART modeling. The Contractor will be asked to perform the following tasks:

- a. Assist VISTAS in finalizing this BART modeling protocol, including the specific methods, assumptions, and configuration for the CALPUFF modeling system (CALMET, CALPUFF, CALPOST) inputs, and outputs.
- b. Provide regional CALMET meteorological outputs ready for CALPUFF modeling for the VISTAS 12-km CMAQ modeling domain. Use annual MM5 meteorological model outputs (12-km or 36-km grid) as provided by VISTAS for 2001, 2002, and 2003<sup>28</sup>. Use surface and upper air observations to assist interpolation to CALMET 12-km grid.
- c. Provide subregional, 4-km CALMET meteorological outputs ready for CALPUFF as requested by VISTAS for those receptor areas where finer grid resolution than 12-km is recommended to address complex terrain. The RFP includes cost requests for subdomains.
- d. As VISTAS States determine is appropriate, and as VISTAS resources allow, run CALPUFF for specific BART-eligible sources to determine if the visibility impact exceeds a threshold of 0.5 dv compared to natural background at any receptor in a Class I area for any 24-hr period. Use CALMET meteorological fields developed in previous tasks and CALPOST to calculate visibility impact.
- e. As VISTAS States determine is appropriate, and as VISTAS resources allow, run CALPUFF to evaluate the visibility benefits from potential BART control measures for specific BART sources.
- f. Report CALPUFF and CALPOST results and interpretation for sources modeled in steps (iv) and (v) above.

## 2. VISTAS is considering using emissions divided by distance (Q/d) as an initial screening method to evaluate sources subject to BART.

VISTAS States asked for comment from VISTAS participants on using emissions divided by distance (Q/d) as a screening approach to determine if a BART-eligible source is subject to BART. Analyses by the Midwest Regional Planning Organization (MRPO)<sup>29</sup> and MANE-VU RPO<sup>30</sup> indicate that for SO2 emissions, Q/d compares favorably with magnitude of impact (in deciviews) projected by the

<sup>&</sup>lt;sup>28</sup> 2001 annual MM5 run at 36 km for EPA, 2002 annual MM5 run at 12 and 36 km for VISTAS, and 2003 annual MM5 run at 36 km by MRPO.

<sup>&</sup>lt;sup>29</sup>"Determination of Sources Subject to BART: Example Screening Analysis for Boundary Waters Canoe Area, Minnesota" by Midwest RPO, dated June 22, 2004 and "Determining Which BART-Eligible Sources are Subject to BART: Summary" by MRPO, dated December 21, 2004

<sup>&</sup>lt;sup>30</sup>"BART Exemption Test Screening Analysis" by Gary Kleiman and John Graham, NESCAUM, dated June 25, 2004 and "Comments on Regulatory Text for Proposed 68 FR 25184 Docket # OAR 2002-0076" by MANE-VU, dated July 15, 2004

CALPUFF model. VISTAS asked for comment on a Q/d with "Q" defined as the combined SO2 and NOx emissions (in allowable annual tons) from all BART-eligible emission units at a single source and "d" as the distance of that source in kilometers (km) from the nearest Class I area boundary. VISTAS States initially recommended using Q/d as a one-sided test where States would presume that a source with Q/d greater than a threshold value would be subject to BART. However, any source with Q/d greater than the threshold value could choose to run CALPUFF to determine if visibility impacts were less than 0.5 dv for a single day (or whatever threshold value is set in EPA final guidance), and thereby not subject to BART. For sources with Q/d less than the threshold value, States simply stated that further analysis would be required and that the source should be in consultation with the State.

Federal Land Managers (FLM) recommended that VISTAS use Q/d with a conservative threshold value to identify sources which clearly would not be subject to BART and to reduce the number of emissions sources requiring detailed CALPUFF analyses of BART control measures. Southern Company commented that, if used, Q/d should be established for each pollutant separately and that Q/d should be a two-sided test that would allow a source to be exempted from further BART analysis if below the threshold. Based on these comments, States will continue dialog with stakeholders on possible application of a Q/d screening analysis. After EPA final BART guidance is issued in April 2005, VISTAS may propose a Q/d screening analysis to EPA for review and comment.

# 3. VISTAS recommends using the full CALPUFF modeling system to assess the visibility impacts of emissions of SO<sub>2</sub> and NO<sub>x</sub>, and components of PM from all other BART-eligible sources.

**a.** Screening Mode: VISTAS intends to provide to the VISTAS modeling community the MM5 meteorological fields and geophysical data bases necessary as input to CALMET and the CALMET meteorological field outputs necessary to run CALPUFF. Therefore in the initial draft protocol, VISTAS recommended that because CALPUFF simulations can be run economically on the common CALMET meteorological field, use of CALPUFF in a screening mode offers little benefit in reducing workload and is not recommended.

VISTAS received comment from both FLM and industry that using CALPUFF in screening mode should be retained as an option for those cases where the screening result is unambiguous and there is no need to devote extra resources to a foregone conclusion. VISTAS States will continue dialog with stakeholders concerning use of CALPUFF in screening mode either as an alternative or compliment to a Q/d screening method. Following final EPA BART guidance, VISTAS may propose for EPA review and comment specific cases where CALPUFF might be run in screening mode.

**b. Distance:** CALPUFF should be used for all BART-eligible sources at all transport distances, from a few kilometers to 300 kilometers, from a Class I area. For

sources within 50 km of a Class I area boundary, States have the option to reduce the threshold value for a visibility impact below 0.5 dv.

For sources greater than 200 km from a Class I area boundary, use of the puffsplitting option in CALPUFF may improve representation of horizontal and vertical transport of the plume. (Puff splitting may also be appropriate for even shorter transport distances in complex terrain.) Since puff splitting is demanding of computing resources, it may be appropriate to carry out an initial screening without puff splitting, and then, if the resulting impact marginally exceeds the threshold of 0.5 dv, consider whether to test the impact if puff splitting were applied.

The specific Class I areas to be considered is a source-specific decision. Sources and States should define receptors as part of the source-specific modeling protocol (see section 4.1.3). The receptor grid to be used will be based on those defined by the FLM<sup>31</sup> unless otherwise approved in the source-specific protocol (generally 1 km). Note that a finer receptor grid scale than 1 km may be needed for sources less than 50 km from a Class I area to assure that the receptor grid adequately represents concentrations in the plume.

**c. Meteorological inputs:** MM5 meteorological model outputs for three years (2001, 2002, and 2003) as provided by VISTAS will be used to develop 12-km grid CALMET meteorological fields for the VISTAS 12 x 12 km modeling domain (Figure 4-1). Local surface and upper air measurements will be used to augment modeled data as appropriate. Finer grid subdomains will be defined by States as appropriate to terrain considerations or if a source is less than 50 km from a Class I area.

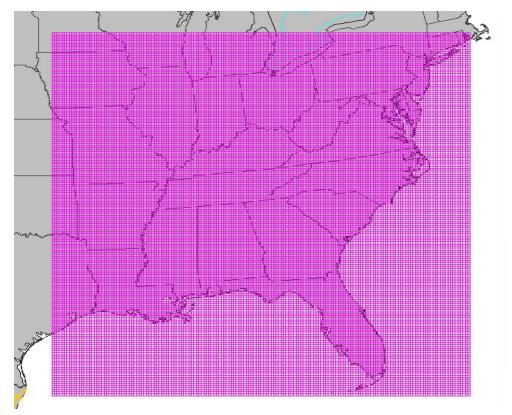
**d. Model Inputs:** Apply CALPUFF for the three model years 2001, 2002, and 2003 using CALMET fields developed for VISTAS.

Use permitted allowable emissions for  $SO_2$ ,  $NO_x$ , and  $PM_{10}$  from the BART-eligible source. Exclude from consideration emissions of less than *de minimis* levels (EPA proposed less than 40 tons per year for  $SO_2$  and  $NO_x$  and less than 15 tons per year for  $PM_{10}$ ). If permitted allowable or potential to emit levels are not available for a BART eligible unit, the State could use 2002 actual emissions (and consider using a lower threshold than 0.5 dv to address added uncertainty). VISTAS received comment that primary sulfate and condensable components of PM should be calculated using available inventory speciation profiles (e.g. AP-42) and modeled using CALPUFF. VISTAS also received comments on the use of de minimis levels and the use of alternative models. These comments will be addressed after EPA issues the final BART guidance in April 2005.

For background concentrations of ozone, use regional monitoring data. For background concentrations of ammonia, use output from VISTAS' revised 2002 run

<sup>&</sup>lt;sup>31</sup> http://www2.nature.nps.gov/air/Maps/Receptors/index.htm

**Figure 4-1.** VISTAS 12 x 12 km air quality modeling grid to be used as basis for 12 km CALMET meteorological model grid.



of the Community Model for Air Quality (CMAQ) model. VISTAS' BART modeling contractor will be asked to recommend the temporal and spatial scales to use for ozone and ammonia inputs to CALPUFF and the feasibility of incorporating measured ammonia data (available from SEARCH and limited time periods at Great Smoky Mountains and Mammoth Cave).

Further details of the CALPUFF model configuration for these simulations will be developed in Section 5 with contributions from the VISTAS BART Modeling Contractor.

e. Use CALPOST to calculate impacts on light extinction at every grid cell in Class I areas of concern. Determine if the 24-hr average impact of the source's emission at any Class I area receptor on any day is an increase in haziness in excess of 0.5 deciviews (dv) relative to natural conditions. Cap RH at 95%, consistent with EPA guidance for tracking progress on regional haze. Use EPA default assumptions for calculating light extinction unless EPA guidance or the IMPROVE equation is revised in 2005 or unless VISTAS States direct otherwise. Define natural conditions using EPA default concentrations, unless the State has determined to revise the

default assumptions for natural background at a Class I area. In this case, relevant revisions should also be incorporated in CALPOST.

f. Use the POSTUTIL postprocessing program to repartition the ammonia and nitric acid concentrations estimated by CALPUFF to reflect the preferential scavenging of ammonia by sulfate and the potential ammonia-limiting effects on nitrate formation. POSTUTIL is intended to improve the estimate of nitrate particle concentrations, however POSTUTIL does not address diurnal variations in NH3 and ammonium nitrate that are seen in monitoring data. Interpretation of results with and without POSTUTIL would provide information on the importance of nitrate for visibility impacts at a Class I.

#### 4. Evaluate whether results are credible and sensible.

Compare CALPUFF results with those of other analyses and use other analysis techniques in a weight-of-evidence approach, as appropriate.

# 5. For sources with substantial VOC emissions [provide threshold?], use a regional grid model to estimate the concentrations of secondary organic aerosol from those emissions.

CALPUFF is currently not configured to address visibility impacts from VOC because secondary organic aerosol formation from VOC is not addressed (although condensable organic carbon can be calculated from PM10.) For those BART sources with significant VOC emissions, VISTAS intends to use a weight of evidence approach using either the CMAQ or CAMx as applied for VISTAS' 12 x 12 km grid to calculate visibility impacts from VOC emissions from all BART sources collectively. Emissions sensitivities run for VISTAS by Georgia Institute of Technology using 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). These results suggest that CMAQ or CAMx could be run with and without VOC emissions from all BART sources in each VISTAS state and the difference in calculated light extinction be interpreted as the impact of VOC emissions from all BART sources in each state. If these impacts are collectively less than 0.5 dy, then these results could be used as evidence that impacts from individual sources in the state would also be less than 0.5 dv. If the combined impacts are greater than 0.5 dv, then additional sensitivities may need to be considered. A source attribution module such as Tagged Species Source Apportionment (TSSA) in CMAQ or Particulate Source Attribution Tool (PSAT) in CAMx, might be considered if application of one of these tools is practical at the time the analysis is done.

Issues yet to be resolved:

a. Should the modified SOA module in CMAQ developed for VISTAS by ENVIRON be used?

- b. What adjustments should be made for excessive initial dispersion of emissions in the 12 x 12 km grid cell where the source is located? Excess diffusion in the first cell is likely to underestimate organic carbon particle levels at the receptors and thus impacts from the source. A plume in-grid treatment could address this artificial diffusion, but is not likely to be feasible in VISTAS' schedule.
- c. How should visibility impacts from VOC emissions calculated at receptors by CMAQ or CAMx be combined with the visibility impacts from other emissions as calculated in CALPUFF and CALPOST? CMAQ and CAMx at 12 km grid is inconsistent with CALPUFF and CALPOST receptor grids of ~1 km.
- d. CMAQ or CAMx is only available for 2002 and would not be available for additional years. EPA would need to approve VISTAS proposed protocol for treating VOC emissions.

#### 4.1.3 Source Specific Modeling Protocol

As noted in Section 2.2.1, the EPA anticipates that a modeling protocol will be prepared, irrespective of whether a State or source owner carries out the modeling. VISTAS states will use this common modeling protocol as the basis for analyses for all sources. VISTAS states will ask each single source to provide a site-specific modeling protocol that includes the source-specific description and parameters required for modeling. If the source is requesting the state to approve exceptions to the common VISTAS modeling protocol, these changes are to be documented in the source-specific protocol and be approved by the State before implementation.

A typical Table of Contents for a single-source modeling protocol is shown in Table 4-1. Each section of the protocol describes the data or tool that will be used or how a task will be undertaken.

Table 4-1 would need to be modified if the source-specific protocol was to cover simultaneous modeling of multiple BART-eligible units at a single source, in which case information should be provided in its Section 2 for each separate unit. Since the material in Section 4 in Table 4-1 overlaps the material in this generic BART modeling protocol document, we have indicated that this document be attached as an appendix and suggest that it be cited as appropriate instead of writing out Section 4 in full.

Note that, after the modeling is completed, the section headings in Table 4-1 can also serve as the basis for a report on the modeling effort and its results.

**Table 4-1.** Sample Table of Contents of a Modeling Protocol for Evaluating Whether aSingle Source is Subject to BART.

#### 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

#### 4.1.4 Alternative Modeling Approaches to Assess Visibility Impacts of BART sources

Other impact assessment options potentially useful for assessing whether a source is subject to BART have not been addressed by EPA's proposed guidance. Examples include alternative modeling approaches such as:

- The SCICHEM (Second-order Closure Integrated Chemistry) plume model<sup>32</sup> developed by EPRI has representations of sulfate and nitrate chemistry that are superior to those of CALPUFF, and it also includes a capability for simulating the formation of secondary organic aerosol (SOA). SCICHEM largely overcomes the criticisms concerning CALPUFF's handling of sulfur and nitrate particle formation. SCICHEM has advanced from its origins as a plume-in-grid model to become a fully independent puff model with advanced diffusion and chemistry capabilities. Since SCICHEM is more sophisticated than CALPUFF, the computing resources needed to apply it are greater and the time required for each modeling run is longer. SCICHEM has not yet been submitted for EPA approval and therefore has not been designated as an approved model, although the earlier version without chemistry, SCIPUFF, is approved as an alternative model.<sup>33</sup>
- A regional photochemical model with source apportionment capability for secondary particulate matter, such as CMAQ with TSSA (Tagged Species Source Apportionment) or CAMx with PSAT (PM Source Apportionment Technology), operated at a sufficiently fine grid resolution that artificial diffusion effects do not cause large errors when simulating the chemical reactions in a single-source plume. TSSA and PSAT are both still under development and evaluation, though, and do not yet have full capabilities, such as for source apportionment of SOA.
- A regional photochemical model with plume-in-grid simulation of individual source plumes, which permits use of a coarser grid than that required for the TSSA or PSAT source apportionment approaches. EPRI is submitting to EPA a demonstration of a plume-in-grid module for CMAQ in winter 2005.

These three approaches are not in routine use today, however, and thus applying them would involve some degree of learning and experimentation, as well as obtaining regulatory agency approval for their use. Because of the limited time available, these methods will not be discussed further here as options for routine use by the VISTAS States. However, a source operator always has the option of performing more refined modeling with the concurrence of the relevant regulatory agency.

<sup>&</sup>lt;sup>32</sup> SCICHEM: A New Generation Plume-in-Grid Model. Report TR-113097. EPRI, Palo Alto, CA. June 1999.

<sup>&</sup>lt;sup>33</sup> http://www.epa.gov/scram001/tt22.htm#altmod

EPA's draft guidance suggested that PLUVUEII could be used in cases where a source is less than 50 km from a Class I area. PLUVUEII addresses plume optics and does not address regional haze. VISTAS has not attempted in this protocol to address methods to apply PLUVUEII for BART sources or to interpret results in the context of regional haze. Sources that want to petition States to use PLUVUEII should provide proposed modeling protocol for State review and decision whether to allow PLUVUEII.

# 4.2 Evaluate Potential Visibility Improvements from the Application of BART

As part of the BART assessment, CALPUFF is to be applied again to assess the improvements in visibility that can be expected from the application of BART. In general this impact assessment would use the same approach as that described in Section 4.1.

The principal difference is in the interpretation of the results. Whereas the analysis of whether a source was subject to BART evaluated its daily impact against the monthly natural conditions calculated from EPA's default concentration estimates, the assessment of visibility improvements is to assess the average impact on the 20% haziest days before and after application of BART (69 FR 25227).

The question also arises whether the findings of the initial modeling analyses (if they were performed and the source was not declared subject to BART on the basis of a Q/d screening analysis alone) could not be used to reduce the number of modeling runs that will be required to the analyses of improvements. Such economy is desirable because the BART assessment could require modeling of several alternative approaches to BART. For example, could the modeling be limited to those Class I areas where the original impact exceeded 0.5 dv (compared to natural background) on any single day at any single receptor? Or, since 20% haziest days differ from average days, when the nearest Class I areas within 200 km be considered or only the closest Class I areas?

## 4.3 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. The proposed BART guidance does not specify the method to be used for this modeling. Assumptions would need to be made how emissions under a cap and trade scenario would differ from source-by-source BART control implementation. From a technical perspective, either CALPUFF applied to every source or a regional air quality model could be used to determine the difference in visibility at each impacted Class I area due to the two alternative assumptions. If the expected distribution of emissions is different under the two approaches, then "dispersion modeling" of all sources must be used to 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" (69 FR 25231).

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 a federal program (e.g. Clean Air Interstate Rule, CAIR, or Clear Skies Initiative, CSI, legislation) targeting 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. This demonstration is planned for late spring/summer 2005 and will indicate benefits from assumed BART controls. Because BART controls will not be finalized by the States at this point, the analyses will be indicative of potentials 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 SO2 trading program is better than BART, an acceptable modeling methodology assessing the effectiveness of a cap and trade program, remains unclear. VISTAS intends to review results of the planned regional haze control strategies discussed above and to evaluate progress by EPA and WRAP to define appropriate methods for assessing a trading program prior to deciding if and how to demonstrate the benefits of a regional cap and trade program.

## 5 CALPUFF Modeling Considerations and Recommended Configuration

[Details to be developed in cooperation with contractor hired by VISTAS and consistent with final BART guidance. A few samples of topics to be covered are indicated in the outline below. In some cases different methods and discussions will be required for the initial impact analysis and for the control benefits evaluation.]

### 5.1 CALMET

- Years to be modeled: 2001, 2002, 2003
- Based on MM5 meteorological model outputs provided by VISTAS and augmented as recommended in the final protocol with observational data
- Grid scale: based on 12 km grid over VISTAS domain, with potential for finer grids in subdomains to be defined in VISTAS BART modeling protocol. Source may request approval of finer grid..
- Need for terrain blocking?

## 5.2 CALPUFF

- Emission input specifications, point or area source
- Modeling domain for each source of interest; list of Class I areas for which visibility impacts are considered
- Receptors at Class I area(s), based initially on recommendations from Federal Land Managers, modified as recommended by Modeling Protocol.
- Ambient concentrations of ozone and ammonia derived from observations for ozone and CMAQ 2002 annual modeling for ammonia
- Assignment of part of PM<sub>10</sub> condensibles to sulfate, nitrate, OC particles
- Deviations from default settings -- e.g., simplify deposition, include puff splitting
- Special considerations at very short source-receptor distances -- downwash, gravitational deposition. When, if ever, is plume visibility model needed?

## 5.3 CALPOST

- Visibility impact calculation method to be used
- Specifications for f(RH)
- Specifications for natural background concentrations of components of PM
- Application of POSTUTIL
- Values of ground-level 24-hr-average light extinction compared to natural conditions

## 5.4 Presentation of Results

- Forms of tables, graphs, and maps
- Identification of causes of uncertainty and estimates of that uncertainty (including error caused by ignoring VOCs)

## 6 Quality Assurance Plan

## 6.1 QA Responsibilities

- Source owner/operator
- State agency
- Modeling contractor
- VISTAS -- Project Officer, Technical Coordinator, and Workgroups

## 6.2 Data Bases to be Used

- Quality control procedures
- Limitations

## 6.3 CALMET

- Implications of principal assumptions e.g. terrain blocking
- Verification of model settings
- Quality control and evaluation of credibility of output meteorological fields
- Evaluation of model performance vs. ambient meteorological measurements
- Estimated uncertainties

## 6.4 CALPUFF

- Implications of principal assumptions e.g., puff splitting, background concentrations of ozone and ammonia
- Verification of model settings
- Quality control and evaluation of credibility of output species concentration fields
- Estimated uncertainties

## 6.5 CALPOST

- Implications of principal assumptions e.g., visibility impact calculation method (MVISBK), ammonia limiting (POSTUTIL)
- Verification of model settings
- Quality control and evaluation of credibility of visibility impact estimates
- Estimated uncertainties

## 6.6 Quality Assessment

- Overview and synthesis of assumptions, limitations, errors, uncertainties, and confidence in the CALPUFF modeling system and its results
- Implications for interpreting and applying the results of the CALPUFF modeling of (1) source impacts and (2) control benefits.

## APPENDIX A Estimating Light Extinction and Natural Conditions

#### A.1 IMPROVE AND EPRI Light Extinction Formulas

The IMPROVE/EPA extinction formula,

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

is the formula prescribed by the EPA for estimating light extinction (in units of Mm<sup>-1</sup>) from measured concentrations of components of particulate matter and relative humidity. Equation A-1 is the same as Equation 3-1 in the body of this document. Note that the CALPOST notation of OC is used for organic carbonaceous matter, which is labeled OMC in the same formula when it is presented by IMPROVE or the EPA. Definitions of the other terms in the formula can be found in connection with Equation 3-1.

Equation A-1 is known to often underestimate extinction at high concentrations and overestimate it at low concentrations. EPRI has reviewed recent IMPROVE data in an effort to upgrade the accuracy of the formula for estimating light extinction and has proposed revisions to the IMPROVE/EPA coefficients.<sup>34</sup> They conclude that some extinction efficiencies vary with the corresponding component concentrations. As a result of additional work, EPRI has presented further refinements in a recent paper.<sup>35</sup> They have demonstrated that the formula using the new coefficients has much smaller biases in estimating measured extinction (actually light scattering determined by integrating nephelometers) from measured component concentrations at IMPROVE sites than the biases achieved using the standard (IMPROVE) coefficients in Equation A-1.

Table A-1 lists the coefficients (extinction efficiencies) that EPRI has developed for each term in Equation A-1 and compares them with the IMPROVE/EPA coefficients that are currently shown in Equation A-1. (*Caution:* This table uses the notation of Equation A-1, which is that of CALPOST but is not totally consistent with that of IMPROVE and of EPRI.)

<sup>&</sup>lt;sup>34</sup> *Review of the U.S. Environmental Protection Agency Default Implementation Guideline for the Regional Haze Rule.* Technical Report 1011119, EPRI, Palo Alto, CA. September 2004.

<sup>&</sup>lt;sup>35</sup> *Light Extinction Reconstruction in IMPROVE*. P. Ryan, D. Lowenthal, and N. Kumar. Presented at A&WMA Specialty Conference on Regional and Global Perspectives in Haze: Causes, Consequences, and Controversies, Asheville, NC. 26-29 October 2004.

Components	IMPROVE Coefficients	EPRI Coefficients
(NH <sub>4</sub> ) <sub>2</sub> SO <sub>4</sub>	3	1.2 if [ions] < 0.5 $\mu$ g/m <sup>3</sup> 1.5[ions] <sup>0.3</sup> if [ions] $\ge$ 0.5 $\mu$ g/m <sup>3</sup> and $\le$ 20 $\mu$ g/m <sup>3</sup> 3.7 if [ions] $\ge$ 20 $\mu$ g/m <sup>3</sup>
NH <sub>4</sub> NO <sub>3</sub>	3	Identical to the sulfate coefficient
OMC	4	<i>2.2 [1.43 OMC]</i> <sup>0.3</sup> Also, multiply OMC in Equation A-1 by 1.43
Soil	1	1
Coarse Mass	0.6	0.6
EC	10	10

Table A-1. Comparison of IMPROVE and EPRI Coefficients for Equation A-1

In Table A-1, *[ions]* represents the sum of ammonium sulfate and ammonium nitrate mass concentrations, i.e., *[ions]* = *[ammonium sulfate]* + *[ammonium nitrate]*. *[OC]* represents the concentration of carbonaceous organic matter, which is assumed by CALPOST to be 1.4 x the measured concentration of organic carbon alone. All concentrations are in  $\mu$ g/m<sup>3</sup> and all coefficients are in units of m<sup>2</sup>/g. Note that when the formula is used to calculate the extinction impact of a source, then the value of *[ions]* should be that of the background plus the source, while the *[ammonium sulfate]* and *[ammonium nitrate]* values Equation A-1 are those due to the source alone.

To summarize the changes introduced by the EPRI formula, it introduces (1) a coefficient for the ammonium sulfate and ammonium nitrate terms that depends on the total combined concentrations of both; and (2) increases the OC term by a factor of 1.43 and introduces a coefficient for the OC term that depends on the OC concentration.<sup>36</sup>

Note that if the sum of the ammonium sulfate and ammonium nitrate concentrations lies in the range  $0.5 \ \mu g/m^3 \le [ions] \le 20 \ \mu g/m^3$ , then the first line of the extinction formula given at the beginning of this memo simplifies to  $1.5 \ f(RH) \{ [ammonium sulfate] + [ammonium nitrate] \}^{1.3}$  when the EPRI coefficients are used. Note also that when the formula is used to calculate the extinction impact of a source, then the value of [ions] should be that of the background plus the source, while the [ammonium sulfate] and [ammonium nitrate] values in the equation should be those due to the source alone.

<sup>&</sup>lt;sup>36</sup> Using the IMPROVE notation, [OC] represents the organic carbon concentration measured in the laboratory. IMPROVE multiplies the laboratory value by a factor of 1.4 to account for the oxygen, hydrogen, halocarbons, and other matter that are attached to the carbon to make up hydrocarbons. Recent work suggests strongly that the factor of 1.4 is too low. EPRI concluded that the factor should be 2.0, which means that the current factor of 1.4 should be multiplied by 1.43. So, in the notation of CALPOST, where [OC] is defined to include the whole of the hydrocarbons, the new [OC] is 1.43 times the old [OC].

According to EPRI, its OMC extinction efficiency formula should also have limits on its range of applicability. Since actual OMC concentrations don't usually approach zero, a lower limit may not be needed in practice. The upper limit is yet to be determined, but will probably not be of consequence for Class I areas.

In response to the issues raised by the EPRI analyses, IMPROVE has commissioned a panel to review its light extinction formula in light of current knowledge. A report is expected in the summer of 2005. Presumably any changes that are made by IMPROVE will also be reflected in the EPA's approach and in CALPOST calculations of source impacts.

## A.2 Natural Conditions

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 climatologicallyrepresentative 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.

Refinements to the default natural conditions values are also possible, and are allowed by the EPA. 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 (e.g., the 2.0 recommended by EPRI); (2) Increasing the estimates of natural conditions extinction on the 20% haziest days to better reflect the statistical distribution of extinction; and (3) Including sea salt in the IMPROVE/EPA formula.

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% haziest days, which are of relevance only for the assessment of the benefits of the application of BART. It slightly increases the default haziness on those days and therefore reduces the absolute deciview impact of a source's emissions, but it has no effect on the change in haziness (in dv) imputed to application of BART at a source and therefore is not of great practical importance for the BART assessment process.

The sea salt adjustment applies to the description of natural conditions, and has effect mainly near the seacoast. A default concentration of sea salt would have to be developed to accompany the values recommended by the EPA for the other constituents in Equation A-1.

One additional adjustment to natural conditions that is appropriate for BART assessments is to use a correct value of the Rayleigh scattering coefficient for clear air, instead of the default 10 Mm<sup>-1</sup> that is in Equation 3-1 and the IMPROVE equation. The default value is appropriate for an elevation of 1600 m (about 5000 ft). Since the correct value at sea level is about 12 Mm<sup>-1</sup>, so the default value could never be attained at low altitude sites and the relative impact of a source on haze would be overstated by using the default Rayleigh value.<sup>37</sup>

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 A-1, whether those of EPRI or those that result from the current review by IMPROVE, should be reflected in natural conditions extinction estimates.<sup>38</sup>

<sup>&</sup>lt;sup>37</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.

<sup>&</sup>lt;sup>38</sup> A comprehensive discussion of alternative approaches to estimating natural conditions in the VISTAS region appears in the paper, *Evaluating Natural Background Visibility and Reasonable Progress Goals in the VISTAS Region*. I. Tombach and P. Brewer. Submitted to the Journal of the Air & Waste Management Association, January 2005.