

**Appendix 9-4: CAMx Modeling Protocol, Screening Analysis of Potentially
BART-Eligible Sources in Texas**

Revised Draft Final Modeling Protocol

**Screening Analysis of
Potentially BART-Eligible
Sources in Texas**

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1.0 INTRODUCTION

OVERVIEW

The final version of United States Environmental Protection Agency's (EPA) Regional Haze Regulations was published in the *Federal Register* (FR) on July 6, 2005 (70 FR 39104). One of the provisions of the program is the requirement that certain existing stationary sources emitting visibility-impairing air pollutants install and operate the Best Available Retrofit Technology (BART). The regulations require case-by-case BART determination to define specific emissions limitations representing BART and schedules for compliance for each source subject to BART. These requirements would be part of the SIP revisions that each state must submit to EPA by December 17, 2007. EPA's BART Rule requirements are summarized below, particularly with respect to the modeling analyses that are required to determine (a) if a source is BART-eligible, and (b) what levels of emissions controls might be necessary for sources shown to cause or contribute to visibility impairment at federally-protected Class I areas. This summary is based on EPA's BART guidelines (EPA, 2005) and BART modeling protocols prepared by Visibility Improvement State and Tribal Association of the Southeast (VISTAS) (2005) and Central Regional Air Planning Association (CENRAP) (Alpine and ENVIRON, 2005).

Regional Haze Rule and BART Guidelines

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

The BART guidelines were written primarily for the benefit of state, local and Tribal agencies, and describe a process for making the BART determinations and establishing the emission limitations that must be included in their SIPs or Tribal implementation plans (TIPs). The guidelines provide a process for making BART determinations that states can use in implementing the regional haze BART requirements on a source-by-source basis. States must

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

A BART eligible source or existing stationary facility means any stationary source of air pollutants, including any reconstructed source, which: (a) "was not in operation prior to August 7, 1962, and was in existence on August 7, 1977," (b) "has the potential to emit 250 tons per year or more of any air pollutant" and (c) falls within one or more of 26 specifically listed source categories (40 CFR Section 51.301). BART controls are required for any BART-eligible source that can be reasonably expected to cause or contribute to impairment of visibility in any of the 156 federal parks and wilderness (Class I) areas protected under the regional haze rule. Air quality modeling is an important tool available to the states in determining whether a source can be reasonably expected to contribute to visibility impairment in a Class I area.

In EPA's August 1, 2005 proposed rulemaking (70 FR 44154), entitled "Revisions to Provisions Governing Alternative to Source-Specific Best Available Retrofit Technology Determinations," the agency provided states with a process to show that an emissions trading program may be used as an alternative to applying BART.

Role of Air Quality Models

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

Option 1: Individual Source Attribution. States can use dispersion modeling to determine that an individual source cannot reasonably be anticipated to cause or contribute to visibility impairment in a Class I area and thus is not subject to BART. Under this option, states can analyze an individual source's impact on visibility as a result of its emissions of SO₂, NO_x and direct PM emissions. Because some dispersion models cannot currently be used to estimate the predicted impacts on visibility from an individual source's emissions of volatile organic compounds (VOC) or ammonia, states may elect to use a more qualitative assessment to determine on a case-by-case basis, which sources of VOC or ammonia emissions may be likely to impair visibility and should therefore be subject to BART review. EPA approved models should be used to predict the visibility impacts from a single source at a Class I area.

Option 2: Use of 'Model' Plants. Under this option, analysis of model (or prototypical) plants could be used to exempt certain BART-eligible sources that share specific characteristics. This type of analysis is used to identify the types of small sources that do not cause or contribute to visibility impairment for purposes of BART, and thus should not be subject to a BART review. Different Class I areas may have different characteristics, however, so care should be used to ensure that the criteria developed are appropriate for the applicable cases. The guidance (EPA, 2005) suggests that states could use modeling analyses of representative plants to reflect groupings of

specific sources with important common characteristics and based on these analyses, states may determine that certain types of sources may clearly be anticipated to cause or contribute to visibility impairment whereas others do not.

EPA's 'Model' plants example in their BART guidance pertains to exempting sources whose sulfur dioxide (SO₂), nitrogen oxides (NO_x) or SO₂ plus NO_x emissions are less than 500 tpy and are greater than 50 kilometers (km) from any Class I area, or for sources whose emissions are less than 1,000 tpy and are greater than 100 km from any Class I area. EPA directed that states may (if they so choose) use the example cited in the Guidelines to exempt sources with no further analysis. In other words, states that establish 0.5 deciviews (dv) as a contribution threshold may exempt sources that emit less than 500 tpy of NO_x or SO₂ (or combined NO_x and SO₂) with no further analysis, as long as these sources are located more than 50 km from any Class I area. Also, states that establish 0.5 deciviews as a contribution threshold may exempt sources that emit less than 1,000 tpy of NO_x or SO₂ (or combined NO_x and SO₂) with no further analysis, as long as these sources are located more than 100 km from any Class I area.

Option 3: Cumulative Modeling. States may also submit to EPA a demonstration, based on an analysis of overall visibility impacts, that emissions from BART-eligible sources in your state, considered together, are not reasonably anticipated to cause or contribute to any visibility impairment in a Class I area. Therefore, no source should be subject to BART. States may do this on a pollutant by pollutant basis or for all visibility-impairing pollutants to determine if emissions from these sources contribute to visibility impairment.

This modeling protocol discusses the use of this third option to exempt potential BART-eligible sources' VOC and particulate matter (PM) emissions from BART and screen non-electric generating units (NEGU) potential BART-eligible sources' SO₂ and NO_x emissions to eliminate those that have insignificant visibility impacts from further BART analysis.

While EPA identifies several options for determining whether or not a source is "subject to BART," the most credible method is the use of dispersion modeling. Air quality modeling allows a state or source operator to analyze an individual source's impact on visibility as a result of its emissions of SO₂, NO_x and direct PM emissions.

EPA assumes in the BART guidance that dispersion modeling cannot currently be used to estimate the predicted impacts on visibility from an individual source's emissions of VOC or ammonia. Instead, EPA suggests a more qualitative assessment to determine on a case-by-case basis, which sources of VOC or ammonia emissions may be likely to impair visibility and should therefore be subject to BART review. The primary difficulty in using California Puff Model (CALPUFF) for VOCs is that the CALPUFF modeling system, recommended as the BART modeling platform, does not adequately treat PM formation from VOCs. Use of photochemical grid models to assess the visibility impacts of VOC emissions provides a quantitative and more scientifically defensible approach than a qualitative assessment.

A primary difficulty in estimating visibility impairment resulting from ammonia is uncertainties in the ammonia emissions inventories. These uncertainties result in modeled impacts on PM levels that are not as reliable as the results of modeling other PM components. While ammonia

emissions from industrial facilities are relatively well-characterized, livestock operations and soil are major sources of ammonia emissions, and their quantification is highly uncertain. In 70 FR 39104, EPA concluded that the decision whether to consider ammonia as a visibility-impairing pollutant in a specific case where a potential BART source actually emits more than 250 tpy of ammonia is best left to the state.

EPA Guidance on Air Quality Models

The BART determination under the Regional Haze Rule seeks to quantify the impact of source emissions of SO₂, NO_x, and direct PM (PM_{2.5} and/or PM₁₀) on hourly and daily visibility impairment at receptors located within downwind Class I areas. Since visibility is defined in the context of light extinction, which itself is determined by atmospheric concentrations of specific fine particulate species (like sulfate, nitrate, organic carbonaceous matter, elemental carbon, other fine particles and coarse mass), logic dictates that the modeling method(s) used must be capable of simulating these components reliably.

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

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

So, on the one hand, EPA maintains that CALPUFF is the "best regulatory modeling application currently available for predicting a single source's contribution to visibility impairment" and notes, "it is the only EPA-approved model for use in estimating single source pollutant

concentrations resulting from the long range transport of primary pollutants.” On the other hand, only regional grid models with appropriate chemistry are to be used in developing PM_{2.5} and Regional Haze SIPs. EPA has attempted to reconcile these two positions in the Final BART Rule by asserting that (a) regional models were not developed to treat individual point sources, and (b) CALPUFF’s secondary aerosol chemistry is adequate for estimating relative benefits of controls on BART sources.

More recent developments in photochemical grid modeling should alleviate some of the concerns related to using them for single-source visibility assessment. In particular, the use of finer grid spacing and new PM Plume-in-Grid (PiG) modeling techniques can extend the grid model’s applicability to assess the visibility impacts of a single source and groups of sources. As photochemical grid models include state-of-science representation of chemistry, this allows for the quantitative assessment of the visibility impacts of VOC emissions.

Steps in the BART Modeling Process

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

Identify BART-Eligible Sources. The first step is to identify whether a source is BART-eligible based on its source category, when it was put in service, and the magnitude of its emissions of one or more “visibility-impairing” air pollutants. The BART guidelines list 26 source categories of stationary sources that are BART-eligible. Sources must have been put in service between August 7, 1962 and August 7, 1977 in order to be BART-eligible. Potential emissions of 250 tpy or more of a visibility-impairing air pollutant are required to make a source eligible for BART. Qualifying pollutants include primary particulate matter (PM₁₀) and gaseous precursors to secondary fine particulate matter such as SO₂ and NO_x. Whether ammonia and VOCs should be included as visibility-impairing pollutants for BART eligibility is left for the states to determine on a case-by-case basis. The guidance states that high molecular weight VOCs with 25 or more carbon atoms and low vapor pressure should be considered as primary PM_{2.5} emissions and not VOCs for BART purposes.

Determine Sources Subject to BART. Next, one determines whether a BART-eligible source can be excluded from BART controls by demonstrating that the source cannot be reasonably expected to cause or contribute to visibility impairment in a Class I area. EPA’s preferred approach is an assessment with the CALPUFF modeling system (or other appropriate model) followed by comparison of the estimated 24-hr visibility impacts against a threshold above estimated natural conditions to be determined by the states. The threshold to determine whether a single source “causes” visibility impairment is set at 1.0 deciview change from natural conditions over a 24-hour averaging period in the final BART rule (70 FR 39118). Any exceedance of this threshold would trigger a BART determination. The guidance also states that the proposed threshold at which a source may “contribute” to visibility impairment should not be higher than 0.5 deciviews, although depending on factors affecting a specific Class I area, it may be set lower than 0.5 deciviews.

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

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

Note that for states under the PM_{2.5} provisions of the Clean Air Interstate Rule (CAIR), EPA has noted that CAIR satisfies the BART requirements for Electrical Generating Units' (EGU) SO₂ and NO_x emissions. However, since CAIR does not address VOC and PM emissions, a state still needs to determine whether an EGU's VOC and/or PM emissions contributes significantly to visibility impairment at any Class I area and, if so, address the rest of the BART requirements.

According to the BART guidance, a modeling protocol should be submitted for all modeling demonstrations regardless of the distance from the BART-eligible source to the Class I area. EPA's role in the development of the protocol is only advisory as the "states better understand the BART-eligible source configurations" and factors affecting their particular Class I areas (70 FR 39126).

CALPUFF Modeling Recommendations

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

CALPUFF is recommended for ascertaining whether a source may be exempted from BART. If a source is determined to be subject to BART, CALPUFF or another appropriate model should be used to evaluate the improvement in visibility resulting from the application of BART controls. Emissions reflecting periods of start-up, shutdown, and malfunction are not to be considered in determining the appropriate emission rates. The EPA recommends that the state use the highest 24-hour average actual emission rate for the most recent five-year period (excluding periods with start-up, shutdown, and malfunctions). Visibility improvements may be evaluated on a pollutant-specific basis. States are encouraged to account for the magnitude, frequency, and duration of the contributions to visibility impairment caused by the source when assessing whether the source is reasonably anticipated to cause or contribute to visibility impairment at a Class I area.

One approach being considered by several Regional Planning Organization (RPOs) (e.g., Midwest RPO, Western Regional Air Partnership-WRAP and VISTAS) is to perform a weight-of-evidence analysis using a photochemical grid model (e.g., CAMx and/or CMAQ) to assess whether VOC emissions from all potential BART-eligible point sources in a state contribute to visibility impairment. If the impact of eliminating all VOC emissions from all potential BART-eligible point sources in a state is shown to be less than 0.5 dv, then, logically, the impact of any one potential BART-eligible source would be less than 0.5 dv. Some RPOs are considering weight-of-evidence modeling with Community Multiscale Air Quality Modeling System (CMAQ) or Comprehensive Air Quality Model with extensions (CAMx) to address ammonia in the same way.

Alternative Models for BART Analyses

All air quality models potentially suited to BART analysis share a common foundation: the species-conservation (or atmospheric diffusion) equation. Source-oriented air quality models, including CALPUFF, derive from this equation that applies equally to one source or a million or more sources. The distinction lies in how the various terms are treated (CAMx, CMAQ) or neglected (CALPUFF) in the governing equations and the choice of coordinate system (Lagrangian or Eulerian). As shown in the next section, much of the simplicity of the CALPUFF model derives from the fact that many chemical and physical processes known to influence visibility are simply ignored. In contrast, comprehensive regional models treat these processes in detail, albeit at the expense of greater computer resources and data needs. EPA's BART guidance allows for the use of alternative models on a case-by-case basis.

EPA's dismissal of regional scale ignores a very substantial body of research and model development carried out at the agency and elsewhere in the U.S. over the past 20 years. Although grid models have generally been applied at geographic scales ranging from a multi-state to the continental scale, and were not initially designed to simulate individual point sources, modern one-atmospheric regional photochemical grid models, employing nested grid (Kumar and Russell, 1996) and Plume-in-Grid techniques (Karamanchandani et al., 2002; ENVIRON, 2005), are fully applicable to the analysis of point source plumes, most especially when reactive atmospheric chemistry occurs. If they were not, then they would not be reliable in simulating the combined effects of the wide array of anthropogenic and biogenic emissions that cause gas phase, particulate, secondary aerosol, and visibility air pollution problems. Furthermore, the convergence of fast commodity-based Linux computer clusters and recently-developed regional modeling emissions, meteorological, and air quality data bases make application of these modeling platforms no longer a research or academic exercise. While regional scale modeling

clearly requires expertise to perform properly, the actual program costs to conduct a CMAQ or CAMx regional modeling study are quite comparable with, and often less than, a traditional Prevention of Significant Deterioration (PSD) modeling study using the Industrial Source Complex Model (ISC), CALPUFF, or American Meteorological Society/Environmental Protection Agency Regulatory Model Improvement Committee Model (AERMOD). Given grid nesting and Plume-in-Grid technology, modern regional models are applicable to a very broad range of scales from 10-20 km to continental scale. In fact, regional photochemical grid models have been applied with grid spacing down to hundreds of meters on occasion (Kemball-Cook, Emery and Yarwood, 2005). Regional photochemical grid models are clearly more appropriate than CALPUFF for cumulative modeling requirements such as in the determination of the aggregate contribution of all-BART-eligible sources to visibility impairment. And as confirmed in EPA's fine particulate and regional haze modeling guidance discussed previously (EPA, 2001) and clearly shown by Morris and co-workers (2003; 2005), regional photochemical grid models, such as CMAQ and CAMx, provide a much more accurate and technically correct representation of the formation of secondary PM species, such as SO₄, NO₃ and secondary organic aerosols (SOA), than CALPUFF.

Still, for the vast majority of potential BART-eligible sources the application of the CALPUFF modeling system will in all likelihood be sufficient to address the needs of the source owner, the state, and the approving agency (EPA and the Federal Land Manager-FLM). However, for the specific BART exemption screening analysis being undertaken in this study, a photochemical grid model is more appropriate than the single-source CALPUFF model for the following reasons:

- There are a large number of potential BART-eligible sources in Texas, and the CAMx runs planned will allow the efficient screening of many sources in a scientifically defensible manner;
- For most potential BART-eligible sources in Texas, the Class I areas where visibility impacts will be estimated are between 97 and 654 km from the source;
- TCEQ is trying to identify which of the many potential BART-eligible sources satisfy the three criteria for being BART-eligible. If many of these sources can be determined to make an insignificant contribution to visibility impairment at Class I areas as a group, resources can then be focused on those sources determined most likely to impact visibility in Class I areas;
- Use of a photochemical grid model would allow the quantitative assessment of the visibility impacts due to potential BART-eligible sources' VOC and PM emissions, and;
- Use of a photochemical grid model will provide an evaluation of the cumulative impact of BART-eligible sources on visibility in Class I areas.

PURPOSE

The Texas Commission on Environmental Quality (TCEQ) is currently identifying which sources in Texas may be subject to the BART requirements. TCEQ has compiled a list of potential BART-eligible sources and desires to perform a screening analysis using an appropriate technique to eliminate sources or precursor pollutants that clearly do not contribute significantly to visibility impairment at any Class I area so is therefore exempt from the BART process. TCEQ is currently evaluating their list of sources against the three BART-eligible criteria. The screening analysis will test whether it is appropriate to exclude VOC and PM emissions and groups of potential BART-eligible sources from the list based on their visibility impairment

contributions. The resulting screened Texas potential BART-eligible sources list would be more manageable, allowing the TCEQ to focus their efforts on determining whether BART controls are needed for the remaining BART-eligible sources.

This modeling protocol describes an initial screening analysis that is aimed at determining the following:

- Whether VOC and/or PM emissions from potential BART-eligible sources in Texas can be shown to not contribute significantly to visibility impairment at Class I areas so may be exempt from the BART process; and
- Whether there are groups of non-EGU potential BART-eligible sources whose total SO₂ and NO_x emissions can be shown to not contribute significantly to visibility impairment at Class I areas so each source may be exempt from BART.

The Texas BART exemption screening analysis would build off the regional photochemical modeling (Morris et al., 2005d) being conducted by CENRAP). In particular, the CENRAP 2002 36 km CAMx modeling database would be enhanced to include a 12 km grid over Texas and vicinity, and CAMx zero-out modeling will be conducted to determine whether potential BART-eligible VOC and PM emissions can be shown to not contribute significantly to visibility impairment at any Class I area. CAMx PM Source Apportionment Technology (PSAT) modeling would also be conducted for groups of potential BART-eligible sources' SO₂ and NO_x emissions. Sources in groups that are shown not to contribute significantly to visibility impairment at any Class I area would be excluded. Note that a new version of CAMx will be used in this work that has incorporated PM chemistry and PSAT within its Plume-in-Grid (PiG) module that will be used to treat the early chemical evolution of potential BART-eligible sources SO₂ and NO_x emissions. This approach is fully consistent with the CENRAP draft BART Modeling Protocol (Alpine Geophysics, 2005).

2.0 MODELING APPROACH

This section describes the modeling approach and databases that will be used to perform the BART exemption screening analysis of potential BART-eligible sources in Texas. There are two elements that will be performed under this work:

- Screening analysis of the potential visibility impacts at Class I areas due to all potential BART-eligible sources VOC and PM emissions; and
- Screening analysis for groups of potential BART-eligible non-EGU sources' SO₂ and NO_x emissions to determine whether the group's visibility impacts at Class I areas are not significant, in which case the visibility impacts from each individual source in the group is not significant.

Both elements of the screening analysis will use the same 36/12 km 2002 annual database. The VOC and PM emission screening analysis will be performed using emissions zero-out modeling, whereas the group of sources' SO₂ and NO_x emissions screening analysis will be performed using an updated version of the PSAT.

2002 ANNUAL 36/12 KM MODELING DATABASE

The Texas BART screening analysis exemption modeling was performed using CAMx (ENVIRON, 2005) and the 2002 annual regional photochemical modeling database developed as part CENRAP. CENRAP has developed a 2002 annual modeling database for CAMx on the 36 km unified national RPO grid that covers the continental United States. This database was developed following the procedures outlined in the CENRAP Modeling Protocol (Morris et al., 2004) and CENRAP modeling Quality Assurance Program Plan (QAPP) (Morris and Tonnesen, 2004). The CENRAP preliminary base case model performance evaluation results for the CAMx model on the national 36 km grid using the CENRAP Base A emissions is given in Morris et al., (2005d). The CENRAP Modeling Protocol, QAPP, and preliminary Base A evaluation reports provide details on the development of the CENRAP 2002 36 km annual modeling database. Below, additional information is provided on enhancements to the CENRAP database for use in the Texas BART exemption screening analysis.

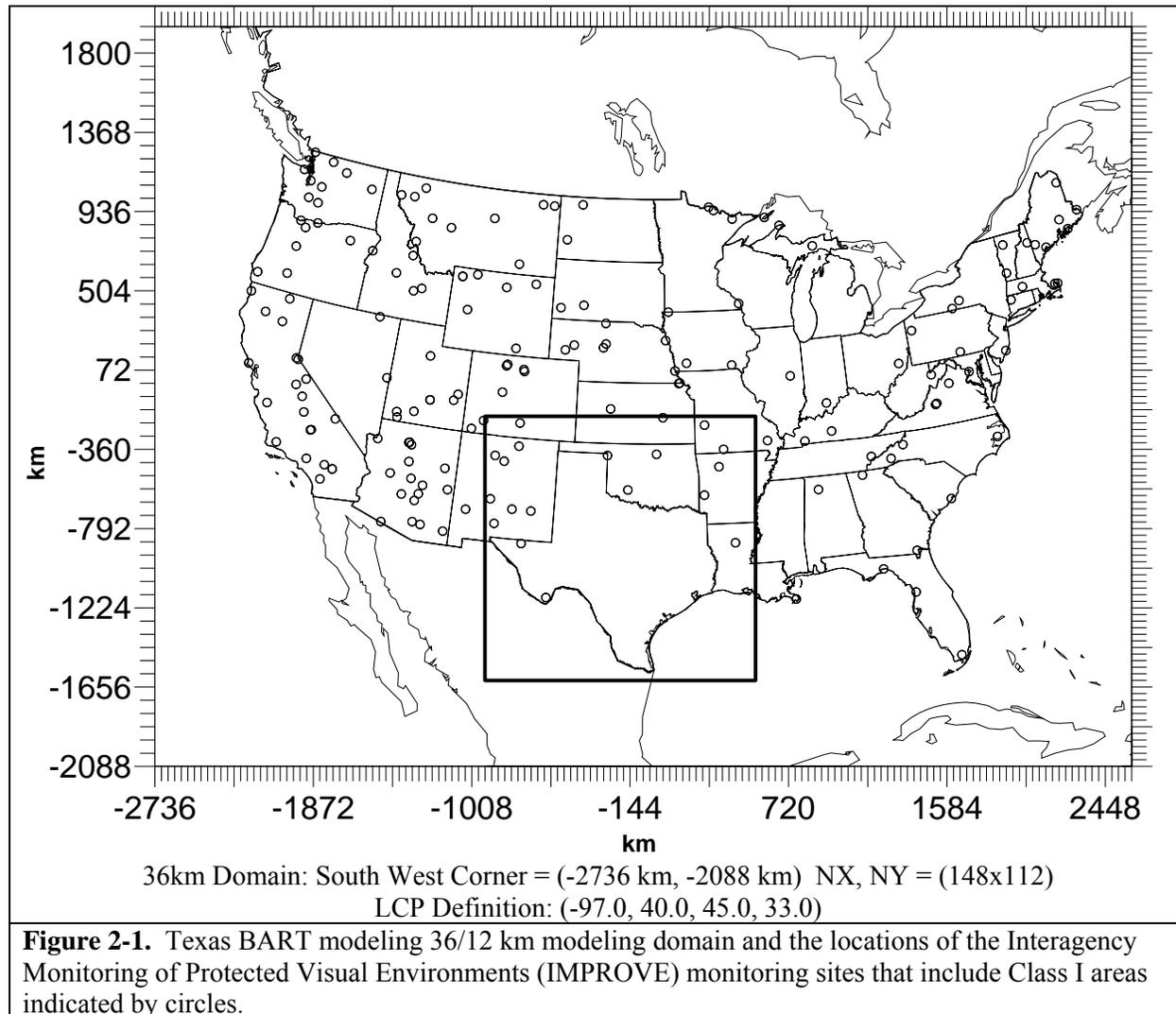
Enhancements to the CENRAP 2002 Modeling Database

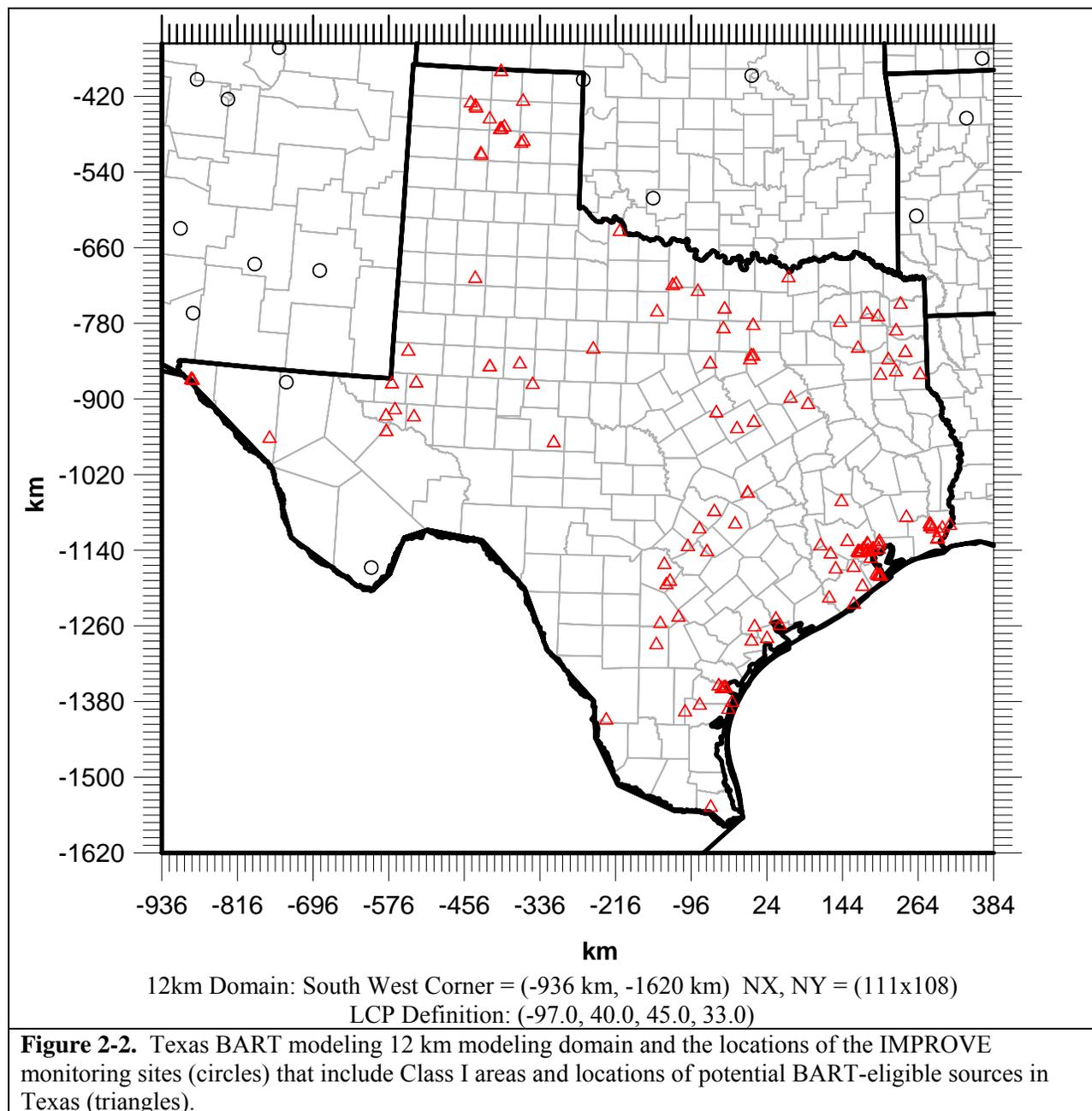
The CENRAP 2002 36 km annual CAMx evaluation using the Base A emissions and CAMx Version 4.20 is reported in Morris and co-workers (2005d) with additional model performance evaluation displays available on the CENRAP modeling Website (<http://pah.cert.ucr.edu/aqm/cenrap/cmaq.shtml#camx>). CENRAP is currently updating the CAMx 2002 36 km base case simulation using the Base B base case emissions and CAMx version 4.30. The Base B base case database and CAMx Version 4.30 will be the starting point for the Texas BART exemption modeling analysis.

The CENRAP Base B 2002 36 km annual CAMx photochemical modeling database will be updated to include a 12 km nested-grid that covers Texas and Class I areas in and near Texas including:

- National Parks: Big Bend (BIBE), Guadalupe Mountains (GUMO), and Carlsbad Caverns
- Wildlife Refuges: Salt Creek (SACR) and Wichita Mountains (WIMO)
- Wilderness Areas: White Mountain (WHIT), Caney Creek (CACR), Upper Buffalo (UPBU), and Hercules-Glade (HEGL).

Figure 2-1 displays the 36/12 km nested grid structure being proposed for the CAMx BART exemption modeling analysis. The locations of the potential BART-eligible sources and Class I areas within the 12 km modeling domain are shown in Figure 2-2. The CAMx flexi-nesting feature will be used to incorporate the 12 km Texas grid within the CENRAP 36 km modeling domain. Full flexi-nesting will be invoked in which CAMx internally interpolates all of the meteorological, emissions and other inputs from the 36 km grid to the 12 km grid.





ENHANCEMENTS TO THE PM SOURCE APPORTIONMENT TECHNOLOGY

For the potential BART-eligible group of sources SO_2 and NO_x emissions screening analysis, the CAMx PSAT will be used. PSAT is currently being updated to be compatible with the CAMx PiG module. The next section describes the technical formulation of the PSAT source apportionment technique and the enhancements to the CAMx PiG and PSAT to make them compatible with each other.

PSAT Formulation

PSAT is designed to source apportion the following PM species modeled in CAMx:

- Sulfate (SO₄)
- Particulate nitrate (NO₃)
- Ammonium (NH₄)
- Particulate mercury (Hg(p))
- Secondary organic aerosol (SOA)
- Six categories of primary particulate matter (PM)
 - Elemental carbon (EC)
 - Primary organic aerosol (POA)
 - Fine crustal PM (FCRS)
 - Fine other primary PM (FPRM)
 - Coarse crustal PM (CCRS)
 - Coarse other primary PM (CPRM)

PSAT performs PM source apportionment for each user defined source group. A source group consists of a combination of a geographic regions and emissions source category. Examples of source regions include states, nonattainment areas, and counties, whereas examples of source categories include mobile sources, biogenic sources, elevated point sources and even an individual source. The user defines a geographic source region map to specify the source regions. The user then inputs each separate source category as separate gridded low-level emission and/or elevated point source emission inputs. The model then determines each source group by overlaying the source categories on top of the source region map.

The PSAT “reactive tracers” that are added for each source category/region (*i*) are described below. In general, a single tracer can track primary PM species whereas secondary PM species require several tracers to track the relationship between gaseous precursors and the resulting PM. Particulate nitrate and secondary organics are the most complex species to apportion because the emitted precursor gases (NO, VOCs) are several steps removed from the resulting PM species (NO₃, SOA). The PSAT tracers for each type of PM are listed below. The PSAT convention is that tracer names for particulate species begin with the letter “P.”

Sulfur

- SO_{2*i*} Primary SO₂ emissions
 PS_{4*i*} Particulate sulfate ion from primary emissions plus secondarily formed sulfate

Nitrogen

- RGN_{*i*} Reactive gaseous nitrogen including primary NO_x (NO + NO₂) emissions plus nitrate radical (NO₃), nitrous acid (HONO) and dinitrogen pentoxide (N₂O₅).
 TPN_{*i*} Gaseous peroxy acetyl nitrate (PAN) plus peroxy nitric acid (PNA)
 NTR_{*i*} Organic nitrates (RNO₃)
 HN3_{*i*} Gaseous nitric acid (HNO₃)
 PN3_{*i*} Particulate nitrate ion from primary emissions plus secondarily formed nitrate
 NH3_{*i*} Gaseous ammonia (NH₃)
 PN4_{*i*} Particulate ammonium (NH₄)

Secondary Organic Aerosol

- ALK_{*i*} Alkane/Paraffin secondary organic aerosol precursors
- ARO_{*i*} Aromatic (toluene and xylene) secondary organic aerosol precursors
- CRE_{*i*} Cresol secondary organic aerosol precursors
- TRP_{*i*} Biogenic olefin (terpene) secondary organic aerosol precursors
- CG1_{*i*} Condensable gases from toluene and xylene reactions (low volatility)
- CG2_{*i*} Condensable gases from toluene and xylene reactions (high volatility)
- CG3_{*i*} Condensable gases from alkane reactions
- CG4_{*i*} Condensable gases from terpene reactions
- CG5_{*i*} Condensable gases from cresol reactions
- PO1_{*i*} Particulate organic aerosol associated with CG1
- PO2_{*i*} Particulate organic aerosol associated with CG2
- PO3_{*i*} Particulate organic aerosol associated with CG3
- PO4_{*i*} Particulate organic aerosol associated with CG4
- PO5_{*i*} Particulate organic aerosol associated with CG5

Mercury

- HG0_{*i*} Elemental Mercury vapor
- HG2_{*i*} Reactive gaseous Mercury vapor
- PHG_{*i*} Particulate Mercury

Primary Particulate Matter

- PEC_{*i*} Primary Elemental Carbon
- POA_{*i*} Primary Organic Aerosol
- PFC_{*i*} Fine Crustal PM
- PFN_{*i*} Other Fine Particulate
- PCC_{*i*} Coarse Crustal PM
- PCS_{*i*} Other Coarse Particulate

PSAT includes a total of 32 tracers for each source group (*i*) if source apportionment is applied to all types of PM. Since source apportionment may not always be needed for all species, the PSAT implementation is flexible and allows source apportionment for any or all of the chemical classes in each CAMx simulation (i.e. the SO₄, NO₃, NH₄, SOA, Hg and primary PM classes listed above). For example, source apportionment for sulfate/nitrate/ammonium requires just nine tracers per source group.

One fundamental assumption in PSAT is that PM should be apportioned to the primary precursor for each type of PM. For example, SO₄ is apportioned to SO_x emissions, NO₃ is apportioned to NO_x emissions, NH₄ is apportioned to NH₃ emissions, etc. As a source apportionment method, PSAT must account for all modeled sources of a PM species. Consider two model species A and B that are apportioned by reactive tracers *a_i* and *b_i*, respectively. Reactive tracers must be included for all sources of A and B including emissions, initial conditions and boundary conditions so that complete source apportionment is obtained, i.e., $A = \sum a_i$ and $B = \sum b_i$.

In PSAT, the general approach to modeling change over a model time step Δt is illustrated for a chemical reaction $A \rightarrow B$. The general equation for species destruction is:

$$a_i(t + \Delta t) = a_i(t) + \Delta A \frac{a_i}{\sum a_i}$$

Here, the relative apportionment of A is preserved as the total amount changes. This equation applies to chemical removal of A and also to physical removal of A by processes such as deposition or transport out of a specific grid cell.

The general equation for species production (e.g. chemical production by the chemical reaction $A \rightarrow B$) is:

$$b_i(t + \Delta t) = b_i(t) + \Delta B \frac{a_i}{\sum a_i}$$

Here, production of B inherits the apportionment of the precursor A . The same equation applies for “production” of B in a specific grid cell due to emissions or transport. For the case where B increases due to emissions, a_i is the apportionment of the emissions inventory. For the case where B increases due to transport, a_i is the apportionment of the upwind grid cell.

In some cases, source category specific weighting factors (w_i) must be added to the equation for species destruction:

$$a_i(t + \Delta t) = a_i(t) + \Delta A \frac{w_i a_i}{\sum w_i a_i}$$

An example is chemical decay of the aromatic VOC tracers (ARO), which must be weighted by the average OH rate constant of each ARO_{*i*}. ARO tracers for different source groups have different average VOC reactivities because the relative amounts of toluenes and xylenes differ between source categories.

In some cases, source category specific weighting factors (w_i) must be added to the equation for species production:

$$b_i(t + \Delta t) = b_i(t) + \Delta B \frac{w_i a_i}{\sum w_i a_i}$$

An example is chemical production of condensable gases (CG1 or CG2) from aromatic VOC tracers, which must be weighted by aerosol yield weighting factors. The aerosol yield weighting factors depend upon the relative amounts of toluenes and xylenes in each source group.

Several aerosol reactions are treated as equilibria, $A \leftrightarrow B$. If A and B reach equilibrium at each time step, it follows that their source apportionments also reach equilibrium:

$$a_i(t + \Delta t) = [a_i(t) + b_i(t)] \left(\frac{A}{A + B} \right)$$

$$b_i(t + \Delta t) = [a_i(t) + b_i(t)] \left(\frac{B}{A + B} \right)$$

Examples are the equilibrium between gas phase nitric acid and aerosol nitrate, gas phase ammonium and aerosol ammonium, and condensable organic gases (CG) and secondary organic aerosols (SOA).

The PSAT source apportionment technique has been extensively tested and evaluated against other source apportionment techniques (e.g., ENVIRON, 2005; Morris et al., 2005; Yarwood et al., 2004).

Updates to the PSAT Formulation

The CAMx PSAT and PiG algorithms were updated to treat the near-source chemistry of secondary PM formation and to be compatible with each other. The PiG module now treats full-science aerosol chemistry and dynamics in addition to gas-phase chemistry and has been extended to PSAT and Ozone Source Apportionment Technology (OSAT.) The formulation of the full-science PiG is described below.

Modeling photochemistry is a highly non-linear problem because chemical rates for most compounds depend upon their ambient concentrations. Ambient concentrations in turn depend on how well the modeling grid resolves emissions, transport, and chemical history. Thus, grid resolution plays a vital role in the ability of the model to properly characterize photochemical conditions. Increasing resolution should, in theory, lead to a better model as the time/space discretization tends toward a continuum. However, practical and theoretical considerations suggest that the lower limit on horizontal grid spacing is about 1000 meters for Eulerian air quality models such as CAMx. Nevertheless, even higher resolution is often necessary to adequately simulate chemistry within concentrated point source plumes.

As a result, many modern Eulerian models contain a Plume-in-Grid sub-model that tracks individual plume segments (or puffs) in a Lagrangian sense, accounting for plume-scale dispersion and chemical evolution, until such time as puff mass can be adequately represented within the larger grid model framework. It is important to understand that the inclusion of a Lagrangian puff model within an Eulerian grid model is a forced construct. The formulations of the two modeling approaches are fundamentally different and there is no theoretically “correct” methodology. This explains the variety of Plume-in-Grid methodologies that are in use today. The CAMx PiG module was recently updated in Version 4.4 of the model.

The new PiG approach in CAMx treats the full suite of gas-phase photochemistry, aqueous-phase chemistry and aerosol phase chemistry and dynamics. Chemical processes are simulated within each plume segment using an “incremental chemistry” approach, whereby puffs carry the incremental contributions of the puff relative to the grid concentrations. Incremental puff concentrations can be positive or negative, depending upon the species and stage of plume evolution. A similar chemistry approach is used in the Second-order Closure Integrated puff model (SCIPUFF) with CHEMistry (SCICHEM) Lagrangian model (EPRI, 2000). The approach lends itself to incorporating chemistry for particulates as well.

Basic Puff Structure and Diffusive Growth

The CAMx PiG releases a stream of plume segments (puffs) from a point source specified in the CAMx input file by setting the point source stack diameter to a negative value. Each puff possesses a longitudinal length and directional orientation defined by the separation of a leading and a trailing point. Initial separation of these points is determined by the wind vector at final

plume rise. Each point is then subsequently and independently transported through the gridded wind fields, which directly accounts for puff stretching and changes to centerline orientation due to deforming shears. The official "position" of each puff is defined by the center point of each puff between the endpoints. This position defines the grid cell in which the puff resides for the calculation of diffusion and chemistry.

Like other puff models, the shape of each puff is characterized by a spread tensor, which is defined from a set of Gaussian standard deviations (so-called "sigmas") along the three spatial axes (σ_x , σ_y , σ_z). Diffusive growth is defined by the growth in these sigma values. The total cross-sectional width extends $\pm 1.5\sigma$ from puff centerline. The limits of $\pm 1.5\sigma$ result in an average concentration across the Gaussian distribution that nearly equals a uniformly mixed concentration across that distance. The total longitudinal length is the distance between the puff endpoints $\pm 1.5\sigma_y$. Horizontal area is calculated using the formula for an ellipse. Different vertical constructs are employed for Greatly Reduced and Simplified Dynamics (GREASD) and Incremental Reactions for Organics and NO_x (IRON) PiG, as described later in this section. Figure 2-3 presents a schematic representation of each puff in horizontal cross-section.

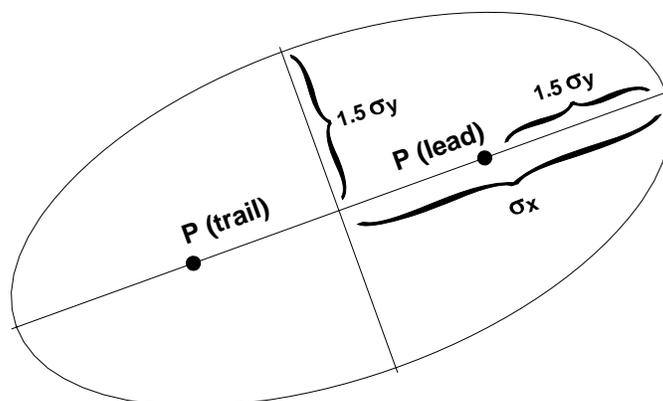


Figure 2-3. Schematic representation of CAMx PiG puff shape in the horizontal. Directional orientation of the puff is arbitrary, and evolves during the aging of the puff according to wind direction, shears and diffusive growth along its trajectory.

We have developed an explicit solution approach for puff growth that shares SCICHEM theory and concepts (EPRI, 2000), but includes some simplifications. SCICHEM solves predictive spatial moment equations with second-order closure that relate the evolution of the puff spread tensor ($\sigma_{ij} = \sigma_i \times \sigma_j$) to resolved mean shears and turbulent velocity statistics. The Reynolds-averaged second-moment transport equation is given as:

$$\frac{d\sigma_{ij}}{dt} = \sigma_{ik} \frac{\partial \bar{u}_j}{\partial x_k} + \sigma_{jk} \frac{\partial \bar{u}_i}{\partial x_k} + \frac{\langle x'_i \overline{u'_j c'} \rangle}{Q} + \frac{\langle x'_j \overline{u'_i c'} \rangle}{Q}$$

where \bar{u} is the mean wind vector component, the primed values represent turbulent fluctuations from the mean, and the angle brackets denote integrals over space. The Reynolds averaging process always introduces higher-order fluctuation correlations, and this is given by the turbulent flux moments $\langle x' \overline{u' c'} \rangle$, where $\overline{u' c'}$ represents the turbulent flux of concentration. It is these last two diffusion terms that SCICHEM solves in its second-order closure scheme.

For sub-puff scale turbulence, SCICHEM employs the restriction that the only off-diagonal component of $\langle x' \overline{u' c'} \rangle$ to be considered is the symmetric horizontal term ($i=x, j=y$), and then only for the large-scale (meso to synoptic) contribution to puff deformation when puff scale reaches such dimensions. In CAMx, we ignore this off-diagonal flux moment term altogether since puff mass is ultimately introduced to the grid when puff size is at the grid scale (1-50 km in practically all applications), and thus puffs never reach spatial scales at which this term becomes important. SCICHEM also makes the assumption that the horizontal turbulence is isotropic, $\langle x' \overline{u' c'} \rangle = \langle y' \overline{v' c'} \rangle$. This results in a single diffusivity equation for both x and y directions, and a single diffusivity for the z direction:

$$K_x = K_y = \frac{\langle y' \overline{v' c'} \rangle}{Q}$$

$$K_z = \frac{\langle z' \overline{w' c'} \rangle}{Q}$$

In our approach for CAMx, we have adopted the SCICHEM second-order tendency equations to model the time-evolution of puff turbulent flux moments (represented by diffusivities $K_x=K_y$ and K_z) and their contribution to the evolution of puff spread (represented by the diagonal components of the puff spread tensor, $\sigma_x^2 = \sigma_y^2$ and σ_z^2). The off-diagonal contributions to puff spread were ignored, since they are unnecessary in the context of the CAMx PiG. Puff spread is defined for puff depth (σ_z) and puff width (σ_y); the latter is also added to the longitudinal length to allow for diffusive growth along the puff centerline. We account for the effects of wind shears in the evolution of lateral spread, but assume that the evolution of vertical spread is solely the result of turbulent fluxes.

The resulting two Reynolds-averaged second-moment transport equations for CAMx PiG are:

$$\frac{d\sigma_z^2}{dt} = 2K_z$$

$$\frac{d\sigma_y^2}{dt} = 2\sigma_y^2 D + 2\sigma_y \sigma_z \left(\frac{du^2}{dz} + \frac{dv^2}{dz} \right)^{1/2} + 2K_y$$

where D is deformation of horizontal wind (see Section 2).

The SCICHEM tendency equation for the horizontal turbulent flux moment is:

$$\frac{d}{dt} \langle y'v'c' \rangle = Qq^2 - A \frac{q}{\Lambda} \langle y'v'c' \rangle$$

where $A = 0.75$, $q^2 = \overline{v'v'}$, and Λ is the horizontal turbulent length scale. Separate equations are given for two different boundary layer turbulence scales (shear- and buoyancy-produced), such that:

$$\langle y'v'c' \rangle = \langle y'v'c' \rangle_{shear} + \langle y'v'c' \rangle_{buoyancy}$$

Within the surface-based boundary layer, the horizontal velocity variance is given by:

$$q_{buoyancy}^2 = 0.13 w_*^2 [1 + 1.5 \exp(z / z_i)]$$

$$q_{shear}^2 = 2.5 u_*^2 (1 - z / z_i)$$

where u_* is the friction velocity, w_* is the convective velocity scale, z is height above the surface, and z_i is the height of the surface-based boundary layer. The horizontal turbulent length scale is given by:

$$\frac{1}{\Lambda_{shear}^2} = \frac{1}{(0.3 z_i)^2} + \frac{1}{(0.65 z)^2}$$

$$\Lambda_{buoyancy} = 0.3 z_i$$

In the stable boundary layer, only the shear components of q^2 and Λ are applied. Above the boundary layer, SCICHEM applies rough approximations for the velocity variance and turbulent length scale: $q^2 = 0.25 \text{ m}^2/\text{s}^2$, and $\Lambda = 1000 \text{ m}$.

The SCICHEM tendency equation for the vertical turbulent flux moment is

$$\frac{d}{dt} \langle z' \overline{w'c'} \rangle = A \frac{q_v}{\Lambda_v} (QK_z^{eq} - \langle z' \overline{w'c'} \rangle)$$

where $q_v^2 = \overline{w'w'}$, Λ_v is the vertical turbulent length scale, and K_z^{eq} is the equilibrium diffusivity. Whereas a specific equation for K_z^{eq} is formulated for SCICHEM, we have chosen to specify the value of this parameter from the gridded fields of vertical diffusivity in CAMx. Again SCICHEM gives separate equations for shear- and buoyancy-produced turbulence scales.

Within the surface-based boundary layer, the vertical velocity variance is given by

$$q_v^2 \Big|_{shear} = 1.5 u_*^2 (1 - z / z_i)$$

$$q_v^2 \Big|_{buoyancy} = 1.1 w_*^2 (z / z_i)^{2/3} (1.05 - z / z_i)$$

The vertical turbulent length scale for both shear and buoyancy is equal to Λ_{shear} given above for horizontal length scale. Above the boundary layer, SCICHEM again applies rough approximations for the velocity variance and turbulent length scale:

$$q_v^2 = 0.01 \text{ m}^2/\text{s}^2, \text{ and } \Lambda_v = 10 \text{ m.}$$

The external variables needed by IRON PiG to complete the dispersion calculations include z_i , u_* and w_* . All of these are available from an internal module in CAMx that calculates these boundary layer similarity theory parameters. Thus, no additional parameters are needed to be input to the model.

Puff Transport

A fresh set of new puffs are released from all PiG point sources within the modeling domain for the duration of the smallest time step among the master and all nested grids. The length of each puff is determined by the combination of the mean total wind speed at the height of final plume rise and time step. Limits are placed on maximum extruded length based on half the finest resolution in the given simulation. If winds and time-steps are such that the maximum allowed length is violated, then several puffs are extruded from a given stack per time step. The orientation of the puff length is along the total wind vector. Total puff volume is determined by stack volumetric flow rate in conjunction with growth due to turbulent entrainment following the SCICHEM approach. Initial σ_y and σ_z are explicitly calculated from this entrainment calculation.

Effects of wind divergence on plume deformation are treated in an explicit manner within the CAMx PiG using a “chained puff” approach (Figure 2-4). Points at the leading and trailing edges of the puff centerline are individually transported through the gridded wind fields, which directly accounts for puff stretching and changes to centerline orientation due to deforming shears. Since PiG puffs can extend over multiple layers, layer density-weighted average wind components are determined for each endpoint based on the vertical coverage of the puff, and these are used for advection of those points. GREASD PiG puffs are not allowed to expand

beyond the depth of the layer in which the centerpoint resides, so only the single layer wind components are used to advect the endpoints.

The "chain" aspect means that at least initially (as puffs are extruded from the stack) the trailing point of a puff emitted at time t will be the leading point of a puff emitted at time $t+dt$. However, as the puffs are advected downstream, the leading point of one puff will deviate from the trailing point the puff behind it due to evolving puff depth and wind fields. Puff volume is conserved in convergent/divergent wind fields. Puff endpoints may move closer together or further apart, in wind fields that are slowing or accelerating downstream. We compute puff endpoint separation changes and then adjust puff widths and depths to maintain constant puff volume. The change in computed puff endpoint spacing defines puff length tendencies, then puff depth tendencies are computed from grid-resolved vertical wind shear (dw/dz), and finally we determine the puff width tendencies required to conserve puff volume.

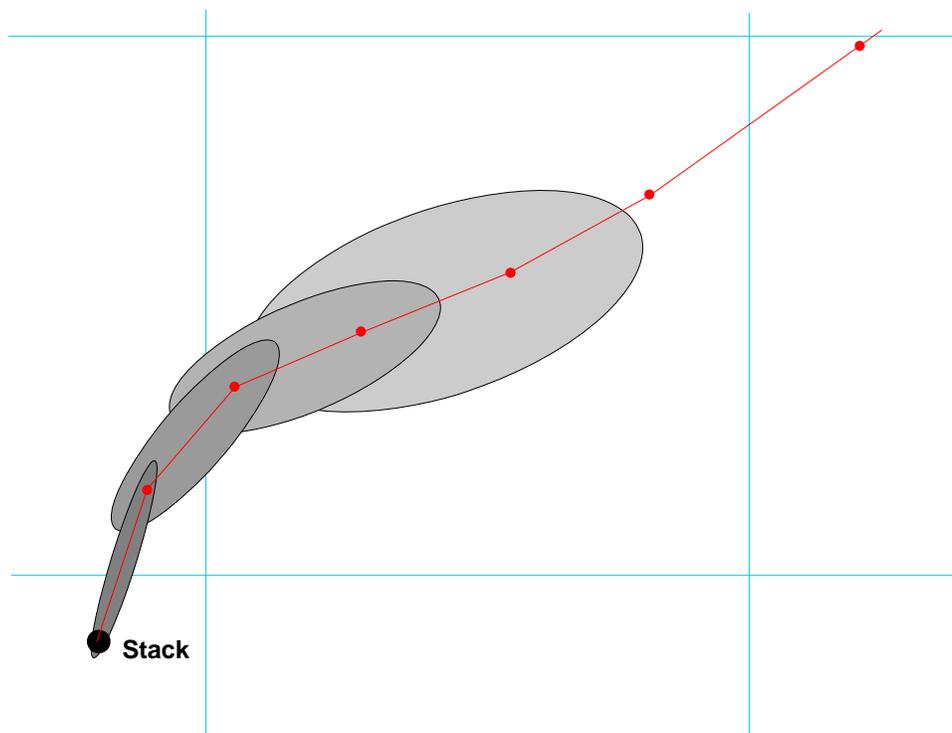


Figure 2-4. Schematic representation of a chain of PiG puffs emitted from a point source into an evolving gridded wind field. The red line connected by dots represents puff centerlines, with dots representing leading and trailing points of each puff. The CAMx computational grid is denoted by the blue lines.

The official "position" of each puff is defined by the center point of each puff between the endpoints. This position defines which grid domain and grid cell the puff resides for the calculation of diffusion and chemistry. This definition holds even if the puff is sufficiently long that the endpoints are in different grid cells (or even different grid domains if near a domain boundary). With our definition for termination when horizontal area approaches grid cell area, the extents of the puff length should not extend across more than two grid cells.

PiG Chemistry

The primary goal of the new PiG formulation in CAMx Version 4.4 was to include a more complete treatment of chemistry in point source pollutant plumes, while secondarily improving puff-grid mass exchange and adding additional features central for treating toxic pollutants not normally carried by the standard CAMx chemical mechanisms. Several approaches have been developed to treat photochemistry within point source plume models. One of the more elegant methodologies is the incremental chemistry idea embodied in the SCICHEM model (EPRI, 2000). However, we found that the implementation of incremental chemistry in SCICHEM is very complex, especially in its handling of the chemistry of overlapping puffs. In adopting this innovative approach for the new PiG, it was necessary to reformulate the physical and chemical configuration of the PiG puffs and to utilize an accurate numerical solution approach based on the Livermore Solver for ordinary differential equations (LSODE) chemical solver.

The Concept of Incremental Chemistry

For a second-order reaction between puff species A and B , the total reaction rate is the following:

$$R_T = k(P_A)(P_B) \quad (1)$$

where P_A and P_B are the total puff concentrations of each species. The total puff concentrations can be expressed as the sum of the background and puff perturbation concentrations:

$$P_A = (c_A + C_A)$$

$$P_B = (c_B + C_B)$$

where C is the ambient concentration and c is the puff increment concentration. Thus the reaction rate is found to be:

$$R_T = k(c_A + C_A)(c_B + C_B)$$

or

$$R_T = k(c_A c_B + C_A c_B + c_A C_B + C_A C_B)$$

If we subtract the rate of change of the background,

$$R_{Ambient} = kC_A C_B \quad (2)$$

by assuming that it is explicitly and separately treated by the grid model, we obtain the reaction rate for the puff increments:

$$R_p = k(c_A c_B + C_A c_B + c_A C_B) \quad (3)$$

Equation 3 is the basis of SCICHEM incremental chemical kinetic solver. One problem with this approach is the mixed terms, C_{ACB} and c_{ACB} . Most chemical solver packages are designed to solve rate equations for total concentration, as in Equation 1. Thus, for the new PiG we developed an alternative numerical solution scheme for puff perturbation chemistry. We note that the CAMx chemical solver can be independently applied to the rate equation for total puff concentrations, Equation 1, and to the rate equation for ambient concentrations, Equation 2. By subtraction of the two solutions, we obtain the solution to rate Equation 3. This requires no modification to, and is obviously completely self-consistent with, the CAMx chemical solvers. Once the incremental puff reaction rates are obtained they are applied to the incremental puff mass to calculate the new (adjusted for chemistry) incremental concentrations. These new puff increments are subsequently advected and dispersed by the transport portions of the PiG code.

Puff Constructs for Incremental Chemistry

The new PiG sub-model includes three new constructs designed specifically to facilitate the incremental chemistry approach:

- Treatments to handle puff-grid information exchange for puffs spanning multiple model layers;
- The concept of “virtual dumping” to handle the chemical impacts of large puffs that can overlap other puffs within a given grid column; and
- The concept of multiple puff “reactor” cells to account for the chemical effects of concentration distributions within each puff.

Each of these is described below.

Puff Layer Spanning

The new PiG is designed to chemically process point source plume mass within streams of puffs until such time that each puff can be adequately resolved on the *horizontal* grid. Unlike the previous versions of the PiG approach, where the vertical layer structure dictates puff leaking and ultimately termination, the approach in new PiG leads to the necessity that puffs be allowed to vertically span multiple grid model layers before they reach horizontal grid scales. This introduces technical implications for defining “background” concentrations and ambient conditions for puff chemistry, as well as for transferring plume incremental mass to the grid. The solution employed in the new PiG is to:

- 1) Assume that the vertical distribution of puff concentration is always uniform;
- 2) Distribute puff mass transfer (via “leaking” and “dumping”) to the grid according to the puff fractional coverage across each model layer and by density-weighting; and
- 3) Determine mean background concentrations and other ambient conditions (e.g., temperature, humidity, etc.) over the puff vertical span via similar fractional layer-density weighting.

PiG puffs are considered to be elliptical in the horizontal, with the minor axis spanning the cross-wind puff width (defined as $\pm 1.5\sigma_y$), and the major axis spanning the along-wind puff length (defined as length $\pm 1.5\sigma_y$ on each end). This is similar to GREASD PiG. However, given the complications associated with multiple layer spanning and mass-weighting of ambient inputs and dumped mass, puffs are rectangular and uniform in the vertical, with total puff depth defined as $\pm 1.5\sigma_z$.

Horizontally, the mean background concentration and ambient conditions are taken from the single host grid column containing each puff center point, even if the puff is large and/or spans a horizontal cell interface.

Chemistry Solution

In summary, chemistry is solved for each PiG puff “reactor” in three steps:

- 1) The layer-mean background (grid + overlapping puff) concentrations and environmental conditions over the volume occupied by the puff are stored and then chemically updated via the LSODE gas-phase chemistry mechanism;
- 2) The pre-updated mean background concentrations are added to the puff increments and the total concentrations are chemically updated; and
- 3) The updated results from step 1 are subtracted from the updated results of step 2 to provide the updated incremental concentrations.

An important consequence of this approach is that the incremental puff mass may be positive or negative. For example, a high- NO_x puff that is destroying ambient ozone will have negative ozone increments. The puff increments are subsequently advected and dispersed by the transport portions of the IRON PiG code. The updated background concentrations, which include “virtual dumps” of mass from large puffs, are used for reference only in the puff incremental chemistry algorithm; the actual grid concentrations are updated in the grid chemistry routine.

Puff Dumping and PiG Rendering

Mass transfer from puff to grid can happen in two ways: slowly, termed “leaking,” or suddenly, termed “dumping.” As described earlier, all mass is transferred from the PiG to the vertical grid structure in a density-weighted fashion according to each puff’s fractional layer coverage. The process of leaking ensures that puff mass is transferred to the grid continuously, rather than in discrete lumps of pollutants with very different concentrations than those in the grid. The idea behind puff leakage is to account for turbulent shearing of mass from the main plume and its subsequent dispersion to the grid scale. This rate of transfer should be directly proportional to the puff size relative to the grid scale. The user can control whether a puff is leaked or not, and for Texas BART screening modeling, we have assumed the default mode in which puffs are not leaked to the grid. This will allow the full-science PiG plume model to treat the chemistry of the BART point source plumes as plume chemistry until the plume size is commensurate to the grid cell size, rather than the early dilution of the plume emissions across the grid when the puff is leaked.

Puff leakage is controlled by comparing the horizontal area of a puff to a specified leakage parameter, defined as a fraction of horizontal grid cell area. When a puff is first emitted, there is no leakage. As the puff grows in volume, the concentrations within the reactors are reduced accordingly by dilution. When the puff area exceeds the leakage onset parameter, a fraction of the mass in each puff reactor is transferred to the grid. This fraction is determined by the relative exceedance of the leakage parameter; initial leakage is slow as the exceedance is relatively small, but leakage rates grow as the puff continues to grow beyond the leakage parameter.

The reduced mass from leakage is compensated by a reduced effective volume, so that concentrations are not artificially diluted by leakage (an essential chemical imperative). Thus, two distinct volumes are tracked: the actual volume (defined by the puff spread sigmas) and the effective volume. While these are identical before leakage, they obviously deviate after leakage is initiated, and thereafter the relative deformation of the actual puff volume (via diffusion, shearing, etc.) is used to scale the deformation of effective puff volume.

Eventually the horizontal span of the puff will exceed the grid cell area, and the remaining mass is then dumped all at once to the grid. However, because of the combination of photochemical processing and leakage, by the time a puff dumps the potential for producing numerical shocks is much reduced. Furthermore, if the puff exceeds a user-defined maximum age, puff mass is transferred to the grid. Also, puff mass is dumped to the grid model when the chemical maturity of the puff is such that plume-scale chemistry is no longer appropriate.

While the mass confined to the puffs at any given time has not yet affected the grid concentrations, it will eventually, so it can be somewhat misleading to sequester this mass from visualizations of a model simulation. The puff mass can be optionally incorporated into the model average output files for visualization purposes (referred to as “PiG rendering”). Rendering employs a “virtual dump” of the puff masses into the average concentration array each time step. As described for chemistry, virtual puff mass is added as an increment over the entire grid column according to fractional layer-density weighting over puff depth, thus diluting its concentrations relative to that within the puff. The actual puff mass remains within the puffs over the course of their lifetimes. This visualization is available for 3-D average output files, and can produce some rather startling effects in output displays, including very narrow virtual plumes, or streaks, representing mass moving through the grid in sub-grid puffs, but not subject to grid-scale eddy diffusion.

High Resolution Puff Sampling

PiG optionally employs surface-layer puff sampling of concentration species on a user-defined grid of arbitrary horizontal resolution, similarly to the way nested grids are defined. Sampling grids are entirely passive, and intended to provide a display of the plume concentrations at scales much smaller than typically used for the finest computational grids (i.e., <1 km), primarily around and downwind of a source complex. Sampled PiG concentrations are time-averaged like the output concentrations provided on the computational grids, and are written to files with similar format so that they may be readily viewed and manipulated with CAMx post-processing software. Additional information on configuring and using PiG sampling grids is provided in Section 5.

Given that the puffs constantly evolve via diffusive growth and reshaping due to deforming shears, the sampling procedure includes trigonometric calculations to define which sampling

points are influenced by each puff. This influence is determined according to the puffs' two-dimensional horizontal Gaussian shape shown in Figure 2-3. To include a sufficiently large percentage of mass across each puff for sampling, limits of $\pm 3\sigma_y$ in both horizontal dimensions are used to define the puffs' total elliptical area coverage. Puffs are only sampled if they extend vertically into the model's surface layer.

3.0 PROCEDURES FOR VOC AND PM EMISSIONS BART SCREENING ANALYSIS

The first screening analysis will estimate the cumulative visibility impacts at Class I areas due to VOC and PM emissions from all potential BART-eligible sources in Texas. Two CAMx 36/12 km simulations will be conducted for the 2002 annual period:

- 2002 BART Base Case Emissions Scenario; and
- 2002 BART VOC and PM Emissions Zero-Out Scenario.

The 2002 BART base case emissions scenario will be based on the CENRAP 2002 typical base case emissions scenario. The BART guidelines require that BART modeling use the actual maximum 24-hour emissions for each BART-eligible source. The CENRAP 2002 typical scenario contains average actual emissions for all sources. The maximum 24-hour actual emission rates are not readily available for most sources. Thus, to account for the differences between maximum 24-hour actual and average typical actual, the average typical actual emissions for potential BART-eligible sources in the CENRAP 2002 typical base case emissions scenario will be doubled. This provides a conservative estimate of maximum 24-hour emissions for these sources.

Visibility impacts will be calculated at each Class I area using the differences in 24-hour PM concentrations between the two scenarios above following the procedures given in EPA's BART modeling guidance (EPA, 2005) and in the Federal Land Managers Air Quality Related Values Workgroup report (FLAG, 2000). The FLAG (2000) procedures were developed to estimate visibility impacts at Class I areas from proposed new sources as part of the Prevention of Significant Deterioration (PSD) and New Source Review (NSR) process and were adapted to BART. These procedures use the Interagency Monitoring of Protected Visual Environments (IMPROVE) reconstructed mass extinction equation (Malm et al., 2000), only instead of using measured PM concentrations from an IMPROVE monitor, incremental PM concentrations from the differences in the CAMx 2002 BART base case and 2002 BART VOC/PM zero-out runs will be utilized in the equation.

The IMPROVE reconstructed mass extinction equation is used to estimate visibility at Class I areas using IMPROVE monitoring data and has also been used for evaluating visibility impacts at Class I areas due to new sources using modeling output of a single source or group of sources. The total light extinction due to a source (b_{source}), in units of inverse Megameters (Mm^{-1}), is assumed to be the sum of the light extinction due to the source's individual PM species concentration impacts times a extinction efficiency coefficient plus Rayleigh (i.e., blue sky) background, that is assumed to be 10 Mm^{-1} .

$$b_{\text{source}} = b_{\text{SO}_4} + b_{\text{NO}_3} + b_{\text{OC}} + b_{\text{EC}} + b_{\text{soil}} + b_{\text{coarse}} + b_{\text{ray}}$$

$$b_{\text{SO}_4} = 3 [(\text{NH}_4)_2\text{SO}_4]f(\text{RH})$$

$$b_{\text{NO}_3} = 3 [\text{NH}_4\text{NO}_3]f(\text{RH})$$

$$b_{\text{OC}} = 4 [\text{OMC}]$$

$$b_{\text{EC}} = 10 [\text{EC}]$$

$$b_{\text{Soil}} = 1 [\text{Soil}]$$

$$b_{\text{coarse}} = 0.6 [\text{Coarse Mass}]$$

$$b_{\text{ray}} = 10 \text{ Mm}^{-1}$$

Here $f(\text{RH})$ are relative humidity adjustment factors. EPA BART modeling guidance recommends that Class I area specific monthly average $f(\text{RH})$ values be used (EPA, 2005; 2003a), which is what we will use in this study. The concentrations in the square brackets are in $\mu\text{g}/\text{m}^3$ and are based on the differences in concentrations between the 2002 BART base case and 2002 BART VOC/PM zero-out case. Although CAMx explicitly models ammonia and ammonium, the IMPROVE extinction equation assumes that SO_4 and NO_3 are completely neutralized by ammonium. The OMC in the above equation is Organic Matter Carbon. When using IMPROVE measurements, the current IMPROVE extinction equation assumed an OMC/OC ratio of 1.4 (i.e., the IMPROVE Organic Carbon, or OC, measurement is multiplied by 1.4 to obtain OMC). Since CAMx directly models OMC, the 1.4 factor is not needed. The following species mappings will be used to map the CAMx species to those used in the IMPROVE reconstructed mass extinction equation given above:

$$\begin{aligned} [(\text{NH}_4)_2\text{SO}_4] &= 1.375 \times \text{PSO}_4 \\ [\text{NH}_4\text{NO}_3] &= 1.290 \times \text{PNO}_3 \\ [\text{OMC}] &= \text{POA} + \text{SOA}_1 + \text{SOA}_2 + \text{SOA}_3 + \text{SOA}_4 \\ [\text{EC}] &= \text{PEC} \\ [\text{Soil}] &= \text{FPRM} + \text{FCRS} \\ [\text{Coarse Mass}] &= \text{CPRM} + \text{CCRS} \end{aligned}$$

Here PSO_4 and PNO_3 are the CAMx particulate sulfate and nitrate species. POA is the CAMx primary Particulate Organic Aerosol species, whereas SOA_1 -4 are the four Secondary Organic Aerosol species carried in CAMx. Primary Elemental Carbon is represented by PEC in CAMx. CAMx carries two species that represent the other $\text{PM}_{2.5}$ components (i.e., fine particles that are not SO_4 , NO_3 , EC or OC), one for the crustal (FCRS) and the other for the remainder of the primary emitted $\text{PM}_{2.5}$ species (FPRM). Similarly, CAMx carries two species to represent Coarse Mass ($\text{PM}_{2.5-10}$), one for crustal (CCRS) and one for other (CPRM).

The Haze Index (HI) for the source is calculated in deciviews (dv) from the source's extinction plus natural background using the following formula:

$$\text{HI}_{\text{source}} = 10 \ln[(b_{\text{source}} + b_{\text{natural}})/10]$$

The source's HI is compared against natural conditions to assess the significance of the source's visibility impact. EPA guidance lists natural conditions (b_{natural}) by Class I areas in terms of Mm^{-1} (EPA, 2003b) and assumes clean conditions with no man-made or weather interference. The visibility significance metric for evaluating BART sources is the change in deciview (del-dv) from the source's and natural conditions haze indices:

$$\begin{aligned} \text{del-dv} &= \text{HI}_{\text{source}} - \text{HI}_{\text{natural}} = 10 \ln[(b_{\text{source}} + b_{\text{natural}})/10] - 10 \ln[b_{\text{natural}}/10] \\ &= 10 \ln[(b_{\text{source}} + b_{\text{natural}})/b_{\text{natural}}] \end{aligned}$$

The visibility impacts from the CAMx BART VOC/PM zero-out run will first be calculated using all PM species. Depending on these results, then separate visibility calculations may be made using just those PM species that may be associated with the elimination of the BART VOC emissions (i.e., PSO_4 , PNO_3 , SOA_1 , SOA_2 , SOA_3 and SOA_4) and then just those species associated with the elimination of the primary PM emissions (i.e., PSO_4 , PNO_3 , POA , PEC ,

FCRS, FPRM, FCRS and CCRS). Note that SO₄ and NO₃ are associated with both VOC and PM: VOC through photochemical reactivity and formation of secondary PSO₄/PNO₃; and primary emitted PSO₄/PNO₃ for PM emissions.

The del-dv impacts will be calculated at all 12 km receptor grid cells in which the 12 km grid intersects any portions of a Class I area. For each day, the maximum del-dv impact across all 12 km grid cells that intersect a Class I area will be used to represent the visibility impact for that day at that Class I area.

The EPA BART guidance suggests that a significance threshold to determine whether a source significantly contributes to visibility impairment at a Class I area should be no greater than 0.5 dv. Thus, if the del-dv due to all potential BART-eligible sources VOC and PM emissions at every Class I area and for all days from 2002 are < 0.5 dv, then VOC and PM emissions from all potential BART-eligible sources would not contribute significantly to visibility impairment and therefore the VOC and PM emissions from each individual potential BART source would not be significant. Under these conditions, VOC and PM emissions no longer need to be considered in the BART analysis for Texas.

If there are any days in 2002 for which the del-dv is greater than 0.5 dv in the BART VOC/PM zero-out screening analysis, the results would be examined in more detail including the analysis of the frequency, magnitude and duration of the visibility impacts. The BART guidance suggests comparing the 98th percentile del-dv at any Class I area with the 0.5 dv significant threshold to determine whether a significant visibility impact would reasonably be expected to occur. Using one year of modeling results (2002), the 98th percentile would correspond to the eighth highest 24-hour average visibility impact at each Class I area. A separate assessment of the contribution of VOC versus PM related PM species may also be performed to determine whether one precursor pollutant or the other is the cause of the del-dv exceeding the 0.5 dv significance threshold. TCEQ will also attempt to identify whether a particular source or group of sources are responsible for the exceedance of the visibility threshold. Additional VOC/PM zero-out runs may be performed using subgroups of potential BART-eligible sources. For example, not including a source that is believed responsible for the visibility threshold exceedance or separating the potential BART-eligible sources into EGU and non-EGU groups.

BART Screening Analysis for PM Emissions Only

If BART screening analysis is desired for primary PM emissions by themselves, then it is much simpler and more computationally efficient to run an inert CAMx simulation with the potential BART-eligible primary PM emissions as input. Gas-phase species and gas-, aqueous- and aerosol-phase chemistry do not affect the primary PM species so these species and chemistry do not need to be simulated when looking at the primary PM impacts. In this case, the BART PM emissions are processed and simulated by the model and only one inert simulation needs to be conducted. Chemistry is turned off in CAMx by setting the "Chemistry" option in the CAMx input file to ".false."

PROCEDURES FOR SCREENING BART SOURCES SO₂ AND NO_x EMISSIONS

The screening analysis for potential BART-eligible non-EGU sources SO₂ and NO_x emissions will use the updated PM Source Apportionment Technology (PSAT) in CAMx and the 2002 36/12 km modeling database described in Section 2. The non-EGU potential BART-eligible sources will be divided up into approximately 10 source groups for the PSAT screening analysis. CAMx/PSAT will be run for the 2002 annual year on the 36/12 km grid with each potential BART-eligible source flagged to use the new PSAT PiG feature.

As described for the zero-out run, if the del-dv due to all sources in a source group at every Class I area and for all days from 2002 is < 0.5 dv, then each individual potential BART-eligible source in the source group would not contribute significantly to visibility impairment. Therefore, the SO₂ and NO_x emissions from each individual potential BART source would not be subject to BART.

At this time we are only considering performing the potential BART-eligible source group PSAT modeling for SO₂ and NO_x emissions from sources that are not Electrical Generating Units (EGUs). As Texas is covered under the PM_{2.5} provisions of the Clean Air Interstate Rule (CAIR) and EPA BART guidance (EPA, 2005) states that CAIR satisfies the BART SO₂ and NO_x requirements for CAIR PM_{2.5} States, then only SO₂ and NO_x emissions from non-EGU potential BART-eligible sources need be considered in this screening analysis.

VISIBILITY IMPACTS FROM PSAT

The sulfate and nitrate families of PSAT source apportionment tracers will be invoked for the PSAT BART screening analysis. The visibility impacts at each Class I area will be calculated in a similar manner as described in Section 3, only the PSO₄ and PNO₃ concentrations from each PSAT BART source group will be used in the extinction equation that is then used to calculate the haze index (HI) and change in deciview (del-dv) from natural conditions due to the SO₂ and NO_x emissions from all of the potential BART-eligible sources in each source group. In this case the IMPROVE reconstructed mass extinction equation for each potential BART-eligible source group will only include the sulfate and nitrate components, as well as Rayleigh background:

$$b_{\text{group}} = b_{\text{SO}_4} + b_{\text{NO}_3} + b_{\text{ray}}$$

$$b_{\text{SO}_4} = 3 [(\text{NH}_4)_2\text{SO}_4]f(\text{RH})$$

$$b_{\text{NO}_3} = 3 [\text{NH}_4\text{NO}_3]f(\text{RH})$$

$$b_{\text{ray}} = 10 \text{ Mm}^{-1}$$

Here f(RH) are the monthly average relative humidity adjustment factors from EPA's guidance (EPA, 2003a). The concentrations in the square brackets are in μg/m³ and are the sulfate and nitrate from the PSAT output for each potential BART-eligible PSAT source group (i) that are assumed to be fully neutralized by ammonium:

$$[(\text{NH}_4)_2\text{SO}_4] = 1.375 \times \text{PS4}_i$$

$$[\text{NH}_4\text{NO}_3] = 1.290 \times \text{PN3}_i$$

The haze index for the source group is calculated in deciview from the source groups extinction plus natural background using the following formula:

$$HI_{\text{group}} = 10 \ln[(b_{\text{group}} + b_{\text{natural}})/10]$$

The source's HI is compared against natural conditions to assess the significance of the source's visibility impact. EPA guidance lists natural conditions (b_{natural}) by Class I areas in terms of Mm^{-1} (EPA, 2003b) and assumes clean conditions with no man-made or weather interference. The visibility significance metric for evaluating BART sources is the change in deciview (del-dv) from the source's and natural conditions haze indices:

$$\text{del-dv} = HI_{\text{group}} - HI_{\text{natural}} = 10 \ln[(b_{\text{group}} + b_{\text{natural}})/10] - 10 \ln[b_{\text{natural}}/10]$$

The 0.5 dv significance threshold will be used to assess whether a potential BART-eligible source group does not contribute significantly to visibility impairment. If the del-dv for each day of 2002 and every 12 km grid cell that intersects with any Class I area is less than 0.5 dv, then the source groups SO₂ and NO_x emissions do not contribute significantly to visibility impairment at any Class I area. EPA's BART guidance suggests using the 98th percentile visibility impact at a Class I area in the visibility significance determination using this approach, then a source group would not have a significant contribution to visibility if the 8th highest 24-hour average del-dv at each Class I area is less than 0.5 dv. Under these conditions the SO₂ and NO_x emissions from each individual potential BART eligible source in the source group also does not contribute significantly to visibility at any Class I area so can be exempt from BART.

Selection of Potential BART-eligible Source Groups for PSAT Modeling

TCEQ is currently discussing the optimal approach for selecting non-EGU potential BART-eligible source groups for PSAT modeling. Originally, the thought was to rank the potential BART-eligible sources by emissions (SO₂ and NO_x) over distance from the nearest Class I area (Q/D) and then divide the list up into 10 decile source groups. This approach would include the smallest emitting sources that are furthest from the Class I areas that are most likely to have an insignificant contribution in one source group, with the largest emitting sources closest to the Class I areas that are most likely to have a significant contribution in another source group. Upon further considerations, however, there may be other criteria that should be factored in when defining the potential BART-eligible source groups for PSAT modeling. For example, it may be advantageous to group sources by source type, which might make control strategy planning and defining what BART is for a particular source type easier in later stages of the BART process. Another consideration may be to use one source group for west Texas EGU potential BART-eligible sources in the event EPA grants the Petition for Reconsideration to remove west Texas EGUs from CAIR. The final configuration may be a hybrid of the above considerations and is under review at TCEQ.

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