

Modeling Guidance

**Guidance for the Application of the CAMx Hybrid
Photochemical Grid Model to Assess Visibility Impacts
of Texas BART Sources at
Class I Areas**

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FOREWORD

This document provides guidance to assist BART-eligible sources prepare for the requirements of the BART rule in Chapter 116 adopted by TCEQ. This document does not substitute for any Clean Air Act provision, EPA regulation, or TCEQ regulation, nor is it a regulation itself. Thus, it does not impose binding, enforceable requirements on any party, nor does it assure that TCEQ will approve all instances of its application. The guidance may not apply to a particular situation, depending upon the circumstances. The TCEQ retains the discretion to adopt approaches on a case-by-case basis that differ from this guidance where appropriate. Any decisions by TCEQ regarding a particular modeling analysis will only be made based on the applicable statute and regulations.

This guidance is a living document and may be revised periodically. Updates, revisions, and additional documentation will be provided at <http://www.tceq.state.tx.us>. As noted above, TCEQ cannot assure that actions based upon this guidance will be fully approvable in all instances. The TCEQ welcomes public comments on this document and will consider those comments in any future revisions of this guidance document, providing such approaches comply with all applicable statutory and regulatory requirements.

Please note several important changes to this guidance:

- In accordance with EPA's BART modeling guidance, Appendix Y of the BART rule (July 6, 2005), **CALPUFF shall be used for** single-source modeling where the distance between the BART source (or potential BART source) and the Class I area is **less than 300 km**. CALPUFF may also be used at distances greater than 300 km, at the source's discretion.
- Since CALPUFF may significantly over predict impacts at greater distances, **CAMx is approved for** situations where the distance is **greater than 300 km**.
- In all cases, modeling **protocols must be approved in advance** by the TCEQ.
- Either CAMx or CALPUFF models may be used for the engineering analysis at any distance between a source and a Class I area.

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GLOSSARY OF ACRONYMS

AERMOD	American Meteorological Society/Environmental Protection Agency Regulatory Model Improvement Committee Model
AQRVs	Air Quality Related Values
BART	Best Available Retrofit Technology
b _{natural}	Clean Natural Conditions
b _{source}	Total light extinction due to a source
CAA	Clean Air Act
CAIR	Clean Air Interstate Rule
CALPUFF	California Puff Model
CAMx	Comprehensive Air Quality Model with extensions
CCRS	Coarse Crustal particulate matter
CENRAP	Central Regional Air Planning Association
CMAQ	Community Multiscale Air Quality Modeling System
CPRM	Coarse other Primary particulate matter
del-dv	change in deciview (delta-deciview)
dv	deciviews
EC	Elemental Carbon
EGU	Electrical Generating Units
EPA	United States Environmental Protection Agency
f(RH)	Relative Humidity adjustment factor
FCRS	Fine Crustal particulate matter
FIPS	Federal Information Processing Standard
FLAG	Federal Land Managers Air Quality Related Values Workgroup
FLM	Federal Land Manager
FPRM	Fine other Primary particulate matter
FR	Federal Register
GREASD	Greatly Reduced and Simplified Dynamics
Hg	Mercury
HI	Haze Index
IMPROVE	Interagency Monitoring of Protected Visual Environments
IRON	Incremental Reactions for Organics and Nitrogen Oxides
ISC	Industrial Source Complex Model
km	kilometers
LSODE	Livermore Solver for Ordinary differential Equations
Mm ⁻¹	Inverse Megameters
MRPO	Midwest Regional Planning Organization
MW	Megawatt
NH ₄	Ammonium
NO ₃	Particulate Nitrate
non-EGU	Non-Electrical Generating Units
NO _x	Nitrogen Oxides
NSR	New Source Review
OC	Organic Carbon
OMC	Organic Matter Carbon
OSAT	Ozone Source Apportionment Technology
PEC	Primary Elemental Carbon
PGM	Photochemical Grid Model
PiG	Plume-in-Grid

PLUVUE	Plume Visibility Model
PM	Particulate Matter
PM ₁₀	Particulate Matter with aerodynamic diameters less than 10 microns
PM _{2.5}	Particulate Matter with aerodynamic diameters less than 2.5 microns
POA	Primary Organic Aerosol
PPM	Piecewise-Parabolic Method
PSAT	Particulate Matter Source Apportionment Technology
PSD	Prevention of Significant Deterioration
QAPP	Quality Assurance Program Plan
RH	Relative Humidity
RHR	Regional Haze Rule
RPO	Regional Planning Organization
SCICHEM	Second-order Closure Integrated Puff model with CHEMistry
SCIPUFF	Second-order Closure Integrated Puff model
SIP	State Implementation Plan
SMOKE	Sparse Matrix Operator Kernel Emissions
SO ₂	Sulfur Dioxide
SO ₄	Sulfate
SOA	Secondary Organic Aerosol
TCEQ	Texas Commission on Environmental Quality
TIP	Tribal Implementation Plan
tpy	ton per year
VISTAS	Visibility Improvement State and Tribal Association of the Southeast
VOC	Volatile Organic Compounds
WRAP	Western Regional Air Partnership

INTRODUCTION

OVERVIEW

The final version of United States Environmental Protection Agency's (EPA) Regional Haze Regulations that include the Best Available Retrofit Technology (BART) Guidelines was published in the Federal Register on 6 July 2005 (70 FR 39104; EPA, 2005). One of the provisions of the program is the requirement that certain existing stationary sources emitting visibility-impairing air pollutants install and operate BART. The regulations require case-by-case BART determinations to define specific emissions limits representing BART. The regulations also establish schedules for compliance for each source subject to BART. These requirements will be part of the State Implementation Plan (SIP) revisions that Texas must submit to EPA by 17 December 2007. Sources are subject to BART if they can be reasonably anticipated to cause or contribute to visibility impairment at a Class I area. Once a source is determined to be subject to BART, an engineering analysis and determination of the degree of visibility improvement due to BART controls must be performed. The EPA BART Guidelines suggest several potential methods for determining whether a source is subject to BART and the methods for determining what the expected visibility benefits of the BART controls will be, including dispersion modeling.

For the subject to BART assessment, EPA BART Guidelines state that "You can use CALPUFF, or another EPA approved model, to predict the visibility impacts from a single source at a Class I area" (EPA, 2005). For the visibility improvement determination, EPA BART Guidelines state "Use CALPUFF, or other appropriate dispersion model to determine the visibility improvement expected at a Class I area from the potential BART control technology applied to the source" (EPA, 2005). For the subject to BART modeling, cumulative modeling may also be conducted to show that no source in a State is subject to BART. This cumulative BART exemption modeling may be done "on a pollutant by pollutant basis or for all visibility-impairing pollutants to determine if emissions from these sources contribute to visibility impairment" (EPA, 2005). BART Guidelines suggest using California Puff Model (CALPUFF) or a photochemical grid model to perform the cumulative group exemption modeling, but notes "if you wish to use a grid model, you should consult with the appropriate EPA Regional Office to develop an appropriate modeling protocol" (EPA, 2005).

The purpose of this document is to provide sources in Texas with guidelines for preparing a modeling protocol and modeling analysis using the Comprehensive Air Quality Model with extensions (CAMx) grid model. Sources also have the option to use CALPUFF. See TCEQ's BART webpage for information on the Texas CALPUFF Modeling Guidelines (<http://www.tceq.state.tx.us/implementation/air/sip/bart/haze.html>).

Sources performing modeling will be required to submit a modeling protocol to the TCEQ for approval. Protocols must also be made available concurrently to EPA and Federal Land Managers (FLM) for their review.

The report accompanying the source-specific subject-to-BART screening analysis should provide a clear description of the modeling procedures and the results of the analysis. An electronic archive that includes the full set of inputs and model output fields should also be included with the report.

TCEQ BART Screening Exemption Modeling

TCEQ has performed cumulative group BART screening exemption modeling (Morris and Nopmongcol, 2006) using the Comprehensive Air Quality Model with extensions (CAMx). CAMx is a photochemical grid model (PGM) that incorporates the latest scientific advances including current state of science treatment of transport, dispersion deposition and chemical transformation (gas-phase and aqueous-phase chemistry and aerosol chemistry and dynamics). As required in the EPA BART Guidelines, a modeling protocol was prepared (ENVIRON, 2005) and distributed to EPA and the FLMs prior to the BART cumulative exemptions screening analysis for their review. Three types of BART screening exemption modeling were conducted (Morris and Nopmongcol, 2006):

- BART sources Volatile Organic Compounds (VOC) zero-out modeling to ascertain whether or not Texas BART VOC emissions cause or contribute to visibility impairment on any Class I areas;
- BART sources primary particulate matter (PM) zero-out and chemically inert modeling to ascertain whether or not BART primary PM emissions cause or contribute to visibility impairment on any Class I areas; and
- BART sources SO₂ and NO_x modeling using the PM Source Apportionment Technology (PSAT) and the Plume-in-Grid (PiG) subgrid-scale point source model.

Concerns have been raised regarding the use of PGMs for single source assessments, such as a BART visibility assessment. These concerns revolve around:

(1) PGMs can only resolve the dynamics and chemistry of a point source plume to the grid resolution specified and use of a high resolution grid (e.g., 100 m to 1 km) to resolve a plume would require extensive model inputs and model run times; and

(2) to assess the impacts of a source two runs have to be performed, a base case with the source and a zero-out case where the emissions of the source are eliminated. As PGM runs are already more costly than a source-oriented plume model, like CALPUFF, the need to do multiple zero-out runs to assess the individual impacts of multiple sources is quite costly. Recent advances in the CAMx model development have alleviated these concerns regarding the use of PGMs for single source assessments as follows (Morris, Emery and Yarwood, 2006):

- Implementation of the PM Source Apportionment Technology (PSAT) that allows the separate tracking of individual source PM impacts so that the individual impacts from many different sources can be obtained cost-effectively in one run;
- The threading of the PSAT PM source apportionment through the full-chemistry PiG module so that the early plume chemistry and plume dynamics can be tracked by the subgrid-scale PiG module until the plume size is commensurate with the grid resolution when the plume can be adequately simulated by the grid model; and

- Implementation of flexi-nesting whereby finer nests can be specified inside of a coarser grid and the model can interpolate some or all of the model inputs from the coarse grid, which allows better resolution of point source plume chemistry and dispersion.

Purpose

Although CAMx now has the capability to cost-effectively estimate the air quality and visibility impacts of individual sources, being that it is a relatively new technology, the procedures for performing such a single source assessment using CAMx/PSAT/PiG are not fully documented. Thus, this document will provide guidance in the application of CAMx for single source assessments as needed for BART, New Source Review (NSR) and Prevention of Significant Determination (PSD) assessments. The TCEQ BART screening exemption modeling is used as an example approach for these types of assessments.

BACKGROUND

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 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.

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

In EPA's 1 August 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. Texas, however, will not be participating in this program.

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 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 may be most useful in identifying 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' plant example in their BART guidance pertains to exempting sources whose SO₂, NO_x or SO₂ plus NO_x emissions are less than 500 tons per year (tpy) and are greater than 50 km from any Class I area, or for sources whose emissions are less than 1,000 tpy and are greater than 100 kilometers (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 as a contribution threshold may exempt sources that emit less than 500 tons per year 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 1000 tons per year 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. Texas used the model plant option as an initial screening method of its BART sources.

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 and thus no source should be subject to BART. You may do this on a pollutant by pollutant basis or for all visibility-impairing pollutants to determine if emissions from these sources contribute to visibility impairment.

While EPA identifies several options for determining whether 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 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 – sulfate, nitrate, organic carbonaceous matter, elemental carbon, other fine particles and coarse mass – 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 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 a 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 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, "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 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, as well as, more accurate and scientifically correct treatment of secondary PM formation (e.g., sulfates and nitrates) and regional transport and dispersion.

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 7 August 1962 and 7 August 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 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 to 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.

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 contribute 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 (EPA, 2003c). 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.

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. The atmospheric diffusion equation applies equally to many 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). 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 modeling ignores a 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 databases 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, today, quite comparable with and often less than a traditional PSD modeling study using plume models, such as Industrial Source Complex Model (ISC), CALPUFF, or The 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 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. 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; 2006), 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 sulfate (SO₄), nitrate (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 FLM.) However, for the BART modeling in Texas, a photochemical grid model (PGM) 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 screening BART exemption runs 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 are estimated are a great distance from the source. The sources that have not yet screened out of BART, based on the CAMx runs already performed on behalf of TCEQ, are between 97 and 654 km from the nearest Class I area. Of the 67 sources remaining, 50 are more than 300 km from the nearest Class I area;
- TCEQ has conducted analyses to identify which of the many potential BART-eligible sources satisfy the three criteria for being BART-eligible. Some of these sources have been determined to make an insignificant contribution to visibility impairment at Class I areas as a group, resources can now be focused on those sources determined most likely to impact visibility in Class I areas (Morris and Nopmongcol, 2006);
- Use of a PGM allows for the quantitative assessment of the visibility impacts due to potential BART-eligible sources' VOC and PM emissions;
- Use of a PGM provides an evaluation of the cumulative impact of BART-eligible sources on visibility in Class I areas; and
- Use of a hybrid PGM that uses a full-chemistry PiG module for near-source plume chemistry and dynamics and a three-dimensional grid model for plume chemistry, transport and dispersion at farther downwind distances contains all of the scientific advantages of both CALPUFF and a PGM while treating secondary PM formation using full-science algorithms at all scales.

2.0 CAMx BART MODELING APPROACH

In this section we describe the general modeling approach used to perform the BART screening analysis of potential BART-eligible sources in the state of Texas using the CAMx PGM. This modeling approach is used as an example for how the CAMx, with its PSAT and PiG features, can be used to perform single source or groups of sources visibility assessments as part of the BART exemption and visibility improvement steps. The approach could also be used for air quality and Air Quality Related Values (AQRVs) assessments from proposed new or modified sources as part of the NSR and PSD process (Morris, Emery and Yarwood, 2006). There are two elements that were performed in the Texas BART screening exemption modeling using CAMx:

- 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 significant or not.

Both elements of the screening analysis used the same 36/12 km 2002 annual database. The VOC and PM emission screening analysis was performed using emissions zero-out modeling and inert primary PM modeling, whereas the group of sources' SO₂ and NO_x emissions screening analysis was performed using the PSAT that has been implemented in the full-chemistry PiG. The SO₂ and NO_x emissions analysis could also include the PM PSAT family of source apportionment tracers (and SOA/VOC family as well) and could also be applied for EGU sources.

VERSION OF CAMx

CAMx Version 4.4β (V4.4β) was used in the Texas BART screening exemption modeling analysis. CAMx V4.4β is an updated version to CAMx V4.31 (ENVIRON, 2005) that is currently (August 2006) publicly available on the CAMx website for no cost (www.camx.com). CAMx V4.4β includes several updates to CAMx V4.31, including the implementation of the PSAT within the full-science PiG. CAMx V4.4β is available on request, but is undergoing final testing and will be posted to the CAMx website with an updated user's guide and test case shortly (late summer or early fall 2006).

2002 ANNUAL 36/12 KM MODELING DATABASE

The Texas BART screening analysis exemption modeling was performed using a 2002 annual regional photochemical modeling database that was developed as part of the Central Regional Air Planning Association (CENRAP) regional haze work. CENRAP has developed a 2002 annual modeling database for CAMx on the 36 km unified national Regional Planning Organization (RPO) grid that covers the continental US. 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 we provide additional information related to 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 has updated the CAMx 2002 36 km Base A emissions to Base B and CAMx version 4.30. The Base B base case database was the starting point for the Texas BART exemption modeling screening analysis.

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

- Big Bend, Guadalupe Mountains, Carlsbad Caverns National Parks;
- Salt Creek Wichita Mountains Wildlife Refuges and White Mountain; and
- Caney Creek, Upper Buffalo and Hercules Glade Wilderness Areas.

Figure 2-1 displays the 36/12 km nested grid structure that was used in the Texas 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 was used to incorporate the 12 km Texas grid within the CENRAP 36 km modeling domain. Full flexi-nesting was invoked in which CAMx internally interpolates all of the meteorological, emissions and other inputs from the 36 km grid to the 12 km grid. This option has the desired effect of allowing the BART point source plumes' chemistry, transport and dispersion to be represented and resolved by the higher resolution 12 km grid after treatment of their near-source plume chemistry and dynamics using the subgrid-scale PiG module when plume size is below 12 km.

If BART or similar assessments using CAMx are desired, a new 12 km grid flexi-nest could be defined focused on the selected states and nearby Class I areas.

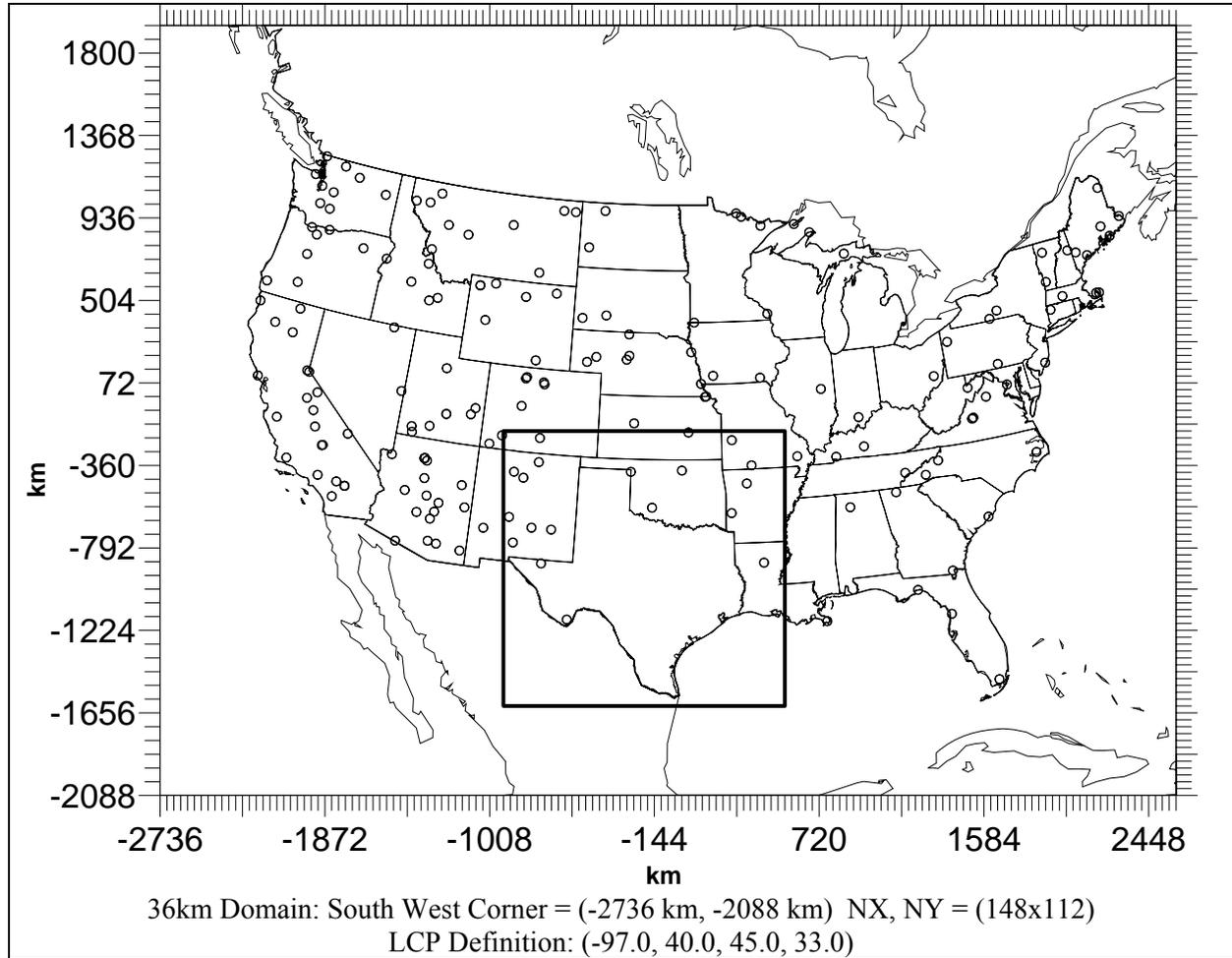


Figure 2-1. Texas BART modeling 36/12 km modeling domain and locations of the IMPROVE monitoring sites that include Class I areas (indicated by circles).

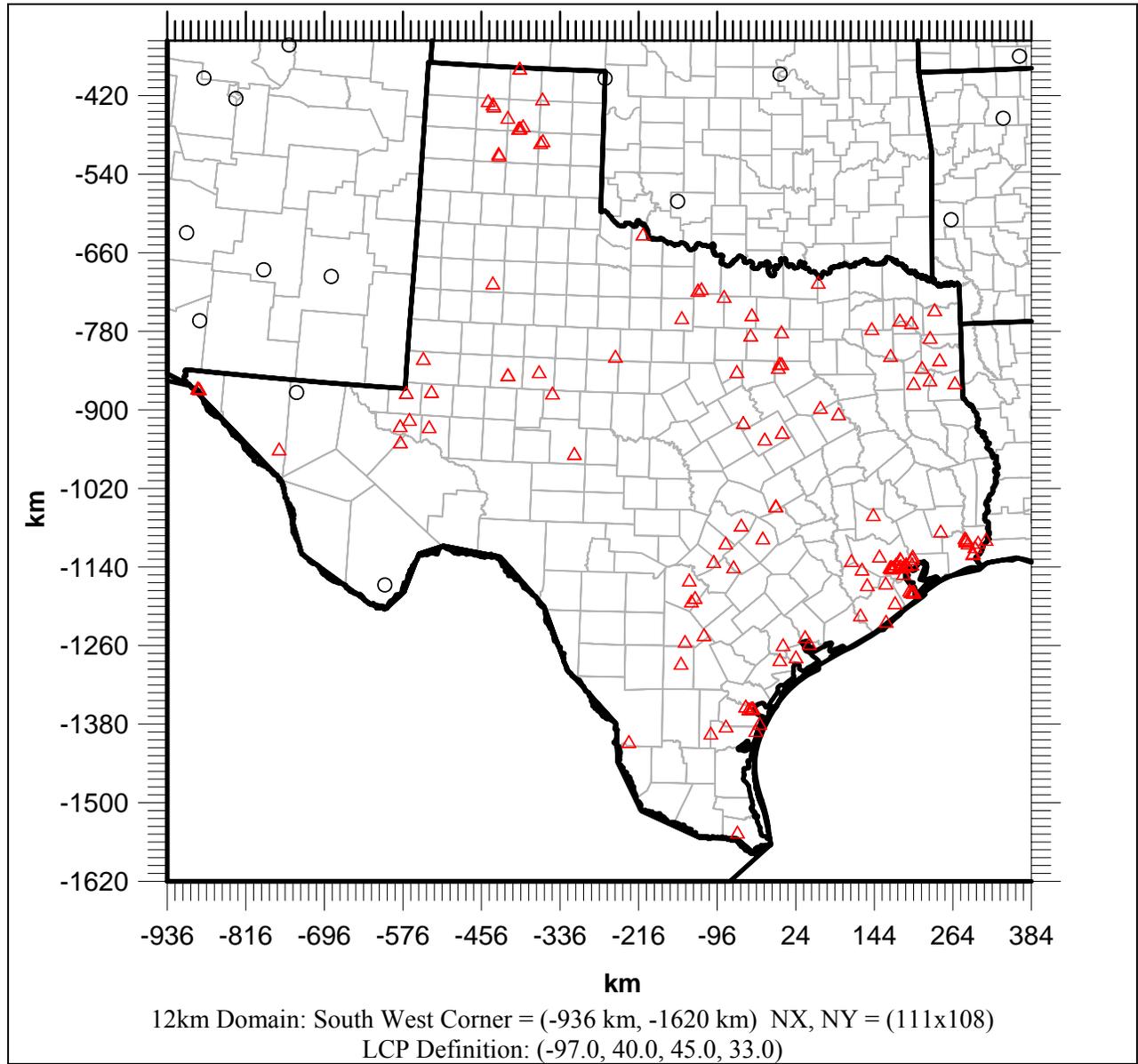


Figure 2-2. Texas BART modeling 12 km modeling domain and locations of the IMPROVE monitoring sites (indicated by circles) that include Class I areas and locations of potential BART-eligible sources in Texas (indicated by triangles).

ENHANCEMENTS TO THE PM SOURCE APPORTIONMENT TECHNOLOGY

To estimate the air quality and/or visibility impacts from a single source or group of sources, the CAMx model PSAT is used. PSAT was updated to be compatible with the CAMx PiG module (CAMx V4.4β). Below we describe 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 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 region 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 or 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_x, VOCs) are several steps removed from the resulting PM species (NO₃, SOA). The PSAT tracers for each type of PM are listed below. 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 9 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_i) which must be weighted by the average hydroxyl radical (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 ARO 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 AND NEW FULL-SCIENCE CHEMISTRY PiG

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.

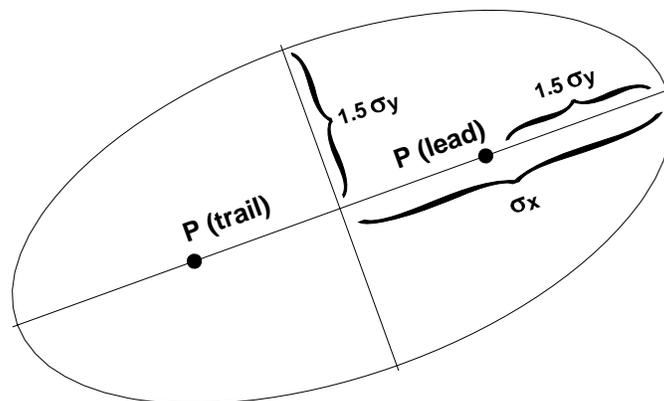


Figure 2-3. Schematic representation of CAMx PiG puff shape in the horizontal. Directional orientation of the puff is arbitrary, and evolves during the aging of the puff according to wind direction, shears and diffusive growth along its trajectory.

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:

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

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 $\langle x' \bar{u}' c' \rangle$, where $\bar{u}' c'$ 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 $\langle x' \bar{u}' c' \rangle$ 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, $\langle x' \bar{u}' c' \rangle = \langle y' \bar{v}' c' \rangle$. This results in a single diffusivity equation for both x and y directions, and a single diffusivity for the z direction:

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

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

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). Note that we ignore the off-diagonal contributions to puff spread, 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:

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

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:

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

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.

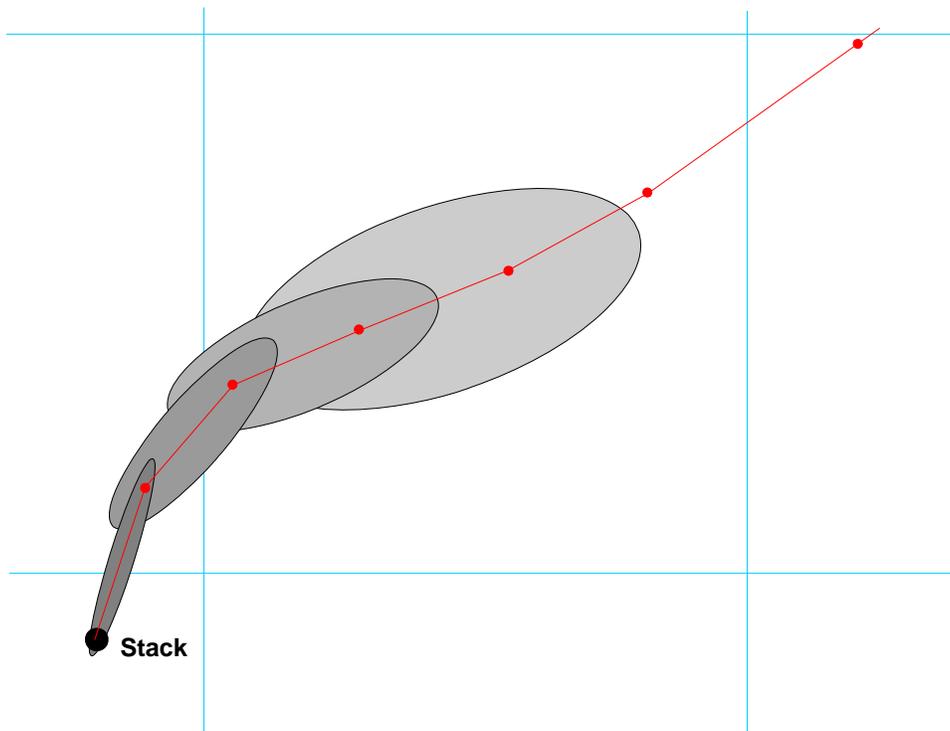


Figure 2-4. Schematic representation of a chain of PiG puffs emitted from a point source into an evolving gridded wind field. The red line connected by dots represents puff centerlines, with dots representing leading and trailing points of each puff. The CAMx computational grid is denoted by the blue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

This section presents the procedures that can be used to perform cumulative BART screening exemption modeling for combined VOC and PM emissions and for PM emissions alone. Details on the steps needed to perform this analysis, selection of the recommended CAMx options and scripts and computer operation notes are provided in Chapter 5.

OVERVIEW OF APPROACH

One type of BART screening analysis using CAMx would be to estimate the cumulative visibility impacts at Class I areas due to VOC and PM emissions from all potential BART-eligible sources. To address impacts due to both VOC and NO_x emissions 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.

For the Texas screening analysis, the 2002 BART Base Case Emissions Scenario was based on the CENRAP 2002 Typical Base Case emissions scenario, although other base case scenarios could also be used (e.g., 2002 Western Regional Air Partnership/WRAP, Visibility Improvement State and Tribal Association of the Southeast/VISTAS, Midwest RPO base cases, CAIR 2001 base case, etc.). The EPA BART guidelines require that BART modeling use the maximum actual 24-hour emissions for each BART-eligible source (excluding start up and shut down). The 2002 base case scenarios typically contain 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 2002 Base Case emissions scenario were doubled as recommended by EPA Region 6. Doubling the average emissions provides a conservative estimate of maximum 24-hour emissions for most sources.

Visibility Calculations

Visibility impacts are calculated at each Class I area using the differences in 24-hour PM concentrations between the 2002 Base Case and 2002 BART Sources VOC and PM Emissions Zero-Out Case scenarios following the procedures given in EPA's BART modeling guidance (EPA, 2005) that are based on 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 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 an extinction efficiency coefficient:

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

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

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

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

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

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

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

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). 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 (OMC). 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 are used to map the CAMx species to those used in the IMPROVE reconstructed mass extinction equation given above:

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

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

$$[\text{OMC}] = \text{POA} + \text{SOA1} + \text{SOA2} + \text{SOA3} + \text{SOA4} + \text{SOA5}$$

$$[\text{EC}] = \text{PEC}$$

$$[\text{Soil}] = \text{FPRM} + \text{FCRS}$$

$$[\text{Coarse Mass}] = \text{CPRM} + \text{CCRS}$$

Here PSO_4 and PNO_3 are the CAMx particulate sulfate and nitrate species. POA is the CAMx primary Particulate Organic Aerosol species, whereas SOA1-5 are the five 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 coarse PM (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:

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

Here, b_{natural} is the Class I area specific clean natural visibility background where EPA's default values will be used in this analysis (EPA, 2003b).

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 area 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 can be calculated using all PM species to assess the visibility impacts due to the elimination of both VOC and PM emissions. Separate visibility calculations may be made using those PM species that may be associated with the elimination of the BART VOC emissions (i.e., SOA1, SOA2, SOA3, SOA4 and SOA5) and then those species associated with the elimination of the primary PM emissions (i.e., PSO4, PNO3, POA, PEC, FCRS, FPRM, FCRS and CCRS).

The del-dv impacts will be calculated at all Class I areas of interest. For each day, the maximum del-dv impact in a Class I area will be used to represent the visibility impact for that day at that Class I area.

Significance Threshold

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.

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 should 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 significance 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.

The separate assessment of the contribution of VOC (SOA1-5) versus primary PM related PM species should be examined to determine whether one precursor pollutant or the other is the cause of the del-dv exceeding the 0.5 dv significance threshold.

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.” (see Appendix A or B for example CAMx run control input files).

4.0 PROCEDURES FOR SCREENING BART SOURCES USING PSAT AND PiG

This section discusses the procedures for using CAMx with the PSAT and full-chemistry PiG subgrid-scale plume module for single source or multiple source BART or similar (e.g., NSR/PSD) modeling. Although the Texas PSAT/PiG BART screening analysis addressed impacts of SO₂ and NO_x emissions from BART non-EGU sources, the general approach can be used for all visibility impairing pollutants (i.e., NO_x, SO₂, PM, VOC and NH₃) as well as for both EGU and non-EGU sources. However, the PSAT computational requirements for simulating Secondary Organic Aerosol (SOA) formation from VOCs are more extensive than for the other PSAT families (see Chapter 2). In addition, the contributions of SOA due to BART type source VOC emissions to visibility impairment at Class I areas is extremely small. Thus, if VOC emissions are an issue, it is recommended that they first be addressed through a zero-out run as described in Chapter 3.

Specifics on the steps and options to be specified for running CAMx/PSAT/PiG for BART and similar assessments are provided in Chapter 5.

SUMMARY OF APPROACH

The updated PSAT that includes the new PiG module in CAMx Version 4.4 (and later versions) is used in the single source or multiple source BART analysis. For the Texas application, the 2002 36/12 km modeling database described in Section 2 was used. The Texas CAMx/PSAT/PiG source apportionment divided the non-EGU potential BART-eligible sources into several source groups for the screening analysis. CAMx/PSAT was 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 in Chapter 3, 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.

Visibility Impacts from PSAT

In the Texas CAMx/PSAT/PiG BART modeling, the sulfate (SO₄) and nitrate (NO₃) families of PSAT source apportionment tracers were invoked for the PSAT BART screening analysis. However, in the discussion below we try to be more general and include a discussion of how you would use the PSAT tracers for the primary PM and SOA PSAT families of PM source apportionment. However, as noted above, it is highly desirable to screen out the VOC emissions (and primary PM if possible) as a significant visibility contributor as the computational requirements of the PSAT SOA family of tracers is greater than the other PSAT families.

The visibility impacts at each Class I area will be calculated in a similar manner as described in Section 3 that uses the IMPROVE reconstructed mass extinction equation. Only concentrations from each PSAT BART source group will be used to calculate the Haze Index (HI) and change in deciview (del-dv) from natural conditions.

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

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

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

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

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

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

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

Here $f(\text{RH})$ are the monthly average relative humidity adjustment factors from EPA's guidance (EPA, 2003a). The concentrations in the square brackets are in $\mu\text{g}/\text{m}^3$ and are the concentrations from the PSAT output for each potential BART-eligible PSAT source group (i) with sulfate and nitrate assumed to be fully neutralized by ammonium. Using the PSAT species naming convention (see Chapter 2) these concentrations are as follows:

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

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

$$[\text{OMC}] = \text{POA}_i + \text{PO1}_i + \text{PO2}_i + \text{PO3}_i + \text{PO4}_i + \text{PO5}_i$$

$$[\text{EC}] = \text{PEC}_i$$

$$[\text{Soil}] = \text{PFC}_i + \text{PFN}_i$$

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

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

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:

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

The 0.5 dv significance threshold is used to assess whether a potential BART-eligible source or source group contributes 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 SO_2 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 .

5.0 DETAILS ON MODELING PROCEDURES

This section provides the details on the modeling procedures discussed in Chapters 4 and 5 for a single BART source or a group of BART sources, or a similar type of modeling analysis using CAMx. Example CAMx run scripts for a base case run as used in the Texas VOC and PM zero-out run is provided in Appendix A, and an example CAMx run script for a Texas BART PSAT/PiG modeling analysis is provided in Appendix B.

VOC AND PM ZERO-OUT MODELING

The CAMx VOC and PM zero-out modeling of BART emissions is conceptually straight forward and involves two runs: a base case simulation and a simulation with all VOC and PM emissions from the BART sources eliminated. For the Texas BART screening analysis, the CENRAP 2002 36 km Base B base case was the starting point for the analysis. The EPA BART Guidelines require the use of maximum actual 24-hour emission rates. Sources will need to determine their actual 24-hour maximum emission rate for use in their modeling analyses. The first step in the analysis is the Sparse Matrix Operator Kernel Emissions (SMOKE) emissions processing of the BART sources 24-hour maximum emission rates.

Compiling Emissions

1. Process the base case emissions with all emissions using SMOKE.
2. Separate BART sources 24-hour maximum actual VOC and PM emissions from 2002 base case emissions.
3. Separately process VOC and PM emissions from BART sources alone using SMOKE.
4. Zero-Out BART VOC and PM emissions inputs are obtained by subtracting the BART VOC and PM emissions (Step 3) from the base case emissions (Step 1).

Once the base case with the 24-hour maximum actual BART VOC and PM emissions and zero-out BART VOC and PM emissions model-ready emission inputs have been prepared, CAMx modeling and post-processing is performed in the following steps:

Running and Post-Processing CAMx

1. Perform CAMx runs for both zero-out and 24-hour maximum actual BART VOC and PM emissions scenarios.
2. Post-process the CAMx BART modeling results. This step involves extracting concentration data from the hourly average concentrations output files (*avrg and *favrg) which have a binary format (refer to the CAMx user's guide) and calculating 24-hour average concentrations from the hourly concentrations.

3. For each Class I area, calculate the change in 24-hour average concentrations of SOA (SOA1-4) from 24-hour maximum actual scenario and the zero-out scenario. Repeat the same steps to obtain two 24-hour average PM (non-SOA species) concentrations.
4. Calculate the mass extinction (b_{source}) and the difference in deciview (del-dv) from the source's and natural conditions haze indices. The formulation is described in Chapter 4.
5. Compare the 98th percentile del-dv at any Class I area with the 0.5 dv significance threshold. The delta deciview at the 98th percentile would correspond to the eighth highest 24-hour average visibility impact at each Class I area during the modeled year.

Appendix A lists an example CAMx script for the 2002 base case with 24-hour maximum actual Texas BART VOC and PM emissions. The script for the 2002 zero-out BART VOC and PM emissions would be similar, with the file names changed for the output files and the point source emission inputs. Changes from the standard CENRAP 2002 Base Case CAMx modeling script are:

- File names and locations to conform with current modeling;
- Addition of a second grid nest centered over Texas using a 12 km resolution grid (e.g., Number_of_Grids = 2,); and
- Specifying no input files for the second grid so that full flexi-nesting of the 12 km grid inputs from the 36 km grid will be used.

The differences in concentrations at each Class I receptor area will be extracted from the binary output files from the two CAMx runs. The visibility calculations described in Chapter 4 can then be performed using an Excel spreadsheet.

PSAT MODELING

PSAT apportions PM components among several source groups as specified by the user. Source groups consist of a source region, defined by a source region map provided as input, and source categories, that are defined by the low-level and point source emission inputs that can be input for each of the PSAT source category. For example, the source region map could divide the domain into 10 different geographic areas (e.g., states) and separate emissions files could be provided for 4 source categories (e.g., biogenic, mobile, area or point) resulting in 40 source groups to be tracked (initial and boundary conditions are always tracked as two source groups).

For the PSAT BART modeling, each BART source or group of BART sources for which separate PM source apportionment is desired needs to be separately identified as a unique source group in the PSAT run. One way of doing this is to have multiple sets of the point source emission inputs with the first one being all point sources with their full emissions, the second one would be all point sources but with all emissions set to zero except those for the first BART source group, the third one would have all point source emissions zeroed-out except the second BART source group, etc. The CAMx PSAT could then be run using these different point source emissions source groups as inputs for each PSAT source group and with a source region map that included one region for the whole modeling domain.

However, for the Texas BART PSAT screening modeling we used an alternative approach using the PSAT/OSAT “point source override” feature. This was done by having a source region map with one source region for the entire domain and assigning a separate source region value in the point source input file that will override the source region that the point source resides in. In addition, a negative flag has to be set for source stack diameters in order for the BART point source to receive the PiG treatment. PSAT outputs require significant disk space. An annual run can take up to 450 gigabytes (GB) (excluding the deposition and the restart (*.depn and *.inst.1.) files. The steps for setting up the BART PSAT emissions are as follows:

Compiling Emissions

1. Process emissions from BART sources separately from non-BART sources. If there is more than one source group, the BART emission file must carry facility information including Federal Information Processing Standard (FIPS) codes, plant ID and stack ID to cross reference each point source to a point index list. In SMOKE, users have an option to create an elevated-point source input file in an ASCII format that contains all of this necessary information.
2. Assign the point index for each source group in the (unused) kcell¹ value on the point source file to a unique value for that source group.
3. Use maximum 24-hour actual NO_x and SO₂ emissions for the BART sources.
4. Set the stack diameters negative for the BART sources for PiG treatment.
5. Steps 2-4 can be accomplished by using “PIGSET_BART” program which outputs a binary CAMx-ready point source file.
6. Append BART emissions to non-BART emissions. This step can be achieved by using “PTSMRG” program.
7. Make a duplicate of the emission file and rename the copy. This step is necessary because the PSAT source apportionment tool needs to read the same emission file as the CAMx host model and once the CAMx main module is accessing it you can not open the file again for reading by PSAT.

Once the PSAT emission files have been generated, then CAMx can be run to obtain separate PM source apportionment modeling results for each individual BART source or group of BART sources as desired. Appendix B lists an example CAMx script for one of the Texas PSAT source apportionment model simulations. The screening analysis demonstrated that Texas BART sources’ VOC emissions are insignificant to the visibility impairments at Class I areas (Morris and Nopmongcol, 2006). In addition, this screening analysis indicated that only some facilities contribute significantly to the visibility impairments. Consequently, for the Texas BART screening modeling, PSAT was run only for the SO₄ and NO₃ families of PSAT tracers. This approach, however, could be extended to the PM and SOA families as well.

Running CAMx with PSAT

8. Create a fixed-width format ASCII receptor definition input file. This file contains the location of Class I areas in the coordinate system of the CAMx grid. For example:

¹ The kcell value for each stack is contained in the time-variant portion of the elevated point source file. The value is typically ignored, except as flag for OSAT/PSAT point source override.

- POINT BAND1 -831.124 -424.425
9. Generate source area region maps for a master grid and nested grids. The source area mapping file assigns each grid cell to a specific geographic source region. The format of this file is an array of integer numbers (3i) corresponding to the CAMx domain (refer to the CAMx's user guide). For PSAT run, assign the same unique number, which is different from BART source groups, to every grid cell. For example, if BART source groups range from 1-10, assign number 11 to every grid cell in the source region map file. This unique number represents a group number of area and non-BART sources. Point source override in CAMx will discard this number and replace it with a user-specified BART source groups.
 10. PSAT is invoked within the CAMx control file. In the &CAMx_Control namelist module, the variable Probing_Tool must be set to "PSAT" and Pig_Submodel must be set to "GREASD".
 11. In the &SA_Control namelist, provide the name of SA_Receptor_Definitions and SA_Source_Area_Map files. For Texas application set PSAT_Treat_SULFATE_Class and PSAT_Treat_NITRATE_Class to "true" for SO₄ and NO₃ PSAT families.
 12. Emission and meteorological inputs are optionally provided for the nested grid. If these files are not supplied, the Flexi-Nest algorithm within CAMx will interpolate the missing fields from the parent grid. In the Texas screening analysis case, 12 km Flexi-Nest was turned on.
 13. Perform CAMx 36/12km run. 15 spin-up days is recommended.
 14. PSAT output is in the receptor concentration file (*.sa.receptor) which contains information for all receptors and all 24 hours for each simulation day. This is a text format that users can use any scripting language to extract the data.
 15. Post processing of BART results to estimate visibility for each Class I area is conducted as follows. First, use 24-hour average concentrations of sulfate and nitrate to calculate the mass extinction (b_{source}). Second, calculate the Haze Index (HI) and the change in deciview (del-dv) from the source's and natural conditions HI. The formulations of these two steps are described in Chapter 4. Finally, compare the 98th percentile del-dv at any Class I area with the 0.5 dv significant threshold. The deciview that the 98th percentile would correspond to is the eighth highest 24-hour average visibility impact at each Class I area.

The example CAMx script in Appendix B for a Texas PSAT SO₄ and NO₃ run is similar to the standard CENRAP CAMx 2002 base case script with the following changes:

- File names and locations were changed to be consistent with current applications;
- Number of grids changes to 2 with a 12 km grid added over Texas and surrounding regions;
- No input files specified for 12 km grid so that full flexi-nesting can be used;
- The "Probing Tool" option is set to PSAT; and
- The BOTT advection solver (BOTT, A. 1989) is specified rather than Piecewise-Parabolic Method (PPM).

The PPM solver was used in the zero-out runs. However, the BOTT advection solver was used in the PSAT run because it is more computationally efficient.

COMPUTATIONAL REQUIREMENTS

This section provides some example CAMx configurations for 36/12 km domain with flexi-nesting and associated system requirements when run on a dual-processor LINUX Power Management (PM) (with Operations and Management Platform-OMP).

Table 5-1. Example of computer requirements on a dual-processor Athlon 2800+ (2.1 Ghz) PC.

Run	Configuration	Memory	Disk Usage (excluding *inst.1 and *depn)	CPUs	Execution Time
VOC and PM zero-out	Chemistry turned on (Mechanism 4 CF)	356mB	255 MB/episode day	2	4 hrs/episode day
PM zero-out	Chemistry turned off	245mB	46.5 MB/ episode day	2	20 mins/ episode day
PSAT	10 Point Source Groups	1278mB	1.25 GB/ episode day	2	6.5 hrs/ episode day

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Appendix A

Example CAMx Run Script for a
Base Case or Zero-Out Run

```

#!/bin/csh
#
# CAMx 4.4beta OMP
#
setenv NCPUS 2
setenv MPSTKZ 128M
limit stacksize unlimited
#
set EXEC      =
"/disk52/tceq.bart/camx/src.v4.30.bart2/CAMx.tceq.bart.pg_linux"
#
set RUN       = "v4.30.tceq.bart.12FE"
set CHEM      = "/disk52/cenrap/camx/inputs/others"
set LUSE      = "/disk52/cenrap/camx/inputs/landuse"
set AHOMAP    = "/disk52/cenrap/camx/inputs/ahomap"
set PHOT      = "/disk52/cenrap/camx/inputs/tuv"
set ICBC      = "/disk52/cenrap/camx/inputs/icbctc"
set MET       = "/disk52/cenrap/camx/inputs/met"
set EMIS      = "/disk52/tceq.bart/camx/input/emis"
set OUTPUT    = "/swamp4/tceq.bart/camx/outputs/cen02b/Q1_double"
#
mkdir -p $OUTPUT
#
# --- set the dates and times ----
#
set STARTDATE = 2002001
set ENDDATE   = 2002090

set JDATE = $STARTDATE

while ( $JDATE <= $ENDDATE )

set RESTART = "true"
if ( $JDATE == $STARTDATE ) set RESTART = "true"

@ YESTERDAY = $JDATE - 1
if ( $YESTERDAY == 2002000 ) set YESTERDAY = 2001365
set YYYY = `j2g $JDATE | awk '{print $1}'`
set MM   = `j2g $JDATE | awk '{print $2}'`
set DD   = `j2g $JDATE | awk '{print $3}'`

#
# --- Create the input file (always called CAMx.in)
#
cat << ieof > CAMx.in

&CAMx_Control

Run_Message      = 'CAMx 4.30 Mech 4 CF - TCEQ.BART 36-12kmFE'

!--- Model clock control ---

Time_Zone        = 0,                ! (0=UTC,5=EST,6=CST,7=MST,8=PST)
Restart          = .${RESTART}.,
Start_Date_Hour = ${YYYY},${MM},${DD},0000, ! (YYYY,MM,DD,HHHH)
End_Date_Hour   = ${YYYY},${MM},${DD},2400, ! (YYYY,MM,DD,HHHH)

Maximum_Timestep = 20.,              ! minutes
Met_Input_Frequency = 60.,          ! minutes
Ems_Input_Frequency = 60.,          ! minutes

```

```

Output_Frequency      = 60.,           ! minutes

!--- Map projection parameters ---

Map_Projection        = 'LAMBERT'      ! (LAMBERT,POLAR,UTM,LATLON)
UTM_Zone              = 0,
POLAR_Longitude_Pole  = 0.,           ! deg (west<0,south<0)
POLAR_Latitude_Pole   = 0.,           ! deg (west<0,south<0)
LAMBERT_Central_Meridian = -97.,      ! deg (west<0,south<0)
LAMBERT_Center_Longitude = -97.,      ! deg (west<0,south<0)
LAMBERT_Center_Latitude = 40.,        ! deg (west<0,south<0)
LAMBERT_True_Latitude1 = 45.,         ! deg (west<0,south<0)
LAMBERT_True_Latitude2 = 33.,         ! deg (west<0,south<0)

!--- Parameters for the master (first) grid ---

Number_of_Grids       = 2,
Master_Origin_XCoord  = -2736.,       ! km or deg, SW corner of cell(1,1)
Master_Origin_YCoord  = -2088.,       ! km or deg, SW corner of cell (1,1)
Master_Cell_XSize     = 36.,          ! km or deg
Master_Cell_YSize     = 36.,          ! km or deg
Master_Grid_Columns   = 148,
Master_Grid_Rows      = 112,
Number_of_Layers(1)   = 19,

!--- Parameters for the second grid ---

Nest_Meshing_Factor(2) = 3,          ! Relative to master grid
Nest_Beg_I_Index(2)    = 51,         ! Relative to master grid
Nest_End_I_Index(2)    = 87,         ! Relative to master grid
Nest_Beg_J_Index(2)    = 14,         ! Relative to master grid
Nest_End_J_Index(2)    = 49,         ! Relative to master grid
Number_of_Layers(2)    = 19,

!--- Model options ---

Diagnostic_Error_Check = .false.,     ! True = will stop after 1st timestep
Advection_Solver       = 'PPM',       ! (PPM,BOTT)
Chemistry_Solver       = 'CMC',       ! (CMC,IEH)
PiG_Submodel           = 'GREASD',    ! (None,GREASD,IRON)
Probing_Tool           = 'None',      ! (None,OSAT,GOAT,APCA,DDM,PA,RTRAC)
Chemistry              = .true.,
Dry_Deposition         = .true.,
Wet_Deposition         = .true.,
Staggered_Winds       = .true.,
Gridded_Emissions     = .true.,
Point_Emissions        = .true.,
Ignore_Emission_Dates = .true.,

!--- Output specifications ---

Root_Output_Name       = '$OUTPUT/camx.$RUN.$JDATE',
Average_Output_3D     = .false.,
HDF_Format_Output     = .false.,
Number_of_Output_Species = 35,
Output_Species_Names(1) = 'NO',
Output_Species_Names(2) = 'NO2',
Output_Species_Names(3) = 'O3',
Output_Species_Names(4) = 'PAN',
Output_Species_Names(5) = 'NXOY',

```

```

Output_Species_Names(6) = 'CO',
Output_Species_Names(7) = 'HONO',
Output_Species_Names(8) = 'HNO3',
Output_Species_Names(9) = 'NTR',
Output_Species_Names(10) = 'SO2',
Output_Species_Names(11) = 'SULF',
Output_Species_Names(12) = 'NH3',
Output_Species_Names(13) = 'HCL',
Output_Species_Names(14) = 'CG1',
Output_Species_Names(15) = 'CG2',
Output_Species_Names(16) = 'CG3',
Output_Species_Names(17) = 'CG4',
Output_Species_Names(18) = 'CG5',
Output_Species_Names(19) = 'PNO3',
Output_Species_Names(20) = 'PSO4',
Output_Species_Names(21) = 'PNH4',
Output_Species_Names(22) = 'POA',
Output_Species_Names(23) = 'SOA1',
Output_Species_Names(24) = 'SOA2',
Output_Species_Names(25) = 'SOA3',
Output_Species_Names(26) = 'SOA4',
Output_Species_Names(27) = 'SOA5',
Output_Species_Names(28) = 'PEC',
Output_Species_Names(29) = 'FPRM',
Output_Species_Names(30) = 'FCRS',
Output_Species_Names(31) = 'CPRM',
Output_Species_Names(32) = 'CCRS',
Output_Species_Names(33) = 'NA',
Output_Species_Names(34) = 'PCL',
Output_Species_Names(35) = 'PH2O',

```

!--- Input files ---

```

Chemistry_Parameters = '$CHEM/CAMx4.3.chemparam.4_CF',
Photolysis_Rates    = '$PHOT/tuv.cenrap36km.${YYYY}${MM}.20051013.txt',
Initial_Conditions  = '$ICBC/ic.cenrap36km.CAMx',
Boundary_Conditions = '$ICBC/bc.cenrap36km.CAMx.$JDATE',
Top_Concentrations  = '$ICBC/topc.cenrap36km.CAMx',
Albedo_Haze_Ozone   = '$AHOMAP/ahomap.${YYYY}${MM}.20051013.txt',
Point_Sources       =
'$EMIS/double/CAMx.pt.tceq_double.RPO_US36.cen02b.$JDATE',
Master_Grid_Restart = '$OUTPUT/camx.$RUN.$YESTERDAY.inst.2',
Nested_Grid_Restart = '$OUTPUT/camx.$RUN.$YESTERDAY.finst.2',
PiG_Restart         = '$OUTPUT/camx.$RUN.$YESTERDAY.pig',

Emiss_Grid(1)      = '$EMIS/CAMx.ar.tceq_zero.RPO_US36.cen02b.$JDATE',
Landuse_Grid(1)    = '$LUSE/CAMx.cenrap36km.luse.bin',
ZP_Grid(1)         = '$MET/camx.zp.${YYYY}${MM}${DD}.OB70.bin',
Wind_Grid(1)       = '$MET/camx.uv.${YYYY}${MM}${DD}.OB70.bin',
Temp_Grid(1)       = '$MET/camx.tp.${YYYY}${MM}${DD}.OB70.bin',
Vapor_Grid(1)      = '$MET/camx.qa.${YYYY}${MM}${DD}.OB70.bin',
Cloud_Grid(1)      = '$MET/camx.cr.${YYYY}${MM}${DD}.OB70.bin',
Kv_Grid(1)         = '$MET/camx.kv.${YYYY}${MM}${DD}.CMAQ.kvmin1.0.bin',
Emiss_Grid(2)      = ' ',
Landuse_Grid(2)    = ' ',
ZP_Grid(2)         = ' ',
Wind_Grid(2)       = ' ',
Temp_Grid(2)       = ' ',
Vapor_Grid(2)      = ' ',
Cloud_Grid(2)      = ' ',

```

```
Kv_Grid(2)      = ' ',  
  
&  
!-----  
---  
ieof  
#  
# --- Execute the model ---  
#  
/usr/bin/time $EXEC >& $OUTPUT/camx.$RUN.$JDATE.stdout  
  
@ JDATE++  
if ( $JDATE == 2001366 ) set JDATE = 2002001  
  
end
```

Appendix B

Example CAMx Run Script for a
PSAT BART Analysis using the
SO₄ and NO₃ PSAT Tracers

```

#!/bin/csh
#
# CAMx 4.40beta OMP
#
setenv NCPUS 2
setenv MPSTKZ 128M
limit stacksize unlimited
#
set EXEC      =
"/disk52/tceq.bart/camx/src.v4.40.Mar29/CAMx.tceq.bart.pg_linuxomp"
#
set run = Q1.tceq.psat.oldmet
set RUN      = "v4.40.tceq.bart.12FE"
set CHEM     = "/disk52/cenrap/camx/inputs/others"
set LUSE     = "/disk52/cenrap/camx/inputs/landuse"
set AHOMAP   = "/disk52/cenrap/camx/inputs/ahomap"
set PHOT     = "/disk52/cenrap/camx/inputs/tuv"
set ICBC     = "/disk52/cenrap/camx/inputs/icbctc"
set MET      = "/disk50/tceq_bart/met"
set MAP      = "/disk52/tceq.bart/camx/input/sa"
set EMIS     = "/disk52/tceq.bart/camx/input/emis/psat"
set OUTPUT   = "/swamp6/tceq.bart2/camx/outputs/Q1.psat.tceqbart.12FE.oldmet"
#
mkdir -p $OUTPUT $run
#
# --- set the dates and times ----
#
set STARTDATE = 2001353
set ENDDATE   = 2002364

set JDATE = 2002021

while ( $JDATE <= $ENDDATE )

set RESTART = "true"
if ( $JDATE == $STARTDATE ) set RESTART = "false"

@ YESTERDAY = $JDATE - 1
if ( $YESTERDAY == 2002000 ) set YESTERDAY = 2001365
set YYYY = `j2g $JDATE | awk '{print $1}'`
set Y2 = `echo $YYYY | awk '{printf("%2.2d", $1-2000)}'`
set MM = `j2g $JDATE | awk '{print $2}'`
set DD = `j2g $JDATE | awk '{print $3}'`

# --- Create the input file (always called CAMx.in)
#
cat << ieof > CAMx.in

&CAMx_Control

Run_Message      = 'CAMx 4.40 Mech 4 CF - TCEQ.BART 36-12kmFE'

!--- Model clock control ---

Time_Zone        = 0,                ! (0=UTC,5=EST,6=CST,7=MST,8=PST)
Restart          = .${RESTART}.,
Start_Date_Hour  = ${YYYY}, ${MM}, ${DD}, 0000,    ! (YYYY,MM,DD,HHHH)
End_Date_Hour    = ${YYYY}, ${MM}, ${DD}, 2400,    ! (YYYY,MM,DD,HHHH)

```

```

Maximum_Timestep      = 20.,           ! minutes
Met_Input_Frequency  = 60.,           ! minutes
Ems_Input_Frequency  = 60.,           ! minutes
Output_Frequency     = 60.,           ! minutes

```

!--- Map projection parameters ---

```

Map_Projection        = 'LAMBERT'      ! (LAMBERT,POLAR,UTM,LATLON)
UTM_Zone              = 0,
POLAR_Longitude_Pole  = 0.,           ! deg (west<0,south<0)
POLAR_Latitude_Pole   = 0.,           ! deg (west<0,south<0)
LAMBERT_Central_Meridian = -97.,      ! deg (west<0,south<0)
LAMBERT_Center_Longitude = -97.,     ! deg (west<0,south<0)
LAMBERT_Center_Latitude = 40.,       ! deg (west<0,south<0)
LAMBERT_True_Latitude1 = 45.,       ! deg (west<0,south<0)
LAMBERT_True_Latitude2 = 33.,       ! deg (west<0,south<0)

```

!--- Parameters for the master (first) grid ---

```

Number_of_Grids       = 2,
Master-Origin_XCoord  = -2736.,       ! km or deg, SW corner of cell(1,1)
Master-Origin_YCoord  = -2088.,       ! km or deg, SW corner of cell (1,1)
Master_Cell_XSize     = 36.,         ! km or deg
Master_Cell_YSize     = 36.,         ! km or deg
Master_Grid_Columns   = 148,
Master_Grid_Rows      = 112,
Number_of_Layers(1)   = 19,

```

!--- Parameters for the second grid ---

```

Nest_Meshing_Factor(2) = 3,          ! Relative to master grid
Nest_Beg_I_Index(2)    = 51,         ! Relative to master grid
Nest_End_I_Index(2)    = 87,         ! Relative to master grid
Nest_Beg_J_Index(2)    = 14,        ! Relative to master grid
Nest_End_J_Index(2)    = 49,        ! Relative to master grid
Number_of_Layers(2)    = 19,

```

!--- Model options ---

```

Diagnostic_Error_Check = .false.,     ! True = will stop after 1st timestep
Advection_Solver       = 'BOTT',      ! (PPM,BOTT)
Chemistry_Solver       = 'CMC',       ! (CMC,IEH)
Aerosol_Solver         = 'ISOROPIA',  ! (ISOROPIA,EQSAM)
PiG_Submodel           = 'GREASD',    ! (None,GREASD,IRON)
Probing_Tool           = 'PSAT',      ! (None,OSAT,GOAT,APCA,DDM,PA,RTRAC)
Chemistry               = .true.,
Dry_Deposition          = .true.,
Wet_Deposition         = .true.,
Staggered_Winds        = .true.,
Gridded_Emissions      = .true.,
Point_Emissions        = .true.,
Ignore_Emission_Dates  = .true.,

```

!--- Output specifications ---

```

Root_Output_Name       = '$OUTPUT/camx.$RUN.$JDATE',
Average_Output_3D      = .false.,
HDF_Format_Output      = .false.,
Number_of_Output_Species = 35,
Output_Species_Names(1) = 'NO',

```

```

Output_Species_Names(2) = 'NO2',
Output_Species_Names(3) = 'O3',
Output_Species_Names(4) = 'PAN',
Output_Species_Names(5) = 'NXOY',
Output_Species_Names(6) = 'CO',
Output_Species_Names(7) = 'HONO',
Output_Species_Names(8) = 'HNO3',
Output_Species_Names(9) = 'NTR',
Output_Species_Names(10) = 'SO2',
Output_Species_Names(11) = 'SULF',
Output_Species_Names(12) = 'NH3',
Output_Species_Names(13) = 'HCL',
Output_Species_Names(14) = 'CG1',
Output_Species_Names(15) = 'CG2',
Output_Species_Names(16) = 'CG3',
Output_Species_Names(17) = 'CG4',
Output_Species_Names(18) = 'CG5',
Output_Species_Names(19) = 'PNO3',
Output_Species_Names(20) = 'PSO4',
Output_Species_Names(21) = 'PNH4',
Output_Species_Names(22) = 'POA',
Output_Species_Names(23) = 'SOA1',
Output_Species_Names(24) = 'SOA2',
Output_Species_Names(25) = 'SOA3',
Output_Species_Names(26) = 'SOA4',
Output_Species_Names(27) = 'SOA5',
Output_Species_Names(28) = 'PEC',
Output_Species_Names(29) = 'FPRM',
Output_Species_Names(30) = 'FCRS',
Output_Species_Names(31) = 'CPRM',
Output_Species_Names(32) = 'CCRS',
Output_Species_Names(33) = 'NA',
Output_Species_Names(34) = 'PCL',
Output_Species_Names(35) = 'PH2O',

```

!--- Input files ---

```

Chemistry_Parameters = '$CHEM/CAMx4.3.chemparam.4_CF',
Photolysis_Rates    = '$PHOT/tuv.cenrap36km.${YYYY}${MM}.20051013.txt',
Initial_Conditions  = '$ICBC/ic.cenrap36km.CAMx',
Boundary_Conditions = '$ICBC/bc.cenrap36km.CAMx.$JDATE',
Top_Concentrations  = '$ICBC/topc.cenrap36km.CAMx',
Albedo_Haze_Ozone   = '$AHOMAP/ahomap.${YYYY}${MM}.20051013.txt',
Point_Sources       = '$EMIS/CAMx.FE.pt.tceq_psat.RPO_US36.cen02b.$JDATE',
Master_Grid_Restart = '$OUTPUT/camx.$RUN.$YESTERDAY.inst.2',
Nested_Grid_Restart = '$OUTPUT/camx.$RUN.$YESTERDAY.finst.2',
PiG_Restart         = '$OUTPUT/camx.$RUN.$YESTERDAY.pig',

```

```

Emiss_Grid(1) = '$EMIS/CAMx.ar.cenrapzero.RPO_US36.cen02b.$JDATE',
Landuse_Grid(1) = '$LUSE/CAMx.cenrap36km.luse.bin',
ZP_Grid(1) = '$MET/camx.zp.${YYYY}${MM}${DD}.OB70.bin',
Wind_Grid(1) = '$MET/camx.uv.${YYYY}${MM}${DD}.OB70.bin',
Temp_Grid(1) = '$MET/camx.tp.${YYYY}${MM}${DD}.OB70.bin',
Vapor_Grid(1) = '$MET/camx.qa.${YYYY}${MM}${DD}.OB70.bin',
Cloud_Grid(1) = '$MET/camx.cr.${YYYY}${MM}${DD}.OB70.bin',
Kv_Grid(1) = '$MET/camx.kv.${YYYY}${MM}${DD}.CMAQ.kvmin1.0.bin',
Emiss_Grid(2) = '$EMIS/CAMx.ar.cenrapzero.RPO_US12.cen02b.$JDATE',
Landuse_Grid(2) = ' ',
ZP_Grid(2) = ' ',
Wind_Grid(2) = ' ',

```

```

Temp_Grid(2)      = ' ',
Vapor_Grid(2)    = ' ',
Cloud_Grid(2)    = ' ',
Kv_Grid(2)       = ' ',

&
!-----
---

&SA_Control

SA_File_Root      = '$OUTPUT/camx.$RUN.$JDATE',
SA_Summary_Output = .false.
SA_Master_Sfc_Output = .true.,
SA_Nested_Sfc_Output = .true.,
SA_Stratify_Boundary = .false.,
SA_Number_of_Source_Regions = 11,
SA_Number_of_Source_Groups = 2,
Use_Leftover_Group = .false.,
Number_of_Timing_Releases = 0,
SA_Receptor_Definitions = '$MAP/receptor.tceqbart.txt'
SA_Source_Area_Map(1) = '$MAP/BART_psat_regn_36km.txt'
SA_Source_Area_Map(2) = '$MAP/BART_psat_regn_12km.txt'
SA_Points_Group(1) =
'$EMIS/CAMx.FE.pt.tceq_psat.RPO_US36.cen02b.$JDATE.copy',
SA_Emiss_Group_Grid(1,1) = ' ',
SA_Emiss_Group_Grid(1,2) = ' ',
SA_Points_Group(2) = ' ',
SA_Emiss_Group_Grid(2,1) =
'$EMIS/CAMx.ar.cenrapzero.RPO_US36.cen02b.$JDATE.copy',
SA_Emiss_Group_Grid(2,2) =
'$EMIS/CAMx.ar.cenrapzero.RPO_US12.cen02b.$JDATE.copy',
SA_Master_Restart = '$OUTPUT/camx.$RUN.$YESTERDAY.sa.inst.2',
SA_Nested_Restart = '$OUTPUT/camx.$RUN.$YESTERDAY.sa.finst.2',
PSAT_Treat_SULFATE_Class = .true.
PSAT_Treat_NITRATE_Class = .true.
PSAT_Treat_SOA_Class = .false.
PSAT_Treat_PRIMARY_Class = .false.
PSAT_Treat_MERCURY_Class = .false.
PSAT_Treat_OZONE_Class = .false.

&

ieof
#
# --- Execute the model ---
#
cp CAMx.in $run/camx.$RUN.$JDATE.in
/usr/bin/time $EXEC |& tee $run/camx.$RUN.$JDATE.stdout

@ JDATE++
if ( $JDATE == 2001366 ) set JDATE = 2002001

end

```