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Best Available Retrofit Technology (BART) Modeling Protocol to Determine Sources Subject to BART in the State of Texas

Air Permits Division
Texas Commission on Environmental Quality

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Table of Contents

Summary of Significant Changes iii

I. Introduction 1

II. Background 1

III. BART Air Quality Modeling Approach 2

IV. Class I Areas to Assess 3

V. Air Quality Model and Inputs 6
- **A. Modeling domain** 6
- **B. CALPUFF system implementation** 7
- **C. Meteorological data modeling (CALMET)** 8
- **D. Stack Parameters** 9
- **E. Emissions** 9
- **F. Dispersion modeling (CALPUFF)** 10
- **G. Post-processing (CALPOST)** 11

VI. Visibility Impacts 12

VII. Change in Visibility Due to BART Controls 14

VIII. Reporting 14

References 15
Appendix A – Federal Class I Areas 16
Appendix B – CALPUFF Control File Inputs 18
Appendix C – POSTUTIL Control File Inputs 25
Appendix D – CALPOST Control File Inputs 26

Summary of Significant Changes

General - Removed "draft" wording and made other minor editorial changes throughout the document.

Section V.B - Changed the version of CALPUFF to the EPA approved version.

Section V.B - Changed the version of POSTUTIL to the EPA approved version.

Section V.B - Changed the version of CALPOST to the EPA approved version.

Section V.C - Added information about re-compiling the code when using the CENRAP-developed CALMET dataset.

Section V.E - Clarified that sources performing the source-specific subject-to-BART screening analysis should consider all visibility impairing species.

Section VIII - Added information for including files associated with re-compiling the code with the electronic archive.

I. Introduction

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

The Texas Commission on Environmental Quality (TCEQ) foresees two purposes for this protocol. First, sources may use the protocol to determine if BART-eligible units are subject to BART and must perform a BART analysis. Second, sources that are subject to BART will have this protocol to use as a starting point to conduct modeling required when making a BART analysis.

New BART guidance, both formal and informal, continues to become available from EPA and the Federal Land Managers (FLMs) that oversee visibility in Class I areas. Texas has developed a schedule for completing BART analyses and implementing the BART strategy in order to meet State Implementation Plan (SIP) deadlines. If the state is to meet those deadlines, modeling to determine sources subject to BART and modeling to make BART analyses may need to be done before all final BART guidance from EPA and the FLMs becomes available.

II. Background

Generally, Class I areas are national parks and wilderness areas in which visibility is more stringently protected under the Clean Air Act than any other areas in the United States. The Class I areas are shown in Appendix A.

The BART requirements are a part of the SIP that will be submitted to EPA in late 2007. The SIP is a comprehensive plan of action to increase visibility in the Class I areas and includes reasonable progress goals in addition to the goals established by sources subject to BART.

The BART provisions are a part of the overall plan that focuses on reducing emissions from large sources that, due to age, were exempted from other control requirements in the Clean Air Act. An emissions source is considered eligible for BART if it:

- Falls into one of 26 listed categories;
- Has the potential to emit at least 250 tons per year of any visibility-impairing pollutant (primarily NO_x, SO_2, or PM); and
- Existed on August 7, 1977, yet was not in operation before August 7, 1962.

Thus, the BART provisions do not cover all sources that may cause or contribute to visibility impairment in any Class I area.

According to the BART guidance, an individual source is considered to cause visibility impairment if it has a least a 1.0 deciview (dv) impact on the visibility in a Class I area. A source is considered to contribute to visibility impairment if it has at least a 0.5 dv impact.

The BART guidance allows a state to exempt individual sources from the BART requirements if they do not cause or contribute to any impairment of visibility in a Class I area. Exemption is done through air quality modeling. Although the BART guidance does not dictate how such an analysis must be done, it provides direction, which was used to develop this modeling protocol.

The BART analysis process includes several other steps in addition to the modeling described in this protocol. These steps, none of which are addressed in this document, include detailed analysis of:

- Costs of compliance;
- Energy and non-air quality impacts;
- Existing pollution control technologies in use at the BART-eligible unit;
- Remaining useful life of the units and/or facility; and
- Improvements in visibility expected from the use of BART controls.

III. BART Air Quality Modeling Approach

One of the air quality modeling approaches suggested by EPA in the BART guidance is an individual source attribution approach. Specifically, this entails modeling source-specific BART-eligible units and comparing modeled impacts to a particular deciview threshold (described above).

The modeling approach discussed here is specifically designed for conducting a source-specific subject-to-BART screening analysis. There may be differences between modeling for conducting BART analyses and that for conducting a visibility analysis for a New Source Review permit, which may involve similar emission sources and the same air dispersion model used here.

In preparing this modeling protocol, the TCEQ consulted BART modeling protocols drafted by other organizations to maintain an appropriately consistent approach within the Central States Regional Air Planning Association (CENRAP). The three available BART modeling protocols consulted were:

1. "Best Available Retrofit Technology (BART) Modeling Protocol to Determine Sources Subject to BART in the State of Minnesota," final version March 2006;
2. "Best Available Retrofit Technology (BART) Modeling Protocol to Determine Sources Subject to BART in the State of Kansas," final version June 2006;
3. "Screening Analysis of Potentially BART-Eligible Sources in Texas," developed by ENVIRON International Corporation, December 2005.

This protocol is most similar to the Kansas and Minnesota final protocols. Texas is in EPA Region VI, and they will be reviewing Texas' Regional Haze SIP, of which BART will be a part.

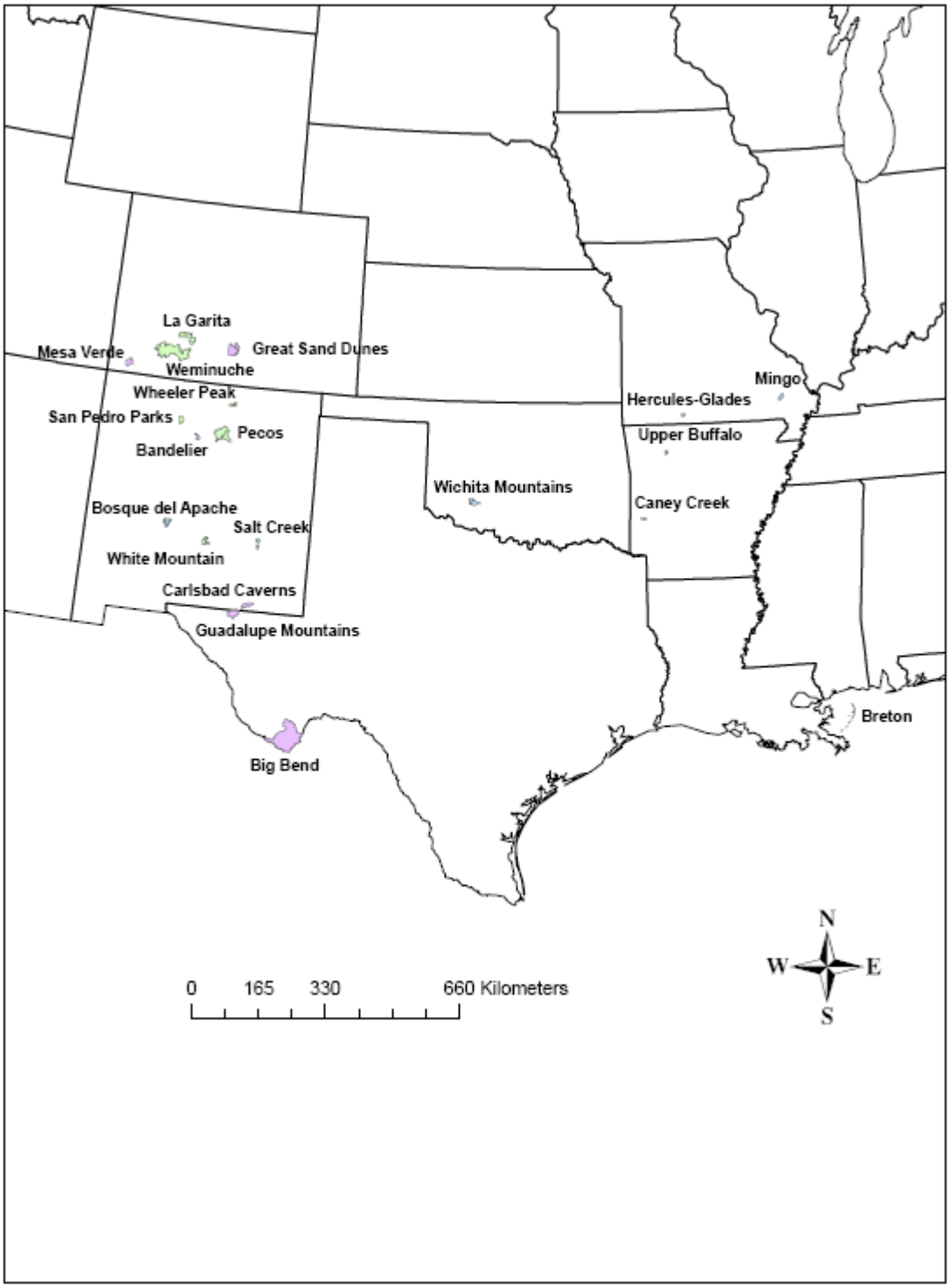
IV. Class I Areas to Assess

Table 1, *Class I Areas Evaluated for BART*, contains the list of Class I areas to be included in the modeling analysis. The list was developed for the subject-to-BART screening evaluation conducted by ENVIRON for the TCEQ. Figure 1, *Location of Class I Areas*, shows the location of each Class I area to be evaluated. Sources conducting the source-specific subject-to-BART screening analysis should include all Class I areas that the ENVIRON screening evaluation showed their source group to have impacts greater than 0.5 dv on visibility.

Table 1 - Class I Areas Evaluated for BART

Class I Area	State	Visibility Monitoring Site Name
Bandelier Wilderness Area	NM	BAND1
Big Bend National Park	TX	BIBE1
Bosque del Apache Wilderness Area	NM	BOAP1
Breton Wilderness Area	LA	BRET1
Caney Creek Wilderness Area	AR	CACR1
Carlsbad Caverns National Park	NM	GUMO1
Great Sand Dunes Wilderness Area	CO	GRSA1
Guadalupe Mountains National Park	TX	GUMO1
Hercules-Glades Wilderness Area	MO	HEGL1
La Garita Wilderness Area	CO	WEMI1
Mesa Verde National Park	CO	MEVE1
Mingo Wilderness Area	MO	MING1
Pecos Wilderness Area	NM	WHPE1
Salt Creek Wildlife Refuges	NM	SACR1
San Pedro Parks Wilderness Area	NM	SAPE1
Upper Buffalo Wilderness Area	AR	UPBU1
Weminuche Wilderness Area	CO	WEMI1
Wheeler Peak Wilderness Area	NM	WHPE1
White Mountain Wilderness Area	NM	WHIT1
Wichita Mountains Wildlife Refuges	OK	WIMO1

Figure 1 - Location of Class I Areas



V. Air Quality Model and Inputs

According to the final Regional Haze Rule's BART guidance, a source "can use CALPUFF or other appropriate model to predict the visibility impacts from a single source at a Class I area." For purposes of the source-specific subject-to-BART screening analysis, the TCEQ recommends the use of CALPUFF. The TCEQ recognizes that CALPUFF has limited ability to simulate the complex atmospheric chemistry involved in the estimation of secondary particulate formation. However, for purposes of this source-specific subject-to-BART screening analysis, the TCEQ recommends the use of CALPUFF for the following reasons:

1. The increased level of effort required for conducting particulate apportionment in the regional scale, full-chemistry Eulerian model (CAMx or CMAQ) to acquire individual source contributions to Class I areas, relative to the simplicity of the CALPUFF model;
2. The limited scope of what this modeling is to determine; and
3. The additional modeling of BART controls that will be conducted as part of the Regional Haze SIP with the CAMx or CMAQ models.

EPA's BART guidance recommends following the EPA's Interagency Workgroup on Air Quality Modeling (IWAQM) guidance, Phase 2 recommendations for long-range transport. The IWAQM guidance was developed to address air quality impacts as assessed through the Prevention of Significant Deterioration (PSD) program at Class I areas, where the source generally is located beyond 50 kilometer (km) of the Class I area. The IWAQM guidance does not specifically address the type of assessment that will occur with the BART analysis.

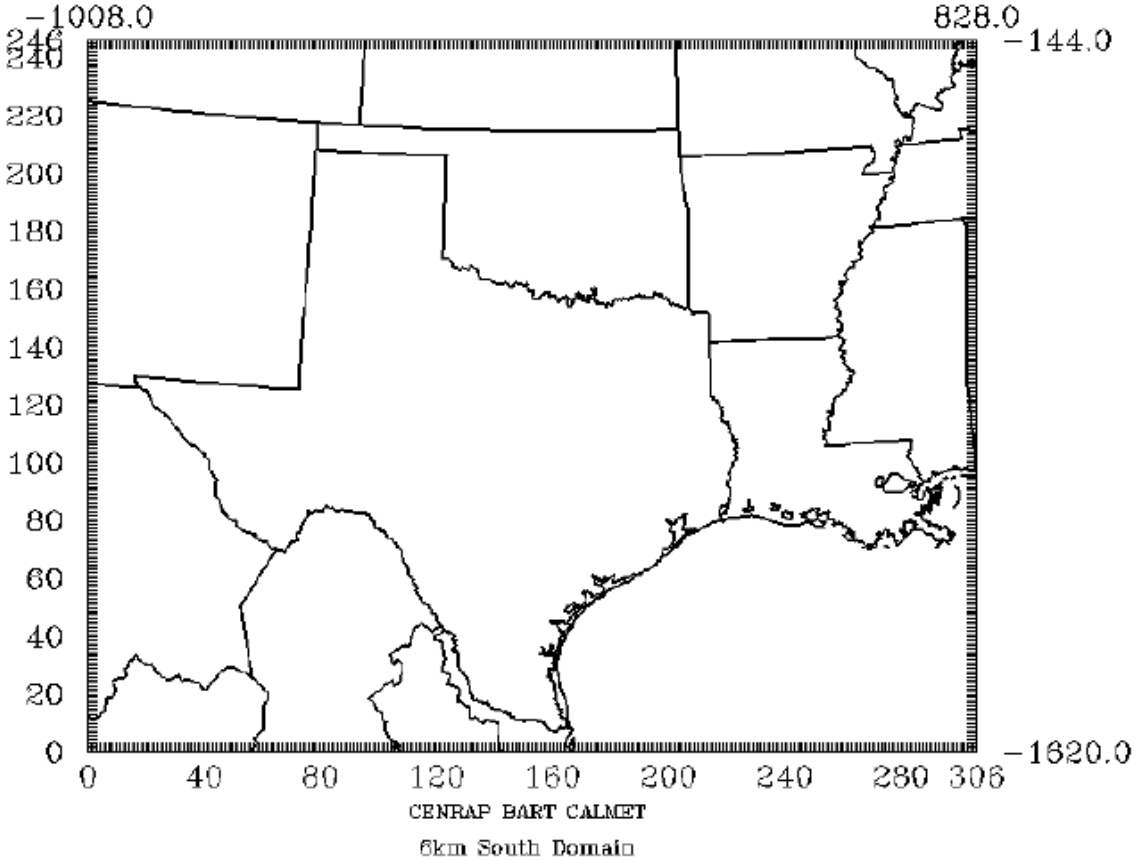
Given the uncertainties of transport and dispersion processes in CALPUFF for distances greater than 300 km, consideration may be given to the CAMx model for determining visibility impacts at Class I areas located 300 km beyond the source in a refined modeling analysis. Below is a list of options for selecting a model to use. The first two apply to the source-specific subject-to-BART screening analysis, and the third is an option for a refined modeling analysis:

1. CALPUFF for Class I areas located within 300 km of the source;
2. CALPUFF for Class I areas located beyond 300 km of the source for a conservative screening analysis; and
3. CAMx for Class I areas located beyond 300 km of the source in a refined analysis.

A. Modeling Domain

The CALPUFF source-specific subject-to-BART screening modeling should be conducted with the CENRAP south 6 km grid. The extent of the proposed CALPUFF domain is shown in Figure 2, *6 km CENRAP South CALPUFF Domain*.

Figure 2 - 6 km CENRAP South CALPUFF Domain



CALPUFF should be applied for three annual simulations spanning the years 2001 through 2003. The IWAQM guidance allows the use of fewer than five years of meteorological data if a meteorological model using four-dimensional data assimilation is used to supply data. See the section on meteorology for more information.

B. CALPUFF System Implementation

There are three main components to the CALPUFF model:

1. Meteorological Data Modeling (CALMET);
2. Dispersion Modeling (CALPUFF); and
3. Post processing (CALPOST).

Versions of the modeling components that may be used in the source-specific subject-to-BART screening analysis are shown in Table 2, *CALPUFF Modeling Components*.

Table 2 - CALPUFF Modeling Components

Processor	Version	Level
TERREL	3.311	030709
CTGCOMP	2.42	030709
CTGPROC	2.42	030709
MAKEGEO	2.22	030709
CALMM5	2.4	050413
CALMET	5.53a	040716
CALPUFF	5.711a	040716
POSTUTIL	1.3	030402
CALPOST	5.51	030709

C. Meteorological data modeling (CALMET)

The 2001-2003 CENRAP-developed CALMET dataset should be used in the source-specific subject-to-BART screening analysis. For additional information on the settings used to develop this dataset, refer to the CENRAP BART Modeling Guidelines document at www.cenrap.org/modeling_document.asp.

Since no observational data were used in the CALMET outputs developed by CENRAP, the prognostic meteorological dataset from MM5 is not supplemented with surface or upper air observations during the CALMET processing. The use of observations is thought to counterbalance smoothing that may occur when using the coarse grid scale of the MM5 data. Both the EPA and FLMs commented on the draft CENRAP guidelines that observations should be used in refined CALPUFF modeling. However, the TCEQ considers this screening modeling to be conservative. Therefore, the TCEQ will not require the use of observational data. Sources may use observational data if they wish to conduct a more refined modeling analysis.

In order to use the CENRAP-developed CALMET dataset, the parameter files for CALPUFF, POSTUTIL, and CALPOST may have to be edited to accommodate the size of the CENRAP-developed CALMET dataset modeling domain. Once the parameter files have been edited, the CALPUFF, POSTUTIL, and CALPOST model code will need to be re-compiled.

D. Stack parameters

Stack parameters required for modeling BART-eligible units are: height of the stack opening from ground, inside stack diameter, exit gas flow rate, exit gas temperature, base elevation above sea level, and location coordinates of the stack. Because the modeling conducted for BART is concerned with long-range transport, not localized impacts, including the effects of building downwash in the source-specific subject-to-BART screening analysis are not necessary. Sources may include the effects of building downwash if they wish to conduct a more refined modeling analysis.

E. Emissions

Emission rates for the BART analyses follow EPA's BART guidance. Specifically, the 24-hour average actual emission rate with normal operations from the highest emitting day of the year should be modeled. Identification of the maximum 24-hour actual emission rates should be made for the most recent four years (2002-2005), according to the following prioritization:

1. Continuous Emissions Monitoring (CEM) data;
2. Facility emissions tests;
3. Emissions factors;
4. Permit limits; or lastly,
5. Potential to emit.

The species that should be modeled and/or emitted in the source-specific subject-to-BART screening analysis are listed in Table 3, *Species Modeled in BART Screening Analysis*. Sources should include all species if the ENVIRON screening evaluation showed any of their source groups to have impacts greater than 0.5 dv on visibility.

Table 3 - Species Modeled in BART Screening Analysis

Species	Modeled	Emitted	Dry Deposited
SO_2	Yes	Yes	Computed-gas
SO_4	Yes	No	Computed-particle
NO_x	Yes	Yes	Computed-gas
HNO_3	Yes	No	Computed-gas
NO_3	Yes	No	Computed-particle
PM-fine	Yes	Yes	Computed-particle
PM-coarse	Yes	Yes	Computed-particle

Note: *In the case of a source where the PM profile for sulfate (SO_4), elemental carbon (EC), and secondary organic aerosols (SOA) are known, SO_4 should be modeled as a separate species in CALPUFF.*

Particle size parameters are entered in the CALPUFF input file for dry deposition of particles. There are default values for "aerosol" species (i.e., SO_4, NO_3, and $PM_{2.5}$). The default value for each of these species is 0.48 µm geometric mass mean diameter and 2.0 µm geometric standard deviation. Where the source is able to supply emissions of $PM_{2.5}$, the default values may be appropriate. However, many sources may not be able to supply $PM_{2.5}$ emissions and will supply what is available, PM_{10} emissions data. In this case, using the default values may underestimate deposition of particulates and overestimate the particulate contribution to visibility. For sources that are not able to supply $PM_{2.5}$ emissions, the source should speciate PM_{10} emissions to $PM_{2.5}$ and PM course by using $PM_{2.5}$/ PM_{10} emission factors, if they are available. If there are no emission factors available, either use the worst-case assumption that all particulate is $PM_{2.5}$ or the source could provide a suggested emissions factor with full scientific documentation.

F. Dispersion modeling (CALPUFF)

The CALMET output is used as input to the CALPUFF model, which simulates the effects of the meteorological conditions on the transport and dispersion of pollutants from an individual source. In general, the default options are used in the CALPUFF model. The CALPUFF model has a puff-splitting option that splits puffs that become large over greater transport distances. The TCEQ recommends that the puff-splitting option not be used in the source-specific subject-to-BART screening analysis.

Detailed information on all CALPUFF settings to be used in the source-specific subject-to-BART screening analysis can be found in Appendix B.

Ozone and ammonia concentrations: Ozone (O_3) and ammonia (NH_3) can be input to CALPUFF as hourly or monthly background values. Background ozone and ammonia concentrations are assumed to be temporally and spatially invariant and will be fixed at 40 and 3 ppb, respectively, across the entire domain for all months. NH_3 concentrations may be derived from regional modeling outputs that CENRAP is currently developing. However, at this time these NH_3 values are not available in a model ready form.

Receptors: Receptors are locations where model results are calculated and provided in the CALPUFF output files. Receptor locations should be derived from the National Park Service (NPS) Class I area receptor database at www2.nature.nps.gov/air/maps/receptors/index.cfm. The discrete receptors are necessary for calculating visibility impacts in the selected Class I areas. The NPS provides receptors in all the Class I areas on a 1 km basis. These receptors should be kept at the 1 km spacing for the BART modeling.

Outputs: The CALPUFF modeling results will be displayed in units of micrograms per cubic meter ($\mu g/m^3$). In order to determine visibility impacts, the CALPUFF outputs must be post-processed.

G. Post-processing (CALPOST)

Hourly concentration outputs from CALPUFF are processed through POSTUTIL and CALPOST to determine visibility conditions. Specifically, POSTUTIL takes the concentration file output from CALPUFF and recalculates the nitric acid and nitrate partition based on total available sulfate and ammonia. CALPOST uses the concentration file processed through POSTUTIL, along with relative humidity data, to perform visibility calculations. For the source-specific subject-to-BART screening analysis, the only modeling results out of the CALPUFF modeling system of interest are the visibility impacts. Please see Appendix C and D for detailed settings for POSTUTIL and CALPOST.

Light extinction: Light extinction must be computed in order to calculate visibility. CALPOST has seven methods for computing light extinction. The BART screening analysis should use Method 6, which computes extinction from speciated particulate matter with monthly Class I area-specific relative humidity adjustment factors. Relative humidity is an important factor in determining light extinction (and therefore visibility) because sulfate and nitrate aerosols, which absorb moisture from the air, have greater extinction efficiencies with greater relative humidity. The BART screening analysis should apply relative humidity correction factors (*f*(RH)s) to sulfate and nitrate concentration outputs from CALPUFF, which can be obtained from EPA's "Guidance for Estimating Natural Visibility Conditions under the Regional Haze Rule (EPA, 2003). The *f*(RH) values for the Class I areas that should be assessed are provided in Table 4, *Monthly Averaged f(RH) Based on Centroid of the Class I Area*.

Table 4 - Monthly Averaged *f*(RH) Based on Centroid of the Class I Area

Class I Area	Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep	Oct	Nov	Dec
Bandelier	2.2	2.1	1.8	1.6	1.6	1.4	1.7	2.1	1.9	1.7	2.0	2.2
Big Bend	2.0	1.9	1.6	1.5	1.6	1.6	1.7	2.0	2.1	1.9	1.8	1.9
Bosque del Apache	2.1	1.9	1.6	1.4	1.4	1.3	1.8	2.0	1.9	1.6	1.8	2.2
Breton	3.7	3.5	3.7	3.6	3.8	4.0	4.3	4.3	4.2	3.7	3.7	3.7
Caney Creek	3.4	3.1	2.9	3.0	3.6	3.6	3.4	3.4	3.6	3.5	3.4	3.5
Carlsbad Caverns	2.1	2.0	1.6	1.5	1.6	1.6	1.8	2.1	2.2	1.8	1.9	2.1
Great Sand Dunes	2.4	2.3	2.0	1.9	1.9	1.8	1.9	2.3	2.2	1.9	2.4	2.4
Guadalupe Mountains	2.0	2.0	1.6	1.5	1.6	1.5	1.9	2.2	2.2	1.8	1.9	2.2
Hercules-Glades	3.2	2.9	2.7	2.7	3.3	3.3	3.3	3.3	3.4	3.1	3.1	3.3
La Garita	2.3	2.2	1.9	1.8	1.8	1.6	1.7	2.1	2.0	1.8	2.2	2.3
Mesa Verde	2.5	2.3	1.9	1.5	1.5	1.3	1.6	2.0	1.9	1.7	2.1	2.3
Mingo	3.3	3.0	2.8	2.6	3.0	3.2	3.3	3.5	3.5	3.1	3.1	3.3
Pecos	2.3	2.1	1.8	1.7	1.7	1.5	1.8	2.1	2.0	1.7	2.0	2.2
Salt Creek	2.1	1.9	1.5	1.5	1.7	1.6	1.8	2.0	2.1	1.8	1.8	2.1
San Pedro Parks	2.3	2.1	1.8	1.6	1.6	1.4	1.7	2.0	1.9	1.7	2.1	2.2
Upper Buffalo	3.3	3.0	2.7	2.8	3.4	3.4	3.4	3.4	3.6	3.3	3.2	3.3
Weminuche	2.4	2.2	1.9	1.7	1.7	1.5	1.6	2.0	1.9	1.7	2.1	2.3
Wheeler Park	2.3	2.2	1.9	1.8	1.8	1.6	1.8	2.2	2.1	1.8	2.2	2.3
White Mountain	2.1	1.9	1.6	1.5	1.5	1.4	1.8	2.0	2.0	1.7	1.8	2.1
Wichita Mountains	2.7	2.6	2.4	2.4	3.0	2.7	2.3	2.5	2.9	2.6	2.7	2.8

The $PM_{2.5}$ concentrations are considered part of the dry light extinction equation and do not have a humidity adjustment factor. The light extinction equation is the sum of the wet sulfate and nitrate and dry components $PM_{2.5}$ plus Rayleigh scattering, which is 10 inverse megameters (Mm^{-1}).

VI. Visibility Impacts

Perceived visibility in deciviews is derived from the light extinction coefficient. The visibility change related to background is calculated using the modeled and established natural visibility conditions. For the BART screening analysis, daily visibility will be expressed as a change in deciviews compared to natural visibility conditions.

The annual average natural levels of aerosol components at each Class I area are shown in Table 5, *Average Annual Natural Levels of Aerosol Components ($\mu g/m^3$)*. Natural conditions

by component in this table are based on whether the Class I area is in the eastern or the western part of the United States. These data are in EPA's "Guidance for Estimating Natural Visibility Conditions under the Regional Haze Rule" (EPA, 2003).

Table 5 - Average Annual Natural Levels of Aerosol Components ($\mu g/m^3$)

Class I Area	Region	SO_4	NO_3	OC	EC	Soil	Coarse Mass
Bandelier	WEST	0.12	0.10	0.47	0.02	0.50	3.00
Big Bend	WEST	0.12	0.10	0.47	0.02	0.50	3.00
Bosque del Apache	WEST	0.12	0.10	0.47	0.02	0.50	3.00
Breton	EAST	0.23	0.10	1.40	0.02	0.50	3.00
Caney Creek	EAST	0.23	0.10	1.40	0.02	0.50	3.00
Carlsbad Caverns	WEST	0.12	0.10	0.47	0.02	0.50	3.00
Great Sand Dunes	WEST	0.12	0.10	0.47	0.02	0.50	3.00
Guadalupe Mountains	WEST	0.12	0.10	0.47	0.02	0.50	3.00
Hercules-Glades	EAST	0.23	0.10	1.40	0.02	0.50	3.00
La Garita	WEST	0.12	0.10	0.47	0.02	0.50	3.00
Mesa Verde	WEST	0.12	0.10	0.47	0.02	0.50	3.00
Mingo	EAST	0.23	0.10	1.40	0.02	0.50	3.00
Pecos	WEST	0.12	0.10	0.47	0.02	0.50	3.00
Salt Creek	WEST	0.12	0.10	0.47	0.02	0.50	3.00
San Pedro Parks	WEST	0.12	0.10	0.47	0.02	0.50	3.00
Upper Buffalo	EAST	0.23	0.10	1.40	0.02	0.50	3.00
Weminuche	WEST	0.12	0.10	0.47	0.02	0.50	3.00
Wheeler Peak	WEST	0.12	0.10	0.47	0.02	0.50	3.00
White Mountain	WEST	0.12	0.10	0.47	0.02	0.50	3.00
Wichita Mountains	WEST	0.12	0.10	0.47	0.02	0.50	3.00

In a cooperative agreement with EPA Regions VI and VII and FLMs, CENRAP guidance deviates from use of the 98th percentile impact. The CALMET datasets as described in this protocol were processed with the "No-Obs" options (i.e., surface and upper air observations were not used in the CALMET wind field interpolation). Aware that exercising CALMET with No-Obs may lead in some applications to potentially less conservatism in the CALPUFF visibility results compared with the use of CALMET with observations, CENRAP has agreed to EPA's recommendation that the maximum visibility impact, rather than the 98th percentile value, should be used for screening analyses using the CENRAP-developed CALMET datasets. This approach should be used in the source-specific subject-to-BART screening analysis.

Sources with modeled maximum impacts below the 0.5 dv threshold are exempt from the remainder of the BART process. Sources with impacts at or above 0.5 dv can either perform refined CALPUFF modeling to show their visibility impact is in fact below the 0.5 dv threshold or continue with the BART process and perform a BART analysis. This analysis will likely include more refined CALPUFF modeling, using observations coupled with the 98th percent impact, finer grid resolution, puff splitting, focused domain, etc.

VII. Change in Visibility Due to BART Controls

Once sources perform their BART analysis and BART emission limits are established, additional CALPUFF modeling should be conducted in order to establish visibility improvement at Class I areas with BART applied. The post-control CALPUFF simulation should be compared to the pre-control CALPUFF simulation by calculating the change in visibility over natural conditions between the pre-control and post-control simulations.

VIII. Reporting

Sources performing refined modeling will be required to submit a modeling protocol to the TCEQ for approval. Protocols must also be made available concurrently to EPA and FLMs for their review. Sources using TCEQ's source-specific subject-to-BART screening modeling protocol will not be required to provide a modeling protocol to the TCEQ. However, sources using the TCEQ's source-specific subject-to-BART screening modeling protocol must provide a modeling protocol to the EPA and FLMs 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 CALPUFF inputs and model output fields should also be included with the report. If the model code is re-compiled, the electronic archive should include all of the edited parameter files and a summary of the steps taken to re-compile the code, including the compiler used.

References

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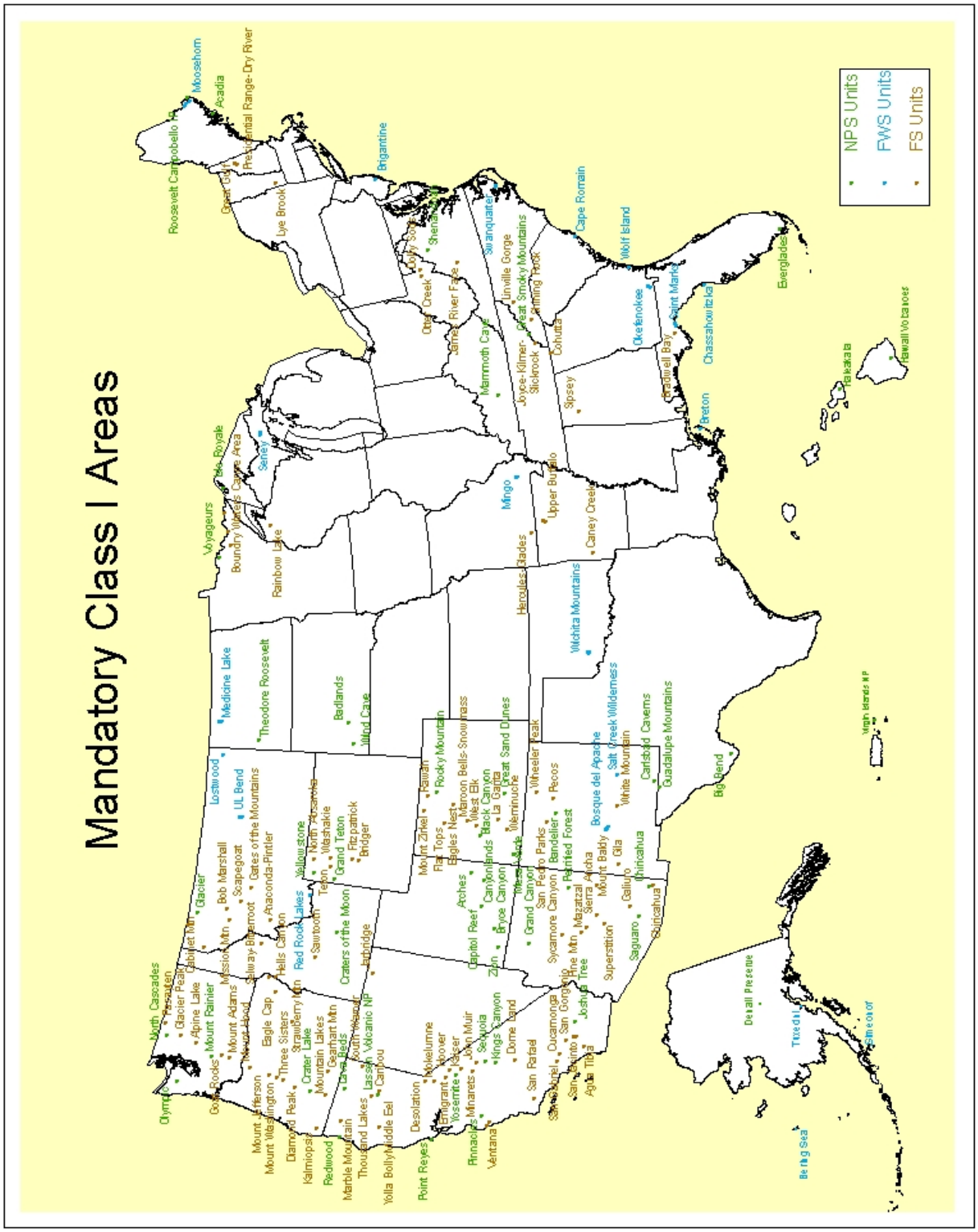
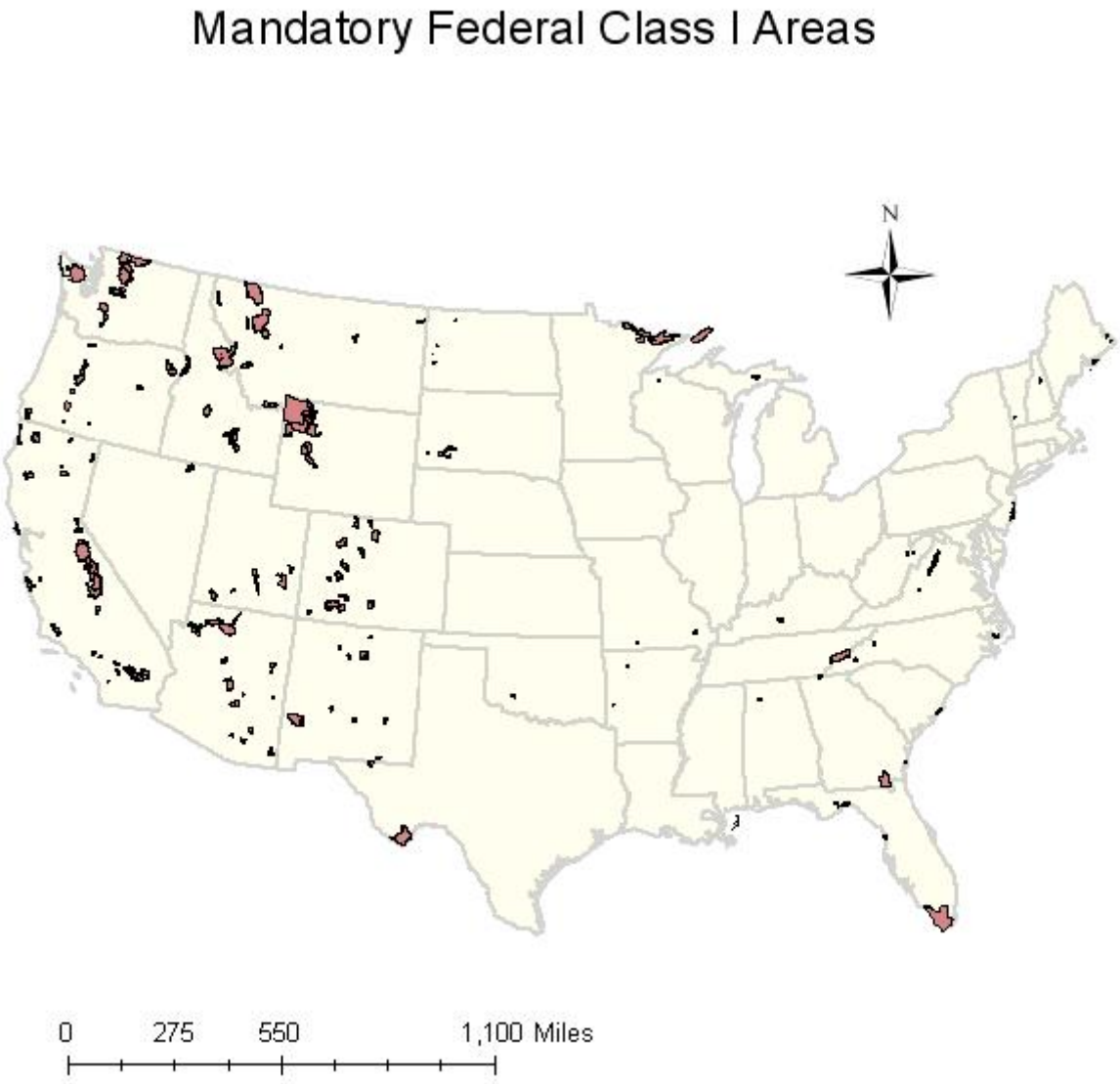
Appendix A – Federal Class I Areas
Map showing locations and names of areas



Appendix A – Federal Class I Areas
Map showing extent of areas



Appendix B – CALPUFF Control File Inputs

Variable	Description	Value	Default	Comments
INPUT GROUP 1: General run control parameters				
METRUN	Control parameter for running all periods in met. File (0=no; 1=yes)	0	Y	
IBYR	Starting year of the CALPUFF run	2002	n/a	2001 and 2003 are the other years modeled
IBMO	Starting month	1	n/a	
IBDY	Starting day	1	n/a	
IBHR	Starting hour	1	n/a	
XBTZ	Base time zone	6.0	n/a	Central Standard Time
IRLG	Length of the run (hours)	8760	n/a	2001=8760hrs, 2003=8748hrs only 12 hrs on 12/31
NSPEC	Total number of species modeled	7	5	
NSE	Number of species emitted	4	3	
METFM	Meteorological data format	1	Y	CALMET unformatted file
AVET	Averaging time (minutes)	60.0	Y	
PGTIME	Averaging time (minutes) for PG - σ_y	60.0	Y	
INPUT GROUP 2: Technical options				
MGAUSS	Control variable determining the vertical distribution used in the near field	1	Y	Gaussian
MCTADJ	Terrain adjustment method	3	Y	Partial plume path adjustment
MCTSG	CALPUFF sub-grid scale complex terrain module (CTSG) flag	0	Y	CTSG not modeled
MSLUG	Near-field puffs are modeled as elongated “slugs”?	0	Y	No
MTRANS	Transitional plume rise modeled?	1	Y	Transitional plume rise computed
MTIP	Stack tip downwash modeled?	1	Y	Yes
MBDW	Method used to simulate building downwash?	1	Y	ISC method
MSHEAR	Vertical wind shear above stack top modeled in plume rise?	0	Y	No
MSPLIT	Puff splitting allowed?	0	Y	No
MCHEM	Chemical mechanism flag	1	Y	Transformation rates computed internally (MESOPUFF II scheme)
MAQCHEM	Aqueous phase transformation flag	0	Y	Aqueous phase not modeled
MWET	Wet removal modeled?	1	Y	Yes
MDRY	Dry deposition modeled?	1	Y	Yes
MDISP	Method used to compute dispersion coefficients	3	Y	PG dispersion coefficients in RURAL & MP coefficients in urban areas
MTURBVW	Sigma-v/sigma-theta, sigma-w measurements used?	3	Y	Use both sigma-(v/theta) and sigma-w from PROFILE.DAT Note: not provided

Variable	Description	Value	Default	Comments
MDISP2	Backup method used to compute dispersion when measured turbulence data are missing	3	Y	PG dispersion coefficients in RURAL & MP coefficients in urban areas
MROUGH	PG sigma-y,z adj. for roughness?	0	Y	No
MPARTL	Partial plume penetration of elevated inversion?	1	Y	Yes
MTINV	Strength of temperature inversion	0	Y	No
MPDF	PDF used for dispersion under convective conditions?	0	Y	No
MSGTIBL	Sub-Grid TIBL module used for shoreline?	0	Y	No
MBCON	Boundary conditions (concentration) modeled?	0	Y	No
MFOG	Configure for FOG model output	0	Y	No
MREG	TEST options specified to see if they conform to regulatory values?	1	Y	Checks made
INPUT GROUP 3: Species list				
CSPEC	Species modeled	SO2 SO4 NOX HNO3 NO3 PM25 PM10	n/a	Modeled: All Emitted: SO2, NOx, PM25, PM10 Dry deposited: SO2(gas), SO4(particle), NOx(gas), HNO3(gas), NO3(particle), PM25(particle), PM10(particle)
INPUT GROUP 4: Map projection and grid control parameters				
PMAP	Map projection	LCC	N	Lambert conformal conic
FEAST	False Easting	0.0	Y	
FNORT	False Northing	0.0	Y	
RLATO	Latitude	40N	n/a	
RLONG	Longitude	97W	n/a	
XLAT1 XLAT2	Matching parallel(s) of latitude for projection	33N 45N	n/a n/a	
DATUM	Datum region for the coordinates	WGS-G	N	WGS-84 GRS 80 spheroid, global coverage (WGS84)
NX NY NZ	<u>Meteorological grid</u>: No. X grid cells in meteorological grid No. Y grid cells in meteorological grid No. vertical layers in meteorological grid	306 246 10	n/a	
DGRIDKM	Grid spacing (km)	6	n/a	
ZFACE	Cell face heights (m)	0, 20, 40,80, 160, 320, 640, 1200,	n/a	

Variable	Description	Value	Default	Comments
		2000, 3000, 4000		
XORIGKM YORIGKM	Reference coordinates of SW corner of grid cell (1,1) (km)	-1008 -1620	n/a	
 IBCOMP JBCOMP IECOMP JECOMP	<u>Computational grid:</u> X index of LL corner Y index of LL corner X index of UR corner Y index of UR corner	 1 1 306 246	n/a	
LSAMP IBSAMP JBSAMP IESAMP JESAMP MESHDN	Logical flag indicating if gridded receptors are used X index of LL corner Y index of LL corner X index of UR corner Y index of UR corner Nesting factor of the sampling grid	F 1	- Y	Receptors are only in the Class I areas assessed
INPUT GROUP 5: Output options				
SPECIES	Species (or group) list for output options	1	n/a	Concentrations saved for SO2, SO4, NOx, HNO3, NO3, PM25, PM10
INPUT GROUP 6: Subgrid scale complex terrain (CTSG) inputs				
NHILL	Number of terrain features	0	Y	
NCTREC	Number of special complex terrain receptors	0	Y	
MHILL	Terrain and CTSG receptor data for CTSG hills input in CTDM format?	2	n/a	Hill data created by OPTHILL & input below in subgroup (6b); receptor data in subgroup (6c) note: no data provided
XHILL2M	Factor to convert horizontal dimensions to meters	1	Y	
ZHILL2M	Factor to convert vertical dimensions to meters	1	Y	
XCTDMKM	X-origin of CTDM system relative to CALPUFF coordinate system, in Km	0	n/a	
YCTDMKM	Y-origin of CTDM system relative to CALPUFF coordinate system, in Km	0	n/a	
INPUT GROUP 7: Chemical parameters for dry deposition of gases				
SPECIES DIFFUSVTY ALPHA STR REACTVTY MESO RES HENRYS C	Chemical parameters for dry deposition of gases	-	Y Y Y Y Y Y	SO2; NOx; HNO3 0.1509 0.1656 0.1628 1000 1 1 8 8 18 0 5 0 0.04 3.5 8.0*E-8
INPUT GROUP 8: Size parameters for dry deposition of particles				
SPECIES GEO. MASS MEAN DIA.	Single species: mean and standard deviation used to compute deposition velocity for	-	n/a	SO4 NO3 PM25 PM10 0.48 0.48 0.48 0.48

Variable	Description	Value	Default	Comments
GEO.STAND DEV.	NINT size-ranges; averaged to obtain mean deposition velocity. Grouped species: size distribution specified, standard deviation as "0". Model uses deposition velocity for stated mean diameter.			2 2 2 2
INPUT GROUP 9: Miscellaneous dry deposition parameters				
RCUTR	Reference cuticle resistance	30	Y	
RGR	Reference ground resistance	10	Y	
REACTR	Reference pollutant reactivity	8	Y	
NINT	Number of particle-size intervals to evaluate effective particle deposition velocity	9	Y	
IVEG	Vegetation state in unirrigated areas	1	Y	
INPUT GROUP 10: Wet deposition parameters				
POLL LIQ PRECIP FRZ PRECIP	Scavenging coefficients	-	Y Y Y	SO2 SO4 NOx HNO3 NO3 3E-5 1E-4 0 6E-5 1E-4 0 3E-5 0 0 3E-5
INPUT GROUP 11: Chemistry parameters				
MOZ	Ozone data input option	0	N	
BCKO3	Monthly ozone concentrations	-	N	12*40
BCKNH3	Monthly ammonia concentrations	-	N	12*3
RNITE1	Nighttime SO2 loss rate	0.2	Y	
RNITE2	Nighttime NOx loss rate	2.0	Y	
RNITE3	Nighttime HNO3 formation rate	2.0	Y	
MH2O2	H2O2 data input option	1	Y	
BCKH2O2	Monthly H2O2 concentrations	-	Y	MQACHEM = 0; not used
BCKPMF OFRAC VCNX	Secondary Organic Aerosol options	-	-	MCHEM = 1; thus, not used
INPUT GROUP 12: Misc. Dispersion and computational parameters				
SYTDEP	Horizontal size of puff beyond which time-dependent dispersion equations (Heffter) are used.	550	Y	
MHFTSZ	Switch for using Heffter equation for sigma z as above	0	Y	
JSUP	Stability class used to determine plume growth rates for puffs above boundary layer	5	Y	
CONK1	Vertical dispersion constant for stable conditions	0.01	Y	
CONK2	Vertical dispersion constant for neutral/unstable conditions	0.1	Y	
TBD	Factor determining transition-point from Schulman-Scire to Huber-Snyder building	0.5	Y	No building downwash used

Variable	Description	Value	Default	Comments
	downwash scheme			
IURB1 IURB2	Range of land use categories for which urban dispersion is assumed	10 19	Y Y	METFM=1; not used
ILANDUIN	Land use category for modeling domain	-	-	METFM=1; not used
ZOIN	Roughness length (m) for modeling domain	-	-	METFM=1; not used
XLAIIN	Leaf area index for modeling domain	-	-	METFM=1; not used
ELEVIN	Elevation above sea level	-	-	METFM=1; not used
XLATIN	Latitude (degrees) for met location	-	-	METFM=1; not used
XLONIN	Longitude (degrees) for met location	-	-	METFM=1; not used
ANEMHT	Anemometer height (m)	-	-	METFM=1; not used
ISIGMAV	Form of lateral turbulence data in PROFILE.DAT	1	Y	Read sigma-v
IMIXCTDM	Choice of mixing heights	-	-	METFM=1; not used
XMXLEN	Maximum length of a slug	1	Y	
XSAMLEN	Maximum travel distance of a puff/slug during one sampling step	1	Y	
MXNEW	Maximum number of slugs/puffs released from one source during one time step	99	Y	
MXSAM	Maximum number of sampling steps for one puff/slug during one time step	99	Y	
NCOUNT	Number of iterations used when computing the transport wind for a sampling step that includes gradual rise	2	Y	
SYMIN	Minimum sigma y for a new puff/slug	1	Y	
SZMIN	Minimum sigma z for a new puff/slug	1	Y	
SVMIN SWMIN	Default minimum turbulence velocities sigma-v and sigma-w for each stability class	-	Y	A B C D E F .5 .5 .5 .5 .5 .5 .2 .12 .08 .06 .03 .016
CDIV	Divergence criterion for dw/dz across puff used to initiate adjustment for horizontal convergence	0, 0	Y	
WSCALM	Minimum wind speed allowed for non-calm conditions. Used as minimum speed returned when using power-law extrapolation toward surface	0.5	Y	
XMAXZI	Maximum mixing height (m)	4000	N	Top interface in CALMET simulation
XMINZI	Minimum mixing height (m)	20	N	
WSCAT	Default wind speed classes	-	Y	1 2 3 4 5 1.54 3.09 5.14 8.23 10.80

Variable	Description	Value	Default	Comments
PLXO	Default wind speed profile power-law exponents for stabilities 1-6	-	Y ISC RURAL	A B C D E F .07 .07 .10 .15 .35 .55
PTGO	Default potential temperature gradient for stable classes E, F (deg K/m)	-	Y	0.020; 0.035
PPC	Default plume path coefficients for each stability class	-	Y	A B C D E F .5 .5 .5 .5 .35 .35
SL2PF	Slug-to-puff transitions criterion factor equal to sigma-y/length of slug	10	Y	
NSPLIT	Number of puffs that result every time a puff is split	3	Y	
IRESPLIT	Time of day when split puffs are eligible to be split once again; this is typically set once per day, around sunset before nocturnal shear develops	-	N	Hour 18 = 1
ZISPLIT	Split is allowed only if last hour's mixing height (m) exceeds a minimum value	100	Y	
ROLDMAX	Split is allowed only if ratio of last hour's mixing ht to the maximum mixing ht experienced by the puff is less than a maximum value	0.25	Y	
NSPLITH	Number of puffs that result every time a puff is split	5	Y	
SYSPLITH	Minimum sigma-y of puff before it may be split	1	Y	
SHSPLITH	Minimum puff elongation rate due to wind shear, before it may be split	2	Y	
CNSPLITH	Minimum concentration of each species in puff before it may be split	1E-7	Y	
EPSSLUG	Fractional convergence criterion for numerical SLUG sampling integration	1E-4	Y	
EPSAREA	Fractional convergence criterion for numerical AREA source integration	1E-6	Y	
DSRISE	Trajectory step-length (m) used for numerical rise integration	1	Y	
HTMINBC	Minimum height (m) to which BC puffs are mixed as they are emitted. Actual height is reset to the current mixing height at the release point if greater than this minimum	500	Y	
RSAMPBC	Search radius (in BC segment lengths) about a receptor for sampling nearest BC puff. BC puffs are emitted with a spacing	10	N	

Variable	Description	Value	Default	Comments
	of one segment length, so the search radius should be greater than 1			
MDEPBC	Near-surface depletion adjustment to concentration profile used when sampling BC puffs?	1	Y	Adjust concentration for depletion
INPUT GROUP 13: Point source parameters				
NPT1	Number of point sources with parameters	-	n/a	
IPTU	Units used for point source emissions	1	Y	
NSPT1	Number of source-species combinations with variable emissions scaling factors	0	Y	
NPT2	Number of point sources with variable emission parameters provided in external file	0	n/a	
INPUT GROUP 14: Area source parameters – Not used				
INPUT GROUP 15: Line source parameters – Not used				
INPUT GROUP 16: Volume source parameters – Not used				
INPUT GROUP 17: Non-gridded (discrete) receptor information				
NREC	Number of non-gridded receptors	0 3996	n/a	147 Bandelier 480 Big Bend 168 Bosque del Apache 40 Breton 80 Caney Creek 256 Carlsbad Caverns 195 Great Sand Dunes 127 Guadalupe Mountains 80 Hercules-Glades 187 La Garita 312 Mesa Verde 47 Mingo 321 Pecos 55 Salt Creek 247 San Pedro Parks 72 Upper Buffalo 744 Weminuche 109 Wheeler Peak 270 White Mountain 59 Wichita Mountains

Appendix C – POSTUTIL Control File Inputs

Variable	Description	Value	Default	Comments
INPUT GROUP 1: General run control parameters				
ISYR	Starting Year	2002	n/a	2001 and 2003 also modeled
ISMO	Starting month	1	n/a	
IDY	Starting day	1	n/a	
ISHR	Starting hour	1	n/a	
NPER	Number of periods to process	8760	n/a	2001=8760 hrs, 2003=8748hrs only 12 hrs on 12/31
NSPECINP	Number of species to process from CALPUFF runs	7	n/a	
NSPECOUT	Number of species to write to output file	7	n/a	
NSPECCMP	Number of species to compute from those modeled	0	n/a	
MDUPLCT	Stop run if duplicate species names found?	0	Y	
NSCALED	Number of CALPUFF data files that will be scaled	0	Y	
MNITRATE	Re-compute the HNO3/NO3 partition for concentrations?	1	N	Yes, for all sources combined
BCKNH3	Default ammonia concentrations used for HNO3/NO3 partition	-	N	12*3
INPUT GROUP 2: Species processing information				
ASPECI	NSPECINP species will be processed	-	n/a	SO2, SO4, NOx, HNO3, NO3, PM25, PM10
ASPECO	NSPECOUT species will be written	-	n/a	SO2, SO4, NOx, HNO3, NO3, PM25, PM10

Appendix D – CALPOST Control File Inputs

Variable	Description	Value	Default	Comments
INPUT GROUP 1: General run control parameters				
METRUN	Option to run all periods found in met files	0	Y	Run period explicitly defined
ISYR	Starting Year	2002	n/a	2001 and 2003 also modeled
ISMO	Starting month	1	n/a	
IDY	Starting day	1	n/a	
ISHR	Starting hour	1	n/a	
NHRS	Number of hours to process	8760	n/a	2001=8760hrs, 2003=8748hrs only 12 hrs on 12/31
NREP	Process every hour of data?	1	Y	Every hour processed
ASPEC	Species to process	VISIB	n/a	Visibility processing
ILAYER	Layer/deposition code	1	Y	CALPUFF concentrations
A, B	Scaling factors X(new) = X(old) *A + B	0, 0	Y	
LBACK	Add hourly background concentrations/fluxes?	F	Y	
MSOURCE	Option to process source contributions	0	Y	
LG LD	Gridded receptors processed? Discrete receptors processed?	F T	N/Y	Receptors located only in the Class I areas assessed
LCT	CTSG Complex terrain receptors processed?	F	Y	
LDRING	Report results by DISCRETE receptor RING?	F	Y	
NDRECP	Flag for all receptors after the last one assigned is set to "0"	-1	Y	
IBGRID JBGRID IEGRID JEGRID	Range of gridded receptors	-1 -1 -1 -1	Y	When LG = T Entire grid processed if all =-1
NGONOFF	Number of gridded receptor rows provided to identify specific gridded receptors to process	0	Y	
BTZONE	Base time zone for the CALPUFF simulation	6	n/a	
MFRH	Particle growth curve f(RH) for hygroscopic species	2	Y	FLAG (2000) f(RH) tabulation. Note: not used
RHMAX	Maximum relative humidity (%) used in particle growth curve	-	N	Not used
LVSO4 LVNO3 LVOC LVPMC LVPMF LVEC	Modeled species to be included in computing light extinction	T T F T T F	Y Y N Y Y N	
LVBK	Include BACKGROUND when ranking for TOP-N, TOP-50, and exceedence tables?	T	Y	
SPECPMC	Species name used for particulates in	PM10	N	

Variable	Description	Value	Default	Comments
SPECPMF	MODEL.DAT file	PM25	N	
EEPMC EEPMF	Modeled particulate species	0.6 1.0	Y Y	
EEPMCBK	Background particulate species	0.6	Y	
EESO4 EENO3 EEOC EESOIL EEEC	Other species	3.0 3.0 4.0 1.0 10	Y Y Y Y Y	
LAVER	Background extinction computation	F	Y	
MVISBK	Method used for background light extinction	6	N	Compute extinction from speciated PM measurements. FLAG RH adjustment factor applied to observed and modeled sulfate and nitrate
RHFAC	Extinction coefficients for hygroscopic species (modeled and background). Monthly RH adjustment factors	-	n/a	See Table 4 in main protocol document
BKSO4 BKNO3 BKPMC BKOC BKSOIL BKEC	Monthly concentrations of ammonium sulfate, ammonium nitrate, coarse particulates, organic carbon, soil and elemental carbon to compute background extinction coefficients	-	n/a	See Table 5 in main protocol document
BEXTRAY	Extinction due to Rayleigh scattering (1/Mm)	10	Y	
IPRTU	Units for all output	3	N	micrograms/cubic meter
L24HR	Averaging time reported	T	n/a	
LTOPN	Visibility: Top "N" table for each averaging time selected.	F	Y	
NTOP	Number of 'Top-N' values at each receptor selected (NTOP must be <=4)	4	Y	
MDVIS	Output file with visibility change at each receptor?	0	Y	Create file of DAILY (24 hour) delta-deciview. Grid model run.