

Example Screening BART Simulation using the VISTAS Regional Domain

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Overview:

A set of sample CALPUFF input files and postprocessing (POSTUTIL and CALPOST) input files illustrating a typical screening-level application of the VISTAS BART protocol on the 12-km VISTAS CALMET domain is described in this memo. These files are available on the CALPUFF web site (www.src.com) on the VISTAS page. In this sample run, CALPUFF, POSTUTIL and CALPOST are run in order to implement the procedure for identifying potential impacts of a single sample source on air quality related values in the Otter Creek Class I Area. Specifically, using the VISTAS CALMET output files for a 1-year period (2002) on the 12-km regional domain, the transport and diffusion of emissions from a single point source is simulated using the CALPUFF model. A version of the CALPUFF model codes that should be used for the BART analysis is provided on the VISTAS page of the CALPUFF web site. The Graphical User Interface (GUI) necessary to implement the procedure, called the CALPUFF PROFESSIONAL GUI or CALPRO is also provided on the web site. Both the GUI and the model codes may be downloaded for free from the web site.

The required OZONE.DAT file is created from a “standard dataset” available on the web site. The SUBDOMN program (available through the CALPRO GUI) should be used to extract the OZONE.DAT files. The preprocessed CALMET output meteorological files required for the run are too large to distribute on the web site. These files can be obtained from the state agencies in the VISTAS region. They are normally distributed on a USB compatible 300 GB external hard drive.

Using POSTUTIL code, speciation of PM₁₀ into filterable and condensable particulates is conducted. Using CALPOST’s Method 6, the concentrations obtained at National Park Service receptors of the Otter Creek Class I area are used to obtain 24-hour changes in deciviews due to the source emissions. These changes in deciviews are referenced to background deciviews values that are provided by the reviewing agency. The peak change in deciviews resulting from these modeled emissions must not exceed 0.5 dv for any 24-hour average period for the screening simulation. See the VISTAS protocol for details.

In addition, although not a required part of the screening analysis, an additional POSTUTIL run can be processed to repartition nitrate and nitric acid using ammonia background on a receptor by receptor and hour by hour basis. A POSTUTIL sample input file and the explanation of the process is provided. This POSTUTIL run would normally be applied as part of the refined analysis, but it is illustrated in this memo using the 12-km screening meteorological dataset.

List of Model Input Information

- Meteorological Domain:**
- Starting time: January 1, 2002, hour 01
 - Run length: 8760 hours, meteorological files provided in 12 monthly runs
 - Map projection: LCC (Lambert Conformal)
 - Datum: NWS-84
 - Projection origin: 40°N, 97°W
 - Matching Parallels: 33°N, 45°N
 - False X, Y at Projection Origin: X = 0.00, Y = 0.00
 - Grid origin: (137.973 km, -1625.974 km)
 - No. grid cells: NX = 160, NY = 172, grid spacing: 12 km
 - No. of vertical layers: 10
 - Cell face heights:
0.,20.,40.,80.,160.,320.,640.,1200.,2000.,3000.,4000.
 - Base time zone: 5 (UTC-05 Eastern Time (US & Canada))

Table 1. Source Properties

Point Source	X (km)	Y (km)	Stack Ht. (m)	Base Elev. (m)	Stack Diam. (m)	Exit Vel. (m/s)	Exit Temp. (°K)	Species Emission Rates					
								SO ₂ (g/s)	SO ₄ (g/s)	NO _x (g/s)	HNO ₃ (g/s)	NO ₃ (g/s)	PM ₁₀ (g/s)
Sample Source	1710.991	-104.144	127.71	10.06	6.10	30.48	402.04	213.82	0.63	593.21	0.0	0.0	22.03

Note: PM₁₀ is not modeled as PM₁₀, it has been broken into different sizes: PM800, PM425, PM187, PM112, PM081, and PM056. The particulate matter species to be entered in CALPUFF are listed below and should be modeled with a unit emission rate, 1g/s:

- PM800 for size 6-10µm
- PM425 for size 2.50-6µm
- PM187 for size 1.25-2.50µm
- PM112 for size 1-1.25µm
- PM081 for size 0.625-1µm
- PM056 for size 0.50-0.625µm

Number of discrete receptors in Otter Creek Wilderness: 122

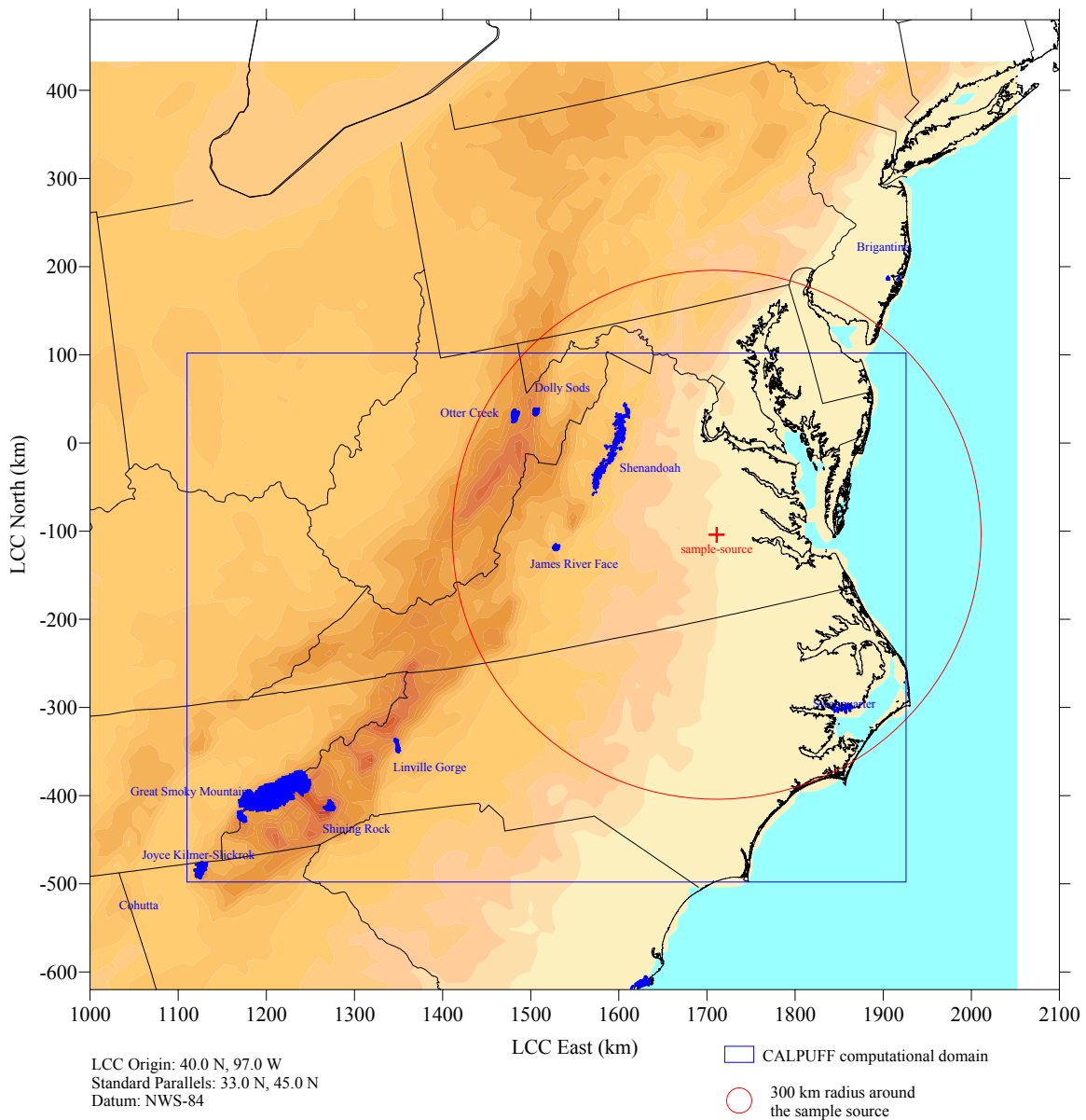


Figure 1. Terrain Elevation (12-km resolution) – Class I areas and a sample source locations. A 300-km radius around the source have been plotted to determine the Class I areas to be analyzed. The application focuses on Otter Creek, one of the five Class I areas that should be analyzed for this sample source.

Class I Visibility Analysis Overview of Steps

- (1) Run SUBDOMN to extract the OZONE.DAT file from the standard dataset.
- (2) Run CALPUFF to model the sample point source.
- (3) Run POSTUTIL to get the new components Elemental Carbon (EC), Soil, Organic Carbon (SOA) and PMC from the six PM categories.
- (4) Run CALPOST for Otter Creek Wilderness Class I area for the sample source using visibility Method 6. Make a table and analyze the results.
- (5) Run POSTUTIL and CALPOST to consider the effects of ammonia limiting and determine if the source can be screened out for this Class I area.

Step 1: CALPUFF Application

The CALPUFF sample control file PUFF2002-SM-R.INP is set-up for modeling a sample source in Virginia and its air quality and visibility impacts on the Otter Creek Wilderness. PG dispersion coefficients are used in the modeling (MDISP=3 and MPDF=0). The properties of the sample source are provided in the spreadsheet SAMPLE-POINT-SOURCE.XLS. Data in this spreadsheet are given in English Units. For the purpose of the CALPUFF modeling, all units are converted to the SI units in the same spreadsheet.

Data files provided:

- PUFF2002-SM-R.INP – sample CALPUFF control file
- SAMPLE-POINT-SOURCE.XLS – spreadsheet with the sample source parameters and emissions rates
- STANDARD2002_O.DAT – standard ozone data file

Steps for running CALPUFF:

- (1) Use COORDS to convert the sample source location listed in “SAMPLE-POINT-SOURCE.XLS” from latitude-longitude to the LCC projection. LCC parameters are provided on page 2 in the “List of Model Input Information”. The results of this conversion should match the LCC X and Y coordinates in Table 1 on page 2. These have already been entered in the sample CALPUFF control file, as well.
- (2) Extract an OZONE.DAT file from the standard dataset using the SUBDOMN program through CALPRO.
 - a- From the CALPRO GUI, select program SUBDOMN from the “Utilities” section of the screen.
 - b- Go to File at the top of the screen and “Change Directory” to your current directory

- c- Go to Input at the top of the screen and select Sequential. If the “shared file” was saved previously, any ‘shared information’ is automatically updated in the “Grid Settings” screen, the first of two screens in SUBDOMN. Check that the grid information is correct by comparing it with the information in the “List of Model Input Information” on page 2. If not, enter the “Grid Setting” using this information. Then, click on the “Next” button at the bottom of the screen.
 - d- In the “Extract Subsets from the Standard Datasets” screen, click on the “X/Y Coordinates” option. Insert the following values (the size of the CALPUFF domain + approximately 50 km outside all borders) to define the box for the ozone data subset: $X_{MIN} = 1060$, $X_{MAX} = 1976$, $Y_{MIN} = -548$, $Y_{MAX} = 152$ (all in kilometers). Type in STANDARD2002_O.DAT for the Input ozone data file, OZ2002VISTAS.DAT and OZ2002VISTAS.LST for the Output ozone data and list files, respectively. Unclick the options for extracting the Surface and Precipitation data files. Click “Extract Data Subsets”.
 - e- In the “SUBDOMN Run Status” click “Run”.
- (3) Run CALPUFF for the Sample Source.
- (4) (Optional) Open CALVIEW and plot CALPUFF domain, source location (red triangle) and receptors location (red crosses), ozone stations locations (blue circles) to check that everything is at the right place. You will need to create a “Shared File” if you have not done so yet to import the grid setting into CALVIEW. Go to “Identify Shared Information” on the main screen of CALPRO to create and save a “shared file”. You can open a Surfer plot to zoom on the CALPUFF domain.

Step 2: POSTUTIL Application - PM speciation

In the CALPUFF run, PM species are broken into several size categories according to the United States Environmental Protection Agency’s (EPA’s) *Compilation of Air Pollutant Emission Factors, Publication AP-42*. The size ranges considered include filterable PM and condensable PM. In the SAMPLE-POINT-SOURCE.XLS spreadsheet, PM emissions are provided for each of these size categories.

Data files provided:

- PMD1-2002-SM-R.INP – sample POSTUTIL control file
- SAMPLE-POINT-SOURCE.XLS – spreadsheet with a sample source parameters and emissions rates
- PM-DISTRIBUTION-SAMPLE-SOURCE.XLS – spreadsheet used to calculate the PM size distribution

Steps for running POSTUTIL:

- (1) In the sample control file, PMD1-2002-SM-R.INP, 11 species are processed and the 6 Particle Matter species (PM800, PM425, PM187, PM112, PM081 and PM056) are transformed in 4 new species - elemental carbon (EC), Soil, Organics (SOA) and PMC, which have different extinction coefficients for visibility impact application. The coefficients used in PMD1-2002-SM-R.INP were computed using the spreadsheet PM-DISTRIBUTION-SAMPLE-SOURCE.XLS.
- (2) A total of 9 species is then output. Note that no meteorological files are needed for this exercise.
- (3) Run POSTUTIL for the sample source.

Step 3: CALPOST Application – Visibility analysis

The CALPOST sample control file VIS-M6-2002-SM-OTCR-R.INP is set up to look at the change in light extinction at the Otter Creek Wilderness due to SO₄, NO₃ and PM₁₀ from the sample source located in Virginia, using visibility Method 6.

Data files provided:

VIS-M6-2002-SM-OTCR-R.INP– sample CALPOST control file

Note:

A monthly background concentration has been entered in the sample control file VIS-M6-2002-SM-OTCR-R.INP. It is entered only for SOIL, as you can see further, the way it is computed makes it suitable to represent background light extinction for all particulates (hygroscopic + non-hygroscopic) at the same time when multiplied by an extinction coefficient of 1.

The natural background light extinction in Table 2, taken from Appendix B of the *Guidance for Estimating Natural Visibility Conditions Under the Regional Haze Rule (2003)* for Otter Creek Wilderness is $b_{back} = 21.14 \text{ Mm}^{-1}$. The annual average value of the Haze Index (HI) is equal to 7.49 dv. The extinction coefficient is expressed in units of inverse megameters (10^{-6} m^{-1}), while haze index is expressed in units of deciviews (dv). Relationship between the extinction coefficient and HI is given by:

$$b_{back} = 10 \cdot e^{\frac{HI}{10}}$$

Total natural background light extinction, b_{back} in Otter Creek, including the Rayleigh scattering coefficient is equal to

$$b_{back} = b_{ray} + b_{soil} = 10 Mm^{-1} + b_{soil} = 21.14 Mm^{-1},$$

Where $b_{ray} = 10 Mm^{-1}$ and b_{soil} represents the extinction for all particulates in the background (hygroscopic or non-hygroscopic).

Hence,

$$b_{soil} = 11.14 Mm^{-1}$$

And since the extinction coefficient for soil C_{soil} is 1.0, the monthly background concentration for soil (BKSOIL) to be put in CALPOST is $11.14 \mu g/m^3$ for every month. Indeed,

$$b_{soil} = C_{soil} \cdot BKSOIL$$

The monthly f(RH) values for each month in Otter Creek as detailed in Table 3 are extracted from Appendix A of *Guidance for Estimating Natural Visibility Conditions Under the Regional Haze Rule (2003)*. These values are also already inserted in the sample control file VIS-M6-2002-SM-OTCR-R.INP.

Run CALPOST using the VIS-M6-2002-SM-OTCR-R.INP control file.

Table 2. Default Natural b_{ext} , (Mm⁻¹), Haze Index, HI (dv), and 10th and 90th Percentile of HI Values (dv)

Class I area	b_{ext} (Mm ⁻¹)	HI Ann. Avg. (dv)	HI Best Days (dv) ^(a)	HI Worst Days (dv) ^(a)
Otter Creek W	21.14	7.49	3.65	11.33

Source: *Guidance for Estimating Natural Visibility Conditions Under the Regional Haze Rule (2003), Appendix B*
^(a) Values for the best and worst days are estimated from a statistical approach described in Section 2.6 of the above document.

Table 3. Monthly f(RH) values based on the Centroid of the Area, for Visibility Method 6 application

Class I area	Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep	Oct	Nov	Dec
Otter Creek W.	3.0	2.8	2.8	2.6	3.2	3.5	3.7	4.1	4.0	3.3	3.0	3.1

Source: *Guidance for Estimating Natural Visibility Conditions Under the Regional Haze Rule (2003), Appendix A*

Results are presented in Tables 4 and 5.

Table 4. Method 6 Visibility results for year 2002

	Max Change in Deciview (dv)	Number of days Exceeding 0.5 dv	Receptor number of Max change	Day with max change
Otter Creek	0.756	2	1	June 20

Table 5. Method 6 Visibility results for year 2002, Ranks 1-8

	Change in Deciview (dv)	Day	Rank
Otter Creek	0.756	Jun 20 (172-0h)	1
	0.544	Dec 18 (353-0h)	2
	0.481	Oct 10 (284-0h)	3
	0.431	Jun 23 (175-0h)	4
	0.390	Jan 19 (020-0h)	5
	0.340	Apr 12 (103-0h)	6
	0.335	Oct 9 (283-0h)	7
	0.224	Mar 26 (086-0h)	8

Step 4: POSTUTIL/CALPOST Application – refined NO₃/HNO₃ repartitioning

In CALPUFF, the scavenging of the available ammonia for nitrate formation is computed on a puff-by-puff basis. Because of multiple puff overlap from an individual source, or several types of sources of a same facility run separately, this approach may tend to overestimate the amount of ammonia available to form nitrate. In order to address the cumulative consumption of ammonia, the CALPUFF chemical module is implemented into POSTUTIL, which repartitions nitric acid and nitrate on a receptor-by-receptor and hour-by-hour basis. All the sources of a same facility need to be included in this run. In this application only one point source is modeled, so only one CALPUFF concentration file is read as MODDAT.

The POSTUTIL input file is provided to illustrate this application. Although this is not a required part of the screening analysis, the file is provided to illustrate the technique that would be normally applied in the refined, fine-resolution simulations. The POSTUTIL runs get new NO₃/HNO₃ equilibrium concentrations for the sample source in the Class I area using BCKNH3 = 0.5ppb on a receptor-by receptor and hour-by-hour basis.

A CALPOST input file is also provided to run CALPOST using Method 6 in order to assess any change in deciview due to the sample source with new NO₃/HNO₃ repartitioning.

Files provided:

NH3-2002-OTCR-SM-R.INP
VIS-M6-2002-SM-OTCR-NH3-R.INP

POSTUTIL:

POSTUTIL repartitions NO₃ and HNO₃ concentrations from the sample source in the modeling domain by using only one NH₃ concentration (0.5ppb) for each hour and each receptor. The 12-km CALMET output files are required for this run of POSTUTIL.

- One concentration file is read as MODDAT: PMD1-2002-SM-R.CON (output of CALPUFF for sample source alone after PM speciation has been done in a previous POSTUTIL run, see step 2 of this exercise)
- There are a total of 9 species to be read from the sample source PMD1-2002-SM-R.CON file, (SO₂, SO₄, NO_x, HNO₃, NO₃, NH₃, EC, SOA, SOIL and PMC). POSTUTIL will output these same 9 species, too. Note that the input species names must match the species names in the CALPUFF files. No new species will be computed from those modeled.
- MNITRATE option is set to 1.

- And since no NH₃ is emitted from the source, NH3TYP is set to 3 (only background NH₃ = 0.5ppb for every month listed as BCKNH3 is used to repartition NO₃/HNO₃).

Run POSTUTIL to repartition NO₃ and HNO₃.

CALPOST:

Run CALPOST using the VIS-M6-2002-SM-OTCR-NH3-R.INP control file. NH3-2002-OTCR-SM-R.DAT is read.

Results are presented in Tables 6 and 7.

Table 6. Method 6 Visibility results after NO₃/HNO₃ repartitioned for year 2002

	Max Change in Deciview (dv)	Number of days Exceeding 0.5 dv	Receptor number of Max change	Day with max change
Otter Creek	0.533	2	6	Dec 18

Table 7. Method 6 Visibility results after NO₃/HNO₃ repartitioned for year 2002, Ranks 1-8

	Change in Deciview (dv)	Day	Rank
	0.533	Dec 18 (353-0h)	1
	0.510	Jun 20 (172-0h)	2
	0.424	Oct 10 (284-0h)	3
Otter Creek	0.412	Jun 23 (175-0h)	4
	0.390	Jan 19 (20-0h)	5
	0.327	Apr 12 (103-0h)	6
	0.302	Oct 9 (283-0h)	7
	0.230	Oct 12 (286-0h)	8