APPENDIX E

Report from

WRAP Regional Modeling Center

for Air Quality Modeling

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Overview

Visibility impairment occurs when fine particulate matter ($PM_{2.5}$) in the atmosphere scatters and absorbs light, thereby creating haze. $PM_{2.5}$ can be emitted into the atmosphere directly as primary particulates, or it can be produced in the atmosphere from photochemical reactions of gas-phase precursors and subsequent condensation to form secondary particulates. Examples of primary $PM_{2.5}$ include crustal materials and elemental carbon; examples of secondary PM include ammonium nitrate, ammonium sulfates, and secondary organic aerosols (SOA). Secondary $PM_{2.5}$ is generally smaller than primary $PM_{2.5}$, and because the ability of $PM_{2.5}$ to scatter light depends on particle size, with light scattering for fine particles being greater than for coarse particles, secondary $PM_{2.5}$ plays an especially important role in visibility impairment. Moreover, the smaller secondary $PM_{2.5}$ can remain suspended in the atmosphere for longer periods and is transported long distances, thereby contributing to regional-scale impacts of pollutant emissions on visibility.

The sources of $PM_{2.5}$ are difficult to quantify because of the complex nature of their formation, transport, and removal from the atmosphere. This makes it difficult to simply use emissions data to determine which pollutants should be controlled to most effectively improve visibility. Photochemical air quality models offer opportunity to better understand the sources of $PM_{2.5}$ by simulating the emissions of pollutants and the formation, transport, and deposition of $PM_{2.5}$. If an air quality model performs well for a historical episode, the model may then be useful for identifying the sources of $PM_{2.5}$ and helping to select the most effective emissions reduction strategies for attaining visibility goals. Although several types of air quality modeling systems are available, the gridded, three-dimensional, Eulerian models provide the most complete spatial representation and the most comprehensive representation of processes affecting $PM_{2.5}$, especially for situations in which multiple pollutant sources interact to form $PM_{2.5}$. For less complex situations in which a few large point sources of emissions are the dominant source of $PM_{2.5}$, trajectory models (such as the California Puff Model [CALPUFF]) may also be useful for simulating $PM_{2.5}$.

Air Quality Models

The WRAP RMC utilized two regulatory air quality modeling systems to conduct all regional haze modeling. A brief discussion of each of these models is provided below.

Community Multi-Scale Air Quality Model

EPA initially developed the Community Multi-Scale Air Quality (CMAQ) modeling system in the late 1990s. The model source code and supporting data can be downloaded from the Community Modeling and Analysis System (CMAS) Center (http://www.cmascenter.org/), which is funded by EPA to distribute and provide limited support for CMAQ users. CMAQ was designed as a "one atmosphere" modeling system to encompass modeling of multiple pollutants and issues, including ozone, PM, visibility, and air toxics. This is in contrast to many earlier air quality models that focused on single-pollutant issues (e.g., ozone modeling by the Urban Airshed Model). CMAQ is an Eulerian model—that is, it is a grid-based model in which the

frame of reference is a fixed, three-dimensional (3-D) grid with uniformly sized horizontal grid cells and variable vertical layer thicknesses. The number and size of grid cells and the number and thicknesses of layers are defined by the user, based in part on the size of the modeling domain to be used for each modeling project. The key science processes included in CMAQ are emissions, advection and dispersion, photochemical transformation, aerosol thermodynamics and phase transfer, aqueous chemistry, and wet and dry deposition of trace species. CMAQ offers a variety of choices in the numerical algorithms for treating many of these processes, and it is designed so that new algorithms can be included in the model. CMAQ offers a choice of three photochemical mechanisms for solving gas-phase chemistry: the Regional Acid Deposition Mechanism version 2 (RADM2), a fixed coefficient version of the SAPRC90 mechanism, and the Carbon Bond IV mechanism (CB-IV).

Comprehensive Air Quality Model with Extensions

The Comprehensive Air Quality Model with extensions (CAMx) model was initially developed by ENVIRON in the late 1990s as a nested-grid, gas-phase, Eulerian photochemical grid model. ENVIRON later revised CAMx to treat PM, visibility, and air toxics. While there are many similarities between the CMAQ and CAMx systems, there are also some significant differences in their treatment of advection, dispersion, aerosol formation, and dry and wet deposition.

Model Versions

Both EPA and ENVIRON periodically update and revise their models as new science or other improvements to the models are developed. For CMAQ, EPA typically provides a new release about once per year. The initial 2002 MPE for WRAP used CMAQ version 4.4, which was released in October 2004. In October 2005 EPA released CMAQ version 4.5, which includes the following updates and improvements to the modeling system:

- A new vertical advection algorithm with improved mass conservation
- Changes in deposition velocities for some PM species
- A new sea-salt emissions model and inclusion of sea salt in the aerosol thermodynamics
- An option to make vertical mixing parameters vary as a function of land use type

The RMC completed the initial CMAQ MPE using CMAQ v.4.4. When version 4.5 was released in October, the modeling was revised and a comparison of the model performance using the two versions was compared. Note that some of the new features in CMAQ v4.5 (e.g., sea salt in the AE4 aerosol dynamics module, and percent urban minimum vertical diffusivity) require the reprocessing of the MM5 data using the new version of MCIP (MCIP v3.0). However, because such reprocessing could potentially jeopardize the WRAP modeling schedule, WRAP elected to operate CMAQ v4.5 using the MM5 data processed using a previous MCIP version, MCIP v2.3, and the AE3 aerosol module that does not include active sea salt chemistry.

ENVIRON releases updated versions of CAMx approximately every two years, or as new features become available. The version used for the comparison of CMAQ and CAMx was CAMx v4.3. There are many similarities between CMAQ and CAMx regarding the science algorithms and chemical mechanisms used, including the CB-IV gas-phase and RADM aqueous-phase chemistries, ISORROPIA aerosol thermodynamics, and PPM horizontal advection scheme.

In the past, the treatment of vertical advection was a major difference between the two models; however, the incorporation of the new mass conservation scheme in CMAQ v4.5 makes its vertical advection algorithm much more similar to that of CAMx.

Major differences between the two models that still exist are in the basic model code, in the treatment of horizontal diffusion SOA formation mechanisms, and in grid nesting (CAMx supports one-way and two-way nesting, whereas CMAQ supports just one-way grid nesting). Both models include process analysis for the gas-phase portions of the model. The publicly released version of CAMx supports ozone and PM source apportionment through its Ozone and PM Source Apportionment Technology (OSAT/PSAT) probing tools, while for CMAQ there are research versions of the model that include Tagged Species Source Apportionment (TSSA) for some PM species (e.g., sulfate and nitrate). There are also research versions of CMAQ and CAMx that support the Decoupled Direct Method (DDM) sensitivity tool for PM and ozone.

The CAMx model is computationally more efficient than CMAQ. However, CAMx is currently supported for use on only a single central processing unit (CPU) and can perform multiprocessing using Open Multi-Processing (OMP) parallelization (i.e., shared memory multiprocessors). CMAQ parallelization, on the other hand, is implemented using Message Passing Interface (MPI) multiprocessing and therefore can be run using any number of CPUs. Depending on the number of model simulations to be performed and the manner in which they are set up, there can be a slight advantage either to CAMx or to CMAQ in regard to computational efficiency.

Model Simulations

In support of the WRAP Regional Haze air quality modeling efforts, the RMC developed air quality modeling inputs including annual meteorology and emissions inventories for a 2002 actual emissions base case, a planning case to represent the 2000-04 regional haze baseline period using averages for key emissions categories, and a 2018 base case of projected emissions determined using factors known at the end of 2005. All emission inventories were developed using the Sparse Matrix Operator Kernel Emissions (SMOKE) modeling system. Each of these inventories has undergone a number of revisions throughout the development process to arrive at the final versions used in CMAQ and CAMx air quality modeling. The development of each of these emission scenarios is documented under the emissions inventory sections of the TSS. In addition to various sensitivities scenarios, the WRAP performed air quality model simulations for each of the emissions scenarios as follows:

- The 2002 base case emissions scenario, referred to as “2002 Base Case” or “Base02”. The purpose of the Base02 inventory is to represent the actual conditions in calendar year 2002 with respect to ambient air quality and the associated sources of criteria and particulate matter air pollutants. The Base02 emissions inventories are used to validate the air quality model and associated databases and to demonstrate acceptable model performance with respect to replicating observed particulate matter air quality.
- The 2000-04 baseline period planning case emissions scenario is referred to as “Plan02”. The purpose of the Plan02 inventory is to represent baseline emission patterns based on average, or “typical”, conditions. This inventory provides a basis for comparison with the

future year 2018 projected emissions, as well as to gauge reasonable progress with respect to future year visibility.

- The 2018 future-year base case emissions scenario, referred to as "2018 Base Case" or "Base18". These emissions are used to represent conditions in future year 2018 with respect to sources of criteria and particulate matter air pollutants, taking into consideration growth and controls. Modeling results based on this emission inventory are used to define the future year ambient air quality and visibility metrics.

Data Sources

The CMAQ model requires inputs of three-dimensional gridded wind, temperature, humidity, cloud/precipitation, and boundary layer parameters. The current version of CMAQ can only utilize output fields from the PSU/NCAR MM5 meteorological model. MM5 is a state-of-the-science atmosphere model that has proven useful for air quality applications and has been used extensively in past local, state, regional, and national modeling efforts. MM5 has undergone extensive peer-review, with all of its components continually undergoing development and scrutiny by the modeling community. In-depth descriptions of MM5 can be found in Dudhia (1993) and Grell et al. (1994), and at http://www.mmm.ucar.edu/mm5. All meteorological data used for the WRAP air quality modeling efforts are derived from MM5 model simulations. The development of these data is documented in (Kemball-Cook, S. et al., 2005)

Emission inventories for all WRAP air quality simulations were developed using the Matrix Operator Kernel Emissions (SMOKE) modeling system. The development of these data has been discussed and documented elsewhere (Tonnesen, G. et al., 2006)

Initial conditions (ICs) are specified by the user for the first day of a model simulation. For continental-scale modeling using the RPO Unified 36-km domain, the ICs can affect model results for as many as 15 days, although the effect typically becomes very small after about 7 days. A model spin-up period is included in each simulation to eliminate any effects from the ICs. For the WRAP modeling, the annual simulation is divided into four quarters, and included a 15-day spin-up period for the quarters beginning in April, July, and October. For the quarter beginning in January 2002, a spin-up period covering December 16-31, 2001, using meteorology and emissions data developed for CENRAP were used..

Boundary conditions (BCs) specify the concentrations of gas and PM species at the four lateral boundaries of the model domain. BCs determine the amounts of gas and PM species that are transported into the model domain when winds flow is into the domain. Boundary conditions have a much larger effect on model simulations than do ICs. For some areas in the WRAP region and for clean conditions, the BCs can be a substantial contributor to visibility impairment.

For this study BC data generated in an annual simulation of the global-scale GEOS-Chem model that was completed by Jacob et al. (http://www-as.harvard.edu/chemistry/trop/geos/) for calendar year 2002 were applied. Additional data processing of the GEOS-Chem data was required before using them in CMAQ and CAMx. The data first had to be mapped to the boundaries of the WRAP domain, and the gas and PM species had to be remapped to a set of species used in the CMAQ and CAMx models. This work was completed by Byun and coworkers (http://www-

as.harvard.edu/chemistry/trop/geos/meetings/2005/ppt/Expanding_Model_Capabilities/GEOS-CMAQ_april_4_Byun.ppt

The CMAQ model options and configuration used for the WRAP 36-km model simulations are described in Tonnesen, G. et al., 2006.

Model Run Specification Sheets

In order to provide documentation for each of the CMAQ and CAMx air quality model simulations conducted by the WRAP RMC during Calendar year 2006, a series of Model Run Specification Sheets were developed. These "Spec Sheets" provide a description of each simulation, the various air quality model options and configurations used and detailed listing and description of the meteorological data and emission inventories for each scenario. These Spec Sheets also provide a means for the RMC to track the development of each of the input data sets and defined the modeling schedule. The purpose of each simulation, and expected results, including their implications, are also included. A link to each of the individual Specification Sheets for the model simulations can be found on the RMC web site at: http://pah.cert.ucr.edu/aqm/308/cmaq.shtml.

2002 Base Case Modeling

Base02 Sensitivity Simulations

The purpose of the 2002 Base Case modeling efforts was to evaluate air quality/visibility modeling systems for a historical episode—in this case, for calendar year 2002—to demonstrate the suitability of the modeling systems for subsequent planning, sensitivity, and emissions control strategy modeling. Model performance evaluation is performed by comparing output from model simulations with ambient air quality data for the same time period. After creating emissions and meteorology inputs for the two air quality models, CMAQ and CAMx, the next step was to perform the visibility modeling and the model performance evaluations, which are described below. A detailed discussion of the results of the CMAQ and CAMx model simulations can be found in Tonnesen, G. et al., 2006. Also documented in Tonnesen, G. et al., 2006 are the results of the model performance evaluation, a model inter-comparison and discussion of various sensitivity simulations. This information was used as the basis for recommending the selection of CMAQ and/or CAMx to complete the remaining modeling efforts in RMC's support of WRAP.

Model Performance Evaluation

The objective of a model performance evaluation (MPE) is to compare model-simulated concentrations with observed data to determine whether the model's performance is sufficiently accurate to justify using the model for simulating future conditions. There are a number of challenges in completing an annual MPE for regional haze. The model must be compared to ambient data from several different monitoring networks for both PM and gaseous species, for an

annual time period, and for a large number of sites. The model must be evaluated for both the worst visibility conditions and for very clean conditions. Finally, final guidance on how to perform an MPE for fine-particulate models is not yet available from EPA. Therefore, the RMC experimented with many different approaches for showing model performance results. The plot types that were found to be the most useful are the following:

- Time-series plots comparing the measured and model-predicted species concentrations
- Scatter plots showing model predictions on the *y*-axis and ambient data on the *x*-axis
- Spatial analysis plots with ambient data overlaid on model predictions
- Bar plots comparing the mean fractional bias (MFB) or mean fractional error (MFE) performance metrics
- "Bugle plots" showing how model performance varies as a function of the PM species concentration
- Stacked-bar plots of contributions to light extinction for the average of the best-20% visibility days or the worst-20% visibility days at each site; the higher the light extinction, the lower the visibility

Examples of each of these MPE metrics and analysis products can be found in Tonnesen, G. et al., 2006. The results of the MPE are available from the WRAP RMC website (http://pah.cert.ucr.edu/aqm/308/eval.shtml)

2002 Planning Scenario

The 2000-04 baseline period planning case scenario is referred to as "Plan02". The purpose of the Plan02 scenario is to simulation the air quality representative of baseline emission patterns based on average, or "typical", conditions. This scenario provides a basis for comparison with the future year 2018 scenario based on projected emissions, as well as to gauge reasonable progress with respect to future year visibility.

Plan02 Simulations Input Data

Input data used for the 2002 Planning model simulations consisted of the same meteorology as for the 2002 Base Case and the Plan02 emission inventories described under the Emissions Modeling section of the TSS.

The setup of the CMAQ model (including science options, run scripts, simulation periods, and ancillary data) for the Plan02 cases was identical to that used in the Base02 modeling, as described in the 2002 MPE report (Tonnesen et al., 2006). In summary, CMAQ v4.5 (released by EPA in October 2005) was used on the RPO Unified 36-km domain. The Carbon Bond Mechanism version 4 (CB4) with RADM aqueous chemistry, the SORGAM organic aerosol algorithm, and all other science algorithms detailed in Tonnesen et al., 2006 were used. Initial condition (IC) data for January 1, 2002, were developed using a 15-day spin-up period (December 16-31, 2001). Boundary condition (BC) data were generated in an annual simulation

of the global-scale GEOS-Chem model that was completed by Jacob et al. (http://www-as.harvard.edu/chemistry/trop/geos/) for calendar year 2002.

Comparison With Base02 Simulations

For each of the three Plan02 emissions datasets, annual visibility modeling was performed using the CMAQ model. This was a key aspect of the QA procedure, since errors in the emissions inventories that might not be apparent during the emissions QA steps might be more readily detected in the results from the CMAQ modeling.

In our initial analysis of the Plan02 scenario, plots were prepared for QA purposes that compared the Plan02a CMAQ results with the Base02a CMAQ results for daily and monthly averages. After revising Plan02a to create Plan02b and Plan02c, additional QA plots were prepared to compare the CMAQ results of each revised Plan02 case to the previous iteration. These were prepared as Program for the Analysis and Visualization of Environmental data (PAVE) spatial plots showing the change in individual $PM_{2.5}$ species concentrations as daily, monthly, and annual averages. The final set of analysis products, available on the RMC web site, include PAVE difference plots comparing the CMAQ-predicted annual average species concentrations from the Plan02c case with those from the Base02b case. Note that these plots are not useful for visibility planning purposes, but are being provided to show the magnitudes of changes when moving from the 2002 Base Case to the 2002 Planning Case—in other words, from the actual emissions for the year 2002 to the "typical-year" emissions created for the final Plan02 scenario. The primary analysis "product" from the Plan02 CMAQ modeling is the use of its output in combination with the CMAQ output from the 2018 modeling to develop the visibility progress calculations and glide path plots, described below.

2018 Model Simulations

The 2018 future-year base case scenario is referred to as "2018 Base Case" or "Base18". The purpose of the Base18 scenario is to simulation the air quality representative of conditions in future year 2018 with respect to sources of criteria and particulate matter air pollutants, taking into consideration growth and controls. Modeling results based on this emission inventory are used to define the future year ambient air quality and visibility metrics.

Base18 Simulation Input Data

Input data used for the 2018 Base Case model simulations consisted of the same meteorology as for the 2002 Base Case and the Base18 emission inventories described under the Emissions Modeling section of the TSS.

The setup of the CMAQ model (including science options, run scripts, simulation periods, and ancillary data) for the Base18 cases was identical to that used in the Base02 modeling, as

described in the 2002 MPE report (Tonnesen et al., 2006). In summary, CMAQ v4.5 (released by EPA in October 2005) was used on the RPO Unified 36-km domain. The Carbon Bond Mechanism version 4 (CB4) with RADM aqueous chemistry, the SORGAM organic aerosol algorithm, and all other science algorithms detailed in Tonnesen et al., 2006 were used. Initial condition (IC) data for January 1, 2002, were developed using a 15-day spin-up period (December 16-31, 2001). Boundary condition (BC) data were generated in an annual simulation of the global-scale GEOS-Chem model that was completed by Jacob et al. (http://www-as.harvard.edu/chemistry/trop/geos/) for calendar year 2002.

Base18 Simulation Results

The purpose of modeling 2018 visibility is to compare the 2018 visibility predictions to the 2002 typical-year visibility modeling results, as discussed below. Some improvements in visibility by 2018 are expected because of reductions in emissions due to currently planned regulations and technology improvements. A brief summary is provided here of the comparison between the 2018 and 2002 results using annual average PAVE spatial plots. The goal of this summary is to convey the scale and spatial extent of changes in key $PM_{2.5}$ species from 2002 to 2018. For planning purposes, on the other hand, states and tribes should focus on the visibility projections and glide path calculations at individual Class I Areas.

Figures 1 through 4 show the annual average concentrations for sulfate, nitrate, $PM_{2.5}$ and model-reconstructed visibility (in deciviews), respectively. In each figure, the bottom two plots show the modeled concentration or deciviews for the Plan02b and Base18b cases, while the top plot shows the change in visibility calculated as Base18b minus Plan02b. The Plan02b results are presented here instead of Plan02c results because these plots had previously been prepared with version B. As the differences between Plan02b and Plan02c are extremely small, new plots prepared using Plan02c would be essentially identical to the results in Figure 1 through 4.

In each of the top plots in the four figures, cool colors indicate areas in which model-predicted visibility improved from 2002 to 2018, while warm colors indicate areas where modeled visibility became worse over that period. Figure 1 shows that reductions in sulfate were largest in the southwest corner of the WRAP region and in Texas and Oklahoma. This results from planned SO_x emissions reductions in the CENRAP region. There were smaller reductions in sulfate in the Los Angeles area, western Washington state, and southern Nevada. There were small increases of sulfate, mostly in Wyoming, due to growth in SO_x emissions. Most regions of the WRAP domain had low concentrations of sulfate in 2002 and little change in sulfate by 2018.

Figure 2 shows the results for nitrate. In the both 2002 and 2018, the modeled nitrate was greatest in California, and there were reduction in nitrate in that state in 2018 because of reductions in mobile-source NO_x emissions. There were small reductions in the Phoenix area as well, also from reductions in mobile-source NO_x emissions.

Figure 3 shows the comparison of $PM_{2.5}$ for 2002 and 2018. In most areas of the WRAP region, changes in $PM_{2.5}$ were less than 1 $\mu g/m^3$. Locations with increases in $PM_{2.5}$ correspond to areas of increased sulfate (see Figure 3-1). Areas with the largest reductions in $PM_{2.5}$ were the areas in California that had large reductions in modeled nitrate in 2018 (see Figure 3-2). Results for other species that contribute to $PM_{2.5}$ are available on the RMC web site at http://pah.cert.ucr.edu/aqm/308/cmaq.shtml#base18bvsplan02b.

Figure 4 compares model-reconstructed visibility for 2002 and 2018. Note that these results are calculated using the modeled relative humidity (RH), so they differ from the results that use site-specific monthly average RH. Nonetheless, the results in Figure 4 are indicative of the direction and magnitude of visibility changes in from 2002 to 2018. Although the largest improvements are in California and the Pacific Northwest, there were improvements throughout the WRAP region. The change in deciviews is more dramatic than the change in $PM_{2.5}$ mass (Figure 3) because the visibility in deciviews is a relative metric, so small mass changes in $PM_{2.5}$ in good visibility areas can result in large relative improvements in visibility.

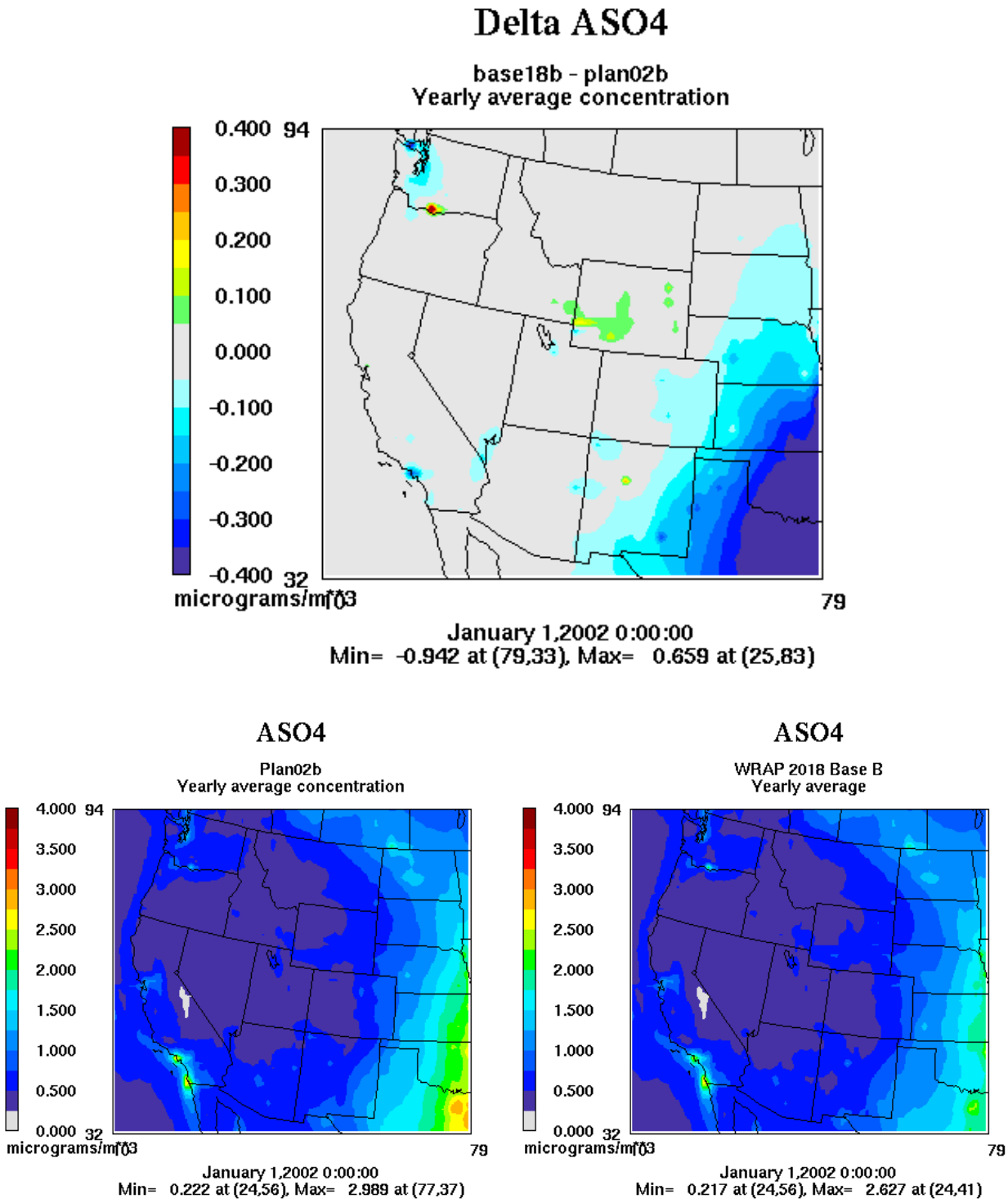


Figure 1. Annual average aerosol sulfate (ASO4) concentration comparisons between Base18b and Plan02b. Top plot: difference between the two (Base18b – Plan02b); bottom left plot: Plan02b results; bottom right plot: Base18b results.

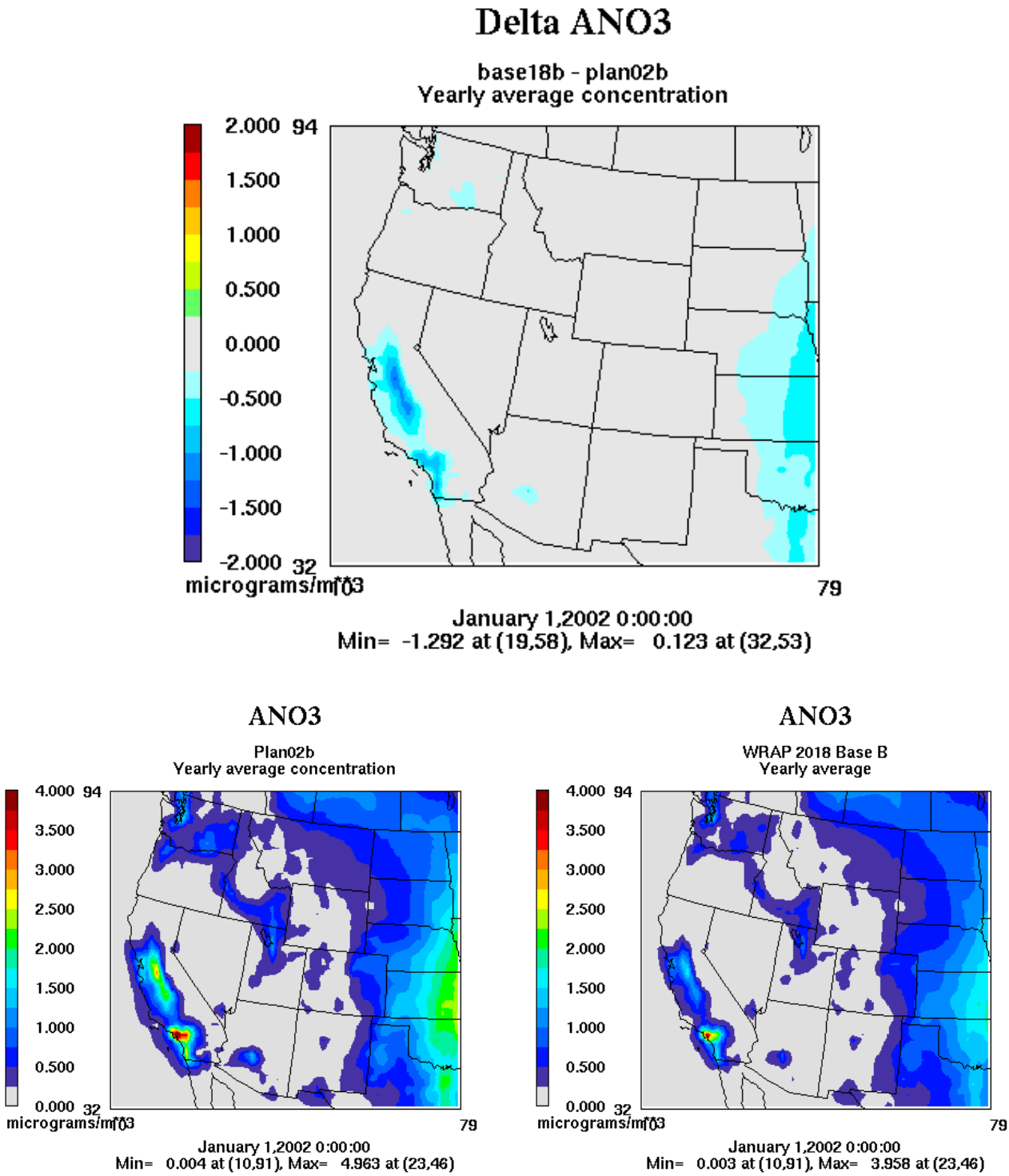


Figure 2. Annual average aerosol nitrate (ANO3) concentration comparisons between Base18b and Plan02b. Top plot: difference between the two (Base18b – Plan02b); bottom left plot: Plan02b results; bottom right plot: Base18b results.

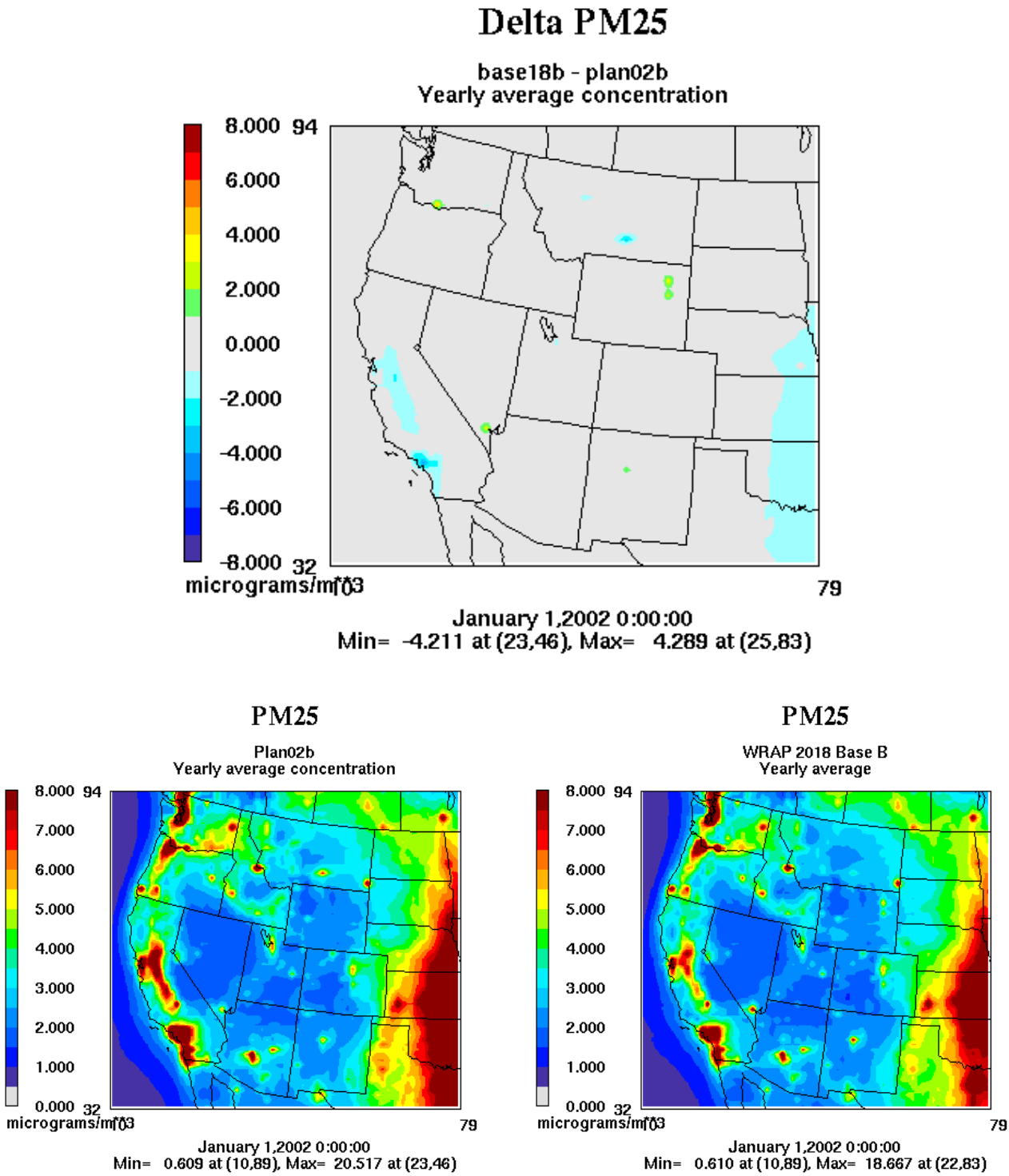


Figure 3. Annual average $PM_{2.5}$ concentration comparisons between Base18b and Plan02b. Top plot: difference between the two (Base18b – Plan02b); bottom left plot: Plan02b results; bottom right plot: Base18b results.

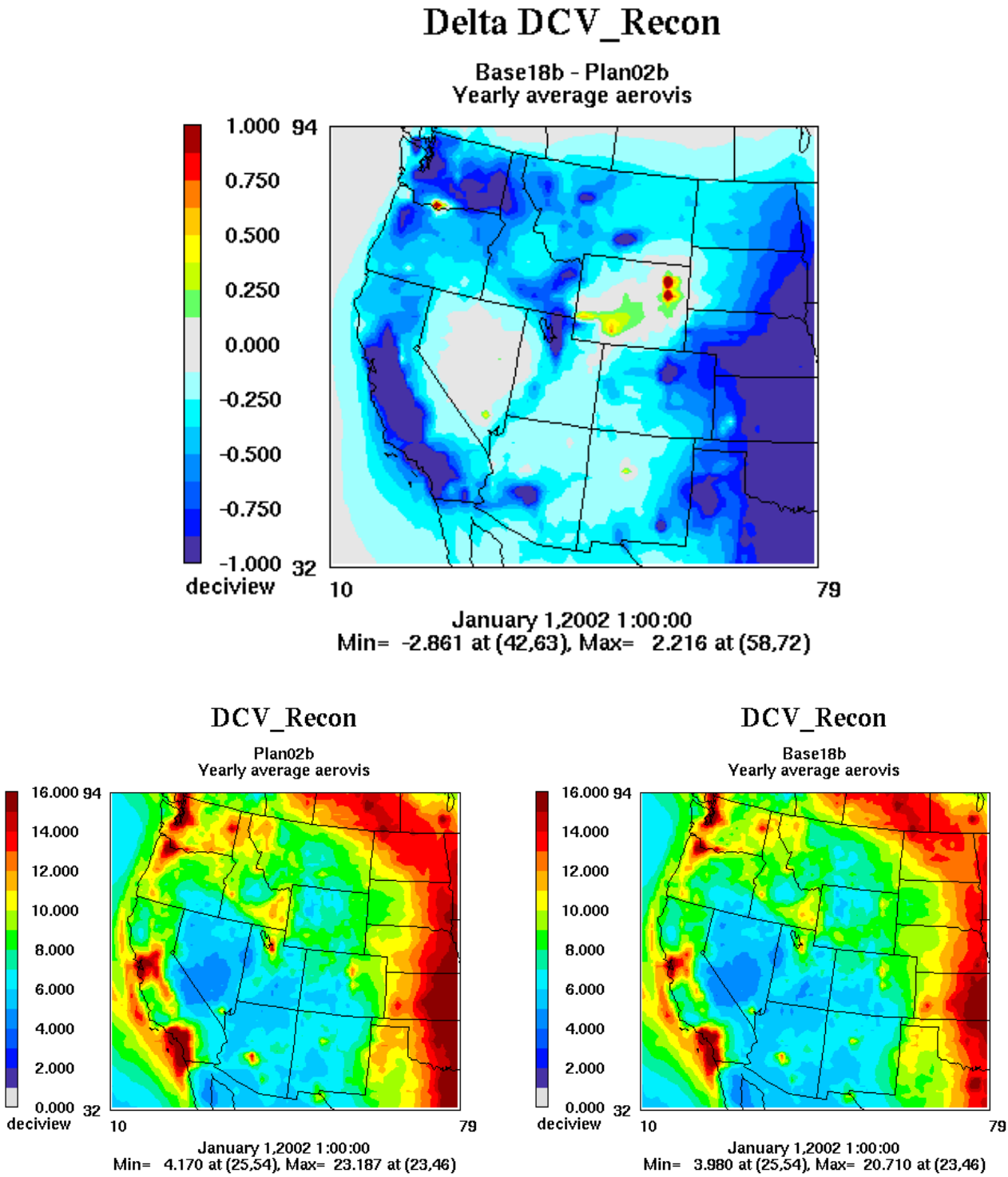


Figure 4. Annual average deciview comparisons between Base18b and Plan02b. Top plot: difference between the two (Base18b – Plan02b); bottom left plot: Plan02b results; bottom right plot: Base18b results.

Visibility Projections

The Regional Haze Rule (RHR) goals include achieving natural visibility conditions at 156 Federally mandated Class I areas by 2064. In more specific terms, that RHR goal is defined as (1) visibility improvement toward natural conditions for the 20% of days that have the worst visibility (termed "20% worst," or W20%, visibility days) and (2) no worsening in visibility for the 20% of days that have the best visibility ("20% best," or B20%, visibility days). One component of the states' demonstration to EPA that they are making reasonable progress toward this 2064 goal is the comparison of modeled visibility projections for the first milestone year of 2018 with what is termed a uniform rate of progress (URP) goal. As explained in detail below, the 2018 URP goal is obtained by constructing a "linear glide path" (in deciviews) that has at one end the observed visibility conditions during the mandated five-year (2000-2004) baseline period and at the other end natural visibility conditions in 2064; the visibility value that occurs on the glide path at year 2018 is the URP goal.

Preliminary WRAP 2018 visibility projections have been made using the Plan02c and Base18b CMAQ 36-km modeling results, following EPA guidance that recommends applying the modeling results in a relative sense to project future-year visibility conditions (U.S. EPA, 2001, 2003a, 2006**).** Projections are made using relative response factors (RRFs), which are defined as the ratio of the future-year modeling results to the current-year modeling results. The calculated RRFs are applied to the baseline observed visibility conditions to project future-year observed visibility. These projections can then be used to assess the effectiveness of the simulated emission control strategies that were included in the future-year modeling. The major features of EPA's recommended visibility projections are as follows (U.S. EPA, 2003a,b, 2006):

- Monitoring data should be used to define current air quality.
- Monitored concentrations of PM_{10} are divided into six major components; the first five are assumed to be $PM_{2.5}$ and the sixth is $PM_{2.5\text{-}10}$.
  - SO_4 (sulfate)
  - NO_3 (particulate nitrate)
  - OC (organic carbon)
  - EC (elemental carbon)
  - OF (other fine particulate or soil)
  - CM (coarse matter).
- Models are used in a relative sense to develop RRFs between future and current predicted concentrations of each component.
- Component-specific RRFs are multiplied by current monitored values to estimate future component concentrations.
- Estimates of future component concentrations are consolidated to provide an estimate of future air quality.

- Future estimated air quality is compared with the goal for regional haze to see whether the simulated control strategy would result in the goal being met.
- It is acceptable to assume that all measured sulfate is in the form of ammonium sulfate [$(NH_4)_2SO_4$] and all particulate nitrate is in the form of ammonium nitrate [NH_4NO_3].

To facilitate tracking the progress toward visibility goals, two important visibility parameters are required for each Class I area:

- *Baseline Conditions:* "Baseline Conditions" represent visibility for the B20% and W20% days for the initial five-year baseline period of the regional haze program. Baseline Conditions are calculated using monitoring data collected during the 2000-2004 five-year period and are the starting point in 2004 for the uniform rate of progress (URP) glide path to Natural Conditions in 2064 (U.S. EPA, 2003a).
- *Natural Conditions:* "Natural Conditions," the RHR goal for 2064 for the Federally mandated Class I areas, represent estimates of natural visibility conditions for the B20% and W20% days at a given Class I area.

Baseline Conditions

Baseline Conditions for Class I areas are calculated using fine and coarse PM concentrations measured at Interagency Monitoring of Protected Visual Environments (IMPROVE) monitors (Malm et al., 2000). Each Class I area in the WRAP domain has an associated IMPROVE PM monitor. The IMPROVE monitors do not measure visibility directly, but instead measure speciated fine particulate ($PM_{2.5}$) and total $PM_{2.5}$ and PM_{10} mass concentrations from which visibility is calculated using the IMPROVE aerosol extinction equation, discussed later.

Visibility conditions are estimated starting with the IMPROVE 24-h average PM mass measurements related to six PM components of light extinction:

- Sulfate [$(NH_4)_2SO_4$]
- Particulate nitrate [$(NH_4NO_3$]
- Organic matter [OMC]
- Light-absorbing carbon [LAC] or elemental carbon [EC]
- Soil
- Coarse matter [CM]

The IMPROVE monitors do not directly measure some of these species, so assumptions are made as to how the IMPROVE measurements can be adjusted and combined to obtain these six components. For example, sulfate and particulate nitrate are assumed to be completely neutralized by ammonium and only the fine mode ($PM_{2.5}$) is speciated to obtain sulfate and nitrate measurements (that is, any coarse-mode sulfate and nitrate in the real atmosphere may be present in the IMPROVE CM measurement). Concentrations for the above six components of

light extinction in the IMPROVE aerosol extinction equation are obtained from the IMPROVE measured species using the formulas shown in Table 1.

Table 1. Definition of IMPROVE components from measured species.

IMPROVE Component	Calculation of Component from IMPROVE Measured Species
Sulfate	1.375 x (3 x S)
Nitrate	1.29 x NO_3^-
OMC	1.4 x OC
LAC	EC
Soil	(2.2 x Al) + (2.49 x Si) + (1.63 x Ca) + (2.42 x Fe) + (1.94 x Ti)
CM	MT – MF

where

- S is elemental sulfur as determined from proton-induced x-ray emissions (PIXE) analysis of the IMPROVE Module A. To estimate the mass of the sulfate ion ($SO_4^=$), S is multiplied by 3 to account for the presence of oxygen. If S is missing then the sulfate (SO_4) measured by ion chromatography analysis of Module B is used to replace (3 x S). For the IMPROVE aerosol extinction calculation, sulfate is assumed to be completely neutralized by ammonium (1.375 x SO_4).

- NO_3^- is the particulate nitrate measured by ion chromatography analysis of Module B. For the IMPROVE aerosol extinction calculation, it is assumed to be completely neutralized by ammonium (1.29 x NO_3).

- The IMPROVE organic carbon (OC) measurements are multiplied by 1.4 to obtain organic matter (OMC), which adjusts the OC mass for other elements assumed to be associated with OC.

- Elemental carbon (EC) is also referred to as light-absorbing carbon (LAC).

- Soil is determined as a sum of the masses of those elements (measured by PIXE) predominantly associated with soil (Al, Si, Ca, Fe, K, and Ti), adjusted to account for oxygen associated with the common oxide forms. Because K is also a product of the combustion of vegetation, it is represented in the formula by 0.6 x Fe and is not shown explicitly.

- MT and MF are total PM_{10} and $PM_{2.5}$ mass, respectively.

Associated with each PM species is an extinction efficiency that converts concentrations (in $\mu g/m^3$) to light extinction (in inverse megameters, Mm^{-1}), as listed below. Sulfate and nitrate are hygroscopic, so relative humidity (RH) adjustment factors, f(RH), are used to increase the

particles' extinction efficiency with increasing RH; this accounts for the particles' taking on water and having greater light scattering. Note that some organic matter (OMC) compounds may also have hygroscopic properties, but the IMPROVE aerosol extinction equation assumes OMC is nonhygroscopic.

$$\beta_{Sulfate} = 3 \times f(RH) \times [sulfate]$$
$$\beta_{Nitrate} = 3 \times f(RH) \times [nitrate]$$
$$\beta_{OM} = 4 \times [OMC]$$
$$\beta_{EC} = 10 \times [EC]$$
$$\beta_{Soil} = 1 \times [soil]$$
$$\beta_{CM} = 0.6 \times [CM]$$

The total light extinction (β_{ext}) is assumed to be the sum of the light extinctions due to the six PM species listed above plus Rayleigh (blue sky) background extinction (β_{Ray}), which is assumed to be 10 Mm^{-1}. This is reflected in the IMPROVE extinction equation:

$$\beta_{ext} = \beta_{Ray} + b_{Sulfate} + \beta_{Nitrate} + \beta_{EC} + \beta_{OMC} + \beta_{Soil} + \beta_{CM}$$

The total light extinction (β_{ext}) in Mm^{-1} is related to visual range (VR) in kilometers using the following relationship:

$$VR = 3912 / \beta_{ext}$$

The RHR requires that visibility be expressed in terms of a haze index (HI) in units of deciview (dv), which is calculated as follows:

$$HI = 10 \ln(\beta_{ext}/10)$$

The equations above, with measurements from the associated IMPROVE monitor, are used to estimate the daily average visibility at each Class I area for each IMPROVE monitored day. For each year from the 2000-2004 baseline period, these daily average visibility values are then ranked from highest to lowest. The "worst days" visibility for each of the five years in the baseline period is defined as the average visibility across the 20% worst-visibility days (highest deciview values); similarly, the "best days" visibility is defined as the average visibility across the 20% best-visibility days (lowest deciview values) for each year. The Baseline Conditions for the best and worst days are defined as the five-year average of the B20% visibility days and of the W20% visibility days, respectively, across the five-year baseline period.

The set of equations given above for relating measured PM species to visibility (light extinction) are referred to as the "Old IMPROVE" equation. The IMPROVE Steering Committee has developed a "New IMPROVE" equation that they believe better represents the fit between measured PM species concentrations and visibility impairment. Although conceptually similar to the Old IMPROVE equation, the New IMPROVE equation includes updates to many of the parameters and the addition of extinctions due to NO_2 absorption and sea salt. 2018 visibility projections and comparisons with the URP glide path goals were performed using both the New and Old IMPROVE equations. The reader is referred elsewhere for details on the New IMPROVE extinction equation (e.g., EPA, 2006a,b).

Mapping Model Results to IMPROVE Measurements

As noted above, future-year visibility at Class I areas is projected by using modeling results in a relative sense to scale current observed visibility for the B20% and W20% visibility days. This scaling is done using RRFs, the ratios of future-year modeling results to current-year results. Each of the six components of light extinction in the IMPROVE reconstructed mass extinction equation is scaled separately. Because the modeled species do not exactly match up with the IMPROVE measured PM species, assumptions must be made to map the modeled PM species to the IMPROVE measured species for the purpose of projecting visibility improvements. For example, in the model's chemistry (which explicitly simulates ammonium), sulfate may or may not be fully neutralized; the IMPROVE extinction equation, on the other hand, assumes that observed sulfate is fully neutralized by ammonium. For the CMAQ v4.5 model (September 2005 release) used in the WRAP RMC modeling, the mapping of modeled species to IMPROVE measured PM species is listed in Table 2.

Table 2. Mapping of CMAQ v4.5 modeled species concentrations to IMPROVE measured components.

IMPROVE Component	CMAQ V4.3 Species
Sulfate	1.375 x (ASO4J + ASO4I)
Nitrate	1.29 x (ANO3J + ANO3I)
OMC	AORGAJ + AORGAI + AORGPAJ + AORGPAI + AORGBJ + AORGBI
LAC	AECJ + AECI
Soil	A25J + A25I
CM	ACORS + ASEAS + ASOIL

Projecting Visibility Changes Using Modeling Results

RRFs calculated from modeling results can be used to project future-year visibility. For the urrent modeling efforts, RRFs are the ratio of the 2018 modeling results to the 2002 modeling results, and are specific to each Class I area and each PM species. RRFs are applied to the Baseline Condition observed PM species levels to project future-year PM levels, which are then used with the IMPROVE extinction equation listed above to assess visibility. The following six steps are used to project future-year visibility for the B20% and W20% visibility days (the discussion below is for W20% days but also applies to B20% days):

1. For each Class I area and each monitored day, daily visibility is ranked using IMPROVE data and IMPROVE extinction equation for each year from the five-year baseline period (2000-2004) to identify the W20% visibility days for each year.
2. Use an air quality model to simulate a base-year period (ideally 2000-2004, but in reality just 2002) and a future year (e.g., 2018), then apply the resulting information to develop

Class-I-area-specific RRFs for each of the six components of light extinction in the IMPROVE aerosol extinction equation.

3. Multiply the RRFs by the measured 24-h PM data for each day from the W20% days for each year from the five-year baseline period to obtain projected future-year (2018) 24-h PM concentrations for the W20% days.
4. Compute the future-year daily extinction using the IMPROVE aerosol extinction equation and the projected PM concentrations for each of the W20% days in the five-year baseline from Step 3.
5. For each of the W20% days within each year of the five-year baseline, convert the future-year daily extinction to units of deciview and average the daily deciview values within each of the five years separately to obtain five years of average deciview visibility for the W20% days.
6. Average the five years of average deciview visibility to obtain the future-year visibility Haze Index estimate that is compared with the 2018 progress goal.

In calculating the RRFs, EPA draft guidance (U.S. EPA, 2001, 2006a) recommends selecting modeled PM species concentrations "near" the monitor by taking a spatial average of PM concentrations across a grid-cell-resolution–dependent NX by NY array of cells centered on the grid containing the monitor. For the WRAP 36-km CMAQ modeling, the model estimates for just the grid cell containing the monitor are used (i.e., NX=NY=1).

For the preliminary 2018 visibility projections, results are presented only for "Method 1," which is the recommended approach in EPA's draft modeling guidance documents (U.S. EPA, 2001, 2006a). In the Method 1 Average RRF Approach, an average RRF for the W20% days from 2002 (Modeled Worst Days) is obtained for the Plan02c and the Base18b CMAQ simulations by averaging the PM concentration components across the Modeled Worst Days and then calculating the (future year):(base year) ratio of the average PM concentrations. For example, if $SO4_{i,j}$ is the measured sulfate concentrations at Class I area j for the i=1,…,N 20% worst visibility days in 2002, then the RRF for sulfate on the W20% days would be obtained as:

$$RRF_j(SO4) = \frac{\frac{1}{N}\sum_{i=1}^{N} SO4_{ij}(2018)}{\frac{1}{N}\sum_{i=1}^{N} SO4_{ij}(2002)} = \frac{\sum_{i=1}^{N} SO4_{ij}(2018)}{\sum_{i=1}^{N} SO4_{ij}(2002)}$$

For each Class I area and each of the W20% days, the average RRF for each PM component would be applied to concentrations for the W20% days from the 2000-2004 baseline period to estimate future-year PM concentrations for each of the W20% days. Extinction and HI would then be calculated to obtain the projected future-year visibility conditions using the procedures given previously.

<u>Glide Path to Natural Conditions</u>

The presumptive visibility target for 2018 is the URP goal that is obtained by constructing a linear glide path from the current Baseline Conditions to Natural Conditions in 2064 (both expressed in deciviews). For instance, Figure 5 displays an example visibility glide path for the Grand Canyon National Park (GRCA) Class I area. EPA's default Natural Conditions value for the W20% days (U.S. EPA, 2003b), shown as the green line, is the 2064 visibility goal at GRCA of 6.95 dv. The blue diamonds at the left of the plot are the annual average current conditions, based on IMPROVE observations for the W20% days as obtained from the Visibility Information Exchange Web System (VIEWS) web site (http://vista.cira.colostate.edu/views/). These annual average visibility values for the 20% worst days allow an assessment of trends and the year-to-year variation in visibility. The Baseline Conditions are the average of the W20% visibility from 2000-2004, which is the starting point for the glide path in 2004 (12.04 dv for GRCA). A linear URP from the Baseline Conditions in 2004 to Natural Conditions in 2064 (sloping pink line with triangles) is assumed, and the value on the glide path at 2018 is the presumptive URP visibility target that the modeled 2018 projections are compared against to judge progress. In this example, the visibility progress goal in 2018 would be 10.85 dv. Meeting this would require a 1.19 dv reduction in visibility by 2018 to meet that milestone year's visibility progress target at the Grand Canyon National Park.

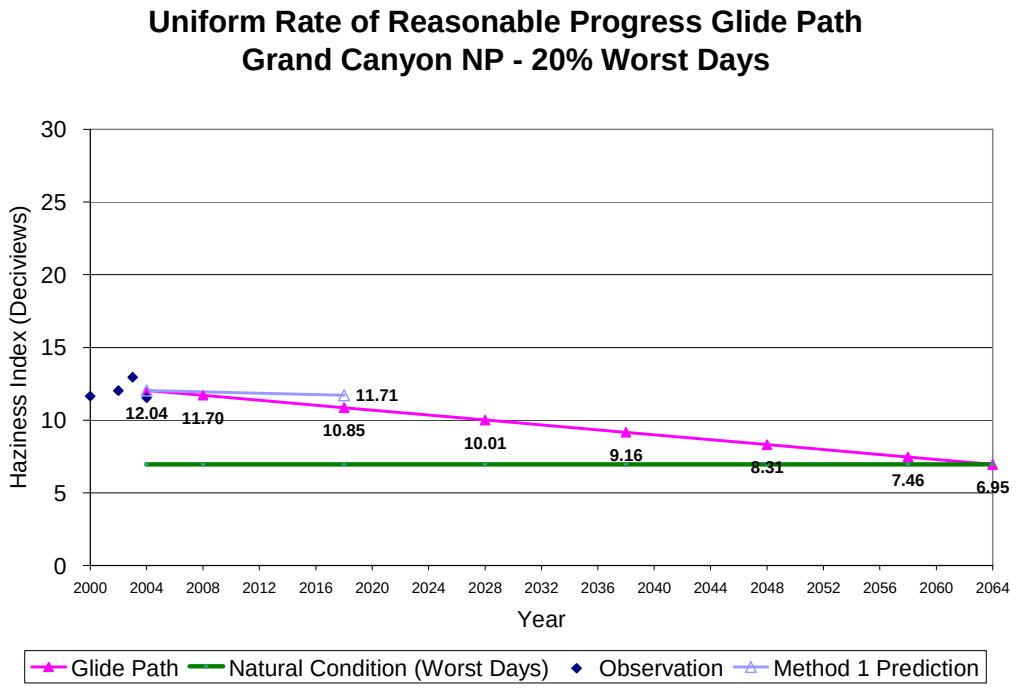


Figure 5. Example of URP glide path using IMPROVE data from the Grand Canyon National Park for the W20% days and comparison with Base18b visibility projections.

Preliminary Visibility Projection Results

For all of the WRAP Class I areas, the RMC performed preliminary 2018 visibility projections and compared them to the 2018 URP goals using the Plan02c and Base18b CMAQ modeling results and the Old and New IMPROVE equations. As an example, Figure 5 above compares the Base18b visibility projections with the URP goal based on the glide path for GRCA and the Old IMPROVE equation. To achieve the 2018 URP goal, the modeled 2018 visibility projection would have to show a 1.19 dv (=12.04-10.85) reduction. However, the modeled 2018 visibility projection shows only a 0.33 dv (=12.04-11.71) reduction by 2018, which indicates that the emission controls simulated in case Base18b would not achieve the modeled URP goal; the 2018 visibility projection achieves only 28% of the goal (28% = 100 x 0.33/1.19). Figure 6 displays the 2018 visibility projections for all WRAP Class I areas, using both the Old and New IMPROVE equations, expressed as a percentage of achieving the URP goal, with values of 100% or greater achieving the goal. Using the procedures outlined above, none of the WRAP Class I areas are projected to achieve their URP goals. There are various reasons for this, such as the presence of W20% days that are dominated by emissions from sources that are not controllable, such as wildfires, dust, and/or international transport. Additional analysis of these results and alternative projection techniques are currently under study.

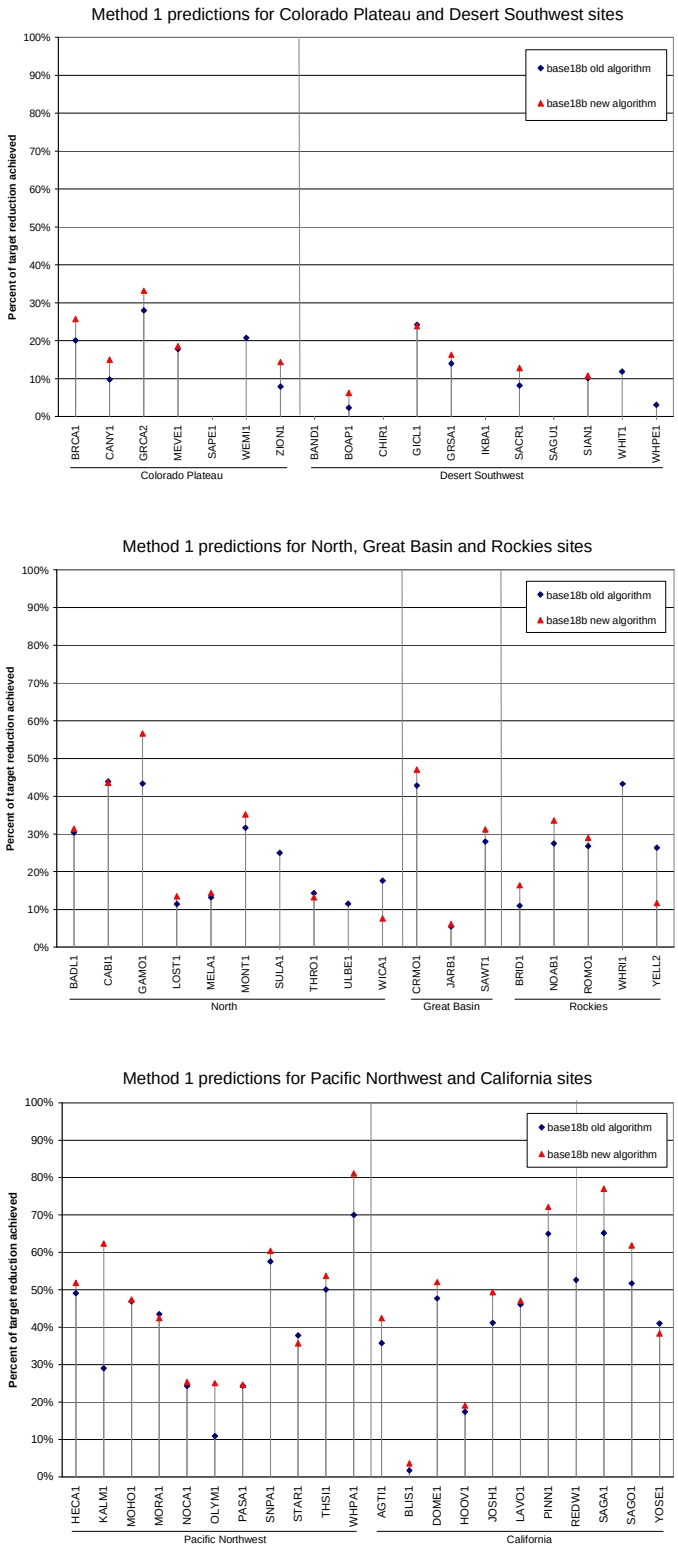


Figure 6. 2018 visibility projections at WRAP Class I areas expressed as a percent of achieving the 2018 URP goal using the Old and New IMPROVE equation and the WRAP Base18c CMAQ 36-km modeling results.

PM Source Apportionment

Impairment of visibility in Class I areas is caused by a combination of local air pollutants and regional pollutants that are transported long distances. To develop effective visibility improvement strategies, the WRAP member states and tribes need to know the relative contributions of local and transported pollutants, and which emissions sources are significant contributors to visibility impairment at a given Class I area.

A variety of modeling and data analysis methods can be used to perform source apportionment of the PM observed at a given receptor site. Model sensitivity simulations have been used in which a "base case" model simulation is performed and then a particular source is "zeroed out" of the emissions. The importance of that source is assessed by evaluating the change in pollutants at the receptor site, calculated as pollutant concentration in the sensitivity case minus that in the base case. This approach is known as a "brute force" sensitivity because a separate model run is required for each sensitivity.

An alternative approach is to implement a mass-tracking algorithm in the air quality model to explicitly track for a given emissions source the chemical transformations, transport, and removal of the PM that was formed from that source. Mass tracking methods have been implemented in both the CMAQ and CAMx air quality models. Initial work completed by the RMC during 2004 used the CMAQ Tagged Species Source Apportionment (TSSA) method. Unfortunately, there were problems with mass conservation in the version of CMAQ used in that study, and these affected the TSSA results. A similar algorithm has been implemented in CAMx, the PM Source Apportionment Technology (PSAT). Comparisons of TSSA and PSAT showed that the results were qualitatively similar, that is, the relative ranking of the most significant source contributors were similar for the two methods. However, the total mass contributions differed. With separate funding from EPA, UCR has implemented a version of TSSA in the new CMAQ release (v4.5) that corrects the mass conservation error, but given the uncertainty of the availability of this update, the CAMx/PSAT source apportionment method was used for the WRAP modeling analysis.

The main objective of applying CAMx/PSAT is to evaluate the regional haze air quality for typical 2002 (Plan02c) and future-year 2018 (Base18b) conditions. These results are used

- to assess the contributions of different geographic source regions (e.g., states) and source categories to current (2002) and future (2018) visibility impairment at Class I areas, to obtain improved understanding of (1) the causes of the impairment and (2) which states are included in the area of influence (AOI) of a given Class I area; and

- to identify the source regions and emissions categories that, if controlled, would produce the greatest visibility improvements at a Class I area.

<u>CAMx/PSAT</u>

The PM Source Apportionment Technology performs source apportionment based on user-defined source groups. A source group is the combination of a geographic source region and an emissions source category. Examples of source regions include states, nonattainment areas, and

counties. Examples of source categories include mobile sources, biogenic sources, and elevated point sources; PSAT can even focus on individual sources. The user defines a geographic source region map to specify the source regions of interest. He or she then inputs each source category as separate, gridded low-level emissions and/or elevated-point-source emissions. The model then determines each source group by overlaying the source categories on the source region map. For further information, please refer to the white paper on the features and capabilities of PSAT (http://pah.cert.ucr.edu/aqm/308/reports/PSAT_White_Paper_111405_final_draft1.pdf), with additional details available in the CAMx user's guide (ENVIRON, 2005; http://www.camx.com).

PM source apportionment modeling was performed for aerosol sulfate (SO_4) and aerosol nitrate (NO_3) and their related species (e.g., SO_2, NO, NO_2, HNO_3, NH_3, and NH_4). The PSAT simulations include 9 tracers, 18 source regions, and 6 source groups. The computational cost for each of these species differs because additional tracers must be used to track chemical conversions of precursors to the secondary PM species SO_4, NO_3, NH_4, and secondary organic aerosols (SOA). Table 3 summarizes the computer run time required for each species. The practical implication of this table for WRAP is that it is much more expensive to perform PSAT simulations for NO_3 and especially for SOA than it is to perform simulations for other species.

Table 3. Benchmarks for PSAT computational costs for each PM species. Run time is for one day (01/02/2002) on the WRAP 36-km domain.

Species	No. of Species Tracers	RAM Memory	Disk Storage per Day	Run Time with 1 CPU
SO_4	2	1.6 GB	1.1 GB	4.7 h/day
NO_3	7	1.7 GB	2.6 GB	13.2 h/day
SO_4 and NO_3 combined	9	1.9 GB	3.3 GB	16.8 h/day
SOA	14	6.8 GB	Not tested	Not tested
Primary PM species	6	1.5 GB	3.0 GB	10.8 h/day

Two annual 36-km CAMx/PSAT model simulations were performed: one with the Plan02c typical-year baseline case and the other with the Base18b future-year case. It is expected that the states and tribes will use these results to assess the sources that contribute to visibility impairment at each Class I Area, and to guide the choice of emission control strategies. The RMC web site includes a full set of source apportionment spatial plots and receptor bar plots for both Plan02b and Base18b. These graphical displays of the PSAT results, as well as additional analyses of these results are available on the TSS under http://vista.cira.colostate.edu/tss/Tools/ResultsSA.aspx

CAMx/PSAT 2002 and 2018 Setup

PSAT source apportionment simulations for 2002 and 2018 were performed using CAMx v4.30. Table 4 lists overall specifications for the 2002 PSAT simulations. The domain setup was identical to the standard WRAP CMAQ modeling domain. The CAMx/PSAT run-time options are shown in Table 5. The CAMx/PSAT computational cost for one simulation day with source tracking for sulfate (SO_4) and nitrate (NO_3) is approximately 14.5 CPU hours with an AMD Opteron CPU. The source regions used in the PSAT simulations are shown in Figure 7 and Table 4. The six emissions source groups are described in Table 6. The development of these emissions data are described in more detail below.

The annual PSAT run was divided into four seasons for modeling. The initial conditions for the first season (January 1 to March 31, 2002) came from a CENRAP annual simulation. For the other three seasons, we allowed 15 model spin-up days prior to the beginning of each season. Based on the chosen set of source regions and groups, with nine tracers, and with a minimum requirement of 87,000 point sources and a horizontal domain of 148 by 112 grid cells with 19 vertical layers, the run-time memory requirement is 1.9 GB. Total disk storage per day is approximately 3.3 GB. Although the RMC's computation nodes are equipped with dual Opteron CPUs with 2 GB of RAM and 1 GB of swap space, the high run-time memory requirements prevented running PSAT simulations using the OpenMP shared memory multiprocessing capability implemented in CAMx.

Table 4. WRAP 2002 CAMx/PSAT specifications.

WRAP PSAT Specs	Description
Model	CAMx v4.30
OS/compiler	Linux, pgf90 v.6.0-5
CPU type	AMD Opteron with 2 GB of RAM
Source region	18 source regions; see Figure 4.1 and Table 4.4
Emissions source groups	Plan02b, 6 source groups; see Table 4.5
Initial conditions	From CENRAP (camx.v4.30.cenrap36.omp.2001365.inst.2)
Boundary conditions	3-h BC from GEOS-Chem v2

Table 5. WRAP CAMx/PSAT run-time options.

WRAP PSAT specs	Description
Advection solver	PPM
Chemistry parameters	CAMx4.3.chemparam.4_CF
Chemistry solver	CMC
Plume-in-grid	Not used

WRAP PSAT specs	Description
Probing tool	PSAT
Dry/wet deposition	TRUE (turned on)
Staggered winds	TRUE (turned on)

Table 6. WRAP CAMx/PSAT source regions cross-reference table.

Source Region ID	Source Region Description[1]	Source Region ID	Source Region Description[1]
1	Arizona (AZ)	10	South Dakota (SD)
2	California (CA)	11	Utah (UT)
3	Colorado (CO)	12	Washington (WA)
4	Idaho (ID)	13	Wyoming (WY)
5	Montana (MT)	14	Pacific off-shore & Sea of Cortez (OF)
6	Nevada (NV)	15	CENRAP states (CE)
7	New Mexico (NM)	16	Eastern U.S., Gulf of Mexico, & Atlantic Ocean (EA)
8	North Dakota (ND)	17	Mexico (MX)
9	Oregon (OR)	18	Canada (CN)

[1]The abbreviations in parentheses are used to identify source regions in PSAT receptor bar plots.

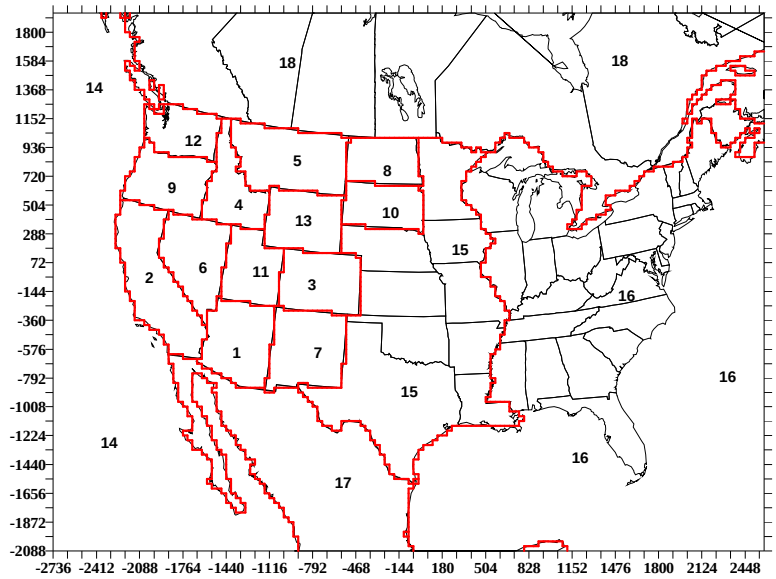


Figure 7. WRAP CAMx/PSAT source region map. Table 6 defines the source region IDs.

Table 7. WRAP CAMx/PSAT emissions source groups.

Emissions Source Groups	Low-level Sources	Elevated Sources
1	Low-level point sources (including stationary off-shore)	Elevated point sources (including stationary off-shore)
2	Anthropogenic wildfires (WRAP only)	Anthropogenic wild fires (WRAP only)
3	Total mobile (on-road, off-road, including planes, trains, ships in/near port, off-shore shipping)	
4	Natural emissions (natural fire, WRAP only, biogenics)	Natural emissions (natural fire, WRAP only, biogenics)
5	Non-WRAP wildfires (elevated fire sources in other RPOs)	Non-WRAP wild fires (elevated fire sources in other RPOs)
6	Everything else (area sources, all dust, fugitive ammonia, non-elevated fire sources in other RPOs)	

PSAT Results

The source apportionment algorithms implemented in CAMx generate output files in the same format as the standard modeled species concentrations files. This typically consists of a two-dimensional, gridded dataset of hourly-average surface concentrations for each source group tracer that gives the contribution of the tracer to all the surface grid cells in the model domain for each hour of the simulation. Three-dimensional instantaneous concentrations are also output for the last two hours of the simulation, which are used to restart the model. Although there are options to output hourly 3-D average tracer concentrations, the model is usually configures to output only the model's surface layer concentrations because of the vast disk storage space needed for the 3-D file output for all the source group contributions.

The source apportionment model results are typically presented in two ways :

- *Spatial plots* showing the area of influence of a source group's PM species contributions throughout the model domain, either at a given hourly-average point in time or averaged over some time interval (e.g., monthly average).
- *Receptor bar plots* showing the rank order of source groupings that contribute to PM species at any given receptor site. These plots also can be at a particular point in time or averaged over selected time intervals—for example, the average source contributions for the 20% worst visibility days.

If the 3-D tracer output files are saved, it is also possible to prepare animations of PM species plumes from each of the source groups. However, these plots are less useful than the others for quantitative analysis, are expensive to produce, and require saving 3-D hourly output, which is disk-space intensive. The primary products of the WRAP PSAT modeling were receptor bar plots showing the emission source groups that contribute the most to the model grid cells containing each IMPROVE monitoring site and other receptor sites identified by WRAP.

Model Sensitivity Simulations

A variety of sensitivity simulations were conducted by the RMC as part of their modeling efforts to support the WRAP in addressing the Regional Haze Rule requirements. These sensitivity simulations are described below.

2002 Clean Case

There are many natural sources of ambient $PM_{2.5}$, both direct emissions of primary $PM_{2.5}$ (such as windblown dust) and emissions of gaseous species that undergo photochemical transformation or condensation to form secondary $PM_{2.5}$. Natural sources of $PM_{2.5}$ are of concern because they represent sources that cannot be controlled. Estimates of natural haze levels have been developed by EPA for visibility planning purposes and are described in *Guidance for Estimating Natural Visibility Conditions Under the Regional Haze Rule* (U.S. EPA, 2003a). These are the natural haze levels to be used in glide path calculations, such as those we performed as part of the visibility projections for 2018. However, the natural haze levels developed by EPA for glide path calculations were based on ambient data analysis, not on visibility modeling. This question thus arises: Would modeled levels of natural haze be consistent with the values estimated by EPA for visibility planning? If the natural haze levels calculated by the model were substantially higher than the levels used for planning purposes, this would make it more difficult for modeling studies to demonstrate progress in attaining visibility goals, because the model would predict haze levels that exceeded EPA's natural haze levels even if all anthropogenic sources of $PM_{2.5}$ were removed from the modeling. The RMC explored this issue by conducting a CMAQ sensitivity "clean conditions" simulation

There are many uncertainties and unknowns regarding natural emissions. There have been only limited studies of natural emissions conditions. It is known that there are very large uncertainties in the categories of natural emissions included in the WRAP emissions inventories, and that some categories of natural emissions are not included at all. Also, it is difficult to know what truly natural emissions would have been like in the absence of human modifications of the environment. For example, wildfire emissions are a large source of natural emissions in our modeling, but how much larger might that source be in the absence of fire suppression efforts? For all of these reasons, it was decided to describe this sensitivity simulation as a "clean conditions" scenario rather than a "natural conditions" scenario. In this simulation, all anthropogenic emissions were removed from the inventory and only those emissions that were defined as biogenic in the 2002 base case (Base02) were included. Thus, this model simulation does not represent true natural conditions. It indicates instead the lowest haze levels that could be achieved in the model if all anthropogenic emissions were zeroed out.

Emission Inventories

The emissions for the clean 2002 sensitivity case were derived from case Base02a. Because it was a sensitivity analysis to test the impacts of natural emissions sources on visibility, it is referred to it as scenario Base02nt, where "nt" refers to natural. The following emissions categories in Base02nt were included:

- *Biogenics:* Generated in case Base02a by BEIS3.12 using SMOKE.

- *WRAP Ammonia:* The Base02a ammonia emissions for the WRAP region were developed with a GIS by ENVIRON. The five emissions category modeled included three anthropogenic sources (domestic animals, livestock, and fertilizer application) and two natural sources (soils and wildlife). Only the two natural sources in scenario Base02nt were used.

- *CENRAP and MRPO Ammonia:* To create ammonia inventory files for only natural sources, we used a list of SCCs representing natural sources to extract the emissions records of these sources from the monthly inventory files that were used in Base02a. it was found that there were no natural ammonia sources in the MRPO monthly inventory files.

- *Natural Area Sources:* The Base02a area-source inventory files included natural sources, such as wildfires and wild animals. These records were extracted from the stationary-area-source inventories. Note that the WRAP area-source files did not include any natural sources.

- *Natural Fires:* Of the five fire categories modeled in Base02a (wildfires, wildland fire use, non-Federal rangeland prescribed fires, prescribed fires [which were split into natural and anthropogenic prescribed for this purpose of this sensitivity], and agricultural fires), only the categories that represent natural fires (wildfires, wildland fire use, and natural prescribed fires) were included.

- *Windblown Dust:* We used the windblown dust inventory that ENVIRON and the RMC developed for use in case Base02a. Additional details on this dust inventory are available at http://www.cert.ucr.edu/aqm/308/wb_dust2002/wb_dust_ii_36k.shtml.

The biogenic and windblown dust emissions from the Base02a SMOKE outputs that are stored at the RMC were used directly. For the fire (including both point and area fires), natural area, and ammonia emissions, these data were reprocessed specifically for scenario Base02nt using the same ancillary data (temporal, chemical, and spatial allocation data) used in case Base02a. QA plots and documentation for scenario Base02nt are posted on the RMC web site at http://pah.cert.ucr.edu/aqm/308/qa_Base02nt36.shtml.

Modeling Results

Figure 8 shows the model-reconstructed light extinction in the clean emissions model simulation. Because the natural fire emissions in the WRAP states were a major component of the clean emissions, the largest visibility impairment is in the regions with natural fire emissions. Contributions to light extinction from natural sources were small in regions without large fire emissions, as evidenced in the eastern U.S., where the extinction was only slightly larger (about 2 Mm^{-1}) than perfectly clean Rayleigh conditions of 10 Mm^{-1}.

Although there are large uncertainties in the natural emissions, and it is known that there are missing types of natural emissions, the components of the natural inventory used in this sensitivity simulation did contribute to relatively large visibility impairment in regions where there were large wildfires. Extinction coefficients as large as 90 Mm^{-1} were simulated in the southern Oregon and northern California regions; this was most likely a result of the large Biscuit fire in Oregon, plus contributions from smaller fires and other natural emissions. These visibility

impairment levels exceed the natural visibility levels specified in the EPA regional haze natural visibility guidance document. It will thus be more difficult for the modeling to demonstrate attainment of progress goals in areas of the country subject to wildfires because of their large contribution to visibility impairment that is not controllable. In other regions of the country for which the inventories lacked large natural fire emissions, the modeled clean visibility was only slightly greater than clean Rayleigh conditions. Note the model results may be overly optimistic in these regions because we lack a complete, accurate natural emissions inventory.

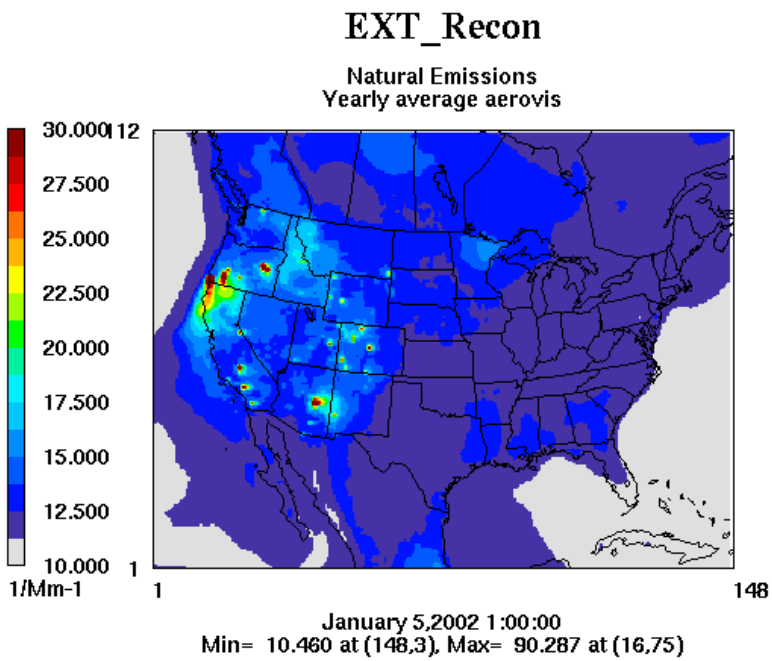


Figure 8. Annual average model-reconstructed "clean conditions" visibility as extinction coefficient.

These results are all very tentative because of the large uncertainties in natural emissions. Considerable effort would be needed to more fully investigate natural conditions in future modeling studies. It will always be difficult to determine and quantify "clean conditions" based on observations because of the pervasive influence of anthropogenic emissions.

Also as part of this sensitivity analysis, the contributors to organic carbon aerosols (OC) for the clean conditions scenario wer4e evaluated. The CMAQ model represents explicitly three classes of organic carbon aerosols:

- *AORGPA:* Primary anthropogenic OC resulting from direct organic mass emissions, such as primary organic aerosol (POA).
- *AORGA:* Secondary anthropogenic OC resulting from aromatic VOCs, such as xylene, toluene, and cresols.

- *AORGB:* Secondary biogenic OC resulting from biogenic VOCs, such as terpenes.

Because it was not cost effective to carry out CAMx/PSAT simulations with OC, the explicit OC results for the clean conditions case were analyzed, and then compared those results to the Base02b case in an attempt to infer the relative contributions of biogenic and anthropogenic VOCs to OC. These results are difficult to interpret for at least two reasons:

- Because of the simplified approach used by CMAQ and the Carbon Bond Mechanism version 4 (CB4) to represent these species, it is not possible to accurately classify all emissions into the CMAQ model as either biogenic or anthropogenic based simply on the species name. Thus, some biogenic OC might be included with AORGA, and some anthropogenic OC might be included in AORB.
- Some fire emissions are classified as anthropogenic, but these emissions might include species such as terpenes that are typically considered biogenic. Using the analysis approach in which all terpenes are assumed biogenic then incorrectly causes some anthropogenic emissions to be labeled biogenic when we use the simplified approach of analyzing OC in terms of AORGPA, AORGA and AORGB.

In spite of these difficulties, however, the results should classify the majority of the emissions correctly as either biogenic or anthropogenic.

For each of the above three components of OC, plots of the annual average mass in the Base02b case were prepared, and then the controllable mass was estimated as the difference between the Base02b case the Base02nt clean emissions scenario. Figure 9 shows the annual average mass of OC contributed from AORGPA in case Base02b (top) and the portion of that mass attributed to controllable emissions (bottom). Comparing these two plots indicates that in the western U.S. there is considerable AORGPA mass that is not controllable. It is likely that much of this mass is from fires, since uncontrollable AORGPA mass is present at the site of large fires in southern Oregon and north of Tucson, AZ.

Figure 10 shows the annual average mass of secondary OC contributed from AORGA in the Base02b case (top) and the portion of that mass attributed to controllable emissions (bottom). These plots indicate that virtually all of the AORGA mass is controllable, since the bottom plot is almost identical to the top plot.

Figure 11 shows the annual average mass of OC contributed from AORGPA in the Base02b case (top) and the portion of that mass attributed to controllable emissions (bottom). These plots indicate that although most of the AORGB mass is not controllable, a significant amount of mass is controllable. It is likely that the controllable AORGB mass results from VOC oxidation chemistry and the larger amount of biogenic mass that is oxidized and subsequently condenses to form OC in the Base02b case. These results indicate that controlling O_3 precursor emissions is effective at reducing a small but significant fraction of the biogenic OC.

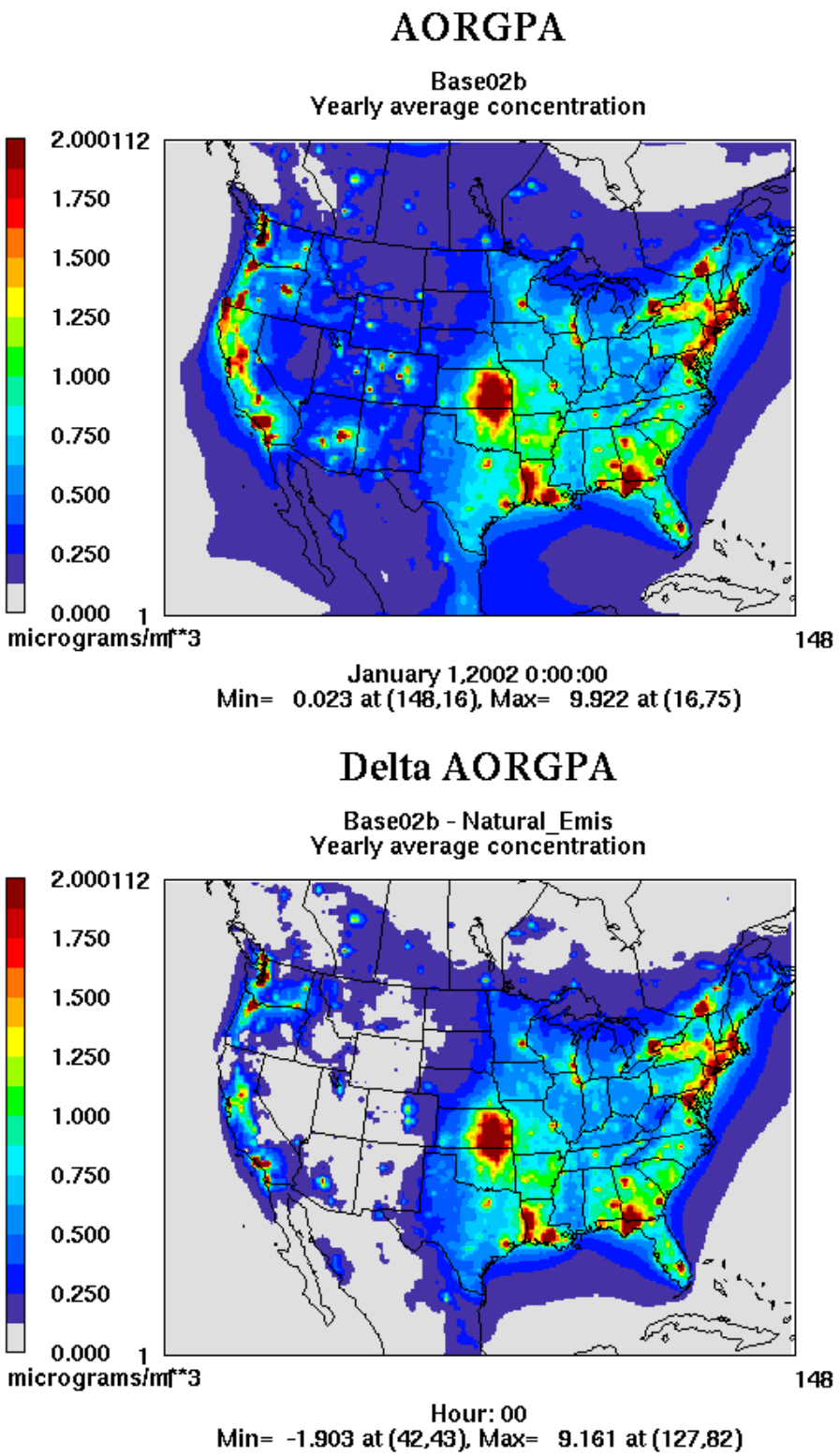


Figure 9. Annual average modeled primary anthropogenic OC (AORGPA) in Base02b (top) and the portion that is "controllable" primary anthropogenic OC (bottom).

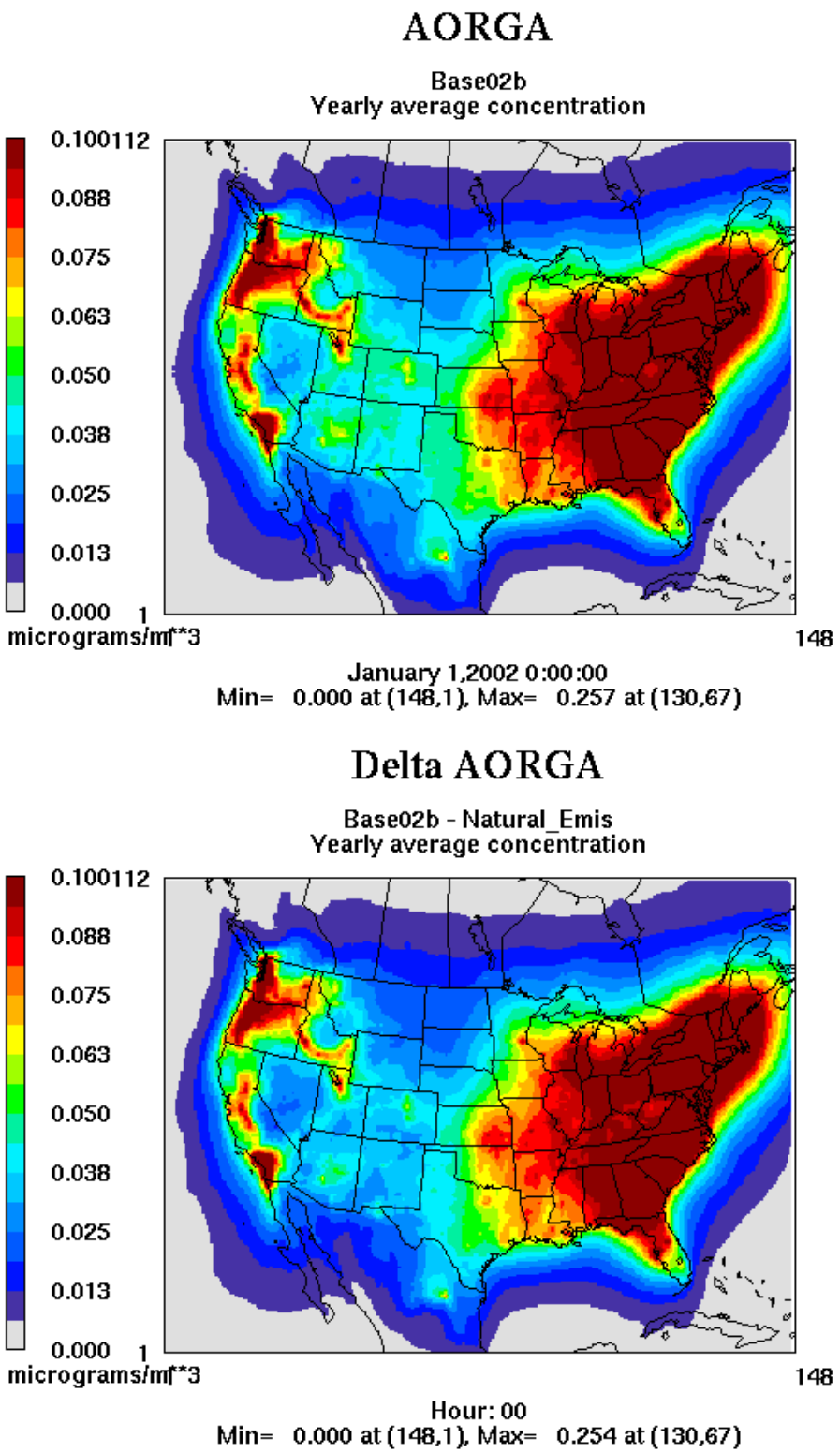
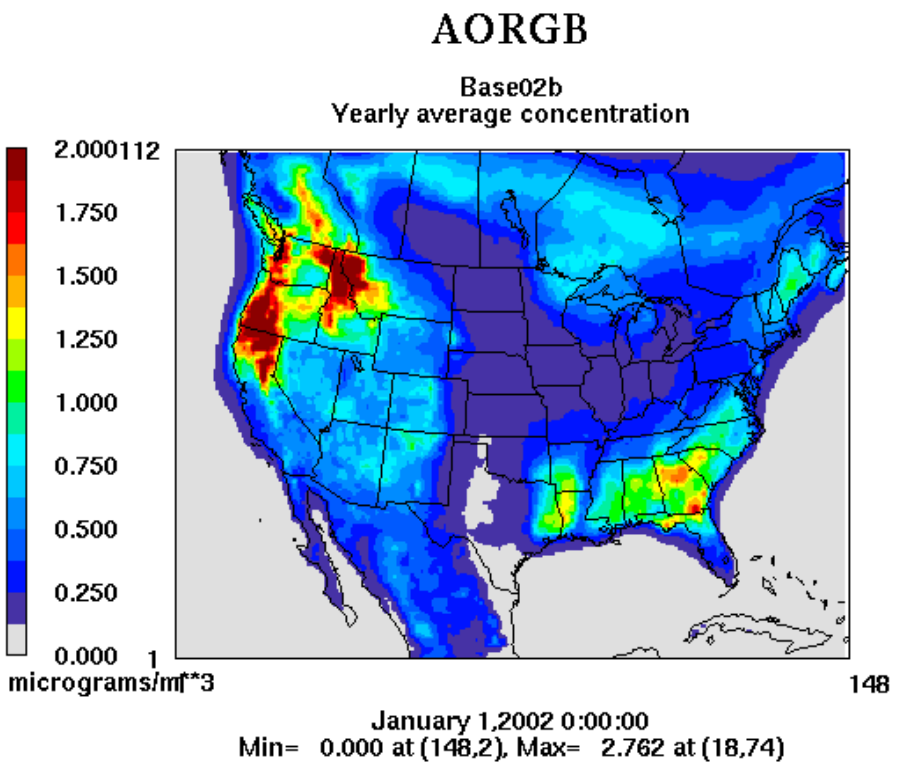


Figure 10. Annual average modeled secondary anthropogenic OC (AORGA) in Base02b (top) and the portion that is "controllable" secondary anthropogenic OC (bottom).



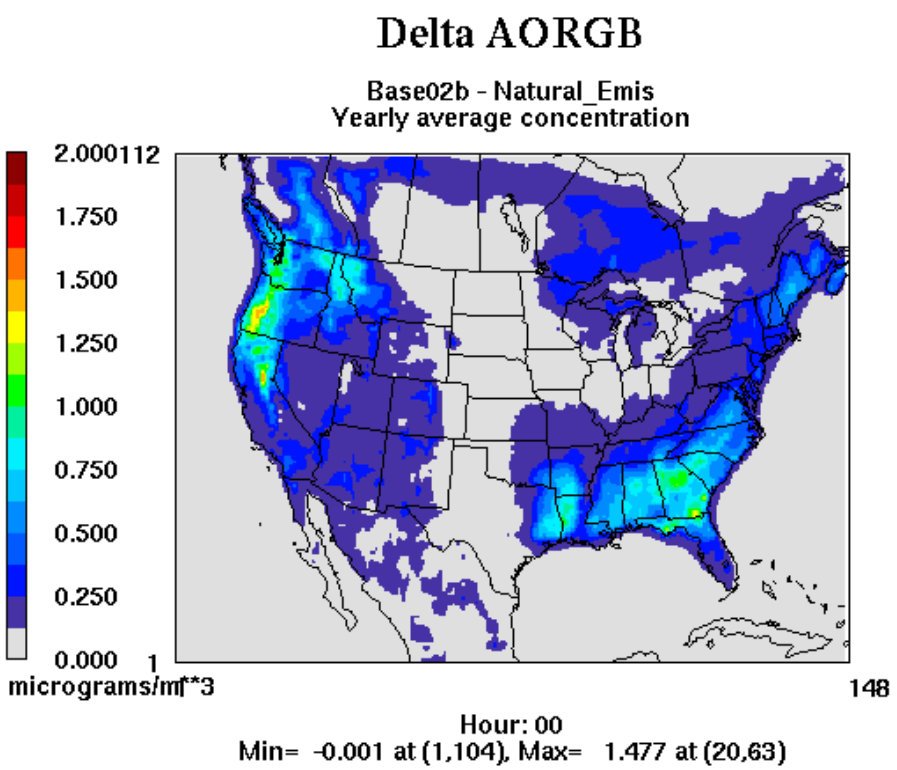


Figure 11. Annual average modeled primary biogenic OC (AORGB) in Base02b (top) and the portion that is "controllable" primary biogenic OC (bottom).

It might be difficult for the WRAP states and tribes to use these results quantitatively in developing emissions control strategies for visibility SIPs and TIPs. However, the results do provide some insight into the relative contributions of biogenic and anthropogenic OC as well as the amount of each that is controllable in the model simulations.

Finally, it is noted that there are uncertainties in the modeled emissions of anthropogenic VOCs, and larger uncertainties in the modeled emissions of biogenic VOCs. It is not possible to evaluate the model performance individually for biogenic and anthropogenic OC because the OC measurements do not distinguish between those two forms. Instead, only comparisons of total modeled OC to total measured OC can be made. Therefore, even when the model achieves good performance for total OC, it is possible that the model may be overpredicting one component of total OC and underpredicting the other. The inability to evaluate model performance for each component of OC increases the uncertainty of the results described here and illustrated in Figures 9 through 11, so caution should be used when drawing conclusions about the sources of OC based on these results.

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