VISTAS. This profile provided state specific updates for home heating emissions and was applied to the full inventory in place of profile 17XX.

Other additions to the Base02G temporal allocation data included updates that made by other RPOs that are applicable to their inventories. These other updates to the temporal allocation files included

- VISTAS continuous emissions monitoring (CEM)-specific profiles for EGUs in the VISTAS states;
- VISTAS agricultural burning profiles;
- Wildfire and prescribed fire profiles developed by VISTAS for the entire U.S.;
- MANE-VU on-road mobile profiles;
- WRAP weekly and diurnal road dust profiles;
- WRAP diurnal wildfire, agricultural fire, and prescribed fire profiles; and
- WRAP on-road mobile weekly and diurnal profiles.

Finally, for all of the monthly and seasonal emissions inventories, we modified the temporal cross-reference files to apply uniform monthly profiles to the sources contained in these inventories. The monthly variability is inherent in monthly and seasonal inventories and does not need to be reapplied through the temporal allocation process in SMOKE. The inventories to which we applied uniform monthly temporal profiles included:

- WRAP, CENRAP, and MRPO non-road mobile sources;
- WRAP on-road mobile sources;
- WRAP road dust; and
- CENRAP anthropogenic ammonia.

2.1.8 Spatial Allocation

SMOKE uses spatial surrogates and SCC cross-reference files to allocate county-level emissions inventories to model grid cells. Geographic information system (GIS)-calculated fractional land use values define the percentage of a grid cell that is covered by standard sets of land use categories. For example, spatial surrogates can define a grid cell as being 50% urban, 10% forest, and 40% agricultural. In addition to land use categories, spatial surrogates can also be defined by demographic or industrial units, such as population or commercial area. Similar to the temporal allocation data, an accompanying spatial cross-reference file associates the spatial surrogates (indexed with a numeric code) to SCCs. Spatial allocation with surrogates is applicable only to area and mobile sources that are provided on a county level basis. Point sources are located in the model grid cells by SMOKE based on the latitude-longitude coordinates of each source. Biogenic emissions are estimated based on 1-km^2 gridded land use information that is mapped to the model grid using a processing program such as the Multimedia Integrated Modeling System (MIMS) Spatial Allocator (CEP, 2004).

We used various sources of spatial surrogate information for the U.S., Canada, and Mexico inventories in the simulations. For the U.S. and Canadian sources, we used the EPA unified

surrogates available through the EFIG web site (EPA, 2005c). For the 36-km grid, EPA provides these data already formatted for SMOKE on the RPO Unified 36-km domain that we used for the simulations. We modified the spatial surrogates for Canada on the RPO Unified 36-km domain by adopting several surrogate categories that were enhanced by the WRAP. Table 2-9 provides details about the new Canadian spatial surrogates that were developed by the WRAP and used for CENRAP simulations. For modeling Mexico, we used Shapefiles developed for the Big Bend Regional Aerosol and Visibility Observations Study (BRAVO) modeling to create surrogates for Mexico on the RPO Unified 36-km domain (EPA, 2005c).

Table 2-9. New Canadian spatial surrogates.

Attribute	Base02a Code	Shapefile	Reference
Land area	950	can_land93_land	Natural Resources Canada (1993) AVHRR land cover data
Water area	951	can_land93_water	Natural Resources Canada (1993) AVHRR land cover data
Forest land area	952	can_land93_forest	Natural Resources Canada (1993) AVHRR land cover data
Agricultural land area	953	can_land93_agri	Natural Resources Canada (1993) AVHRR land cover data
Urban land area	954	can_land93_urban	Natural Resources Canada (1993) AVHRR land cover data
Rural land area	955	can_land93_rural	Natural Resources Canada (1993) AVHRR land cover data
Airports	956	can_airport	U.S. DOT Bureau of Transportation Statistics (2005) NORTAD 1:1,000,000 scale data
Ports	957	can_port	U.S. DOT Bureau of Transportation Statistics (2005) NORTAD 1:1,000,000 scale data
Roads	958	can_road1m	Natural Resources Canada (2001) National Scale Frameworks data
Rail	959	can_rail1m	Natural Resources Canada (1999) National Scale Frameworks data

2.2 Stationary Point Source Emissions

Stationary-point-source emissions data for SMOKE consist of (1) Inventory Data Analyzer (IDA)-formatted inventory files; (2) ancillary data for allocating the inventories in space, time, and to the Carbon Bond-IV chemistry mechanism used in CMAQ and CAMx; and (3) meteorology data for calculating plume rise from the elevated point sources. This section describes where CENRAP obtained these data, how we modeled them, and the types of QA that we performed to ensure that SMOKE processed the data as expected.

2.2.1 Data Sources

For the stationary-point-source inventories in Typ02G and Base18G, we used actual 2002 data developed by the RPOs for the U.S., version 2 of the year 2000 Canadian inventory, and the BRAVO 1999 Mexican inventory. The BRAVO inventory was updated with entirely new inventories for the six northern states of Mexico for stationary area, as well as stationary point, on-road mobile, and off-road mobile sources. Emissions for the southern states of Mexico were included for the first time in CENRAP simulations Typ02G and Base18G. These data were provided by ERG, Inc., who completed an updated 1999 emissions inventory for northern Mexico (ERG, 2006b) and delivered these data to the WRAP. The CENRAP stationary-point inventory consisted of annual county-level and tribal data provided in August of 2005 (Pechan and CEP, 2005e). The WRAP (ERG, 2006a) and VISTAS Base G (MACTEC, 2006) stationary-point inventories consisted of an annual data set and monthly CEM data for selected EGUs. The WRAP and VISTAS provided these data directly to CENRAP. We downloaded the MANE-VU stationary-point inventories from the MANE-VU web sites. MRPO base K data was downloaded and processed for SMOKE modeling by Alpine Geophysics under contract from MARAMA. UCR entered into a nondisclosure agreement with Environment Canada to obtain version 2 of the 2000 Canadian point-source inventory. This inventory represented a major improvement over the version of the data that we had used in the preliminary 2002 modeling.

Reductions anticipated from BART controls for electric generating units (EGU) in Oklahoma, Arkansas, Kansas, and Nebraska were included in projections of 2018 emissions. These anticipated reductions were based on actual operating conditions and estimated control efficiencies from utilities.

Newly permitted coal-fired utilities were included in 2018 projections. Conservatively, no IPM projected new units were removed from the simulation with the addition of the permitted facilities.

Due to missing or clearly erroneous stack parameters, several facilities in CENRAP states were relegated to default stack profiles based on SCC in the NEI QA process. Prioritizing for the largest emissions sources, these default parameters were corrected by CENRAP States and updated files were provided to modeling contractors. Final IDA input files Typ02G and Base18G for point sources reflect State corrections.

For coal-fired point and area sources, The EPA Office of Air Quality and Planning Standards (OAQPS) determined that the organic carbon fraction in the speciation profile code "NCOAL" was not representative of most coal combustion occurring in the U.S. This profile has an organic carbon fraction of 20%, which includes an adjustment factor of 1.2 to account for other atoms (like oxygen) attached to the carbon. OAQPS has reverted back to the profile code "22001" for coal combustion, which has an organic carbon fraction of 1.07% (again including the 1.2 factor adjustment). This is the same profile that EPA used for previous rulemaking efforts including the Heavy Duty Diesel Rule and Non-Road Rule, which were proposed (and publicly reviewed) prior to the introduction of the NCOAL profile.

The consensus in OAQPS is that the NCOAL profile has a high organic carbon percentage because it is based on measurements of combustion of lignite coal. With the exception of Texas, lignite is not widely used in the U.S.. Thus, OAQPS staff stopped relying on this profile as a national default profile. A new coal speciation profile developed based on Eastern bituminous

coal combustion (since much of the coal burned in the U.S. is of this type) is being developed by EPA's Office of Research and Development but was not completed for this study.

The profile recently developed for MRPO by Carnegie Mellon was provided to CENRAP and is representative of combustion of eastern bituminous coal. This profile is a more appropriate profile for most facilities in the U.S. than the default NCOAL profile.

Additionally, the "22001" profile has been flagged as problematic because of the apparent inadvertent switching of the organic carbon and elemental carbon fractions, which are 1.07% and 1.83% respectively. The report discovering the discrepancy in the profile did not offer a clear alternative to correct the problem (MACTEC, 2003).

CENRAP has continued to use the NCOAL factor for facilities burning lignite in North Dakota and Texas. For the remainder of the U.S., the MRPO profile, CMU, was used. The NCOAL factor was modified reducing the organic carbon by half and assigning the remainder to $PM_{2.5}$. The modification was at the request of Texas and was reflective of the original study for the NCOAL factor conducted in Texas (Chow, 2005). Table 2-10 summarizes the $PM_{2.5}$ speciation profiles for the NCOAL, 2201 and CMU speciation profiles for coal burning sources.

Table 2-10. PM 2.5 speciation profiles for coal-burning sources.

Profile	POC	PEC	PNO3	PSO4	PM2.5
NCOAL	0.1000	0.0100	0.0050	0.1600	0.7250
22001	0.0107	0.0183	0.0000	0.1190	0.8520
CMU	0.0263	0.0315	0.0036	0.0447	0.8938

Final simulations used improved temporal allocation and speciation information relative to the preliminary 2002 modeling; the rest of the ancillary data for modeling stationary point sources stayed the same (Mansell et al., 2005).

2.2.2 Emissions Processing

For Typ02G and Base18G simulations we configured SMOKE to process the annual inventories for the U.S., Canada, and Mexico and process hourly CEM data for the VISTAS. We configured SMOKE to allocate these emissions up to model layer 15 (approximately 2,500 m AGL), which roughly corresponds to the maximum planetary boundary layer (PBL) heights across the entire domain throughout the year. As coarse particulate matter (PMC) is not an inventory pollutant but is required by the air quality models as input species, we used SMOKE to calculate PMC during the processing as (PM_{10} - $PM_{2.5}$). With the SMOKE option WKDAY_NORMALIZE set to “No,” we treated the annual inventories based on the assumption that they represent average-day data based on a seven-day week, rather than average weekday data. We also assumed that all of the volatile organic compound (VOC) emissions in the inventories are reactive organic gas (ROG), and thus used SMOKE to convert the VOC to total organic gas (TOG) before converting the emissions into CB-IV speciation for the air quality models. To capture the differences in diurnal patterns that are contained in the CEM temporal profiles for VISTAS and CENRAP states (Base02F), we configured SMOKE to generate daily temporal matrices, as opposed to using a Monday-weekday-Saturday-Sunday (MWSS) temporal allocation approach.

To QA the stationary-point emissions, we used the procedures in the CENRAP emissions modeling QA protocol (Morris and Tonnesen, 2004) and a suite of graphical summaries. We used tabulated summaries of the input data and SMOKE script settings to document the data and configuration of SMOKE for all simulations. These QA graphics are available on the web site at: http://pah.cert.ucr.edu/aqm/cenrap/emissions.shtml

2.2.3 Uncertainties and Recommendations

There were issues with the stationary-point emissions that we left unresolved at the completion of the Typ02G and Base18G emissions modeling either because we did not feel they would have a major impact on the modeling results in CENRAP states or because we did not have alternative approaches and they represented the best available information. Canadian emissions for 2000 were found to have a significant number of missing stack parameters. These stacks when modeled with default parameters frequently resulted in lower plume heights. Stack parameters for 2000 were corrected based on cross referencing sources with the 2005 Canadian inventory for the largest emitting points. Stack parameters for many of the sources with lower emissions remain incorrect, but are assumed to have a less significant impact on CENRAP Class I areas. The 2020 projected emissions for Canada were obtained as air quality model-ready files from EPA. EPA has not confirmed that missing stack parameters were corrected for the projected inventory. It is assumed that they were not corrected and default parameters were used instead. Given confidentiality issues that surround Canadian inventories, EPA processed emissions represent the best available data.

2.3 Stationary Area Sources

Stationary-area-source emissions data for SMOKE consist of IDA-formatted inventory files and ancillary data for allocating the inventories in space, time, and to the Carbon Bond-IV chemistry mechanism used in CMAQ and CAMx. This section describes where we obtained these data, how we modeled them, and the types of QA that we performed to ensure that SMOKE processed the data as expected.

2.3.1 Data Sources

For the stationary area source inventories in the Typ02G and Base18G simulations, we used actual 2002 data developed by the RPOs for the U.S., version 2 of the year 2000 Canadian inventory, and the updated Mexican inventory, http://www.epa.gov/ttn/chief/net/mexico.html. The BRAVO inventory was updated with entirely new inventories for the six northern states of Mexico for stationary area, as well as stationary point, on-road mobile, and off-road mobile sources. Emissions for the southern states of Mexico were included for the first time in CENRAP simulations Typ02G and Base18G. The CENRAP stationary-area inventory consisted of annual county-level and tribal data provided by in August of 2005 (Pechan and CEP, 2005e). The WRAP (ERG, 2006a) and VISTAS Base G (MACTEC, 2006) stationary-area inventories consisted of an annual data set. We downloaded the MANE-VU stationary-area inventories from the MANE-VU web sites. MRPO base K data was downloaded and processed for SMOKE modeling by Alpine Geophysics under contract from MARAMA.

To prepare the stationary-area inventories for modeling, we made several modifications to the files by removing selected sources either to model them as separate source categories or to omit them from simulations completely. Using guidance provided by EPA (EPA, 2004b), we extracted fugitive and road dust sources from all stationary-area inventories for adjustment by transport factors and modeling as separate source categories (see Section 2.8). We also extracted and discarded the stage II refueling sources (Table 2-11) from the U.S. inventories; we modeled these sources with MOBILE6 as part of the on-road mobile-source emissions. We left the stage II refueling emissions in the WRAP stationary-area inventory because the on-road mobile inventory that we received for this region did not contain these emissions.

Table 2-11. Refueling SCCs removed from the non-WRAP U.S. stationary-area inventory.

SCC	Description
2501060100	Storage and Transport Petroleum and Petroleum Product Storage Gasoline Service Stations Stage 2: Total
2501060101	Storage and Transport Petroleum and Petroleum Product Storage Gasoline Service Stations Stage 2: Displacement Loss/Uncontrolled
2501060102	Storage and Transport Petroleum and Petroleum Product Storage Gasoline Service Stations Stage 2: Displacement Loss/Controlled
2501060103	Storage and Transport Petroleum and Petroleum Product Storage Gasoline Service Stations Stage 2: Spillage
2501070100	Storage and Transport Petroleum and Petroleum Product Storage Diesel Service Stations Stage 2: Total
2501070101	Storage and Transport Petroleum and Petroleum Product Storage Diesel Service Stations Stage 2: Displacement Loss/Uncontrolled
2501070102	Storage and Transport Petroleum and Petroleum Product Storage Diesel Service Stations Stage 2: Displacement Loss/Controlled
2501070103	Storage and Transport Petroleum and Petroleum Product Storage Diesel Service Stations Stage 2: Spillage

Other steps that we took to prepare the stationary-area inventories included confirming that there is no overlap between the anthropogenic NH_3 inventory (Section 2.9) and stationary area sources, and moving area-source fires in each regional inventory to separate files. In addition to these inventory modifications we made a few changes to the ancillary data files for simulation Typ02G, as described next.

Simulation Typ02G used improved temporal and spatial allocation information relative to the preliminary 2002 modeling; the rest of the ancillary data for modeling stationary area sources stayed the same as in the preliminary 2002 modeling (Mansell et al., 2005). We adopted enhanced spatial allocation data with additional area-based surrogates for Canada (Table 2-9), and added surrogates for a missing county in Colorado (Broomfield) from WRAP modeling and QA work. The WRAP had noticed when looking at the Canadian data for the preliminary 2002 modeling that forest fire emissions from the Canadian area-source inventory, which are relatively large sources of CO, NO_x, and $PM_{2.5}$, were being allocated to a surrogate for logging activities. They found similar discrepancies for other area and non-road SCCs in Canada. To improve the representation of the Canadian emissions, we adopted several land-area-based surrogates developed by the WRAP, such as forested land area, urban land area, and rural land area, and made the accompanying additions to the spatial cross-reference file to associate inventory SCCs with these surrogates. We also added spatial surrogates for Broomfield County, CO; this county was included in the inventory but was not included in the base EPA surrogates (this county was recently created from portions of other counties).

Improvements to the temporal allocation data for simulation Typ02G included the addition of several FIPS-specific profiles provided by VISTAS and CENRAP contractors (Pechan 2005b). These temporal profiles listed in Table 2-12 targeted mainly fire and agricultural NH_3 sources, such as open burning and livestock operations, respectively.

Table 2-12. New Temporal Profile Assignments for CENRAP Area Source SCCs.

SCC	Description	Month	Week	Diurnal	Recommendation Based on Profile Data for SCC	Description of Similar SCC used to Recommend Profiles
2310001000	Industrial Processes; Oil and Gas Production: SIC 13;All Processes : On-shore; Total: All Processes	262	7	26	2310000000	Industrial Processes;Oil and Gas Production: SIC 13;All Processes;Total: All Processes
2310002000	Industrial Processes;Oil and Gas Production: SIC 13;All Processes : Off-shore;Total: All Processes	262	7	26	2310000000	Industrial Processes;Oil and Gas Production: SIC 13;All Processes;Total: All Processes
2461870999	Solvent Utilization;Miscellaneous Non-industrial: Commercial;Pesticide Application: Non-Agricultural;Not Elsewhere Classified	258	7	26	2461800000	Solvent Utilization;Miscellaneous Non-industrial: Commercial;Pesticide Application: All Processes;Total: All Solvent Types
2805009200	Miscellaneous Area Sources;Agriculture Production - Livestock;Poultry production - broilers;Manure handling and storage	1500	7	26	2805009300	Miscellaneous Area Sources;Agriculture Production - Livestock;Poultry production - broilers;Land application of manure
2805021100	Miscellaneous Area Sources;Agriculture Production - Livestock;Dairy cattle - scrape dairy;Confinement	1500	7	26	2805021300	Miscellaneous Area Sources;Agriculture Production - Livestock;Dairy cattle - scrape dairy;Land application of manure
2805021200	Miscellaneous Area Sources;Agriculture Production - Livestock;Dairy cattle - scrape dairy;Manure handling and storage	1500	7	26	2805021300	Miscellaneous Area Sources;Agriculture Production - Livestock;Dairy cattle - scrape dairy;Land application of manure
2805023100	Miscellaneous Area Sources;Agriculture Production - Livestock;Dairy cattle - drylot/pasture dairy;Confinement	1500	7	26	2805023300	Miscellaneous Area Sources;Agriculture Production - Livestock;Dairy cattle - drylot/pasture dairy;Land application of manure
2805023200	Miscellaneous Area Sources;Agriculture Production - Livestock;Dairy cattle - drylot/pasture dairy;Manure handling and storage	1500	7	26	2805023300	Miscellaneous Area Sources;Agriculture Production - Livestock;Dairy cattle - drylot/pasture dairy;Land application of manure
2810020000	Miscellaneous Area Sources;Other Combustion;Prescribed Burning of Rangeland;Total	3	11	13	2810015000	Miscellaneous Area Sources;Other Combustion;Prescribed Burning for Forest Management;Total

2.3.2 Emissions Processing

For simulations Typ02G and Base18G we configured SMOKE to process the annual stationary-area-source inventories for the U.S., Canada, and Mexico. As PMC is not an inventory pollutant but is required by the air quality models as input species, we used SMOKE to calculate PMC during the processing as (PM_{10} - $PM_{2.5}$). With the SMOKE option WKDAY_NORMALIZE set to "Yes," we treated the annual stationary-area inventories based on the assumption that they represent average weekday data, causing SMOKE to renormalize the data to a seven-day estimate before applying any temporal adjustments. We also assumed that all of the VOC emissions in the inventories are ROG and thus used SMOKE to convert the VOC to TOG before converting the emissions into CB-IV speciation for the air quality models. We configured SMOKE to use a MWSS temporal allocation approach, as opposed to a daily temporal approach.

To QA the stationary-area emissions, we used the procedures in the CENRAP modeling QAPP and Modeling Protocol (Morris and Tonnesen, 2004; Morris et al., 2004a) and a suite of graphical summaries. We used tabulated summaries of the input data and SMOKE script settings to document the data and configuration of SMOKE for all simulations. The graphical QA summaries include, for all emissions output species, daily spatial plots summed across all model layers, daily time-series plots, and annual time-series plots. These QA graphics are available on the UCR/CENRAP web site at http://pah.cert.ucr.edu/aqm/cenrap/emissions.shtml .

2.3.3 Uncertainties and Recommendations

Most of the issues that we encountered with the stationary area sources related to the removal of certain SCCs from the base inventories for inclusion as other source categories or complete omission from simulations. We spent considerable effort on ensuring that we did not have overlap between the area inventory and the other sectors that explicitly represent sources traditionally contained in the area inventory, such as NH_3 and dust.

Both the Canadian and Mexican inventories presented minor problems that we resolved for simulation Typ02G but that can be addressed more thoroughly in future simulations. The Canadian inventory we used contained data only at the province level, essentially equivalent to a statewide rather than county-level inventory. A higher resolution inventory would have allowed us to use higher-resolution and more accurate spatial allocation data. Future modeling that uses Canadian data should move to the newly released municipality-level year 2000 inventories for Canada.

There was a discrepancy between the state and county coding in the Mexican inventory and the SMOKE file that defines acceptable FIPS codes. Differences in the ordering of the Mexican state names between these two data sets led to some of the Mexican inventory sources being mislabeled in the SMOKE QA reports. The state codes in the inventory and spatial surrogate files for two Mexican states were changed to be consistent with the SMOKE country/state/county codes file.

2.4 On-Road Mobile Sources

On-road mobile-source emissions data for SMOKE consist of IDA-formatted emissions and vehicle activity inventory files, and ancillary data for allocating the inventories in space, time, and to the Carbon Bond-IV chemistry mechanism used in CMAQ and CAMx. This section describes where we obtained these data, how we modeled them, and the types of QA that we performed to ensure that SMOKE processed the data as expected.

2.4.1 Data Sources

The SMOKE processing for CENRAP included two approaches for processing on-road mobile sources depending on the source of the data provided. The first approach was to compute mobile emissions values prior to providing them to SMOKE; we call this the pre-computed emissions approach. The second approach was to provide SMOKE with VMT data, meteorology data, and MOBILE6 inputs, and let the SMOKE/MOBILE6 module compute the mobile emissions based on these data; we call this the VMT approach. These approaches are not mutually exclusive for a single SMOKE run; therefore, we performed single SMOKE runs in which both approaches were used as follows:

- Annual VMT for computing CO, NO_x, VOC, SO2, NH3 and PM using MOBILE6 for all CENRAP States.
- Pre-computed, seasonal MOBILE6-based emissions of all pollutants for the 13 WRAP states that included pre-speciated $PM_{2.5}$ data.
- Annual VMT for computing CO, NO_x, VOC, SO2, NH3 and PM using MOBILE6 for the rest of the United States (VISTAS, MRPO and MANE-VU).
- Pre-computed, annual 1999 emissions of all pollutants for Mexico.
- Pre-computed, annual 2000 emissions of all pollutants for Canada.

For the CENRAP states, STI provided VMT data and MOBILE6 input files for all counties in the CENRAP region (Reid et al., 2004a). MOBILE6 input files were provided only for the months of January and July for 2002. MOBILE6 input files for the remaining months of 2002 had to be generated. These data were then processed within SMOKE. Using one set of MOBILE6 input files for each county in the CENRAP states resulted in compute memory requirements that were to large to process all CENRAP states together. Therefore the on-road mobile processing for the CENRAP states was split into two groups for SMOKE processing. The resulting gridded emissions data files were then merged together to obtain an on-road mobile source emissions file for the entire CENRAP region.

For the WRAP states we used actual 2002 data split into California and non-California seasonal inventories that were provided by the WRAP (Pollack et al., 2006). In addition to the standard criteria pollutants, these files contained pre-speciated $PM_{2.5}$ emissions. For the rest of the U.S. we used annual county-level activity and speed inventories with monthly, county-level MOBILE6 inputs, and hourly meteorology to estimate the hourly emissions with the SMOKE/MOBILE6 module. For the non-U.S. inventories, we used version 2 of the year 2000 Canadian inventory and the updated 1999 Mexican inventory pre-computed mobile source emissions.

2.4.2 Emissions Processing

For the Typ02G emissions modeling we configured SMOKE to process the annual on-road mobile emissions inventory data for the WRAP, Canada, and Mexico as pre-computed inventories. For the non-WRAP states, we used the SMOKE/MOBILE6 integration to process the annual activity inventories and monthly, county-based roadway information. The WRAP inventories contained pre-computed speciated PM emissions (Pollack et al, 2006) so the SMOKE PM speciation module was not used. The WRAP on-road mobile inventories were developed to represent seven-day (weekly) average emissions (as compared to the area source inventory, which represented average weekday emissions). As actual weekly average emissions, we configured SMOKE to process the WRAP on-road mobile source emissions by setting WKDAY_NORMALIZE to "No" in which case the emissions are adjusted to represent weekday and Saturday and Sunday emissions (as in contrast to the area sources where the emissions are just adjusted for Saturday and Sunday). We also assumed that all of the VOC emissions in the inventories are ROG and used SMOKE to convert the VOC to TOG before converting the emissions into CB-IV speciation for the air quality models. We configured SMOKE to create day-of-week specific rather than MWSS, temporal profiles because the WRAP on-road mobile temporal profiles contain weekly profiles that vary across the weekdays.

As noted previously, the large number of county roadway inputs for MOBILE6 processed for the non-WRAP portion of the U.S. required us to split the states mobile-source processing into three subsets because of computer memory limitations. Separate MOBILE6 input files were used for each separate county for CENRAP states, where as one MOBILE6 input file was used for several counties outside of the CENRAP region. The three subsets consisted of two sets of SMOKE/MOBILE6 simulations for the CENRAP and a simulation that computed on-road mobile emissions for the MRPO, VISTAS, and MANE-VU states. We configured MOBILE6 to use weekly temperature averaging for computing these emissions within SMOKE.

To QA the on-road mobile emissions, we used the CENRAP emissions modeling QA protocol (Morris and Tonnesen, 2004; Morris et al., 2004a) and a suite of graphical summaries. We used tabulated summaries of the input data and SMOKE script settings to document the data and configuration of SMOKE for simulations Typ02G and Base18G. The graphical QA summaries include, for all emissions output species, daily spatial plots, daily time-series plots, and annual time-series plots. These graphics are available at http://pah.cert.ucr.edu/aqm/cenrap/qa_base02b36.shtml#mb

2.4.3 Uncertainties and Recommendations

We approached the on-road mobile emissions preparation for simulation Typ02G from three different directions, which were based on the form of the input inventories and ancillary emissions data for different regions of the modeling domain:

- The WRAP region used emissions estimates pre-computed with EMFAC for California and MOBILE6 for the rest of WRAP states and processed like area sources with SMOKE adjusted from weekly to day-of-week emissions.
- The CENRAP, VISTAS, MRPO, and MANE-VU states used county-level activity data to compute emissions with the SMOKE/MOBILE6 module.

- The non-U.S. parts of the domain also had pre-computer on-road mobile source emissions so used an area-source approach for processing with SMOKE.

Different approaches for modeling a single emissions sector adds complexity and additional sources of error and inconsistencies to the modeling because of the different assumptions that went into the preparation of the input data. For example, refueling emissions from the on-road mobile sector are represented in the WRAP area-source sector but are computed with MOBILE6 for the rest of the U.S. Not using MOBILE6-based emissions for the non-U.S. portion of the domain neglects the effects of the actual 2002 meteorology on these emissions. Applying MOBILE6 outside of the U.S. is currently not possible because MOBILE6 is instrumented only for calculating emissions for the U.S. automotive fleet. The result of using MOBILE6 to calculate U.S. emissions and not using it to calculate the non-U.S. on-road mobile emissions estimates is that the non-U.S. emissions are not specific to this modeling year and the 2002 meteorological conditions, whereas the U.S. emissions are 2002-specific.

While we used the best available information to compute the on-road mobile emissions for the various portions of the modeling domain, inconsistent approaches for representing these emissions may lead to unnatural emissions gradients along political boundaries. We recommend for future work a unified approach for at least the U.S. inventories, where either we use MOBILE6 in SMOKE for the entire domain (or alternative emissions model such as CONCEPT), or we calculate the emissions with MOBILE6 outside of SMOKE and then use the resulting county-based emissions inventories.

2.5 Non-Road Mobile Sources

Non-road mobile source emissions data for SMOKE consist of annual, seasonal, and monthly IDA-formatted emission inventory files and ancillary data for allocating the inventories in space, time, and to the Carbon Bond-IV chemistry mechanism used in CMAQ and CAMx. This section describes where we obtained these data, how we modeled them, and the types of QA that we performed to ensure that SMOKE processed the data as expected.

2.5.1 Data Sources

The non-road mobile-source inventories in the Typ02G and Base18G emissions modeling used actual 2002 data developed by the RPOs for the U.S., version 2 of the year 2000 Canadian inventory and the improved 1999 Mexican inventory. The U.S. inventories consisted of annual, seasonal, and monthly inventories; the non-U.S. inventories were annual data. Pechan provided the CENRAP inventories divided between annual data for aircraft, locomotive, and commercial marine and annual files for all other non-road sources (Pechan and CEP, 2005e). Minnesota substituted the monthly MRPO Base K non-road inventory for the CENRAP inventory in their state. Iowa substituted the monthly estimates for non-road agricultural sources from the MRPO base K inventory for the CENRAP inventory. Texas provided estimates for 2002 non-road emissions in lieu of the CENRAP prepared inventory. WRAP provided non-road inventories divided between California and non-California seasonal inventories, further subdivided into aircraft, locomotives, shipping, and all other non-road mobile sources (Pollack et al., 2006). Note that the California Air Resources Board uses their own OFFROAD model for California non-

road emissions, whereas the EPA NONROAD model is used for the rest of the states (with the exception of locomotives, aircraft and shipping). With these data WRAP also provided temporal adjustments to apply to the inventories to split them between weekday and weekend emissions. We used these weekday/weekend splits to derive new weekly temporal profiles for the WRAP sources. The MRPO base K monthly non-road inventories were obtained from MRPO in NIF format and were converted to SMOKE format by Wendy Vit of the Missouri DNR. The VISTAS Base G and MANE-VU non-road mobile inventories consisted of annual county-level data (Pechan and CEP, 2005c). We received these inventories directly from the respective RPO inventory representatives. We received the Canadian 2000 inventory version 2 from the U.S. EPA EFIG (EPA, 2005d). For Mexico we used the improved 1999 inventory available at http://www.epa.gov/ttn/chief/net/mexico.html.

Along with adding the WRAP weekday/weekend emissions splits to the temporal allocation files, we also created temporal input files that apply a flat, uniform monthly profile to the monthly and seasonal non-road inventories. With the monthly and seasonal variability inherent in these inventories, we avoided applying redundant monthly profiles by splitting the inventories into seasonal/monthly and annual data. We applied the uniform monthly temporal profiles to the seasonal/monthly inventories and non-uniform monthly temporal profiles to the annual inventories. How the non-road emissions inventory data were split into those with monthly/seasonal emission and those with annual emissions is provided in Table 2-13.

Table 2-13. Non-road mobile-source inventory temporal configuration.

Region	Source	Temporal Coverage
WRAP (non-CA)	Non-road mobile	Seasonal
WRAP (CA)	Non-road mobile	Seasonal
WRAP	Aircraft	Seasonal
WRAP	Locomotive	Annual
WRAP	In-port and near-shore shipping	Annual
CENRAP	All non-road	Annual
CENRAP, IA	Non road Ag.	Monthly
VISTAS	All non-road	Annual
MRPO and MN	All non-road	Monthly
MANE-VU	All non-road	Annual
Canada	All non-road	Annual
Mexico	All non-road	Annual

Iowa elected to use the CENRAP-sponsored inventory for all of the non-road categories except for the agricultural equipment categories provided in Table 2-14. For these agricultural equipment categories, Iowa elected to use the Midwest RPO Base K inventory because this inventory provided improvements to the temporal allocation of emissions for the agricultural sector. The Base K inventory includes monthly emissions. The monthly emissions are used in the SMOKE IDA files for modeling.

Table 2-14. Non-road agricultural emissions categories where the MRPO Base K inventory was used instead of the CENRAP inventory in Iowa.

SCC	SCC Description
22600050xx	Off-highway Vehicle Gasoline, 2-Stroke: Agricultural Equipment (2 SCCs);
22650050xx	Off-highway Vehicle Gasoline, 4-Stroke: Agricultural Equipment (11 SCCs);
22670050xx	LPG : Agricultural Equipment (3 SCCs);
22680050xx	CNG : Agricultural Equipment (3 SCCs); and
22700050xx	Off-highway Vehicle Diesel : Agricultural Equipment (11 SCCs).

Texas provided annual and daily emissions for CO, CO_2, NO_x, VOC, SO_2, PM10-FIL, and PM25-FIL for several oil and gas field equipment non-road categories (Table 2-15). Texas provided authorization to change the pollutant codes from PM10-FIL to PM10-PRI and PM25-FIL to PM25-PRI.

Table 2-15. Non-road oil and gas development equipment categories that Texas provided emissions to be used instead of the CENRAP inventory.

SCC	SCC Description
2265010010	Off-highway Vehicle Gasoline, 4-Stroke : Industrial Equipment: Other Oil Field Equipment;
2268010010	CNG : Industrial Equipment : Other Oil Field Equipment; and
2270010010	Off-highway Vehicle Diesel : Industrial Equipment : Other Oil Field Equipment

Lancaster County Nebraska provided its own non-road inventory for SCC 2260000000 (Off-highway Vehicle Gasoline, 2-Stroke : 2-Stroke Gasoline except Rail and Marine: All). The CENRAP-sponsored inventories for SCCs starting with 226 in Lancaster County were removed to correct double-counting of emissions. This adjustment was made by Pechan for Base02b modeling.

2.5.2 Emissions Processing

We configured SMOKE to process all of the non-road mobile emissions inventory data as area-like inventories using spatial surrogates to grid the county-level emissions. As the WRAP inventories contained pre-computed PM emissions, we did not have to use SMOKE to compute coarse mass PM (PMC). The WRAP non-road mobile inventories represented seven-day average emissions (different from the area inventory, which represented weekday average emissions). As actual weekly average emissions, we configured SMOKE to process them by setting WKDAY_NORMALIZE to "No." For the rest of the non-road mobile inventories we processed the data as weekday average data by setting WKDAY_NORMALIZE to "Yes." We also assumed that all of the VOC emissions in the inventories are ROG and used SMOKE to convert the VOC to TOG before converting the emissions into CB-IV speciation for the air quality models. We configured SMOKE to create MWSS temporal intermediates rather than daily temporal files because the non-road mobile sources do not use weekly temporal profiles that vary across the weekdays, but do have very different emissions on weekdays versus weekend days.

We divided the non-road mobile emissions modeling based on whether the data were annual or seasonal/monthly inventories. This split facilitated the application of uniform monthly temporal profiles to the seasonal/monthly inventories. After processing the non-road emissions as two separate categories, non-road yearly and non-road monthly, we combined them with the rest of the emissions sectors to create model-ready emissions for CMAQ and CAMx.
To QA the non-road mobile emissions we used the procedures in the CENRAP emissions modeling QAPP (Morris and Tonnesen, 2004) and Modeling Protocol (Morris et al., 2004a) and a suite of graphical summaries. We used tabulated summaries of the input data and SMOKE script settings to document the data and configuration of SMOKE for simulations. The graphical QA summaries include, for all emissions output species, daily spatial plots, daily time-series plots, and annual time-series plots. These QA graphics are available at
http://pah.cert.ucr.edu/aqm/cenrap/qa_base02f36.shtml#nr

2.5.3 Uncertainties and Recommendations

We prepared non-road mobile emissions using a combination of inventories having different temporal resolutions and various forms of ancillary data. These different combinations of information may lead to inconsistencies in how these emissions are represented across the modeling domain. In addition, the Canadian inventories contain only province-level information and thus have low-resolution spatial and temporal profiles applied to them. The Mexican non-road emissions are deficient in the number of different SCCs contained in the inventory and the availability of spatial surrogates that are applicable to non-road mobile sources. Improvements to the temporal profiles and spatial surrogates could provide a more consistent approach to representing the non-road emissions across the entire modeling domain.

2.6 Biogenic Sources

Biogenic emissions data for SMOKE consist of input files to the BEIS3 model (EPA, 2004a). BEIS3 is a system integrated into SMOKE for deriving emissions estimates of biogenic gas-phase pollutants from land use information, emissions factors for different plant species, and hourly, gridded meteorology data. The results of BEIS3 modeling are hourly, gridded emissions fluxes formatted for input to CMAQ or CAMx. This section describes the sources of the BEIS3 input data that we used for the Typ02G and Base18G emissions, how we modeled these data and the types of QA that were performed to ensure that SMOKE processed the data as expected.

2.6.1 Data Sources

The BELD3 land use data and biogenic emissions factors that were developed during the WRAP preliminary 2002 modeling were used for the CENRAP biogenic emissions modeling (Tonnesen et al., 2005). These data included BELD3 1-km resolution land use estimates and version 0.98 of the BELD emissions factors. Since the WRAP and CENRAP use the same 36 km Inter-RPO continental U.S. modeling domain, CENRAP was able to leverage of the WRAP work performed previously.

2.6.2 Emissions Processing

We used BEIS3.12 integrated in SMOKE to prepare emissions for the simulations. Most of the preparation for the biogenic emissions processing was completed during the preliminary 2002 modeling (Morris et al., 2005). As the modeling domains did not change from the preliminary 2002 to the final modeling, we re-used the gridded land use data and vegetation emissions factors that we prepared for the preliminary simulations.

To QA the biogenic emissions, we used the CENRAP emissions modeling QAPP (Morris and Tonnesen, 2004) and Modeling Protocol (Morris et al., 2004a) and a suite of graphical summaries. We used tabulated summaries of the input data and SMOKE script settings to document the data and configuration of SMOKE for simulation Base02b. The graphical QA summaries include, for all emissions output species, daily spatial plots, daily time-series plots, and annual time-series plots. These QA graphics are available at http://pah.cert.ucr.edu/aqm/cenrap/qa_base02b36.shtml#b3

2.6.3 Uncertainties and Recommendations

The use of newer versions of BEIS (BEIS3.13) and the new MEGAN biogenic emissions models should be considered in future modeling.

2.7 Fire Emissions

Fire emissions data for SMOKE have traditionally been represented as county-level area-source inventories that were placed in only the first vertical model layer. We advanced the representation of fire emissions for air quality modeling by preparing portions of the inventory data as point sources with specific latitude-longitude coordinates for each fire centroid and pre-computed plume rise parameters that were derived from individual fire characteristics. These new inventories were based on the fire data products prepared by a CENRAP emission contractor (Reid et al., 2004b) and modified by the project team to be properly modeled as point sources. These data consist of annual, daily, and hourly IDA-formatted emissions inventory files and ancillary data for allocating the inventories in space, time, and to the Carbon Bond-IV chemistry mechanism used in CMAQ and CAMx. This section describes where we obtained these data, how we modeled them, and the types of QA performed to ensure that SMOKE processed the fire emissions data as expected.

2.7.1 Data Sources

The fire inventories in the Typ02G emissions inventory were held constant through Base18G. We used actual 2002 fire data developed by the RPOs for the U.S., version 2 of the year 2000 Canadian inventory fire data, and actual 2002 fire data for Ontario, Canada. The inventories used consisted of both area and point source data for the U.S., Canada, and Mexico. Sonoma Technology, Inc. provided the fire emissions for the CENRAP states (Reid et al., 2004b). Air Sciences provided us with the WRAP inventories divided among six different fire categories: wildfires, agricultural fires, wildland fire use, natural prescribed, anthropogenic prescribed, and non-Federal rangeland fires (Air Sciences, 2007a). These inventories consisted of annual, daily, and hourly IDA-formatted files with information on daily emissions totals and hourly plume characteristics for each fire. We received similar fire emission inventories for the other RPOS (Air Sciences, 2007b). We modeled these sources with the rest of the stationary-area-source sector.

CENRAP received data for 54 fires that occurred in Ontario during the year 2002. Information on the data code abbreviations, data definitions, and data units used in the raw data files was obtained from Mr. Rob Luik (Data Management Specialist) at the Ontario Ministry of Natural Resources (Rob.Luik@MNR. gov.on.ca). Emissions for each fire were estimated using the Emission Production Model (EPM)/CONSUME within the BlueSky framework. A fire identification code is needed to track individual fires throughout the processing. The unique fire identification code was created for each fire by concatenating the FIRE_NUMBER and CUR_DIST fields of the original data. The fire identification code also contains the FIPS code of the fire; this information is not used by BlueSky but is needed by BlueSky2Inv, the utility program that converts the BlueSky output to the SMOKE inventory format. The FIPS code 135000 was used for all fires with longitudes east of –90°, and FIPS code 135059 was used for

fires west of –90°. These FIPS codes were used to ensure that the fires would be assigned the correct time zones in later SMOKE processing. Some of the dates provided in the original data included hourly information. In all cases, the hourly information was not used leaving all data at a daily resolution.

2.7.2 Emissions Processing

SMOKE is instrumented to distribute point-source-formatted fire inventories to the vertical model layers either by using a pre-computed plume rise approach or by computing the plume rise dynamically using actual 2002 meteorology. We applied both approaches for modeling point-source fire emissions in simulation Typ02G. For the pre-computed plume rise approach, SMOKE reads an annual inventory file with information on fire locations, a daily inventory file with daily emission totals for each fire, and an hourly inventory file with hourly plume bottom, plume top, and layer 1 fractions for each fire. SMOKE uses this information to locate the fires on the horizontal model grid and to distribute the plume of each fire vertically to the model layers. Because some of these fires have plumes that reach the model top, we set the number of emissions layers for processing these inventories to the full 19 layers of the meteorology. We applied this approach to the point-source fires for the WRAP, CENRAP and VISTAS regions.
The alternative plume rise approach uses information on fuel loading and the heat flux of the fires to distribute the fires vertically to the model layers. The data are provided to SMOKE in the form of an annual inventory with information on fire locations and a daily inventory with daily emission totals for each fire, daily heat flux, and daily fuel loading. We applied this approach to the point-source fires for Ontario, Canada.

All of the point-source fires used diurnal temporal profiles and speciation profiles for VOC and $PM_{2.5}$ developed by Air Sciences (2007a) during the preliminary 2002 modeling (Morris et al., 2005).

We modeled the area-source fires for U.S. and Canada as standard stationary area sources. We applied monthly temporal profiles provided by RPOs, flat weekly temporal profiles, and the diurnal profiles developed by Air Sciences for WRAP fires (Air Sciences, 2007a), and for the rest of the RPOs we used diurnal profiles that were provided by them (Air Sciences, 2007b). We used the forestland area surrogate to distribute these emissions from the county or province level in the inventories to the model grid cells.

To QA the fire emissions, we used the procedure in the CENRAP emissions modeling QA protocol (Environ, 2004) and a suite of graphical summaries. We used tabulated summaries of the input data and SMOKE script settings to document the data and configuration of SMOKE for simulation Typ02G. The graphical QA summaries include, for all emissions output species, daily spatial plots, daily time-series plots, annual time-series plots, and vertical profiles. These QA graphics are available at: http://pah.cert.ucr.edu/aqm/cenrap/qa_typ02g36.shtml.

2.7.3 Uncertainties and Recommendations

We used forestland spatial surrogates to distribute these county level (province level for Canada) data to the model grid. Using spatial surrogates to locate fires is a crude approach that results in the artificial smearing of the emissions over too large an area. This issue can be remedied by

moving to a point-source approach for representing these fires, similar to the approach used by Air Sciences for preparing the WRAP fire inventories.

2.8 Dust Emissions

Dust emissions data for SMOKE have traditionally taken the form of county-level stationary-area-source inventories. As these emissions are correlated to meteorology, land use, and vegetative cover, we made several changes to how dust emissions are simulated by SMOKE to take these parameters into consideration. This section describes where we obtained data for windblown, fugitive, and road dust sources, how we modeled them, and the types of QA performed to ensure that SMOKE processed the data as expected.

2.8.1 Data Sources

For the fugitive dust and road dust inventories in the Typ02G emission scenario, we used actual 2002 data developed by the RPOs for the U.S., version 2 of the year 2000 Canadian inventory, and the BRAVO 1999 Mexican inventory. We extracted the fugitive dust inventories from the stationary-area inventories for each of the RPOs, Mexico, and Canada. Before modeling these data we further divided them into construction/mining sources and agricultural sources. We defined the fugitive dust sources in the Base02f modeling based on guidance provided by EPA (2004b). WRAP provide road dust emission inventories (Pollack et al., 2006). For the rest of the RPOs and Canada, we extracted the road dust SCCs from the stationary-area-source inventories. The BRAVO 1999 Mexico inventory did not contain any road dust SCCs. Table 2-16 lists the SCCs for the various fugitive and road dust sources that we modeled in the Base02f and Typ02G inventories. We applied near-source capture transport factors that are based on county-level vegetative cover to the fugitive and road dust inventories to prepare them for input to the air quality models.

For windblown dust, we used gridded emissions prepared outside of SMOKE using a land use and meteorology-based model developed under funding from the WRAP by ENVIRON and UC-Riverside (Mansell, 2005; Mansell et al., 2005).

Table 2-16. Fugitive and road dust SCCs.

Dust Category	SCCs
Fugitive dust (construction and mining)	2275085000, 2311000000, 2311010000, 2311010070, 2311020000, 2311030000, 2325000000, 2305070000, 2530000020, 2530000100, 2530000120
Fugitive dust (agricultural)	2801000003, 2801000005, 2801000008, 2805001000
Road dust	2294000000, 2296000000

2.8.2 Emissions Processing

We modeled the fugitive and road dust inventories through SMOKE using an area-source approach. We modeled these data on the assumption that they represented weekday, rather than seven-day week, emissions and thus used the SMOKE setting WKDAY_NORMALIZE to convert the data to a seven-day average. We configured SMOKE to compute PMC during the

processing as (PM_{10} - $PM_{2.5}$). Usually the records with dust do not include any other pollutants such as VOC, and NOx. For the few records that did include pollutants other than the PM we

split the records where the PMs processed with dust and the non PMs processed with the area. We configured SMOKE to create MWSS temporal intermediates rather than daily temporal files because the dust sources do not use weekly temporal profiles that vary across the weekdays.
As noted above, we used SMOKE to apply near-source transport factors to the raw fugitive and road dust inventories to prepare them for input to the air quality models. We used U.S. transport factors from work done by Pace (2005) and a 2001 land use/land cover database to develop a SMOKE input file of county and SCC-based transport factors for the U.S., Canada, and Mexico. We applied these factors to create a new set of inventories adjusted for these transport factors for all regions except VISTAS; the VISTAS dust sources that we received already had the transport factors applied to them.

We calculated the windblown dust emissions outside of SMOKE using an internally developed, process-based model. By "process-based" we refer to an emissions model that integrates information about the processes that lead to the emissions of interest, in this case windblown dust. The process-based windblown dust model developed by the WRAP considers wind speeds, precipitation history, and soil types to derive gridded dust fluxes resulting from wind disturbances for the modeling domain. More information on this model, its modes of operation, and the configuration used for simulation Base02a are available in Mansell et al. (2005).
To QA the fire emissions, we used the procedures in the CENRAP emissions modeling QAPP (Morris and Tonnesen, 2004) and Modeling Protocol (Morris et al., 2004a) and a suite of graphical summaries. We used tabulated summaries of the input data and SMOKE script settings to document the data and configuration of SMOKE for Base02f emissions. The graphical QA summaries include, for all emissions output species, daily spatial plots, daily time-series plots, and annual time-series plots. These QA graphics are available at http://pah.cert.ucr.edu/aqm/cenrap/qa_base02f36.shtml#fd for fugitive dust, http://pah.cert.ucr.edu/aqm/cenrap/qa_base02f36.shtml#rd for road dust, and http://pah.cert.ucr.edu/aqm/cenrap/qa_base02b36.shtml#wbd for windblown dust.

2.8.3 Uncertainties and Recommendations

There are several improvements that should be made to the dust emissions modeling in future simulations. We will expand the list of fugitive dust SCCs that we extract from the stationary-area-source inventories for application of transport factors. This expanded list is based on recent work by EPA (2004b). We will also explore improvements to the assumptions that we used for generating emissions with the WRAP windblown dust model. Areas of improvement in the windblown dust model include refinements to the land use data and soil characteristics, additional information about agricultural activities in the WRAP and CENRAP regions, detailed model evaluation on targeted windblown dust case studies, and the application of snow-cover and vegetative transport factors to these emissions (Mansell et al., 2005).

2.9 Ammonia Emissions

Ammonia (NH_3) emissions from agricultural activities are a major source of ammonia and are dependent on many different environmental parameters, such as meteorology, crop and soil

types, and land use. CENRAP developed NH_3 emissions for the CENRAP states (Pechan and CEP, 2005e). Ammonia emissions were estimated for 13 source categories using the Carnegie Mellon University (CMU) model and supplemental technical work; 80% of technical work was dedicated to improving emissions estimates for two source categories—livestock production and fertilizer use. For these two categories, as well as biogenic sources, improvements were made to the activity data and/or emission factors used by the CMU model. For four other source categories (industrial point sources, landfills, ammonia refrigeration, and non-road mobile sources), emissions estimates were prepared independently of the CMU model, and for the remaining six source categories (publicly owned treatment works, wildfires, domestic animals, wild animals, human respiration, and on-road mobile sources), emissions estimates were derived by running the CMU model with no alterations.

CENRAP NH_3 model emissions estimates were combined with data provided by the other RPOs to represent agricultural NH_3 emissions in simulations Typ02G and Base18G.

2.9.1 Data Sources

The WRAP provided NH_3 emissions using the WRAP NH_3 model (Mansell et al, 2005) that generated emissions for the following sectors: domestic sources, wild animals, fertilizers, soils, and livestock. MWRPO provided monthly IDA-formatted inventories reflective of base K to CENRAP that they produced from process-based models of their own, along with temporal profiles and spatial cross-reference information for these sources. Iowa elected to use the MWRPO estimates of NH_3 emissions for fertilizer application, livestock, and wastewater treatment or SCC 28017XXXXX, 28050XXXXX, and 2630020000 respectively. Minnesota reviewed the MWRPO inventory and chose to move forward with the CENRAP developed data set. The rest of the U.S., Canada, and Mexico had agricultural NH_3 emissions contained within their annual stationary-area-source inventories.

2.9.2 Emissions Processing

The WRAP NH_3 emissions were processed outside of SMOKE using the WRAP NH_3 model and provided to CENRAP as gridded, hourly emissions in network common data form (NetCDF) files. CENRAP and MWRPO provided monthly IDA-formatted, county-level NH_3 inventories that were developed separately with process-based models. We modeled these emissions like area sources with SMOKE, applying the temporal profiles and the spatial cross-referencing developed for CENRAP that we received from the MWRPO. The agricultural NH_3 emissions for the rest of the RPOs, Canada, and Mexico are contained within their stationary-area inventories. We applied the SMOKE default temporal profiles and spatial surrogates to all non-process-based NH_3 emissions.

To QA the NH_3 emissions, we used the procedures in the CENRAP modeling QAPP (Morris and Tonnesen, 2004) and Modeling Protocol (Morris et al., 2004a) and a suite of graphical summaries. We used tabulated summaries of the input data and SMOKE script settings to document the data and configuration of SMOKE for simulations Typ02G and Base18G. The graphical QA summaries include, for all emissions output species, daily spatial plots, daily time-series plots, and annual time-series plots. These QA graphics are available at http://pah.cert.ucr.edu/aqm/cenrap/index.shtml

2.9.3 Uncertainties and Recommendations

Like the other emissions categories that have traditionally been represented as stationary area sources, the agricultural NH_3 emissions sector is affected by interregional inconsistencies in the way these emissions are represented.

During the QA of the Base02a emissions, the WRAP discovered a problem with their soil NH_3 estimates. The emission factor for soil NH_3 that were used in developing these data produced too high an emission estimate from this sector. For simulations Base02B through Typ02G, we therefore removed the soil NH_3 sector completely from the WRAP domain. In future simulations we will include these emissions with a revised emission factor for NH_3 emissions from soils.

2.10 Oil and Gas Emissions

Emissions from oil and gas development activities have been poorly characterized in the past. Simulations These emissions have been sporadically reported by some states in their stationary-area-source inventories, but for the most part were missing from our preliminary modeling. In the Typ02G and Base18G simulations, significant effort was made to better represent oil and gas production emissions explicitly as both area and point sources.

2.10.1 Data Sources

Emissions from oil and gas production activities for the CENRAP states were included with the other CENRAP state emission source categories (Pechan and CEP, 2005e). We received oil and gas production emissions inventories for the WRAP states and for tribal lands in the WRAP region as stationary-area-source and stationary-point-source IDA-formatted inventories. ERG, Inc. provided the point-source inventories with the rest of the stationary-point data (ERG, 2006a). ENVIRON provided the area-source oil and gas inventories for non-CA WRAP states and for tribal lands in the WRAP region, along with spatial surrogates for allocating these data to the model grid (Russell and Pollack. 2005). Oil and gas production emissions data for outside of the WRAP region are contained in the stationary-area inventories.

2.10.2 Emissions Processing

We modeled the WRAP point-source oil and gas production emissions in combination with the rest of the stationary-point-source emissions. We modeled the WRAP area-source oil and gas production emissions explicitly as a separate category that included WRAP and tribal inventories. These data represent weekly average emissions and did not require any renormalization within SMOKE. We used spatial surrogates generated by ENVIRON to allocate these annual county-level emissions to the model grid. For all oil and gas emissions, we applied flat temporal profiles to create hourly inputs to CMAQ and CAMx.

2.10.3 Uncertainties and Recommendations

In future 2002 modeling California oil and gas production emissions should be replaced with revised data provided by the California Air Resources Board (CARB). In addition, WRAP has

updated their oil and gas production inventory for the base and future years in a Phase II work effort that substantially improved the emissions inventory estimates (Bar-Ilan et al., 2007).

2.11 MMS Off-shore Gulf of Mexico Emissions

Offshore area point source emissions include emissions in the Gulf of Mexico and off the coast of California that are associated with oil and gas drilling platforms.

2.11.1 Data Sources

We obtained year 2000 IDA-formatted point-source inventories for oil and gas platforms in the Gulf of Mexico from the Minerals Management Service (MMS) web site: http://www.gomr.mms.gov/homepg/regulate/environ/airquality/gulfwide_emission_inventory/2000GulfwideEmissionInventory.html

We combined these with point-source data for coastal California provided to us by CARB during the preliminary 2002 modeling. We also obtained gridded area source emissions for platforms in the Gulf of Mexico from the MMS that we converted to the CENRAP 36-km model grid.

The 2000 MMS Gulf wide Emission Inventory was updated as of June 2006 to account for a change in vessel emissions in the non-point source (non-platform) database file. The point source (platform) emission inventory database file has not changed from the original version. Area source emissions from offshore activities in the Gulf of Mexico were developed from the latest estimates provided by the Minerals Management Service (MMS). The MMS inventory includes both platform and non-platform sources. The non-platform area source emissions estimates are spatially allocated to lease blocks and protraction units throughout the Gulf of Mexico. Temporal and spatial allocation cross-reference data were developed from the MMS inventory data and formatted for input to the SMOKE emissions model by Carolina Environmental Programs. These data were provided to the CENRAP emissions modeling team for implementation within SMOKE. The spatial allocation surrogates were provided for 4-km grid cells. The UCR team used these surrogates and developed surrogates for 36-km grid cells. Because these data are references to lease blocks/protraction units, rather than counties, this source category was processed separately form all other emissions using a customized reference data and SMOKE run scripts.

We modeled the offshore point and area sources as separate categories in the simulations. We used SMOKE to locate the offshore point sources on the model grid and to vertically allocate them into 15 model layers.

To QA the offshore platform emissions, we used the procedures in the CENRAP modeling QAPP (Morris and Tonnesen, 2004) and Modeling Protocol (Morris et al., 20042) and a suite of graphical summaries. We used tabulated summaries of the input data and SMOKE script settings to document the data and configuration of SMOKE for simulation Base02a. The graphical QA summaries include, for all emissions output species, daily spatial plots, daily time-series plots, and annual time-series plots. These QA graphics are available at http://pah.cert.ucr.edu/aqm/cenrap/index.shtml for the point and area sources.

2.11.2 Uncertainties and Recommendations

While the MMS data that we used were an improvement over previously modeled Gulf of Mexico platform inventories, the data were developed for a different modeling application that covered only the extreme northwestern portion of the Gulf, so they are missing large areas of the region of the Gulf that contain drilling platforms. The California offshore inventory represents an initial attempt at compiling an emission inventory for this area and contains very few sources. Future simulations will focus on improving these emissions by expanding the coverage of the offshore platform inventories for both the Gulf of Mexico and the Pacific Coast.

2.12 Off-shore Shipping Emissions

Emission inventory development for regional- and continental-scale air quality modeling has historically neglected offshore emissions sources beyond 25 miles offshore. Concern over the environmental effects of commercial shipping emissions in the Pacific on the coastal states in the WRAP region led to the development of a commercial marine shipping inventory for the Pacific. This inventory of off-shore marine vessels emissions made a substantial difference in some of the coastal western PM estimates (e.g., SO4). VISTAS developed an off-shore marine vessels inventory for the entire modeling domain that included the Pacific and Atlantic Oceans and the Gulf Of Mexico. For Typ02G and Base18G emission inventories CENRAP adopted the offshore shipping inventories developed by VISTAS.

2.12.1 Data Sources

Initially we obtained gridded annual commercial marine shipping emissions for the Pacific on the 36-km model grid from WRAP for inclusion in CENRAP simulations in the Base F modeling (Pollack et al., 2006). The commercial marine inventory contains all of the criteria pollutants contained in the non-road mobile-source inventory: CO, NO_x, VOC, NH_3, SO_2, PM_{10}, and $PM_{2.5}$. This inventory was subsequently updated in the Typ02G and Base18G modeling with the VISTAS off-shore commercial marine emissions inventory that covered the Gulf of Mexico and the Atlantic and Pacific Oceans and was based on the EPA/ARB SOx Emissions Control Area (SECA) program. Dr. James Corbett (University of Delaware) analyzed off-shore marine vessel data and worked with ENVIRON/ICF to convert to gridded emissions for the SECA grid. ENVIRON then provided SO_2, NO_X, PM and VOC emissions for the RPO 36-km grid.

2.12.2 Emissions Processing

The commercial marine shipping inventory was not processed through SMOKE. VISTAS provided the data to the as gridded text files on the 36-km model grid. These data were reformatted to the NetCDF CMAQ input format with a utility developed by UCR. The VOC inventory was converted to CB-IV speciation and the NO_x and $PM_{2.5}$ inventory pollutants to CMAQ input species with SMOKE chemical profiles for commercial shipping sources. No temporal adjustments were applied to these emissions; they use uniform monthly, daily, and diurnal profiles. An SCC for commercial marine vessels within the MMS inventory (SCC CM80002200) was accounted for in the commercial marine inventory developed for VISTAS. The duplicate emissions were removed from the MMS inventory prior to processing emissions

for Base G simulations. The duplicated emissions amounted to 19,000 TPY of NO_X and 3,184 TPY of SO_2. For simulation Typ02G and Base18G we received binary netCDF file from ENVIRON for one day and that day was used for every day of the year.
To QA the commercial marine shipping emissions, we used the procedures in the CENRAP modeling QAPP (Morris and Tonnesen, 2004) and Modeling Protocol (Morris et al., 2004a) and a suite of graphical summaries. The graphical QA summaries include, for all emissions output species, daily spatial plots, daily time-series plots, and annual time-series plots. These QA graphics are available at http://pah.cert.ucr.edu/aqm/cenrap/index.shtml.

2.12.3 Uncertainties and Recommendations

As a first attempt at representing shipping emissions in the Pacific in international waters, the WRAP and VISTAS 2002 commercial shipping inventory is a breakthrough in a historically neglected emissions category. As the RPOs evaluate the effects of these emissions on the air quality modeling, we anticipate that there will be refinements to the temporal profiles and to the vertical allocation of the emissions. Many of the stacks of large commercial ships contained in this inventory extend vertically above the first model layer. Future versions of this inventory should use higher-resolution temporal adjustments and should allocate the emissions to the appropriate model layers. Off-shore marine shipping activity is projected to increase. However, there are also the potential for emission controls on this source category (e.g., SECA program). Given these two off setting activities, the 2002 off-shore marine shipping emissions were assumed to be unchanged going from 2002 to 2018. Better estimates of 2018 marine emissions are being developed that should be considered in future modeling activities.

2.13 2018 Growth and Control

Base18G was based on grown inventories assuming on-the-books control strategies. CENRAP contracted with Pechan to deliver growth and control data for CENRAP and to consolidate growth and control information for other RPOs where available (Pechan, 2005d). The data are applicable to all source categories and pollutants included in the CENRAP 2002 emission inventory. This includes the following pollutants: sulfur oxides (SO_x), oxides of nitrogen (NO_x), volatile organic compounds (VOC), carbon monoxide (CO), ammonia (NH_3), and primary PM_{10} and $PM_{2.5}$. Some source categories were held constant between 2002 and 2018 because either stagnant growth was deemed appropriate or insufficient data was available to adequately project future growth or controls. These source categories include the following:

- Wind Blown Dust from non-agricultural land use categories.
- Emissions from wildfires.
- Emissions from Mexico.
- Global transport sources (i.e., the 2002 GEOS-CHEM boundary conditions).

2.13.1 Data Sources

CENRAP contracted with Pechan to provide growth and control factors to be applied with SMOKE for the CENRAP region (Pechan, 2005d). These growth and control parameters were based on growth estimates derived from EGAS 5.0 and control estimates assumed for

implementation of federal regulations and on-the-books state and local control programs. Emissions projections for electric generating units were developed for the RPOs with the Integrated Planning Model (IPM). The RPO 2.1.9 IPM results were subsequently modified by VISTAS, MRPO and CENRAP to reflect planned new construction and controls. The WRAP provided 2018 EGU estimates developed in coordination with State and Industry stakeholders. VISTAS, MWRPO and the WRAP provided emissions for 2018, having applied growth and control factors outside of SMOKE processing. EPA provided SMOKE processed emissions, applying both growth and controls, for Canada for the year 2020. These emissions were provided on the RPO 36-km grid. However, emissions were inexplicably processed for an alternative vertical structure. Alpine Geophysics, under contract to VISTAS reallocated the emissions through the vertical layers to more accurately reflect the vertical structure applied uniformly by the RPOs. The modified data was obtained directly from Alpine Geophysics. Emissions from Mexico were held constant between the inventory year 1999 and modeled 2002 and 2018. Improvements to the Mexican inventory have been continuously made between generation of the original BRAVO inventory and the present improved 1999 inventory. However, given the continued uncertainties in the improved inventory, no future year projections where attempted by CENRAP.

2.13.2 Emissions Processing

Growth and control factors developed by Pechan (2005d) for Arkansas did not match the final delivered inventory for Arkansas. Arkansas underwent major revisions to point and facility IDs in mid-2005. These updates were not available by the delivery date of the growth and control parameters. In coordination with Arkansas, a cross-walk was developed to correct the point and facility IDs.

The assumptions that went into the development of controls for engines covered under the RICE MACT were not consistent with the final rule. Rule penetration values for CENRAP states were adjusted to more accurately reflect the impact of the final rule.

The impact of the refinery global settlements was not incorporated into CENRAP modeling until the base G simulations. Control assumptions provided by EPA and referenced in EPA CAIR modeling were applied to the 2018 inventory. These reductions primarily impacted SO_2 emissions; however, NO_X reductions were applied in Oklahoma, Louisiana, and Minnesota.

2.13.3 Uncertainties and Recommendations

The impact of control programs is an area of uncertainty that will need continued review as the programs are implemented. Development of growth and control assumptions for Mexico will be necessary for continued refinement of the impact of international transport. CENRAP obtained estimates of increased prescribed burn activity for the Forest Service after processing of the base G simulations was underway. These estimates of increased activity should be reviewed for inclusion in future simulations. EPA developed 2020 estimates of Canadian emissions are assumed to include erroneous stack parameters previously addressed in the 2000 emissions processing. Further review of this data set is recommended.

2.14 2018 Base G C1 Control Sensitivity

CENRAP conducted a control sensitivity evaluating the impact of point source reductions given a maximum dollar per ton control level. The intent of the control sensitivity was to generate information on the impact of possible control strategies in support of the consultation process. The strategies were grouped together under a common set of criteria and not specifically identified by the states. The results of the modeling were not intended to be prescriptive; instead, they were intended to be a starting point for control discussions that would require much greater refinement.

2.14.1 Data Sources

CENRAP contracted with Alpine Geophysics to provide an evaluation of possible additional controls for the 2018 CENRAP point source inventory. These controls were in addition to on-the-books and BART controls assumed in the development of Base18F and Base18G emission scenarios. Base18F IDA files were enhanced with additional information on base level controls. The enhanced dataset was then linked with the control data contained in the 2006 release of EPA's AirControlNet software. Alpine developed cost curves for NO_X and SO_2 in 2005 dollars for the Base18F CENRAP point source inventory. Staff from Iowa DNR and Kansas DHE worked in conjunction to add area of influence data (Alpine Geophysics, 2006) and distance calculations to each Class I area in CENRAP. A variety of dollar per ton control levels were evaluated. CENRAP elected to base the sensitivity on a maximum control cost of $5,000 per ton. This selection was made with the understanding that the cost data under-represented the true cost of retrofit controls and did not take in to consideration more recent market fluctuations impacting costs of controls and construction. CENRAP refined the selection by applying controls to only those sources that met the criteria that the ratio of their emissions in tons per year to their distance to any Class I area in kilometers be less than 5. This distance weighting criteria allowed the sensitivity to focus on those sources with the greatest impact. Additional controls for other RPOs were not considered in this evaluation.

2.14.2 Emissions Processing

Sources considered for control were removed from the IDA files. Growth and control assumptions were applied outside of SMOKE and delivered to UCR as 2018 emissions. Stack parameter changes as a result of additional controls were not considered in this analysis.

2.14.3 Uncertainties and Recommendations

Given uncertainties in control costs more refined analyses should include an evaluation of retrofit control costs under present values.

2.15 Emissions Summaries

Appendix B provides details on the source of the emission files used in the CENRAP Typ02G and Base18G modeling. Also in Appendix B are sample emission summary plots, additional plots are available on the CENREAP modeling website: http://pah.cert.ucr.edu/aqm/cenrap/emissions.shtml.

CENRAP has contracted with E.H. Pechan and Associates to provide emissions summaries used in the final Typ02G and Base18G modeling in Excel spreadsheets and in an Access database that are available on the CENRAP website (http://www.cenrap.org/projects.asp#). Figures 2-3 through 2-9 display the, respectively, SO2, NOx, VOC, PM2.5, PM10, NH3 and CO anthropogenic emissions for the CENRAP states and the Typ02G and Base18G emission scenarios. Emissions are broken down by major source sector. For the state of Texas the emissions are broken by three groups, northeast Texas, southeast Texas and remainder of Texas (west Texas).

For most states, EGUs are the largest contributor to SO2 emissions (Figure 2-3). As EGU SO2 emissions are generally projected to be reduced in the future, most states show a reduction in total SO2 emissions from 2002 to 2018. One exception to this is Louisiana for which non-EGU point source SO2 emissions are greater than for EGU and are projected to increase from 2002 to 2018. The reasons for these increases are unclear, but the growth factors for non-EGU points should be examined more carefully.

NOx emissions are fairly evenly distributed across non-EGU point, EGU point, non-road mobile, on-road mobile and area sources for the 2002 Typ02G emissions scenario (Figure 2-4). In 2018, the contributions of on-road mobile source NOx emissions is reduced dramatically, with some states also showing reductions in EGU NOx emissions as well, resulting in all states exhibiting lower NOx emissions in 2018 than 2002.

VOC emissions are dominated by area, non-road mobile, on-road mobile and non-EGU point sources in both 2002 and 2018 (Figure 2-5). VOC emissions from on-road and non-road mobile source are projected to go down in the future, whereas VOC emissions from non-EGU point and, especially, area sources are projected to increase. Thus, whether a state's total VOC emissions increase or decrease depends on the relative contributions of mobile versus area sources and the level of increase in area source VOC emissions. Note that the VOC emissions listed in Figure 2-5 do not include biogenic VOC emissions that would be greater than the anthropogenic VOC emissions shown in Figure 2-5. Note that because biogenic VOC emissions are processed using the SMOKE/BEIS module on the 36 km grid, state-wide biogenic VOC emissions summaries are not readily available.

Primary $PM_{2.5}$ emissions are primarily from road dust and fugitive dust, and for some states fires (Figure 2-6). Kansas, Oklahoma, Louisiana and Texas all have large contributions from fires not seen in the other states. Road dust and fugitive dust are the most dominate source categories for coarse particulate as well (Figure 2-7).

CENRAP developed a separate ammonia emissions for 13 categories using the CMU model including livestock and fertilizer that dominates the ammonia emissions across the CENRAP

states (Figure 2-8). Several states also have significant ammonia contributions from non-EGU point sources, whereas others do not.

CO emissions are dominated by the on-road and non-road mobile source sectors (Figure 2-9). However, states with fires also see large CO contributions from them as well. On-road mobile source CO emissions are projected to go down substantially from 2002 to 2018, whereas the other source categories are flat.

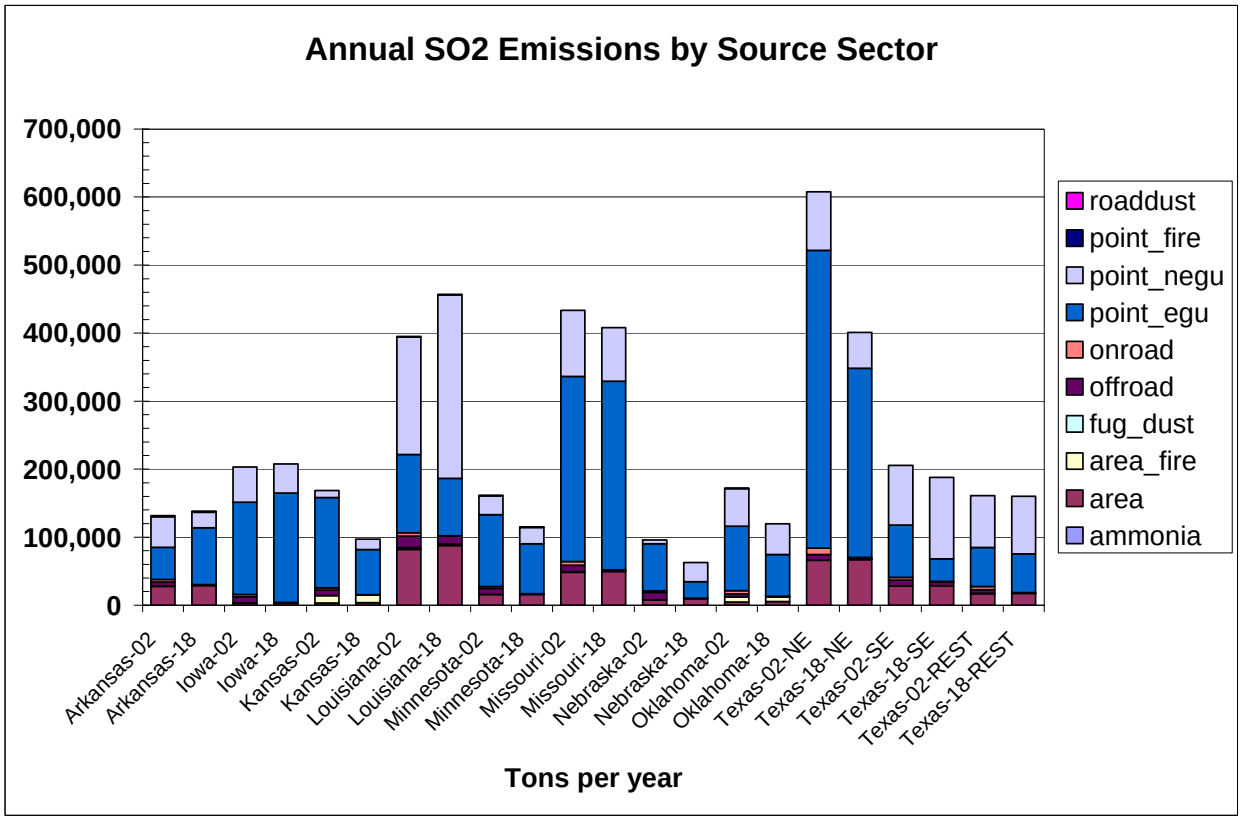


Figure 2-3. Summary of Typ02G and Base18G SO2 emissions by CENRAP state and major source sector (tons per year).

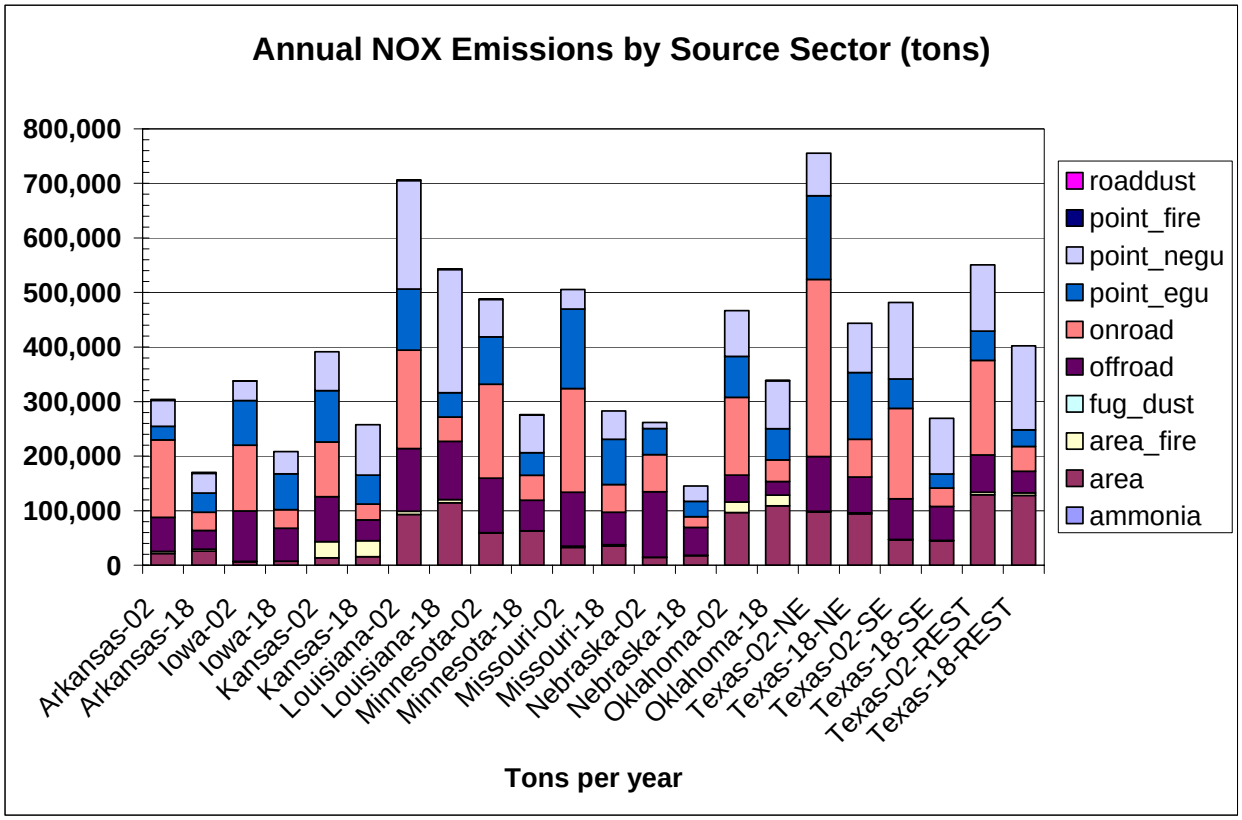


Figure 2-4. Summary of Typ02G and Base18G NOx emissions by CENRAP state and major source sector (tons per year).

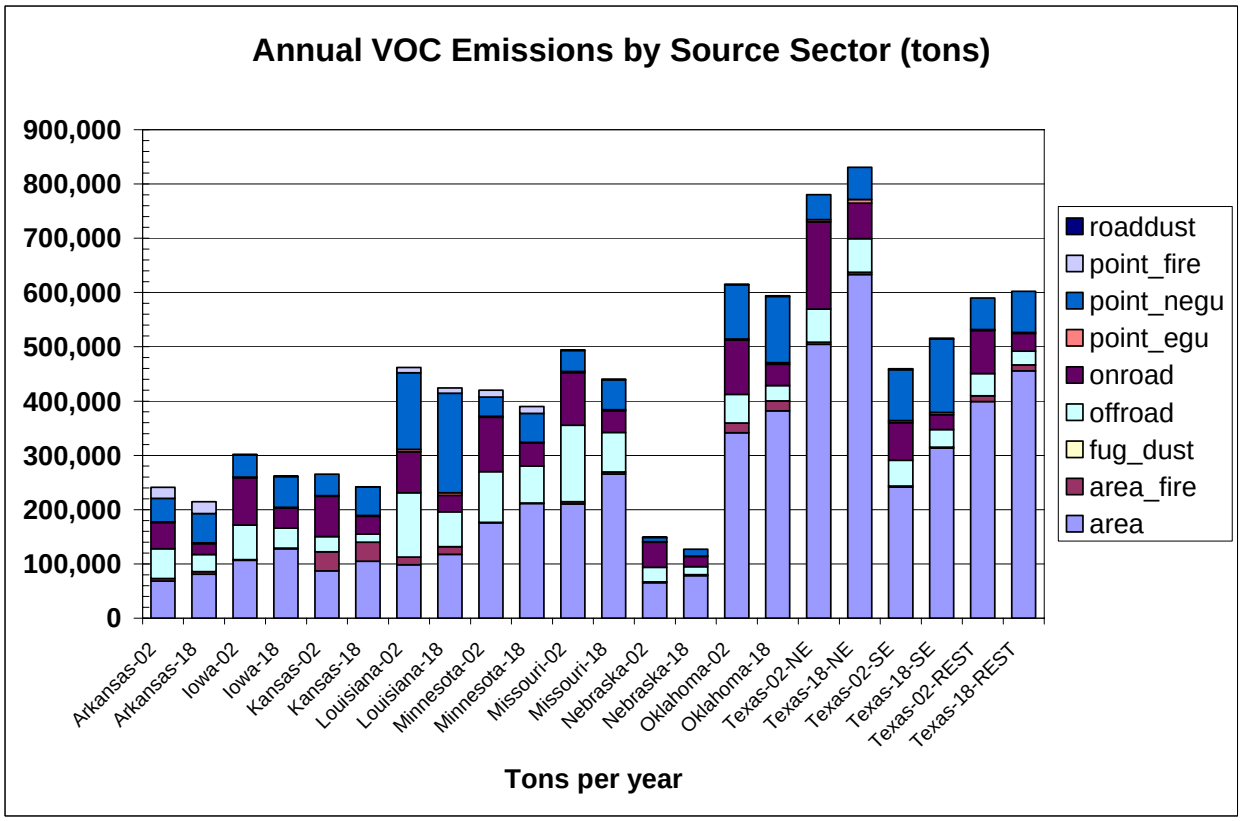


Figure 2-5. Summary of Typ02G and Base18G VOC emissions by CENRAP state and major source sector (tons per year).

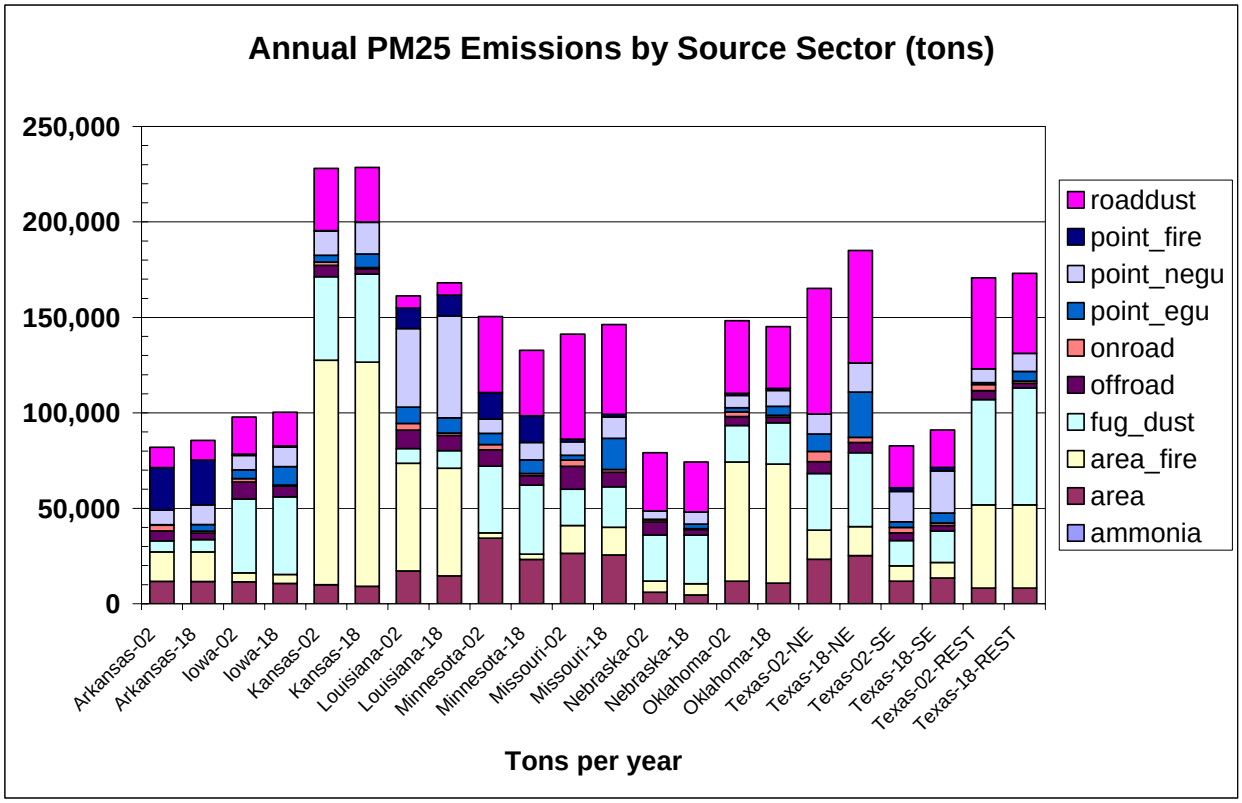


Figure 2-6. Summary of Typ02G and Base18G PM2.5 emissions by CENRAP state and major source sector (tons per year).

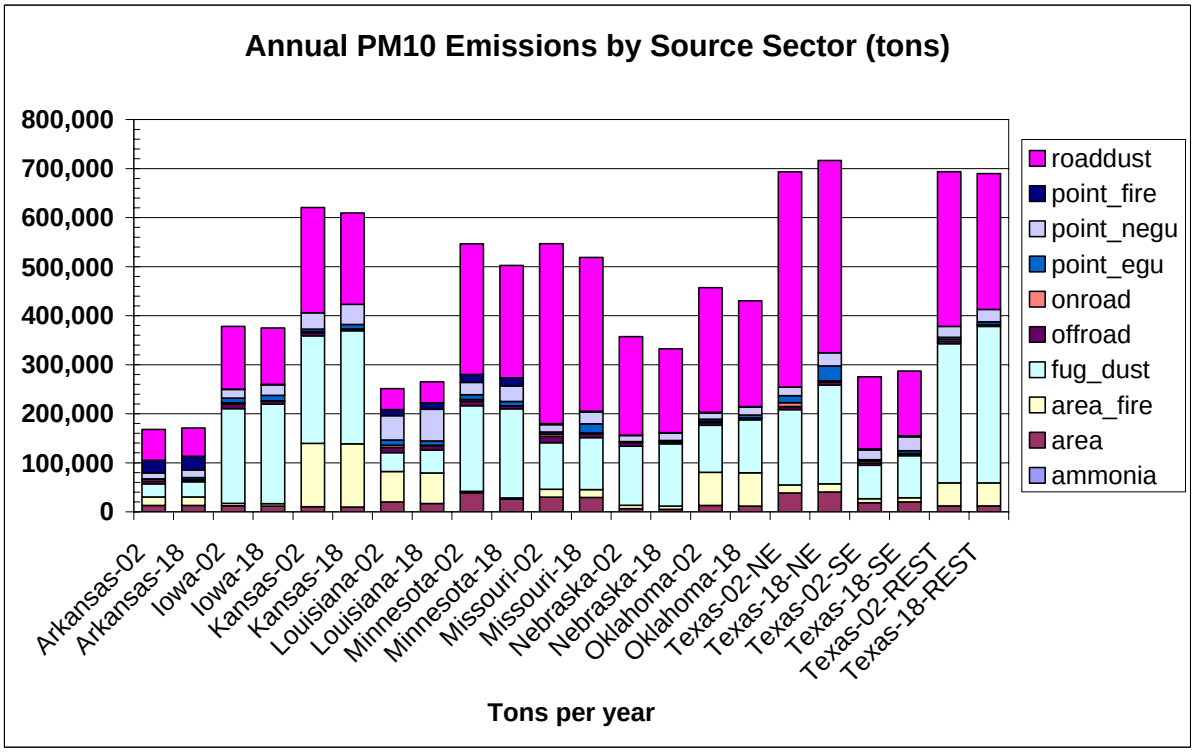


Figure 2-7. Summary of Typ02G and Base18G PM10 emissions by CENRAP state and major source sector (tons per year).

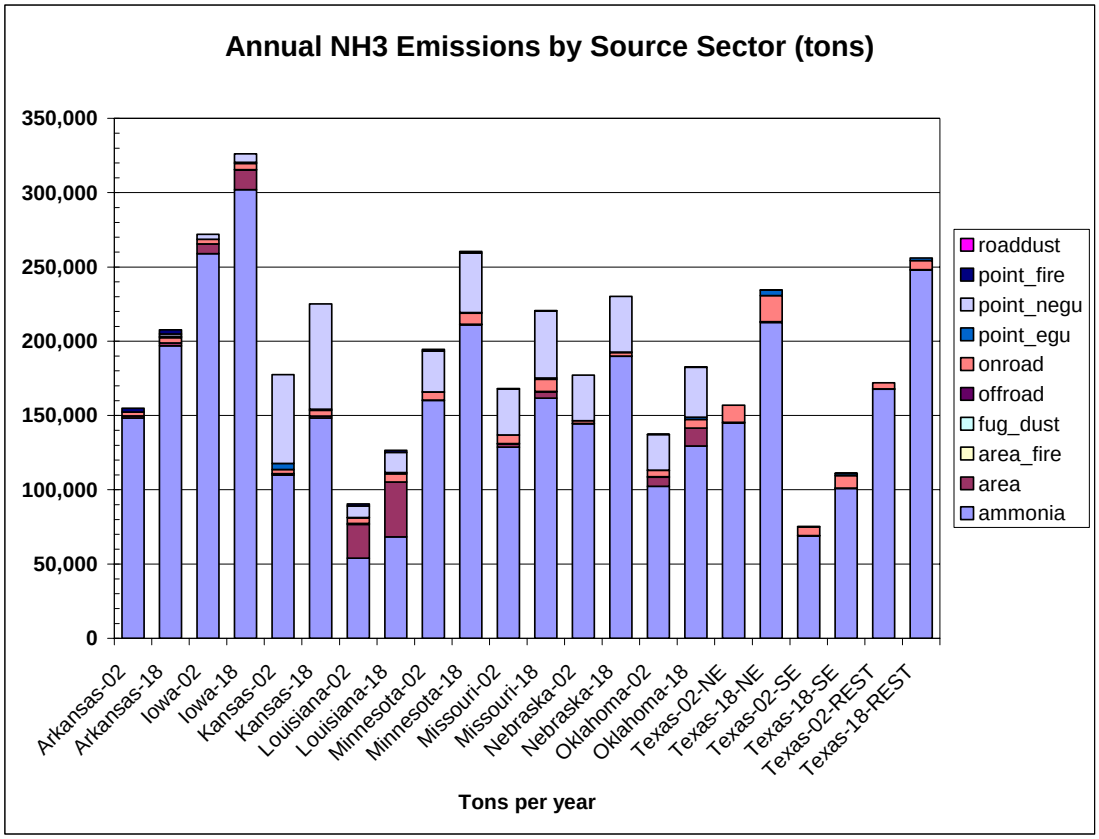


Figure 2-8. Summary of Typ02G and Base18G NH3 emissions by CENRAP state and major source sector (tons per year).

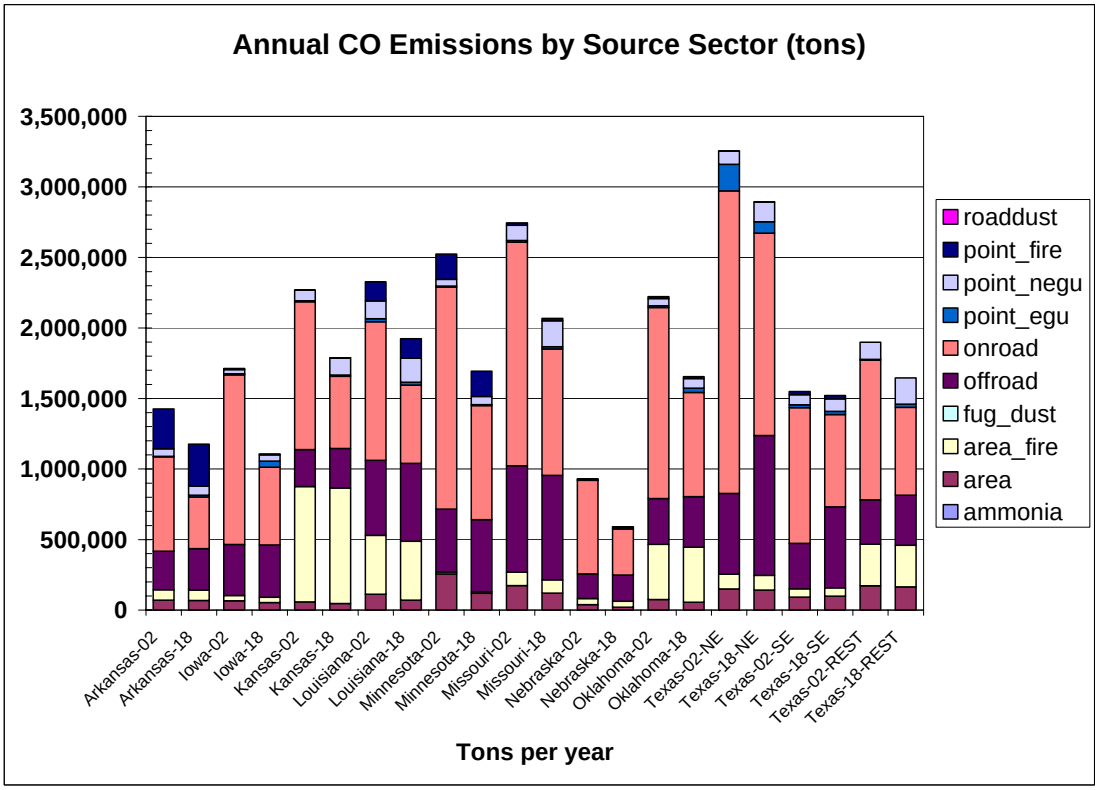


Figure 2-9. Summary of Typ02G and Base18G CO emissions by CENRAP state and major source sector (tons per year).

3.0 MODEL PERFORMANCE EVALUATION

In this Chapter we summarize the CMAQ model performance for the final 2002 36 km Base F base case simulation. Because the 2002 Base F CMAQ simulation produced nearly identical results in the U.S. as the final 2002 Base G simulation and limited resource availability, CENRAP elected not to redo the model evaluation for the 2002 Base G case. This model performance focuses on the ability of the model to predict PM species within the CENRAP region. Details on the model performance are provided in Appendix C. Previously we have documented model performance of interim versions of model base case simulations in reports (Morris et al., 2005) and presentations to the CENRAP Work Groups and POG (e.g., Morris et al., 2006a,b).

3.1 Evaluation Methodology

EPA's integrated ozone, $PM_{2.5}$ and regional haze modeling guidance calls for a comprehensive, multi-layered approach to model performance testing, consisting of the four major components: operational, diagnostic, mechanistic (or scientific) and probabilistic (EPA, 2007). The CMAQ model performance evaluation effort focused on the first two components, namely:

- **Operational Evaluation**: Tests the ability of the model to estimate PM concentrations (both fine and coarse) and the components at PM_{10} and $PM_{2.5}$ including the quantities used to characterize visibility (i.e., sulfate, nitrate, ammonium, organic carbon, elemental carbon, other $PM_{2.5}$, and coarse matter ($PM_{2.5-10}$). This evaluation examines whether the measurements are properly represented by the model predictions but does not necessarily ensure that the model is getting "the right answer for the right reason"; and

- **Diagnostic Evaluation:** Tests the ability of the model to predict visibility and extinction, PM chemical composition including PM precursors (e.g., SOx, NOx, and NH_3) and associated oxidants (e.g., ozone and nitric acid); PM size distribution; temporal variation; spatial variation; mass fluxes; and components of light extinction (i.e., scattering and absorption).

In this final model performance evaluation for the 2002 Typical Base F CMAQ simulation, the operational evaluation has been given the greatest attention since this is the primary thrust of EPA's modeling guidance. However, we have also examined certain diagnostic features dealing with the model's ability to simulate sub-regional, monthly, diurnal, gas phase and aerosol concentration distributions. In the course of the CENRAP air quality modeling and other modeling processes, numerous diagnostic sensitivity tests were performed to investigate and improve model performance. Key diagnostic tests that were performed and the results are discussed on the CENRAP modeling website: http://pah.cert.ucr.edu/aqm/cenrap/index.shtml.

3.2 Ambient Air Quality Data used in the Evaluation

The ground-level model evaluation database for 2002 was compiled by the modeling team using several routine and research-grade databases. The first is the routine gas-phase concentration measurements for ozone, SO_2, NO_2 and CO archived in EPA's Aerometric Information Retrieval System (AIRS) Air Quality System (AQS) database. Other sources of observed information come from the various PM monitoring networks in the U.S. These include the Interagency Monitoring of Protected Visual Environments (IMPROVE); Clean Air Status and Trends Network (CASTNET); EPA Speciation Trends Network (STN) of $PM_{2.5}$ species; and National Acid Deposition Program (NADP). During the course of the CENRAP modeling, the numerous base case simulations were evaluated across the continental U.S. (e.g., Morris et al., 2005). In this section and in Appendix C we focus our evaluation on model performance within the CENRAP region.

3.2 Operational Model Evaluation Approach

The CENRAP modeling databases will be used to develop the visibility State Implementation Plan (SIP) as required by the Regional Haze Rule (RHR). Accordingly, the primary focus of the operational evaluation in this report is on the six components of fine particulate ($PM_{2.5}$) and coarse mass ($PM_{2.5-10}$) within the CENRAP region that are used to characterize visibility at Class I areas:

- Sulfate (SO4);
- Particulate Nitrate (NO3);
- Elemental Carbon (EC);
- Organic Mass Carbon (OMC);
- Other inorganic fine particulate (IP or Soil); and
- Coarse Mass (CM).

The model performance for ozone, precursors, and product species (e.g., SO_4 , NO_3, NH_4 and HNO_3) is also evaluated to build confidence that the modeling system is sufficiently reliable to project future-year visibility.

3.3 Model Performance Goals and Criteria

The issue of model performance goals for PM species is an area of ongoing research and debate. For ozone modeling, EPA has established performance goals for 1-hour ozone: normalized mean bias and gross error of #±15% and #35%, respectively (EPA, 1991). EPA's draft fine particulate modeling guidance notes that performance goals for ozone should be viewed as upper bounds of model performance that PM models may not be able to always achieve and that we should demand better model performance for PM components that make up a larger fraction of the PM mass than those that are minor contributors (EPA, 2001). EPA's final modeling guidance does not list any specific model performance goals for PM and visibility modeling and instead provides a summary of PM model performance across several historical applications that can be used for comparisons, if desired. Measuring PM species is not as precise as ozone monitoring. In fact, the uncertainty in measurement techniques for some PM species is likely to

exceed the more stringent model performance goals, such as those for ozone. For example, recent comparisons of the PM species measurements using the IMPROVE and STN measurement technologies found uncertainties of approximately ∀20% (SO4) to ∀50% (EC) (Solomon et al., 2004).

For the CENRAP modeling we have adopted three levels of model performance goals and criteria for bias and gross error as listed in Table 3-1. Note that we are not suggesting that these performance goals be adopted as guidance. Rather, we are just using them to frame and put the PM model performance into context and to facilitate model performance intercomparison across episodes, species, models and sensitivity tests.

Table 3-1. Model performance goals and criteria used to assist in interpreting modeling results.

Fractional Bias	Fractional Gross Error	Comment
#∀15%	#35%	Ozone model performance goal for which PM model performance would be considered "good" – note that for many PM species measurement uncertainties may exceed this goal.
#∀30%	#50%	Proposed PM model performance goal that we would hope each PM species could meet
#∀60%	#75%	Proposed PM criteria above which indicates potential fundamental problems with the modeling system.

As noted in EPA's PM modeling guidance, less abundant PM species should have less stringent performance goals (EPA, 2001; 2007). Accordingly, we are also using performance goals that are a continuous function of average concentrations, as proposed by Dr. James Boylan at the Georgia Department of Natural Resources (GA DNR), that have the following features (Boylan, 2004):

- Asymptotically approaching proposed performance goals or criteria (i.e., the ∀30%/50% and ∀60%/75% bias/error levels listed in Table 3-1) when the mean of the observed concentrations are greater than 2.5 ug/m^3.

- Approaching 200% error and ∀200% bias when the mean of the observed concentrations are extremely small.

Bias and error are plotted as a function of average concentrations. As the mean concentration approaches zero, the bias performance goal and criteria flare out to ∀200% creating a horn shape, hence the name "Bugle Plots". Dr. Boylan has defined three Zones of model performance: Zone 1 meets the ∀30%/50% bias/error performance goal and is considered "good" model performance; Zone 2 lies between the ∀30%/50% performance goal and ∀60%/75% performance criteria and is an area where concern for model performance is raised; and Zone 3 lies above the ∀60%/75% performance criteria and is an area of questionable model performance.

3.4 Key Measures of Model Performance

Although we have generated numerous statistical performance measures (see Table C-2 in Appendix C) that are available on the CENRAP modeling website, when comparing model performance across months, subdomains, networks, grid resolution, models, studies, etc. it is useful to have a few key measurement statistics to be used to facilitate the comparisons. It is also useful to have a subset of months within the 2002 year that can represent the entire year so that a more focused evaluation can be conducted. We have found that the Mean Fractional Bias and Mean Fractional Gross Error appear to be the most consistent descriptive measure of model performance (Morris et al., 2004b; 2005). The Fractional Bias and Error are normalized by the average of the observed and predicted value (see Table C-2) because it provides descriptive power across different magnitudes of the model and observed concentrations and is bounded by -200% to +200%. This is in contrast to the normalized bias and error (as recommended for ozone performance goals, EPA, 1991) that is normalized by just the observed value so can "blow up" to infinity as the observed value approaches zero. In Appendix C we perform a focused evaluation of model performance for PM and gaseous species and four months of the 2002 year that are used to represent the seasonal variation in performance:

- January
- April
- July
- October

Scatter plots of model predictions and observations for each PM species are presented for each of the four months along with performance statistics and predicted and observed time series plots at each CENRAP Class I area. Summary plots of monthly fractional bias and error are also presented.

3.5 Operational Model Performance Evaluation

A summary of the operational evaluation is presented below. Just the monthly fractional bias performance metrics for each PM species using bar charts and Bugle Plots are presented in this section. The reader is referred to Appendix C for the complete model performance evaluation.

3.5.1 Sulfate (SO4) Model Performance

Figure 3-1 compares the monthly SO4 fractional bias across the CENRAP region for the IMPROVE, STN and CASTNet monitoring networks. An underprediction bias is clearly evident the first 8-10 months of the year. This underestimation bias is greatest across the CASTNet network which persists throughout the year. The SO4 underprediction is not as severe for the STN network and it is minimal by August becoming a slight overprediction in September. For the IMPROVE network, the SO4 fractional bias is < ±20% for the first 2 and last 3 months of the year and ranges from -30% to -50% for the late Spring and Summer months.

Figure 3-1 also includes a Bugle Plot of monthly SO4 fractional bias statistics (for Bugle Plot of fractional gross error see Appendix C) and compares them against the proposed PM model

performance goal and criteria (see Table 3-1). For the STN network, SO4 model performance meets the proposed performance goal for all months. For the IMPROVE network, approximately half of the months achieve the proposed PM performance goal with the other half outside of the goal, but within the performance criteria. Across the CASTNet network, most months are outside of the proposed goal but are within the criteria. The CASTNet fractional bias for some months is right at the performance criteria (≤±60%). With the exception of two IMPROVE months, the monthly SO4 fractional bias performance statistics achieve the proposed PM model performance goal.

3.5.2 Nitrate (NO3) Model Performance

Monthly NO3 model performance across the CENRAP region is characterized by a summer underestimation and winter overestimation bias (Figure 3-2). The summer underestimation bias is more severe, exceeding -100%. Whereas, the winter overestimation bias is approximately 50%. So based on statistics alone, it appears the summer underestimation bias is a bigger concern than the winter overestimation bias. However, the Bugle Plots in the bottom part of Figure 3-2 show that the summer underestimation bias occurs when NO3 is very low and is not an important component of PM and visibility impairment. These summer values occur in the flared horn part of the Bugle Plot and the summer NO3 performance, in most cases, achieves the model performance goal and always achieves the performance criteria. Whereas, the winter overstated NO3 performance for the most part doesn't meet the performance goal and there are some months/networks that also don't meet the performance criteria.

3.5.3 Organic Matter Carbon (OMC) Model Performance

The OMC monthly fractional bias across IMPROVE and STN sites in the CENRAP region are shown in Figure 3-3. The fractional bias for OMC at the IMPROVE sites is quite good throughout the year with values generally within ±20%, albeit with a slight winter overestimation and summer underestimation bias. At the urban STN sites, the model exhibits an underestimation bias throughout the year that ranges from -20% to -50%. The urban underestimation of OMC is a fairly common occurrence and suggests there may be missing sources of organic aerosol emissions in the modeling inventory.

The good performance of the model for OMC at the IMPROVE sites is also reflected in the Bugle Plot (Figure 3-3, bottom) with the bias achieving the proposed PM model performance goal for all months of the year. At the STN sites, however, the OMC bias falls between the proposed PM model performance goal and criteria, with error right at the goal for most months.

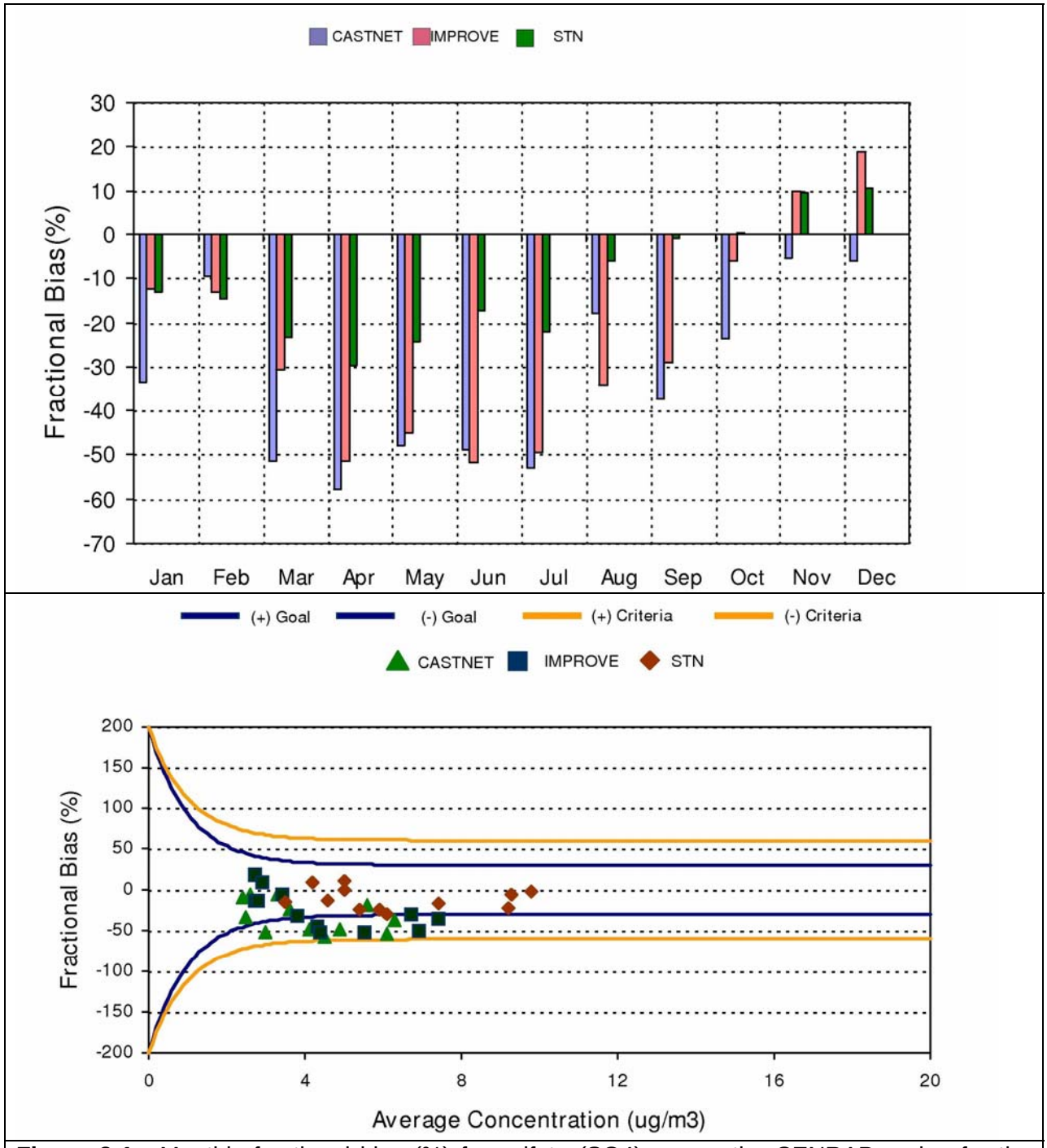


Figure 3-1. Monthly fractional bias (%) for sulfate (SO4) across the CENRAP region for the CMAQ 2002 36 km Base F base case simulation.

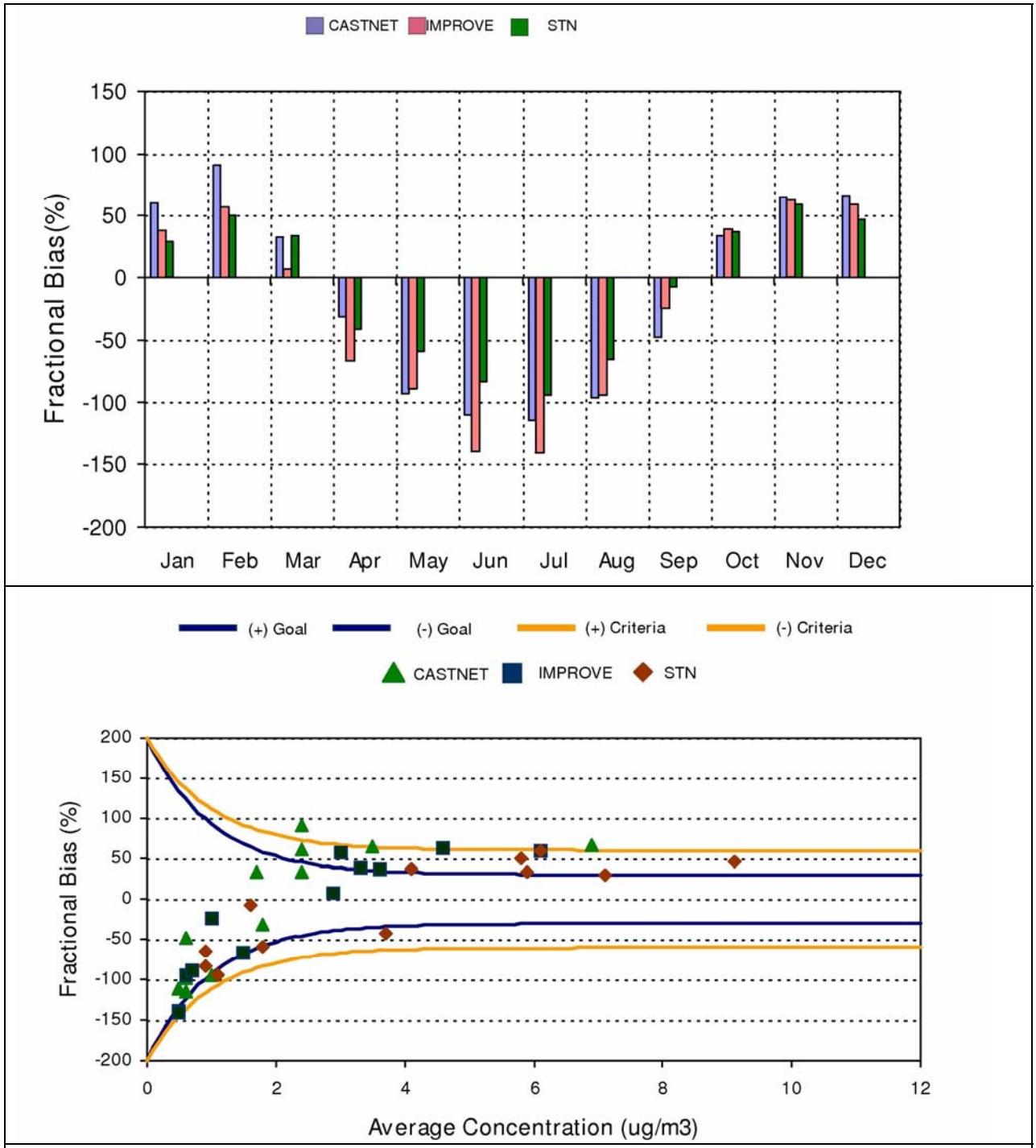


Figure 3-2. Monthly fractional bias (%) for nitrate (NO3) across the CENRAP region for the CMAQ 2002 36 km Base F base case simulation.

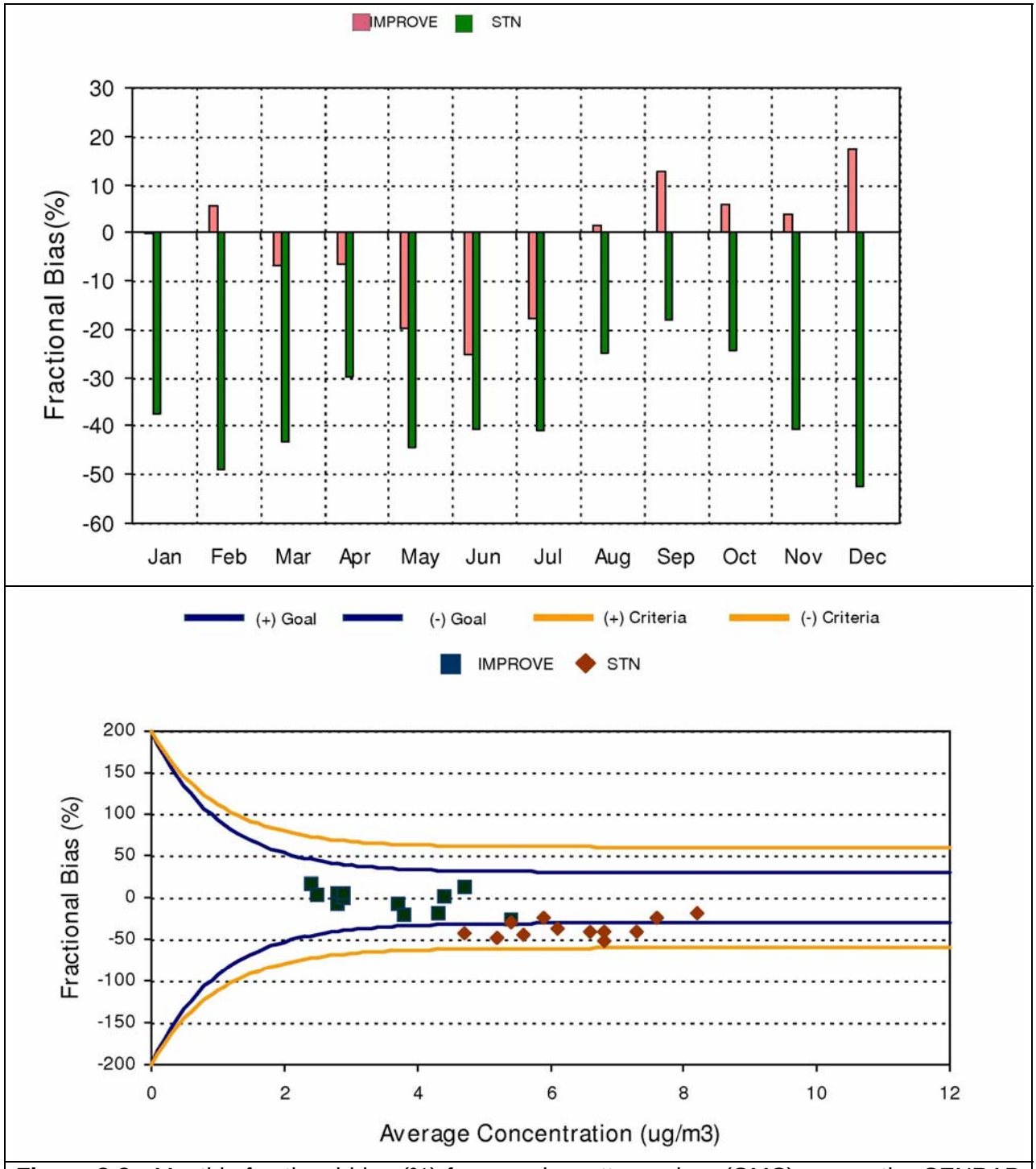


Figure 3-3. Monthly fractional bias (%) for organic matter carbon (OMC) across the CENRAP region for the CMAQ 2002 36 km Base F base case simulation.

3.5.4 Elemental Carbon (EC) Model Performance

The monthly average bias for EC across the IMPROVE and STN monitors in the CENRAP region are shown in Figure 3-4. The STN network exhibits small fractional bias year round, whereas the IMPROVE monitoring network exhibits a large underprediction bias in the summer months (-40% to -70%) and much smaller bias in the winter. The Bugle Plot puts the EC performance in context. The low EC concentrations at the IMPROVE sites results in bias values in the horn of the Bugle Plot. Thus, EC bias achieves the proposed PM performance goal for all months of the year.

3.5.5 Other $PM_{2.5}$ (Soil) Model Performance

Figure 3-5 displays the monthly variation in the Soil fractional bias using IMPROVE measurements in the CENRAP region. During the winter months, the model exhibits a very large (> 100%) overestimation bias. With the exception of July, the summer monthly bias is toward a slight overprediction but generally less than 20%. The July underestimation bias appears to be driven by impacts of high Soil values from wind blown dust events (e.g., see July 2002 discussion in Appendix C). The Bugle Plot indicates that the summer Soil performance achieves the PM performance goal, a few months in the Spring/Fall period fall between the performance goal and criteria and the winter Soil performance exceeds the model performance criteria. Thus, the Soil performance is a cause for concern.

3.5.6 Coarse Mass (CM) Model Performance

The monthly average fractional bias values for CM are shown in Figure 3-6. In the winter the underprediction bias is typically in the -60% to -80% range. In the late Spring and Summer the underprediction bias ranges from -120% to -160%. As this underprediction bias is nearly systematic (i.e., an underprediction almost always occurs), then the fractional errors are the same magnitude as the bias.

The Bugle Plots clearly show that the CM model performance is a problem. The monthly bias exceeds both the performance goal and criteria for almost every month of the year.

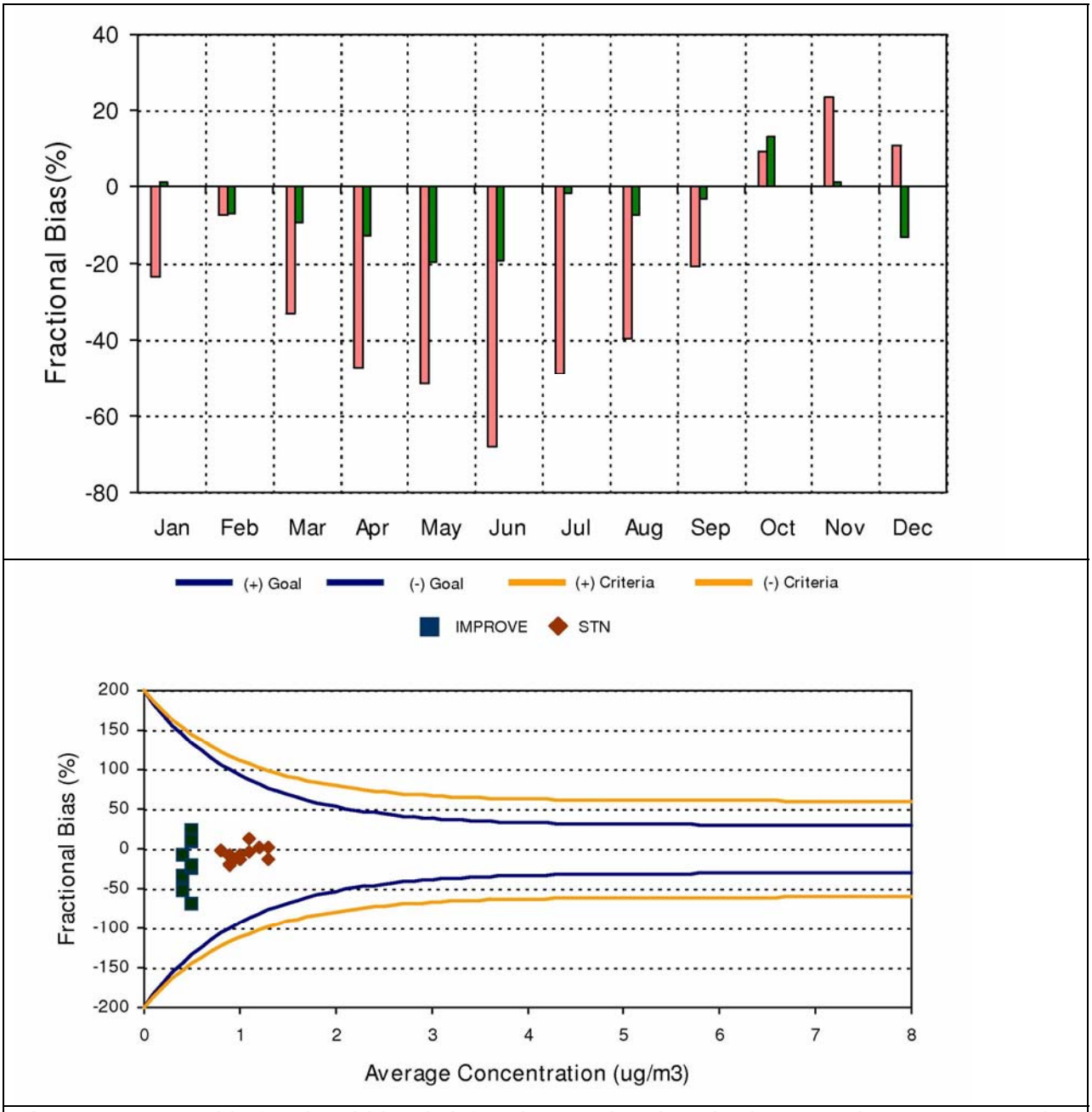


Figure 3-4. Monthly fractional bias (%) for elemental carbon (EC) across the CENRAP region for the CMAQ 2002 36 km Base F base case simulation.

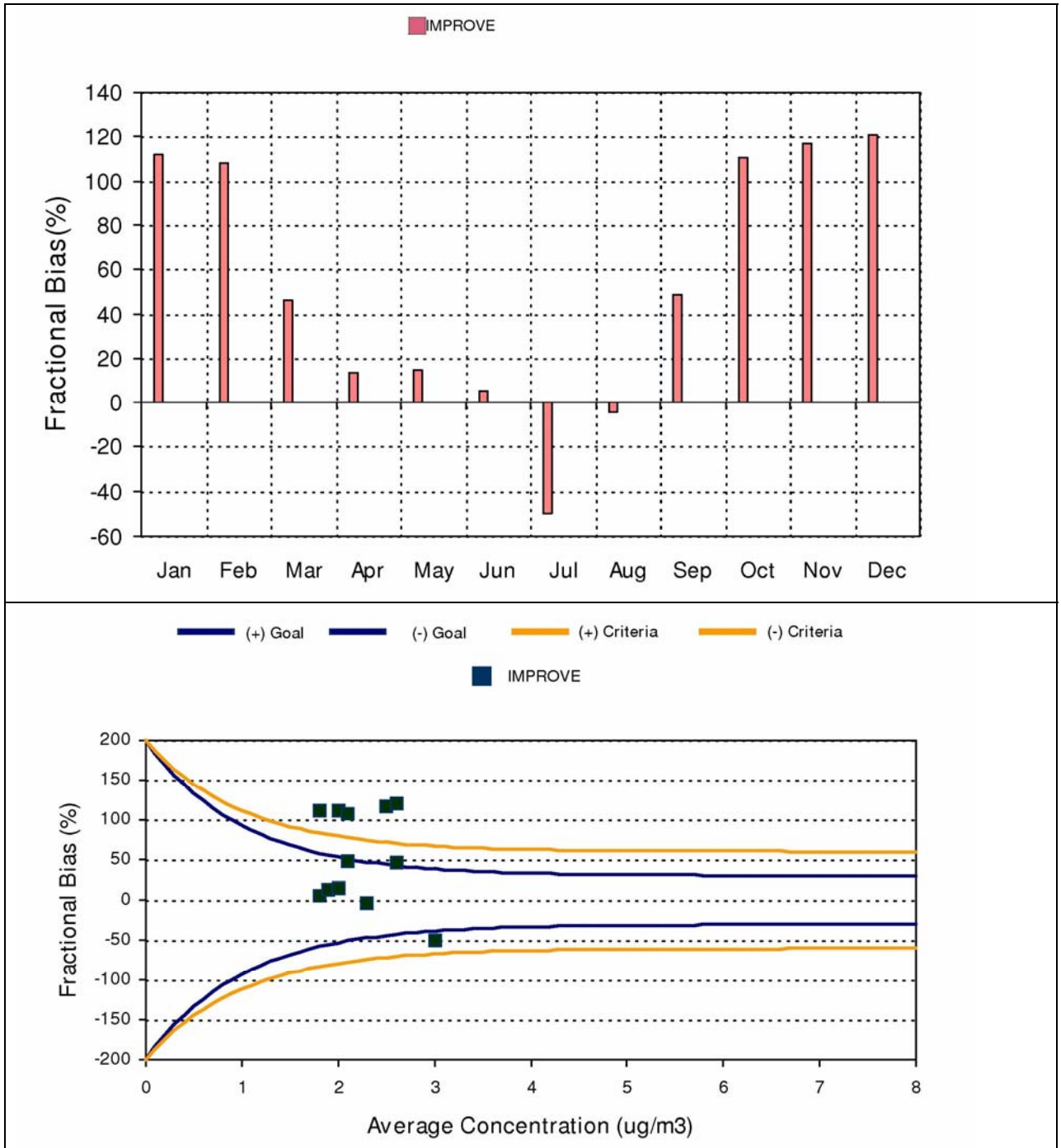


Figure 3-5. Monthly fractional bias (%) for other $PM_{2.5}$ (Soil) across the CENRAP region for the CMAQ 2002 36 km Base F base case simulation.

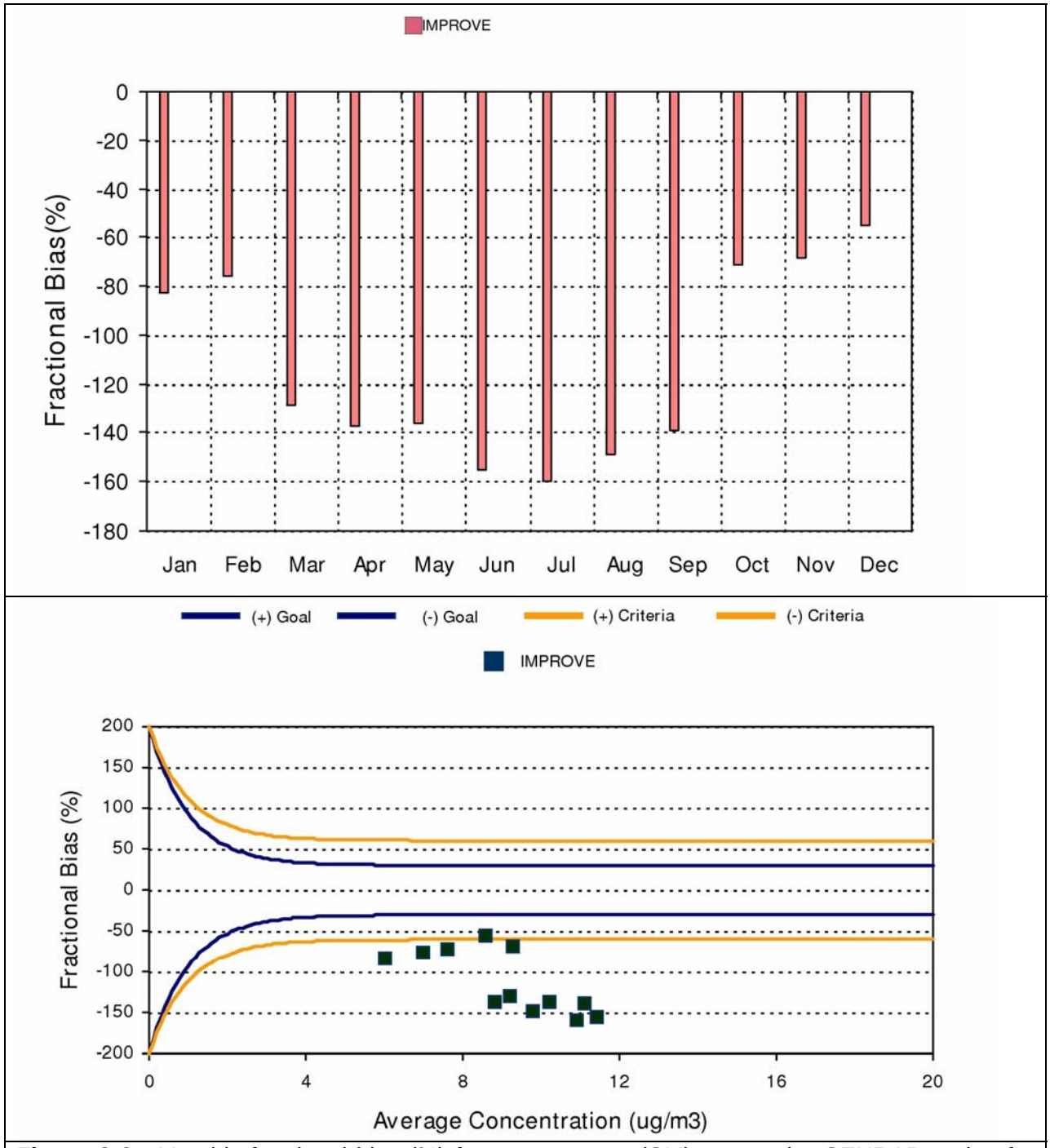


Figure 3-6. Monthly fractional bias (%) for coarse mass (CM) across the CENRAP region for the CMAQ 2002 36 km Base F base case simulation.

3.6 Diagnostic Model Performance Evaluation

The CASTNet and AQS networks also measure gas-phase species that are PM precursor or related species. The diagnostic evaluation of the 2002 36 km Base F CMAQ base case simulation for these compounds and the four seasonal months are presented in Appendix C. The displays for January are provided below as an example; the reader is referred to Appendix C for the rest of the monthly displays.

The CASTNet network measures weekly average samples of SO2, SO4, NO2, HNO3, NO3 and NH4. The AQS network collects hourly measurements of SO2, NO2, O3 and CO. A comparison of the SO2 and SO4 performance provides insight into whether the SO4 formation rate may be too slow or fast. For example, if SO4 is underestimated and SO2 is overestimated that may indicate chemical conversion rates that are too slow. Analyzing the performance for SO4, HNO3, NO3, Total NO3 and NH4 provides insight into the equilibrium of these species. For example, if Total NO3 performs well but HNO3 and NO3 do not, then there may be issues associated with the partitioning between the gaseous and particulate phases of nitrate. Causes for incorrect HNO3/NO3 partitioning could include inadequate ammonia emissions and/or poorly characterized meteorological conditions (e.g., temperature).

3.6.1 Diagnostic Model Performance in January 2002

In January, SO2 is overstated across both the CASTNet and AQS sites with fractional bias values of 38% (Figure 3-7) and 31% (Figure 3-8), respectively. SO4 is understated by -34% across the CASTNet monitors (Figure 3-7) and -12% and -13% for the IMPROVE and STN networks (Figure C-4a). Wet SO4 deposition is also overstated in January (+40%, Figure C-4a). Given that SO2 emissions are well characterized, these results suggest that the January SO4 underestimation may be partly due to understated transformation rates of SO2 to SO4 and overstated wet SO4 deposition.

Total NO3 is overestimated by 35% on average across the CASTNet sites in the CENRAP region in January (Figure 3-7). HNO3 is underestimated (-34%) and particle NO3 is overestimated (+61%) suggesting there are gas/particle equilibrium issues. An analysis of the time series of the four CASTNet stations reveals that NO3, HNO3 and NH4 performance is actually very reasonable at the west Texas site and the HNO3 underestimation and NO3 overestimation bias is coming from the east Kansas, central Arkansas and northern Minnesota CASTNet sites (see Figure C-3 for site locations). One potential contributor for this performance problem could be overstated NH3 emissions. However, the Total NO3 overestimation bias suggests that the model estimated NOx oxidation rate may be too high in January.

The SO2, NO2, O3 and CO performance across the AQS sites in January is shown in Figure 3-8. The AQS monitoring network is primarily an urban-oriented network. So, it is not surprising that the model is underestimating concentrations of primary emissions when a 36 km grid is used. NO2 is underestimated by approximately 5%, and CO by approximately 67%. Ozone is also underestimated on average, especially the maximum values above 60 ppb.

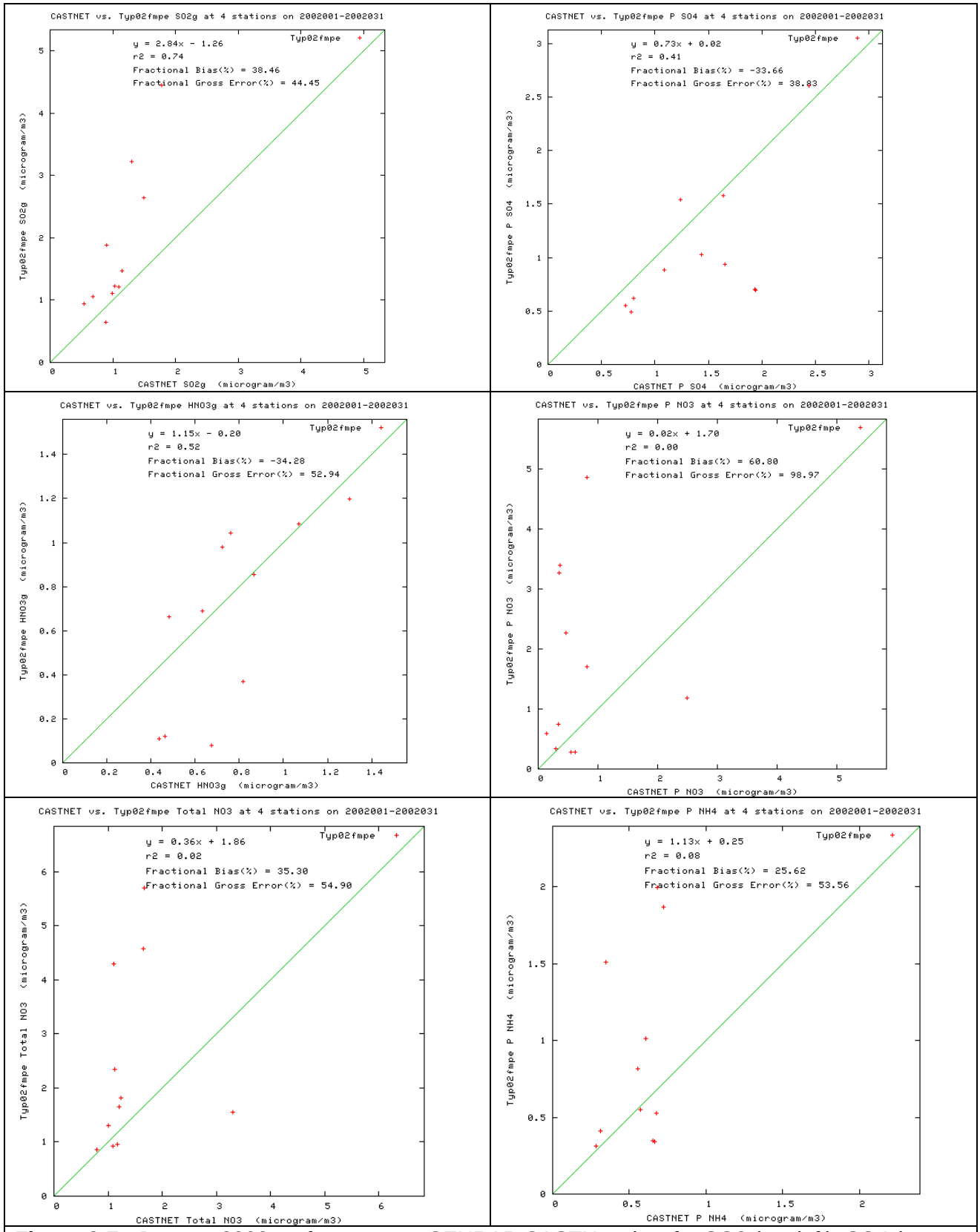


Figure 3-7. January 2002 performance at CENRAP CASTNet sites for SO2 (top left), SO4 (top right), HNO3 (middle left), NO3 (middle right), Total NO3 (bottom left) and NH4 (bottom right).

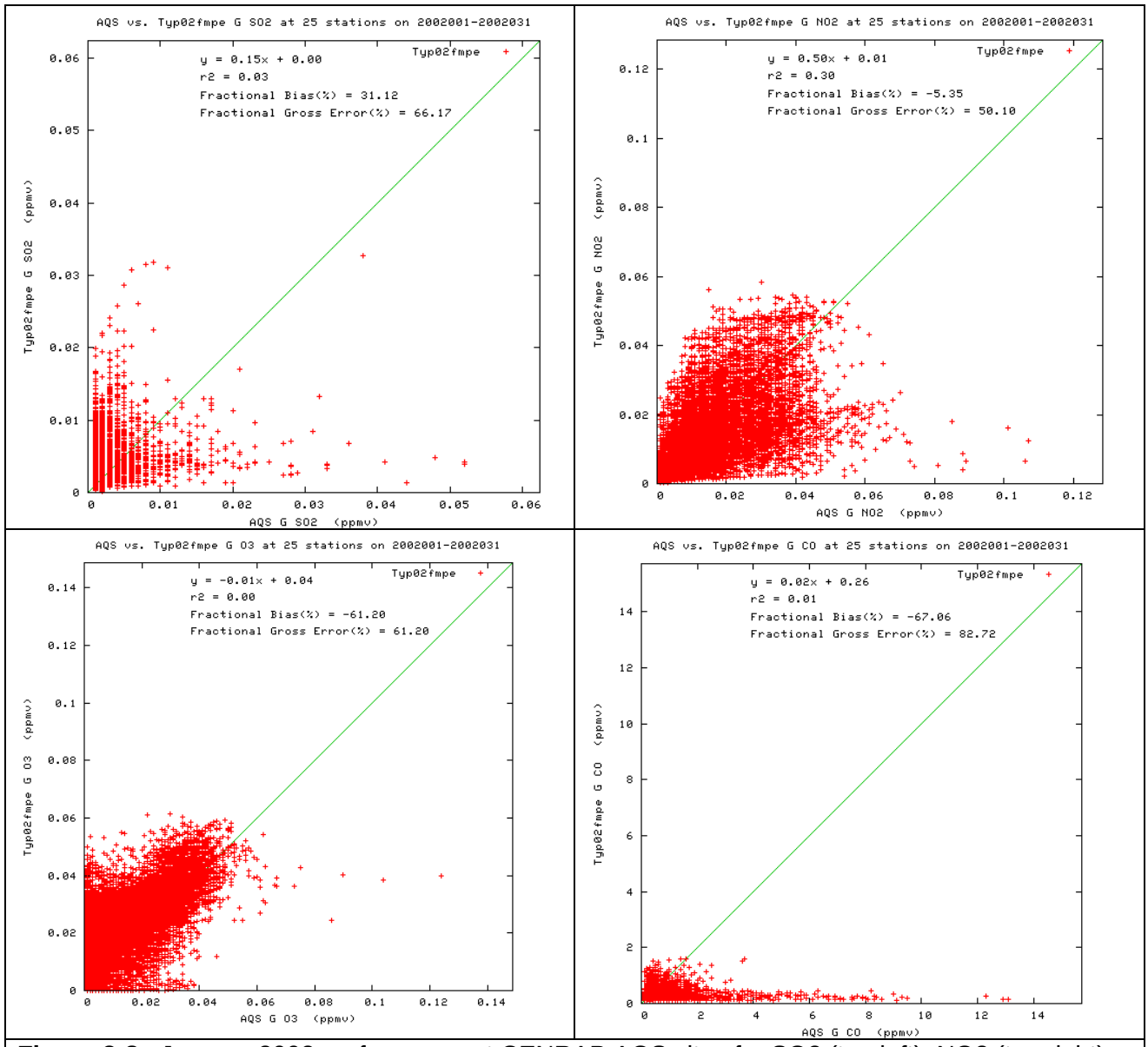


Figure 3-8. January 2002 performance at CENRAP AQS sites for SO2 (top left), NO2 (top right), O3 (bottom left) and CO (bottom right).

3.6.2 Diagnostic Model Performance In April

In April there is an average SO2 overestimation bias across the CASTNet (+15%) and underestimation bias across the AQS (-10%) networks (Figures C-42 and C-43). SO4 is underestimated across all networks by -30% to -58% (Figure C-5a). The wet SO4 deposition bias is near zero. Both SO2 and SO4 are underestimated at the west Texas CASTNet monitor in April suggesting SO2 emissions in Mexico are likely understated.

The HNO3 performance in April is interesting with almost perfect agreement except for 5 modeled-observed comparisons that drives the average underprediction bias of -29% (Figure C-42). On Julian Day 102 there is high HNO3 at the MN, KS and OK CASTNet sites that is not captured by the model. Given that HNO3, NO3 and Total NO3 are all underestimated by about the same amount (-30%), then part of the underestimation bias is likely due to too slow oxidation of NOx.

There is a lot of scatter in the NO2 and O3 performance that is more or less centered on the 1:1 line of perfect agreement with bias values of -8% and -21%, respectively (Figure C-43). CO is underestimated by -72% with the model unable to predict CO concentrations above 1 ppm due to the use of the coarse 36 km grid spacing. Mobile sources produce a vast majority of the CO emissions. So, AQS monitors for CO compliance are located near roadways, which are not simulated well using a 36 km grid.

3.6.3 Diagnostic Model Performance In July

In July SO2 is slightly underestimated across the CASTNet (-5%) and AQS (-12%) networks (Figures C-44 and C-45). SO4 is more significantly underestimated across all networks (-22% to -53%, as shown in Figure C-6a). Since wet deposition SO4 is also underestimated, it is unclear why all sulfur species are underestimated.

The nitrate species are also all underestimated with the Total NO3 bias (-56%) being between the HNO3 bias (-35%) and NO3 bias (-115%). The modeled NO3 values are all near zero with little correlation with the observations, whereas the observed HNO3 and Total NO3 is tracked well with correlation coefficients of 0.74 and 0.76. These results suggest that the July NO3 model performance problem is partly due to insufficient formation of Total NO3, but mainly due to incorrect partitioning of the Total NO3.

Again, there is abundant scatter in the AQS NO2 scatter plot for July (Figure C-45) resulting in a low bias (0%) but high error (65%). Ozone performance also exhibits a low bias (-15%) and error (20%), but the model is incapable of simulating ozone above 100 ppb. Although CO performance in July is better than the previous months, it still has a large underestimation bias of 82%.

3.6.4 Diagnostic Model Performance In October

SO2 is overstated in October across the CASTNet (+28%) and AQS (+33%) sites (Figures C-46 and C-47). Although SO4 is understated across the CASTNet sites (-24%), the bias across the IMPROVE (-6%) and STN (0%) sites are near zero (Figure C-7a).

Performance for HNO3 is fairly good with a low bias (+12%) and error (30%). But NO3 is overstated (+34%) leading to an overstatement of Total NO3 (+37%). The overstatement of NO3 leads to an overstatement of NH4 as well (Figure C-46)

As seen in the other months, NO2 exhibits a lot of scatter resulting in a low correlation (0.22) and high error (61%) but low bias (12%). The model tends to underpredict the high and overpredict the low O3 observations resulting in a -29% bias and low correlation coefficient. CO is also underpredicted (-76%) for the reasons discussed previously.

3.7 Performance at CENRAP Class I Areas for the Worst and Best 20 Percent Days

In this section, and in section C.5 of Appendix C, we present the results of the model performance evaluation at each of the CENRAP Class I areas for the worst and best 20 percent days. Performance on these days is critical since they are the days used in the 2018 visibility projections discussed in Chapter 4. For each Class I area we compared the predicted and observed extinction of the worst and best 20 percent days below. In Appendix C the PM species-specific extinction is also compared for the worst 20 percent days.

3.7.1 Caney Creek (CACR) Arkansas

The ability of the CMAQ model to estimate visibility extinction at the CACR Class I area on the 2002 worst and best 20 percent days is provide in Figures 3-9 and C-48. On most of the worst 20 percent days at CACR total extinction is dominated by SO4 extinction with some extinction due to OMC. On four of the worst 20 percent days extinction is dominated by NO3. The average extinction across the worst 20 percent days is underestimated by -33% (Figure 3-9), which is primarily due to a -51% underestimation of SO4 extinction combined with a 6% overestimation of NO3 extinction (Figure C-48). Performance for OMC extinction at CACR on the worst 20 percent days is pretty good with a -20% bias and 36% error. EC extinction is systematically underestimated. Soil extinction has low bias (-19%) buts lots of scatter and high error (74%), while CM extinction is greatly underestimated (bias of -153%).

On the best 20 percent days at CACR the observed extinction ranges from 20 to 40 Mm^{-1}. Whereas, the modeled extinction has a much larger range from 15 to 120 Mm^{-1}. Much of the modeled overestimation of total extinction on the best 20% days (+44% bias) is due to NO3 overestimation (+94% bias).

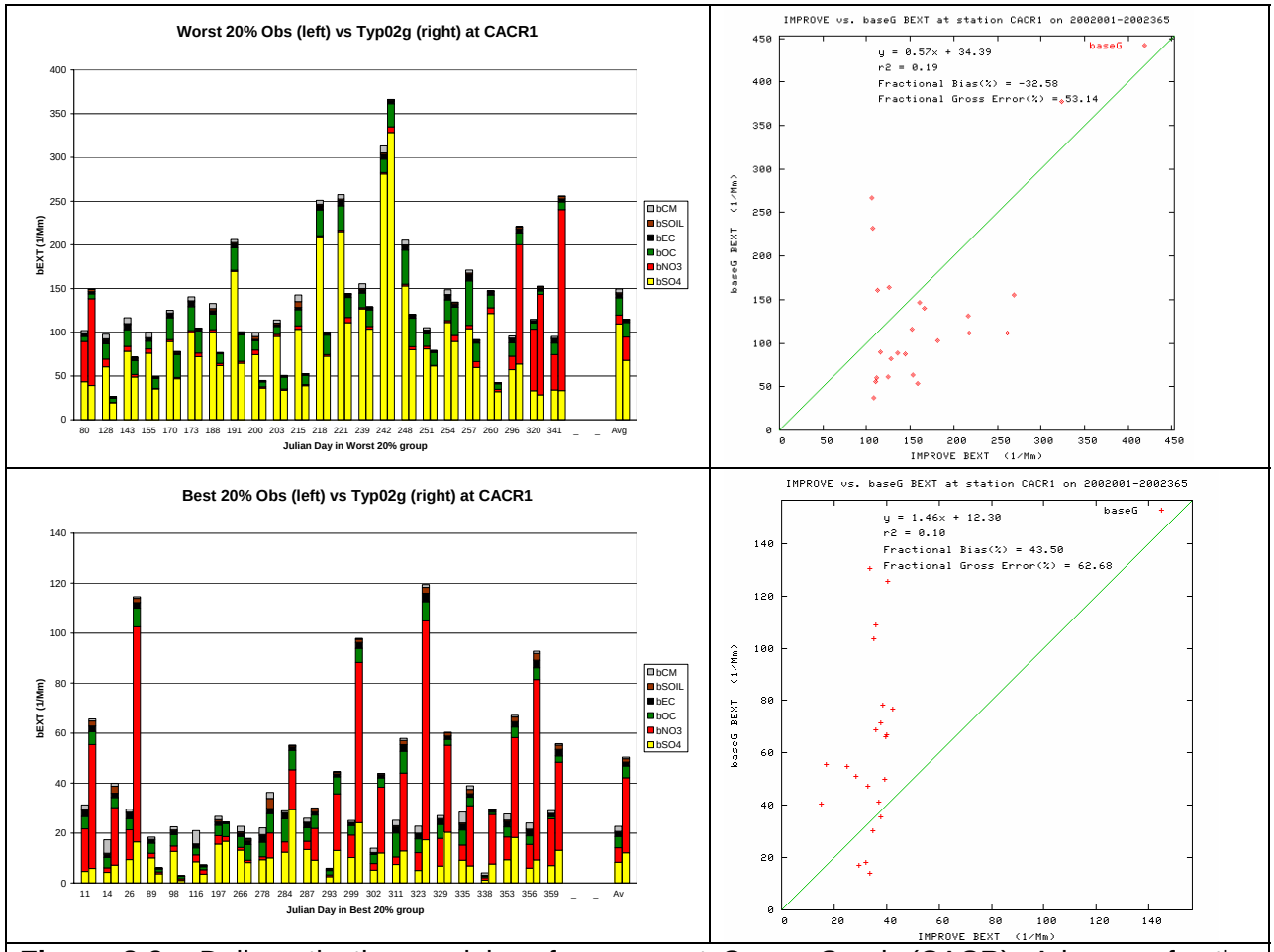


Figure 3-9. Daily extinction model performance at Caney Creek (CACR), Arkansas for the worst (top) and best (bottom) 20 percent days during 2002.

3.7.2 Upper Buffalo (UPBU) Arkansas

Model performance at the UPBU Class I area for the worst and best 20 percent days is shown in Figures 3-10 and C-49. On most of the worst 20 percent days at UPBU, visibility impairment is dominated by SO4, although there are also two high NO3 days. The model underestimates the average of the total extinction on the worst 20 percent days at UPBU by -40% (Figure 3-10), which is due to an underestimation of extinction due to SO4, OMC and CM by -46%, -33% and -179%, respectively.

On the best 20 percent days at UPBU, the model performs reasonably well with a low bias (2%) and error (42%). But again, the model has a much wider range in extinction values across the best 20 percent days (15 to 120 Mm^{-1}) than observed (20 to 45 Mm^{-1}). There are five days in which the modeled NO3 overprediction is quite severe and when those days are removed the range in the modeled and observed extinction on the best 20 percent days is quite similar to the observed, although the model gets much cleaner on the very cleanest modeled days.

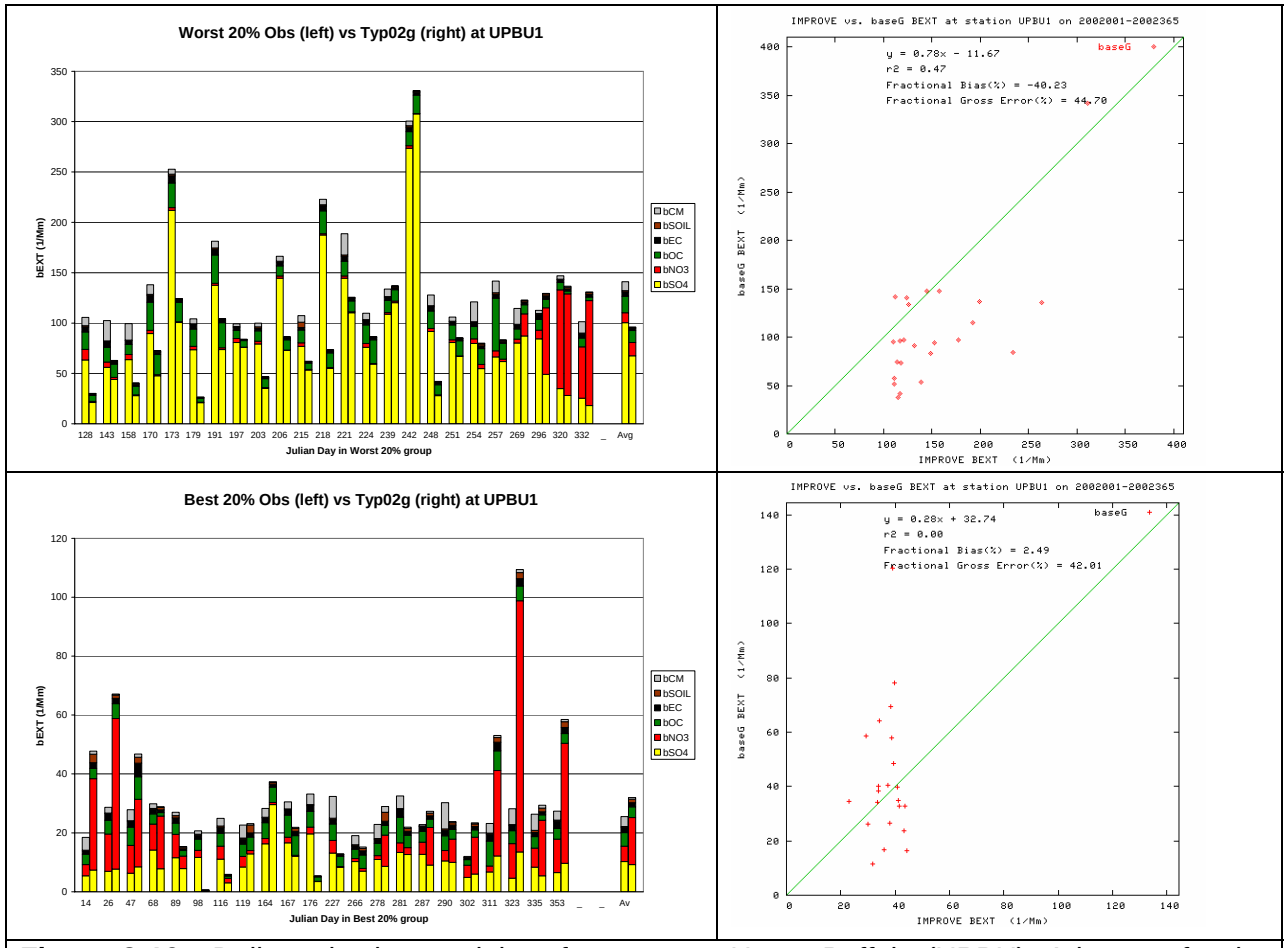


Figure 3-10. Daily extinction model performance at Upper Buffalo (UPBU), Arkansas for the worst (top) and best (bottom) 20 percent days during 2002.

3.7.3 Breton Island (BRET), Louisiana

The observed total extinction on the worst 20 percent days at Breton Island is underestimated by -71% (Figure 3-11), which is due to an underestimation of each component of extinction (Figure C-50) by from -50% to -70% (SO4, OMC and Soil) to over -100% (EC and CM). The observed extinction on the worst 20 percent days ranges from 90 to 170 Mm^{-1}, whereas the modeled values drop down to as low as approximately 15 Mm^{-1}. On the best 20 percent days the range of the observed and modeled extinction is similar (roughly 10 to 50 Mm^{-1}) that results in a reasonably low bias (-22%), but there is little agreement on which days are higher or lower resulting in a lot of scatter and high error (54%).

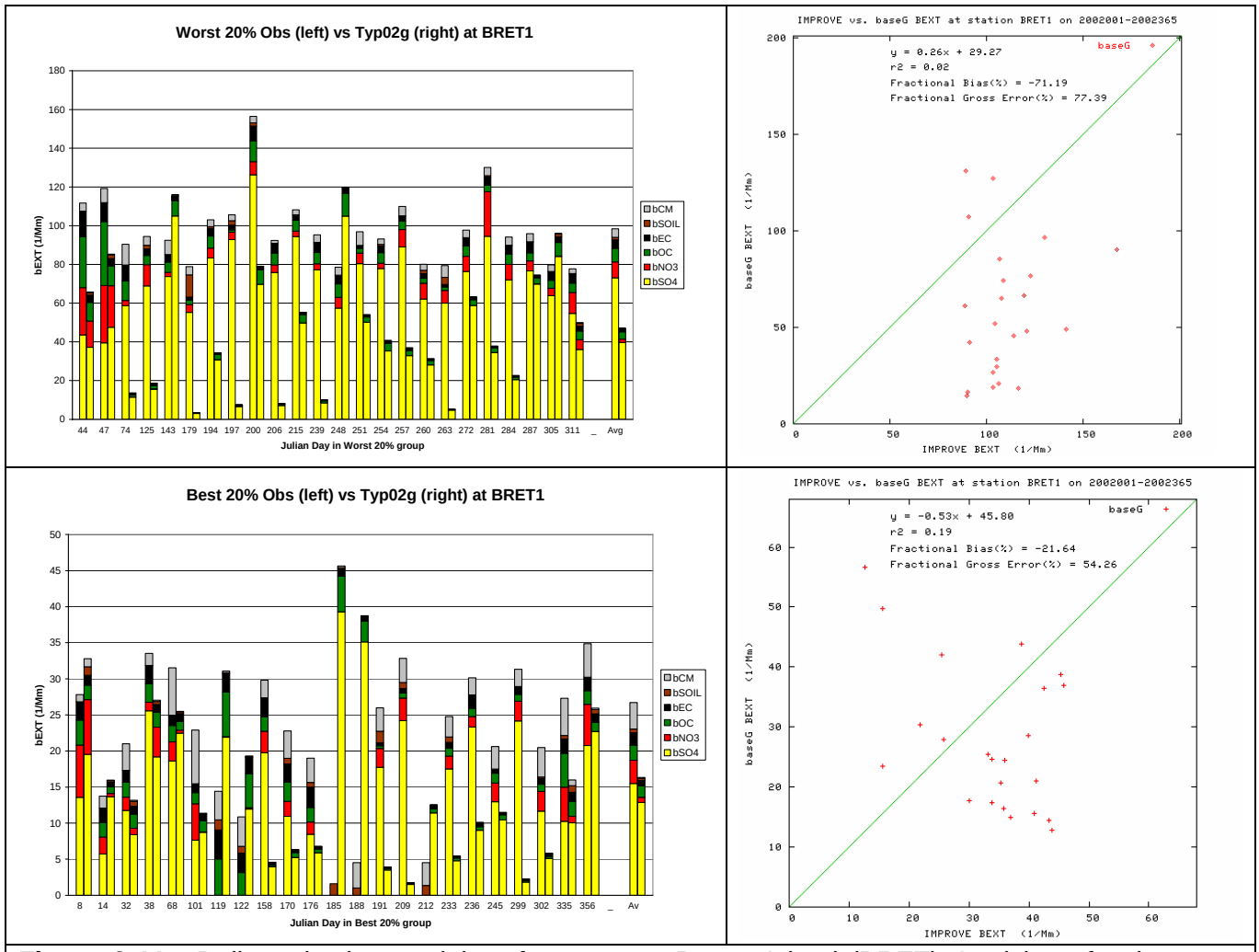


Figure 3-11. Daily extinction model performance at Breton Island (BRET), Louisiana for the worst (top) and best (bottom) 20 percent days during 2002.

3.7.4 Boundary Waters (BOWA), Minnesota

There are three types of days during the worst 20 percent days at BOWA: SO4 days, OMC days and NO3 days (Figure 3-12). The two high OMC days are likely fire impact events that the model captures to some extent on one day and not on the other. On the five high (> 20 Mm^{-1}) NO3 extinction days the model predicts the observed extinction well on three days and overestimates by a factor of 3-4 on the other two high NO3 days. SO4 is underestimated by -43% on average across the worst 20 percent days at BOWA.

With the exception of two days, the model reproduces the total extinction for the best 20 percent days at BOWA quite well with a bias and error value of +14% and 22% (Figure 3-12). Without these two days, the modeled and observed extinction both range between 15 and 25 Mm^{-1}.

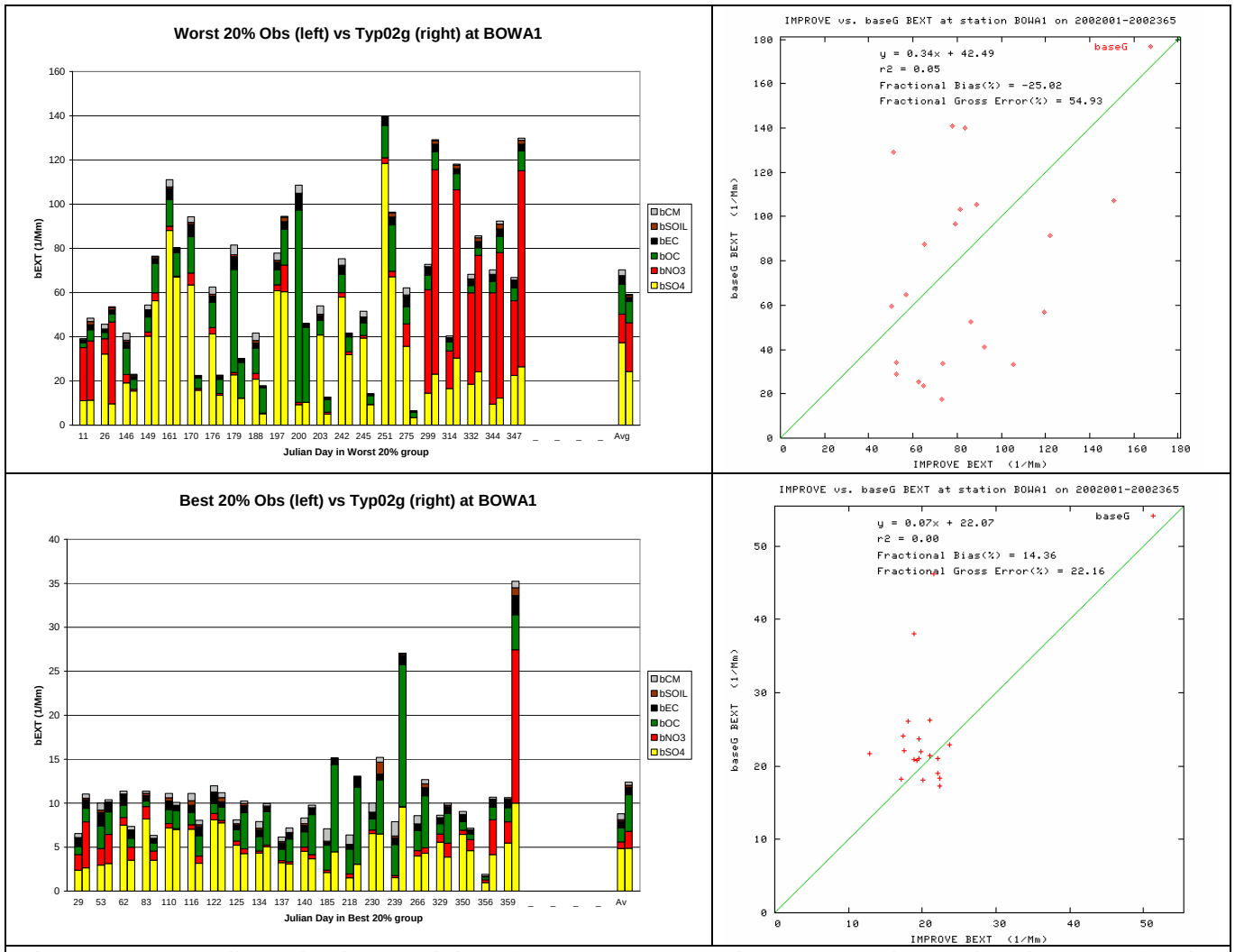


Figure 3-12. Daily extinction model performance at Boundary Waters (BOWA), Minnesota for the worst (top) and best (bottom) 20 percent days during 2002.

3.7.5 Voyageurs (VOYA) Minnesota

VOYA is also characterized by SO4, NO3 and OMC days (Figure 3-13). Julian Days 179 and 200 are high OMC days that were also high OMC days at BOWA again indicating impacts from fires in the area that is not fully captured by the model. SO4 and NO3 performance is fairly good and, without the fire days, OMC performance looks good as well (Figure C-52). On the best 20 percent days there is one day the modeled extinction is much higher than observed and a few others that are somewhat higher, but for most of the best 20 percent days the modeled extinction is comparable to the observed values.

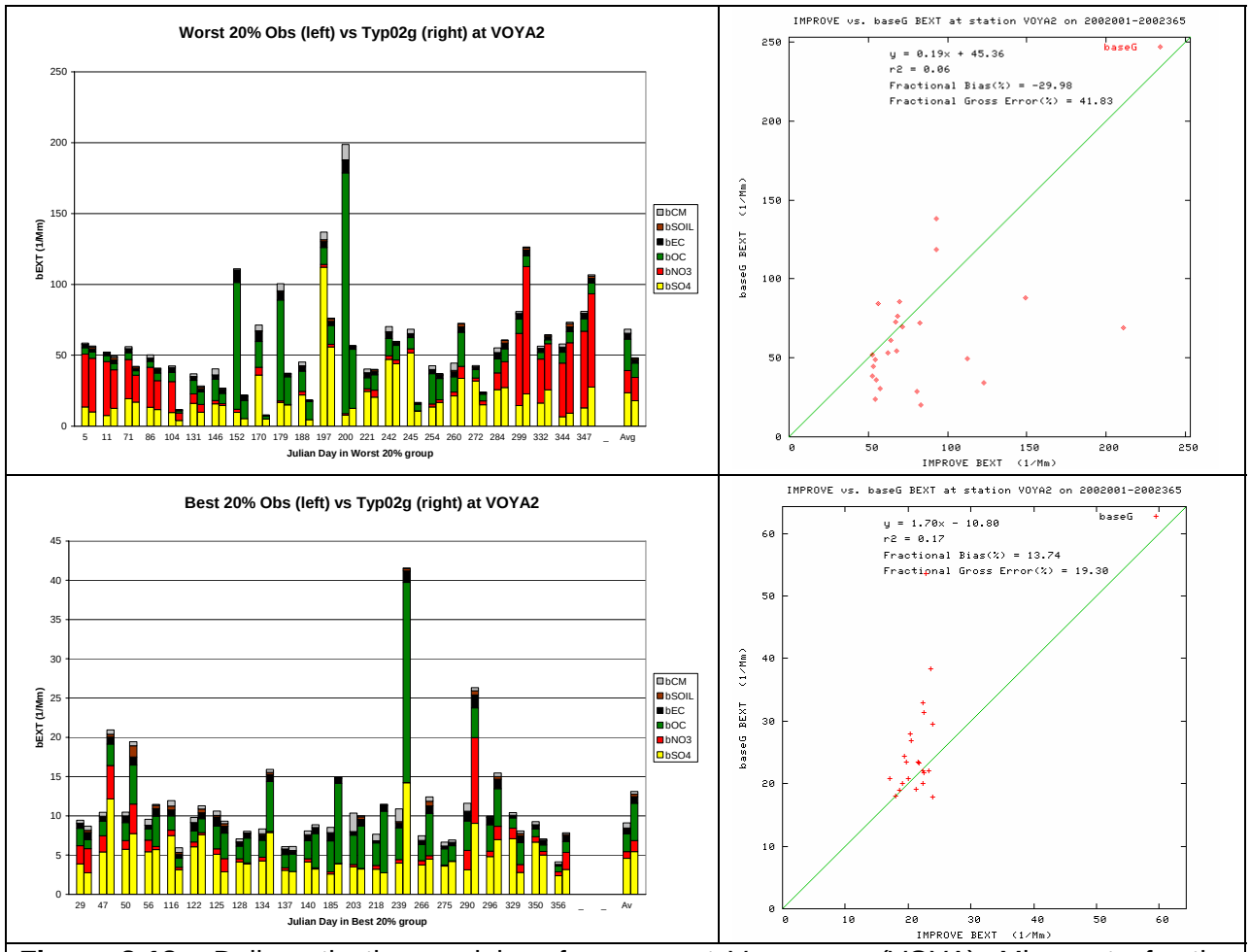


Figure 3-13. Daily extinction model performance at Voyageurs (VOYA), Minnesota for the worst (top) and best (bottom) 20 percent days during 2002.

3.7.6 Hercules Glade (HEGL) Missouri

On most of the worst 20 percent days at HEGL the observed extinction ranges from 120 to 220 Mm^{-1} whereas model extinction ranges from 50 to 170 Mm^{-1} (Figure 3-14). However, there is one extreme day with extinction approaching 400 Mm^{-1} that the model does a very good job in replicating. Over all the days there is a modest underestimation bias in SO4 (-39%) and OMC (-39%) extinction, larger underestimation bias in EC (-62%) and CM (-118%) extinction and overestimation bias in Soil (+30%) extinction (Figure C-53).

On the best 20 percent days there is one day where the model overstates the observed extinction by approximately a factor of four and a handful of other days that the model overstates the extinction by a factor of 2 or so, but most of the days both the model and observed extinction sites are around 40 Mm^{-1} ±10 Mm^{-1}. On the best 20 percent days, when the observed extinction is overstated, it is due to overstatement of the NO3.

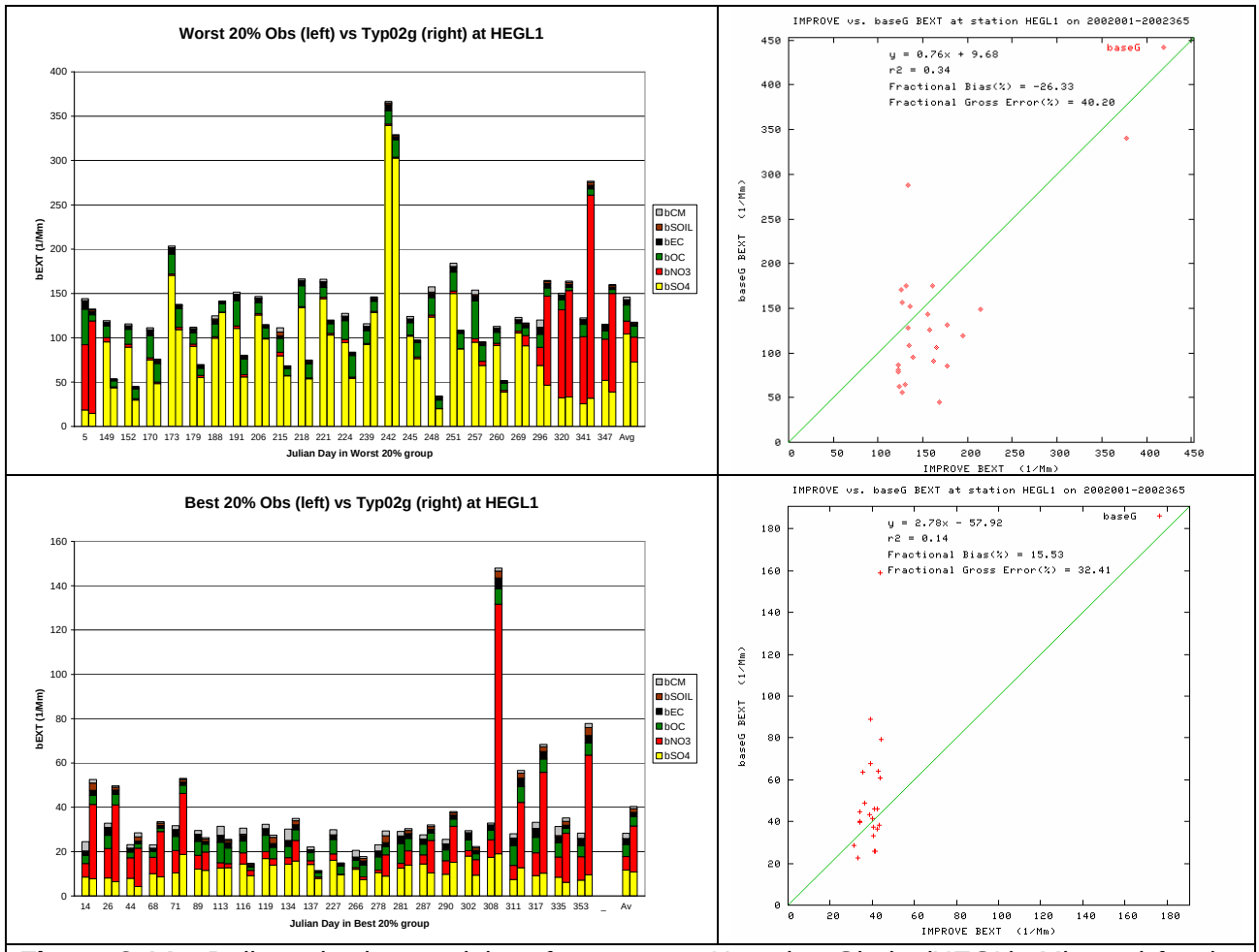


Figure 3-14. Daily extinction model performance at Hercules Glade (HEGL), Missouri for the worst (top) and best (bottom) 20 percent days during 2002.

3.7.7 Mingo (MING) Missouri

The worst 20 percent days at MING are mainly high SO4 days with a few high NO3 days that the model reproduces reasonably well resulting in low bias (+10%) and error (38%) for total extinction (Figure 3-15). The PM species specific performance is fairly good with low bias for SO4 (+4%), good agreement with NO3 on high NO3 days except for one day, low OMC (+23%) and EC (+3%) bias and larger bias in EC (+37%) and CM (-105%) extinction (Figure C-54).

For the best 20 percent days, there is one day the model is way too high due to overstated NO3 extinction and a few other days the model overstates the observed extinction that is usually due to overpredicted NO3, but on most of the best 20 percent days the modeled extinction is comparable to the observed values. This results in low bias (+12%) and error (36%) for total extinction at MING for the best 20 percent days.

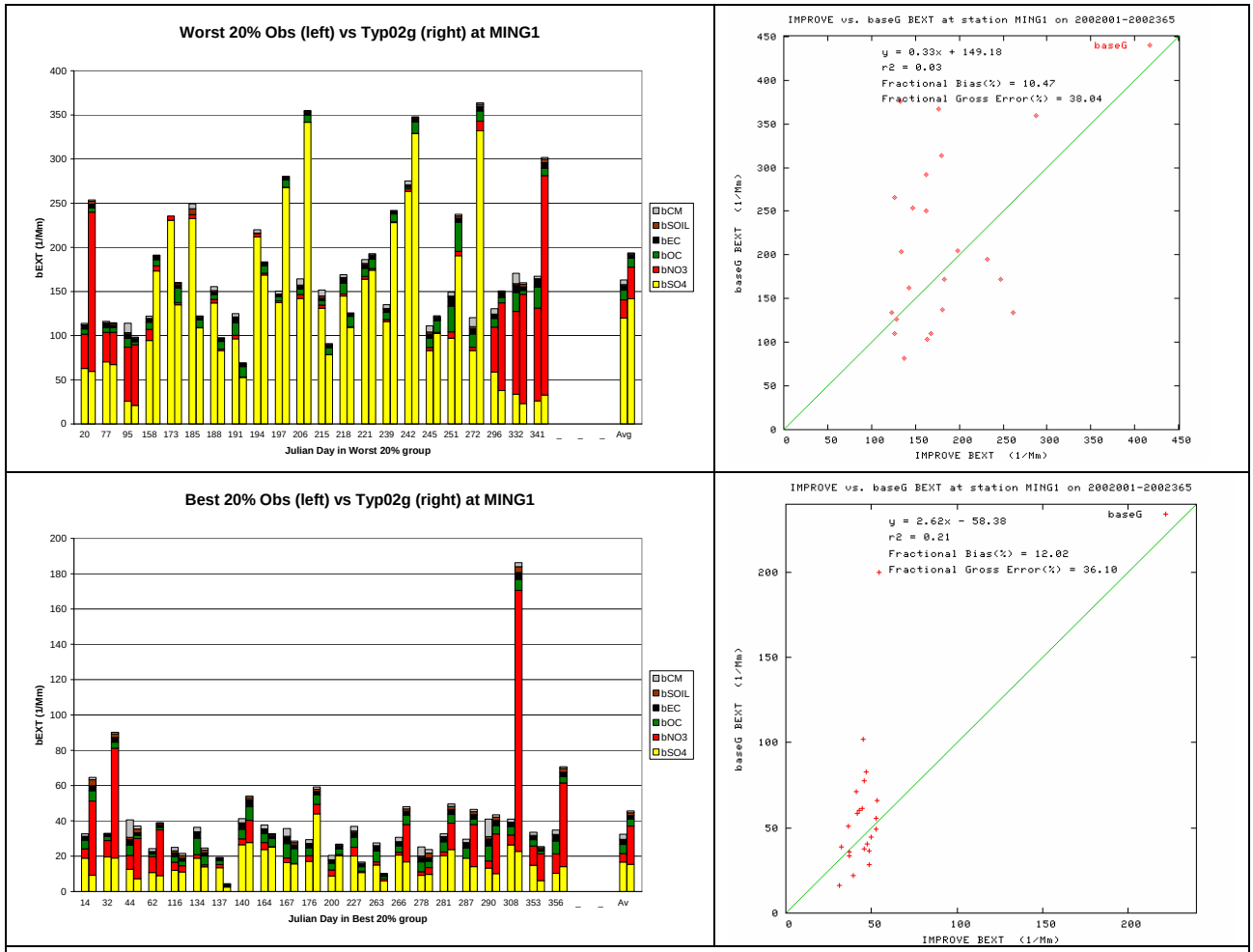


Figure 3-15. Daily extinction model performance at Mingo (MING), Missouri for the worst (top) and best (bottom) 20 percent days during 2002.

3.7.8 Wichita Mountains (WIMO), Oklahoma

With the exception of an overprediction on day 344 due to NO3, observed total extinction on the worst 20 percent days at WIMO is understated with a bias of -42% (Figure 3-16) that is primarily due to an underestimation of extinction due to SO4 (-48%) and OMC (-69%) (Figure C-55).

CMAQ total extinction performance for the average of the best 20 percent days at WIMO is characterized by an overestimation bias (+21%) on most days that is primarily due to NO3 overprediction on several days. Again the modeled range of extinction on the best 20 percent days (12-60 Mm^{-1}) is much greater than observed (20-35 Mm^{-1}).

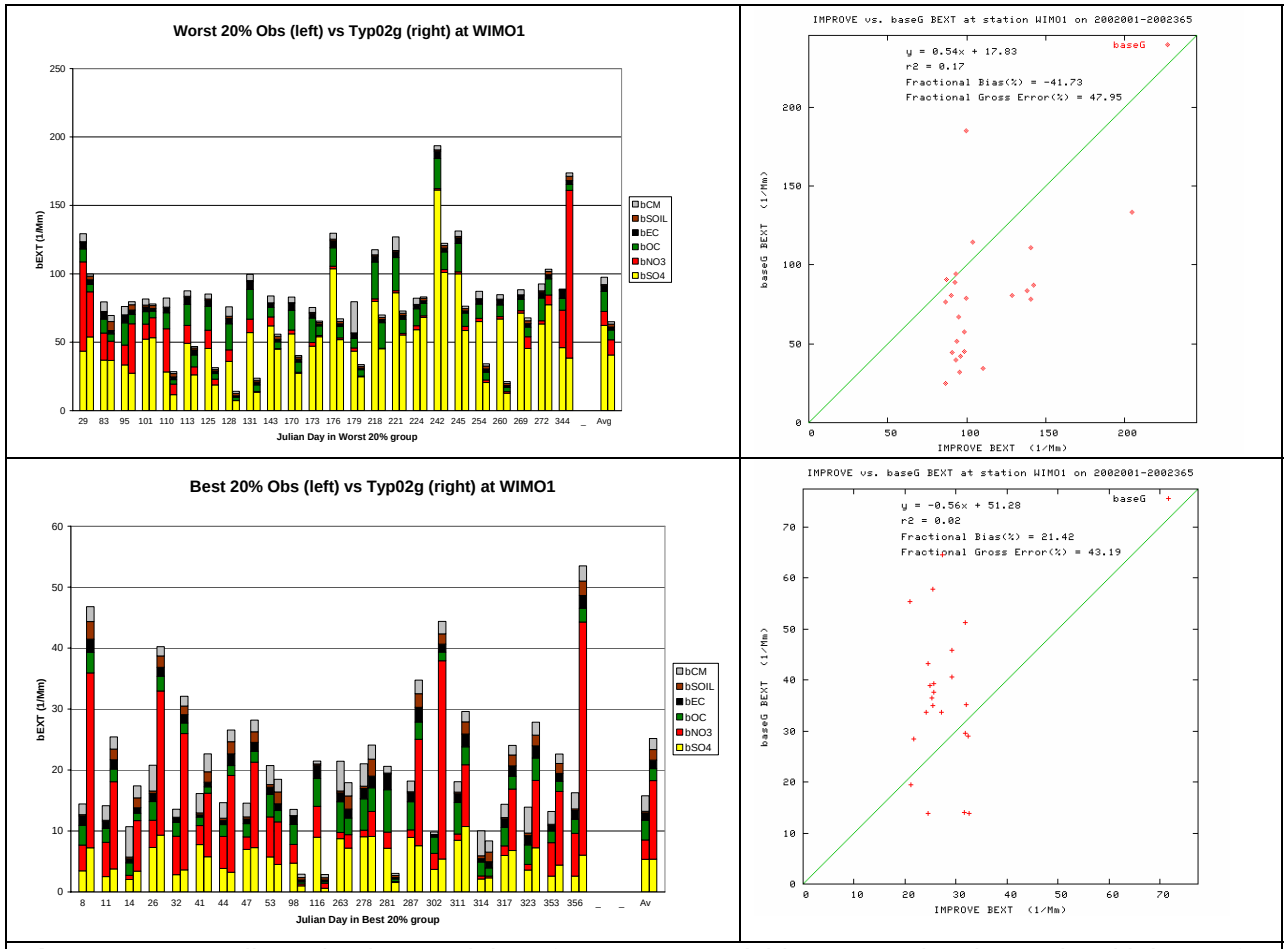


Figure 3-16. Daily extinction model performance at Wichita Mountains (WIMO), Oklahoma for the worst (top) and best (bottom) 20 percent days during 2002.

3.7.9 Big Bend (BIBE) Texas

The observed extinction on the worst 20 percent days at BIBE is underpredicted on almost every day resulting in a fractional bias value of -72% (Figure 3-17). Every component of extinction is underestimated on average for the worst 20 percent days (Figure C-56) with the underestimation bias ranging from -24% (OMC) to -162% (CM). SO4 extinction, that typically represents the largest component of the total extinction is understated by -94%.

The model does a better job in predicting the total extinction at BIBE for the best 20 percent days with average fractional bias and error values of +13% and 19% (Figure 3-17). With the exception of one day that the observed extinction is overestimated by approximately a factor of 2, the modeled and observed extinction on the best 20 percent days at BIBE are both within 12 to 25 Mm^{-1}. However, there are some mismatches with the components of extinction with the model estimating much lower contributions due to Soil and CM.

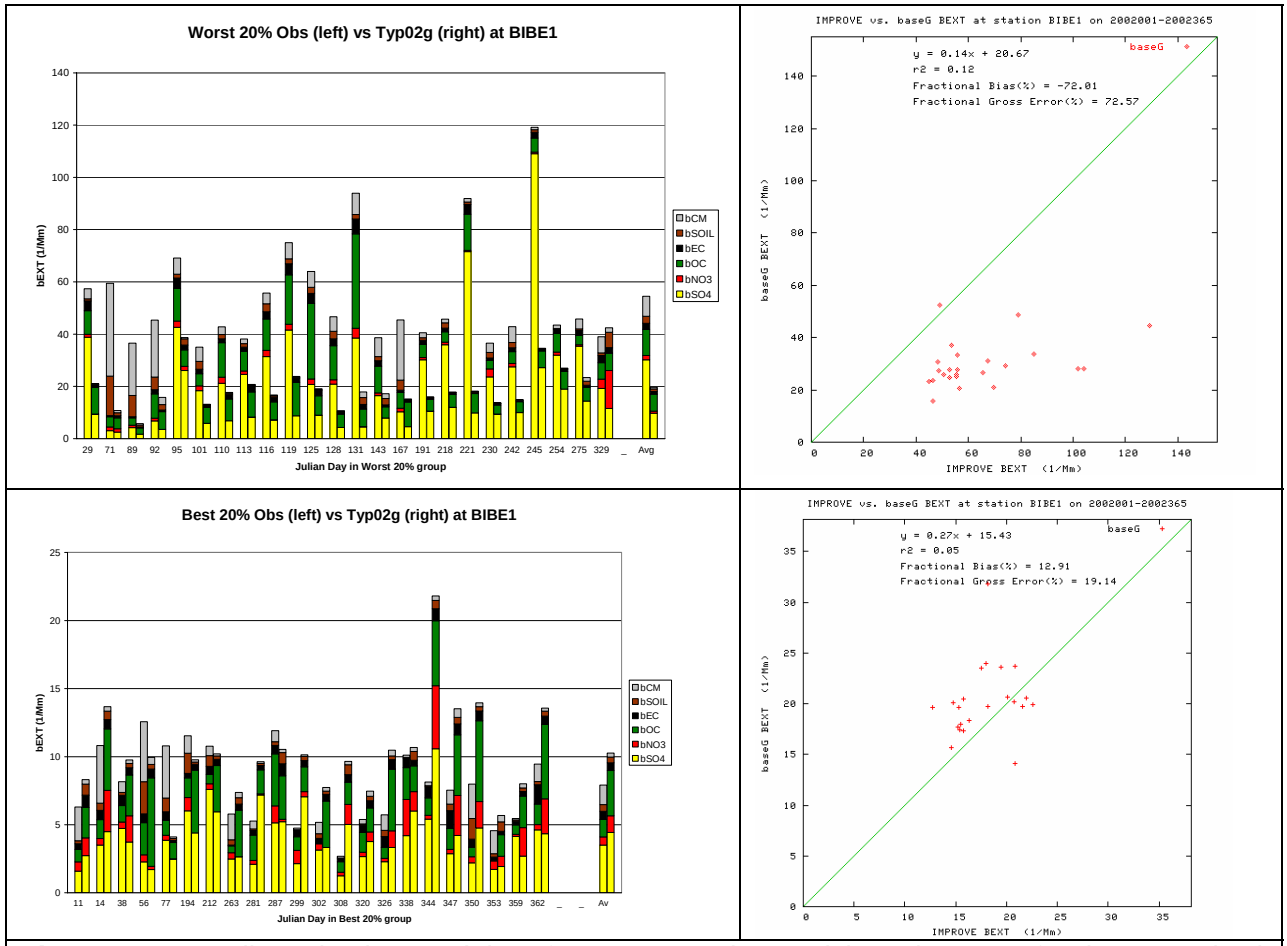


Figure 3-17. Daily extinction model performance at Big Bend (BIBE), Texas for the worst (top) and best (bottom) 20 percent days during 2002.

3.7.10 Guadalupe Mountains (GUMO) Texas

Most of the worst 20 percent days at GUMO are high dust days with high Soil and CM that is not captured by the model (Figure 3-18). Extinction due to Soil and CM on the worst 20 percent days is underestimated by -105% and -191%, respectively (Figure C-57). Better performance is seen on the best 20 percent days with bias and error for total extinction of 8% and 21%, but the model still understates Soil and CM.

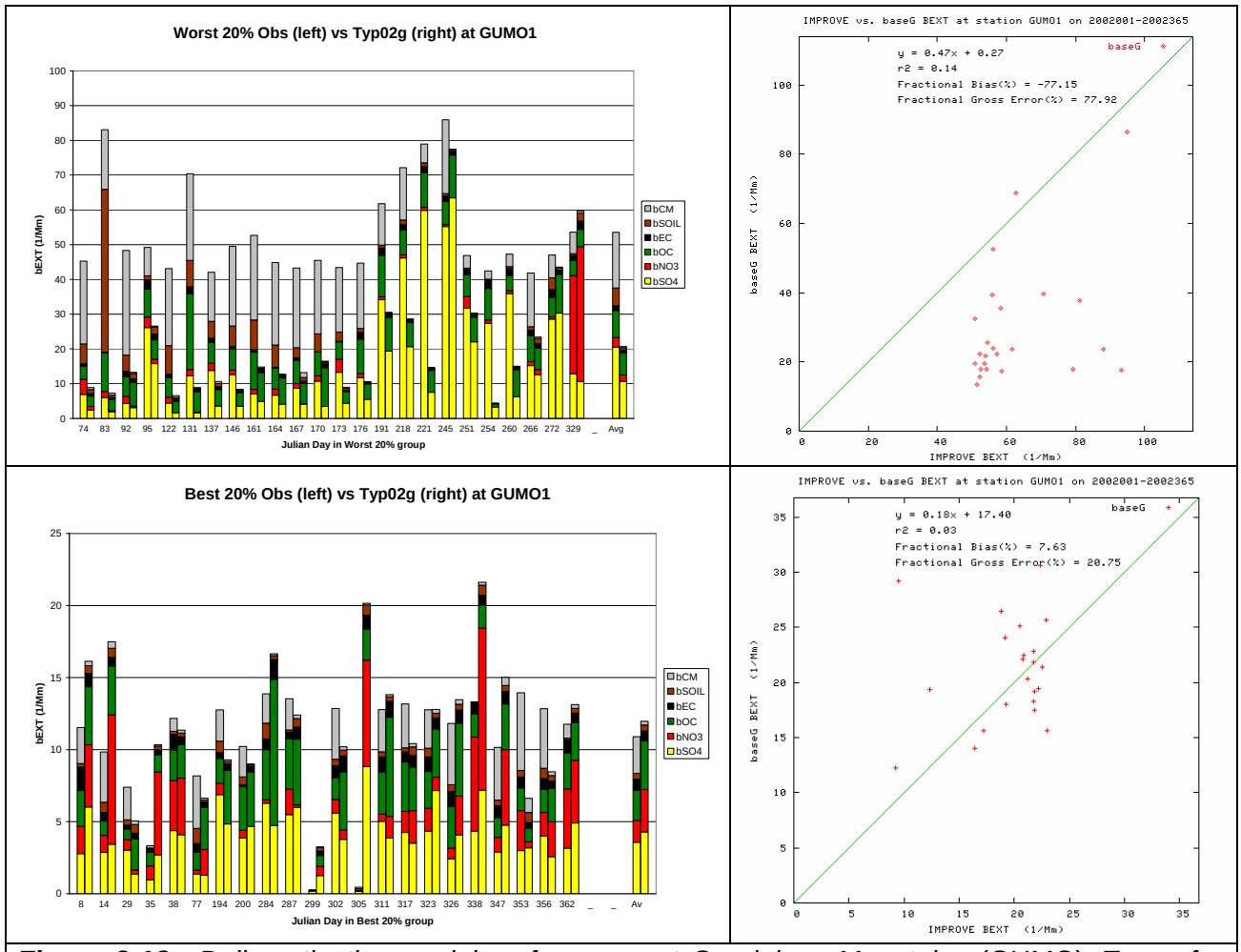


Figure 3-18. Daily extinction model performance at Guadalupe Mountains (GUMO), Texas for the worst (top) and best (bottom) 20 percent days during 2002.

3.8 Model Performance Evaluation Conclusions

The model performance evaluation reveals that the model is performing best for SO4, OMC and EC. Soil performance is mixed with a winter overestimation bias with lower bias and higher error in the summer. CM performance is poor year round. The operational evaluation reveals that SO4 performance usually achieves the PM model performance goal and always achieves the model performance criteria, although it does have an underestimation bias that is greatest in the summer. NO3 performance is characterized by a winter overestimation bias with an even greater summer underestimation bias. However, the summer underestimation bias occurs when NO3 is very low and when it is not an important component of the observed or predicted PM mass concentrations or component of visibility impairment. Performance for OMC meets the model performance goal year round at the IMPROVE sites, but is characterized by an underestimation bias at the more urban STN sites. EC exhibits very low bias at the STN sites and a summer underestimation bias at the IMPROVE sites, but meets the model performance goal throughout the year. Soil has a winter overestimation bias that is outside of the model performance goal and criteria raising questions whether the model should be used for this species. Finally, CM performance is extremely poor with an underprediction bias that is outside of the performance goal and criteria. We suspect that much of the CM concentrations measured at the IMPROVE sites is due to highly localized emissions from fugitive dust sources that are not included in the emissions inventory and would be difficult to simulate using 36 km regional modeling.

Performance for the worst 20 percent days at the CENRAP Class I areas is generally characterized by an underestimation bias. Performance at the BRET, BIBE and GUMO Class I areas for the worst 20 percent days is particularly suspect and care should be taken in the interpretation of the visibility projections at these three Class I areas.

The CMAQ 2002 36 km model appears to be working well enough to reliably make future-year projections for changes in SO4, NO3, EC and OMC at the rural Class I areas. Performance for Soil and especially CM is suspect enough that care should be taken in interpreting these modeling results. The model evaluation focused on the model's ability to predict the components of light extinction mainly at the Class I areas. Additional analysis would have to be undertaken to examine the model's ability to simulate ozone and fine particulate to address 8-hour ozone and $PM_{2.5}$ attainment issues.

4.0 VISIBILITY PROJECTIONS

This section presents the future-year visibility projections for Class I areas within and near the CENRAP states and their comparison with the 2018 Uniform Rate of Progress (URP) point. As noted in Chapter 1, the Regional Haze Rule (RHR) requires states with Class I areas to develop State Implementation Plans (SIPs) that include reasonable progress goals (RPGs) for improving visibility in each Class I area and emission reduction measures to meet those goals. For the initial SIPs due in December 2007, states are required to adopt RPGs for improving visibility from Baseline Conditions. The 2000-2004 five-year period is used to define Baseline Conditions and the first future progress period is 2018. A state is required to set RPGs for each Class I area in the state for two visibility metrics:

- Provide for an improvement in visibility for the most impaired visibility days (i.e., the worst 20 percent days); and

- Ensure no degradation in visibility for the least impaired visibility days (i.e., the best 20 percent days).

The goal of the RPGs is to provide for a rate of improvement sufficient to be on a course to attain "Natural Conditions" by 2064. States are to define controls to meet RPGs every 10 years, starting in 2018, which defines progress periods ending in 2018, 2028, 2038, 2048, 2058 and finally 2064. States will determine whether they are meeting their goals by comparing visibility conditions from one five-year period to another (e.g., 2000-2004 to 2013-2017). As stated in 40 CFR 51.308 (d) (1), baseline visibility conditions, reasonable progress goals, and changes in visibility must be expressed in terms of deciview (dv) units. The haze index (HI) metric of visibility impairment, in deciviews, is derived from light extinction (b_{ext}) as follows:

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

Where light extinction (b_{ext}) is expressed in terms of inverse megameters ($Mm^{-1} = 10^{-6}\ m^{-1}$). Light extinction ($b_{ext}$) is calculated using the observed fine particulate concentrations from the IMPROVE monitors using either the original or the new IMPROVE aerosol extinction equation. Both equations are discussed below.

4.1 Guidance for Visibility Projections

EPA has published several guidance documents that relate to how modeling results should be used to project future-year visibility and how states should define RPGs:

"Guidance on the Use of Models and Other Analyses for Demonstrating Attainment of Air Quality Goals for Ozone, $PM_{2.5}$ and Regional Haze" (EPA, 2007a).

"Guidance for Tracking Progress Under the Regional Haze Rule" (EPA, 2003a).

"Guidance for Estimating Natural Visibility Conditions Under the Regional Haze Rule" (EPA, 2003b).

"Guidance for Setting Reasonable Progress Goals Under the Regional Haze Program" (EPA, 2007b).

The first EPA modeling guidance document listed above (EPA, 2007) discusses the use of modeling results to project future-year visibility. The second EPA guidance document (EPA, 2003a) focuses on monitored visibility, how to define the visibility Baseline Conditions and how to track visibility goals. The third EPA guidance document discusses procedures for defining Natural Conditions for a Class I area. Natural Conditions are the visibility goal for 2064. Although states may propose alternative approaches for defining Natural Conditions, in this section we use the default Natural Conditions at Class I areas (EPA, 2003b; Pitchford, 2006). The final EPA guidance document discusses how states should define their RPGs and their relationship to the 2018 URP point.

The EPA documents discussed above are followed for the visibility projections presented in this section with one notable exception. Some of the EPA documents are based on the original IMPROVE equation (e.g., EPA, 2003a, b). The CENRAP visibility projections are based on the new IMPROVE equation, although projections based on the original IMPROVE equation are also presented as an alternative approach in Chapter 5. EPA guidance allows for using either the original or the new IMPROVE equation (EPA, 2007a; Timin, 2007). CENRAP, along with the other RPOs, have elected to use the new IMPROVE equation for their visibility projections.

4.2 Calculation of Visibility and 2018 URP Point from IMPROVE Measurements

EPA guidance recommends using the model in a relative sense to project future-year visibility conditions (EPA, 2007a). This projection is made using Relative Response Factors (RRFs) that are defined as the ratio of the future-year modeling results to the base-year modeling results. The RRFs are applied to the baseline visibility conditions to project future-year visibility. The major features of EPA's recommended visibility projection approach are as follows (EPA, 2003a,b; 2007a):

- Monitored data are used to define current visibility Baseline Conditions using IMPROVE monitoring data from the 2000-2004 five-year base period.

- Monitored concentrations of PM_{10} are divided into six major components, the first five of which are assumed to be $PM_{2.5}$ and the sixth is coarse mass (CM or $PM_{2.5-10}$).
  - SO4 (sulfate) that is assumed to be ammonium sulfate [$(NH_4)_2SO_4$];
  - NO3 (particulate nitrate) that is assumed to be ammonium nitrate [NH_4NO_3];
  - OC (organic carbon) that is assumed to be total organic mass carbon (OMC)
  - EC (elemental carbon);
  - IP (other fine inorganic particulate or Soil); and
  - CM (coarse mass).

- Models are used in a relative sense to develop RRFs between baseline and future predicted concentrations of each component.

- PM component-specific RRFs are multiplied by observed Baseline monitored values to estimate future-year PM component concentrations.

- Estimates of future-year component concentrations are consolidated to provide an estimate of future-year air quality and visibility using either the original or new IMPROVE equation.

- Future-year model projected visibility is compared with the 2018 point on the URP glidepath to assist in evaluating the visibility improvements.

- It is assumed 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].

In order to facilitate tracking visibility progress, three important visibility concepts are required for each Class I area:

Baseline Conditions: Baseline Conditions represent visibility for the 20 percent best (B20%) and 20 percent worst (W20%) visibility days for the initial five-year baseline period of the regional haze program. Baseline Conditions are calculated using IMPROVE monitor data collected during the 2000-2004 five-year period and are the starting point in 2004 for the URP glidepath and 2018 visibility projections.

Natural Conditions: Estimates of natural visibility conditions for the best 20 percent and worst 20 percent days at a Class I area (i.e., visibility conditions that would be experienced in the absence of human-caused impairment). EPA has defined a set of default Natural Conditions for the original IMPROVE equation (EPA, 2003b) that has been updated to the new IMPROVE equation by the Natural Haze Levels II Committee (Pitchford, 2006) that we have used in this Chapter.

2018 URP Point: The 2018 Uniform Rate of Progress (URP) point is defined by defining a linear glidepath in deciviews starting with the 2000-2004 Baseline Conditions in 2004 and ending at Natural Conditions in 2064. Where the linear glidepath passes through 2018 is the 2018 URP point in deciviews.

4.2.1 Calculation of Visibility from IMPROVE PM Measurements

Baseline Conditions for Class I areas are calculated using the procedures in EPA's guidance document (EPA, 2003a) and fine and coarse particulate matter concentrations measured at IMPROVE monitors (Malm et al, 2000; Debell et al., 2006). Currently, each Class I area in the CENRAP domain has an associated IMPROVE monitor. The IMPROVE monitors do not directly measure visibility, but instead measure speciated fine particulate ($PM_{2.5}$) and total $PM_{2.5}$ and PM_{10} mass concentrations from which visibility is obtained through the IMPROVE equation.

Visibility conditions are estimated starting with the IMPROVE 24-hour average mass measurements for six PM species:

- Sulfate [$(NH_4)_2SO_4$];
- Particulate Nitrate [$(NH_4NO_3$];
- Organic Matter Carbon or Organic Mass by Carbon [OMC];
- Elemental Carbon [EC] or Light Absorbing Carbon [LAC];
- Other fine particulate [Soil]; and
- Coarse Matter or Coarse Mass [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 of light extinction. For example, in the IMPROVE equation sulfate and particulate nitrate are assumed to be completely neutralized by ammonium. In addition, only the fine mode ($PM_{2.5}$) of PM is speciated by the IMPROVE monitor to obtain sulfate and nitrate measurements (that is, any coarse mode sulfate and nitrate in the real atmosphere may be present in the CM IMPROVE measurement). Concentrations for the above six components of light extinction in the IMPROVE equation are obtained from the IMPROVE measured species using the mappings shown in Table 4-1:

Table 4-1. Definition of IMPROVE PM Components from Measured IMPROVE Species.

IMPROVE Component	IMPROVE Measured Species
Sulfate	1.375 x (3 x S)
Nitrate	1.29 x NO_3^-
OMC	1.4*OC (original IMPROVE) and 1.8*OC (new IMPROVE)
LAC	EC
Soil	2.2*AL + 2.49*SI + 1.63*CA + 2.42*FE + 1.94*TI
CM	MT – MF

Where:

- S is elemental sulfur as determined from proton induced x-ray emissions (PIXE) analysis of the IMPROVE Module A[1]. To estimate the mass of the sulfate ion ($SO_4^=$), S is multiplied by 3 to account the presence of oxygen. If S is missing then the sulfate (SO_4) measured by ion chromatography analysis of the 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 the 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 Mass Carbon (OMC) using the original IMPROVE equation and multiplied by 1.8 for the new IMPROVE equation. This adjustment of the measured OC accounts for mass due to other elements in the OMC besides Carbon.
- Elemental Carbon (EC) is also referred to as Light Absorbing Carbon (LAC).

[1] The IMPROVE sampler consists of four independent modules (A, B, C and D). Each module incorporates a separate inlet, filter pack and pump assembly and are controlled by a common timing mechanism. Module A measures fine PM mass and elements. Module B measures sulfate and nitrate ions. Module C measures EC and OC. Module D measures PM_{10} mass. (see http://vista.cira.colostate.edu/improve/ for more details).

- 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. Since K and FE are products of the combustion of vegetation, they are both represented in the formula by 0.6 x Fe and K is not shown explicitly.
- MT and MF are total PM_{10} and $PM_{2.5}$ mass, respectively.

4.2.1.1 Original and New IMPROVE Equations

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}). Sulfate and nitrate are hygroscopic which means that they can absorb water from the atmosphere which changes their extinction efficiency. This is accounted for through relative humidity adjustment factors [f(RH)] that increase the particle's extinction efficiency with increasing RH to account for the particles taking on water Note that some OMC may also have hygroscopic properties, but the IMPROVE equations assume OMC is non-hygroscopic.

There are currently two IMPROVE equations that are used to convert the measured PM concentrations to light extinction, the original (or old) and the new IMPROVE equations.

4.2.1.1.1 Original IMPROVE Equation

The original IMPROVE equation that converts PM species concentrations to light extinction is given as follows:

$$b_{Sulfate} = 3 \times f(RH) \times [Sulfate]$$
$$b_{Nitrate} = 3 \times f(RH) \times [Nitrate]$$
$$b_{EC} = 10 \times [EC]$$
$$b_{OMC} = 4 \times [OMC]$$
$$b_{Soil} = 1 \times [Soil]$$
$$b_{CM} = 0.6 \times [CM]$$

Monthly average f(RH) factors are used as recommended in EPA's guidance (EPA, 2003a). These values are available in the final EPA guidance document (EPA, 2003a) and at: ftp://ftp.saic.com/raleigh/RegionalHaze_2002FRHcurve/fRH_analysis/.

The total light extinction (b_{ext}) is assumed to be the sum of the light extinction due to the six PM species listed above plus Rayleigh (blue sky) background (b_{Ray}) that is assumed to be 10 Mm^{-1}.

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

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

$$VR = 3912 / b_{ext},$$

for b_{ext} in Mm^{-1}.

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

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

4.2.1.1.2 New IMPROVE Equation

The new IMPROVE equation is nonlinear in SO4, NO3 and OMC concentrations accounting for the different light scattering efficiency characteristics as a function of concentrations for these three species. It is expressed as follows:

$$b_{Sulfate} = 2.2 \times f_S(RH) \times [\text{Small Sulfate}] + 4.8\ f_S(RH) \times [\text{Large Sulfate}]$$
$$b_{Nitrate} = 2.4 \times f_S(RH) \times [\text{Small Nitrate}] + 5.1\ f_S(RH) \times [\text{Large Nitrate}]$$
$$b_{EC} = 10 \times [\text{Elemental Carbon}]$$
$$b_{OMC} = 2.8 \times [\text{Small Organic Mass}] + 6.1 \times [\text{Large Organic Mass}]$$
$$b_{Soil} = 1 \times [\text{Fine Soil}]$$
$$b_{CM} = 0.6 \times [\text{Coarse Mass}]$$
$$b_{NaCl} = 1.7 \times f_{SS}(RH) \times [\text{Sea Salt}]$$
$$b_{NO2} = 0.33 \times [NO_2\ (\text{ppb})]$$

The total Sulfate, Nitrate and OMC are each split into two fractions, representing small and large size distributions of those components. As noted in Table 4-1, the OMC is 1.8 times the IMPROVE OC measurement in the new IMPROVE algorithm, compared to 1.4 times the IMPROVE OC measurement in the original IMPROVE equation. New terms have been added for Sea Salt (important for coastal areas and possibly other areas)and for light absorption by NO2 (only used where NO2 observations are available). As none of the CENRAP Class I area IMPROVE sites measure NO2 concentrations, then this component of the new IMPROVE equations was not used. Site-specific Rayleigh scattering for each IMPROVE monitoring site is used in the new IMPROVE equation, as compared to a constant 10 Mm^{-1} value assumed in the original IMPROVE equation.

The apportionment of the Small and Large components of Sulfate, Nitrate and Organic Mass is done as follows:

$$[\text{Large Sulfate}] = [\text{Total Sulfate}] / 20 \times [\text{Total Sulfate}], \text{ for } [\text{Total Sulfate}] < 20\ \mu g/m^3$$

$$[\text{Large Sulfate }] = [\text{Total Sulfate}], \text{ for } [\text{Total Sulfate}] \geq 20\ \mu g/m^3$$

$$[\text{Small Sulfate}] = [\text{Total Sulfate}] - [\text{Large Sulfate}]$$

The same equations are used to apportion Total Nitrate and Total OMC among their Large and Small components.

The total extinction (b_{ext}) in the new IMPROVE equations is the sum of all the extinction components associated with each PM species. The new IMPROVE equation adds Sea Salt and

NO_2 as noted above. In addition, site-specific Rayleigh background is used with the new IMPROVE equation:

$$b_{ext} = b_{Ray} + b_{Sulfate} + b_{Nitrate} + b_{EC} + b_{OMC} + b_{Soil} + b_{CM} + b_{NaCl} + b_{NO2}$$

The Haze Index (HI) and Visual Range (VR) are calculated from the total extinction from the new IMPROVE equation using the same formulas as given above for the original IMPROVE equation.

4.2.1.1.3 Justification for Using the New IMPROVE Equation

The new IMPROVE equation was developed using the latest scientific information on PM species extinction properties combined with fitting reconstructed light extinction based on IMPROVE measured PM and NO2 concentrations with actual co-located measured light extinction (e.g., nephelometer measurements). Figure 4-1 displays example comparisons of 24-hour light extinction using the original and new IMPROVE equations compared against 24-hour nephelometer measurements of light extinction at the Great Smoky Mountains Class I area IMPROVE monitor. The original IMPROVE equation has a bias toward understating light extinction at the high end and overstating it at the low end, whereas the new IMPROVE equation does a better job in estimating light extinction from measured PM at all extinction levels. Because the new IMPROVE equation is based on more recent science and fits the observed light extinction values better, the CENRAP states have elected to perform their primary visibility projections using the new IMPROVE equation. Results using the original IMPROVE equation are presented in Section 5 as an alternative approach.

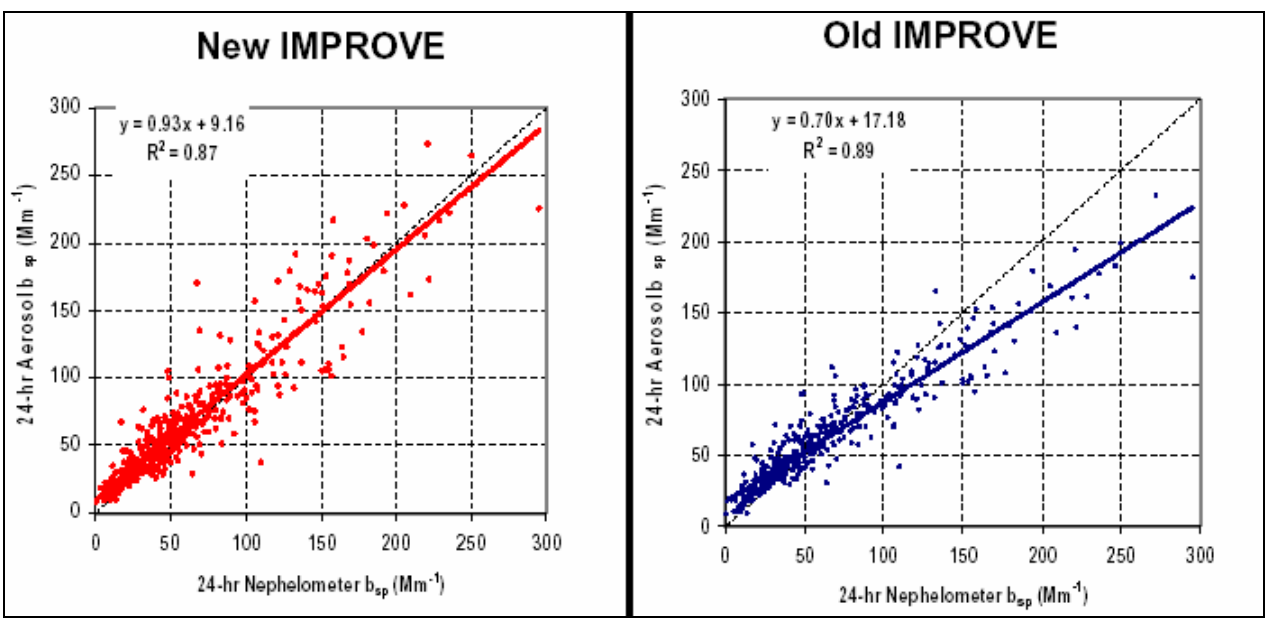


Figure 4-1. Comparisons of observed light extinction with reconstructed light extinction using the new (left) and original (right) IMPROVE equations at the Great Smoky Mountains National Park.

4.2.2 Calculation of the Baseline Conditions

The visibility Baseline Conditions for the worst 20 percent and best 20 percent days is calculated from the IMPROVE observations from the 2000-2004 period for each Class I area following EPA's guidance (EPA, 2003a). The basic procedures for calculating the Baseline Conditions are as follows:

1. Determine whether the observed IMPROVE data for each site and year satisfies EPA's minimal data capture criteria (EPA, 2003a). If there are less than three years with valid data capture for the 2000-2004 Baseline then the Baseline Conditions can not be calculated and data filling is needed.
2. For each year in the 2000-2004 period with sufficient valid data, rank the visibility in terms of extinction or deciview using either the original or new IMPROVE equation and monthly average f(RH) factors (EPA, 2003a).
3. For the worst 20 percent days, extract the 20% most impaired visibility days for each year (similarly for best 20 percent days extract 20% cleanest days). With a complete yearly data capture of IMPROVE 1:3 day sampling frequency this would result in 24 worst 20 percent and 24 best 20 percent days in a year.
4. For each worst 20 percent (or best 20 percent) day in each year, calculate 24-hour average visibility extinction using the IMPROVE measurements and either the original and new IMPROVE equation, convert the daily extinction to daily deciview and then average across each year to get yearly average deciview extinction for the worst 20 percent (or best 20 percent) days for each valid year from the 2000-2004 period.
5. Average the annual average deciview worst 20 percent (or best 20 percent) days deciview across each valid year in the 2000-2004 period (minimum of 3 valid years required) to get the worst 20 percent (or best 20 percent) Baseline Conditions.

4.2.3 Data Filling for Sites with Insufficient Valid Data to Calculate Baseline Conditions

Three CENRAP Class I areas did not contain sufficient IMPROVE observations during the five-year 2000-2004 Baseline to have three valid years of data from which Baseline Conditions could be constructed: Breton Island (BRET), Louisiana; Boundary Waters (BOWA), Minnesota and Mingo (MING), Missouri. For these three Class I areas, data filling was used to obtain sufficient data so that at least three-years of valid data were available from which Baseline Conditions could be calculated. These data filled IMPROVE databases were prepared and made available on the VIEWS website. More information on the data filling procedures can be found at the VIEWS website: (http://vista.cira.colostate.edu/views/).

4.2.4 Natural Conditions

EPA has published default Natural Conditions for Annual Average and the worst 20 percent and best 20 percent days based on the original IMPROVE equation (EPA, 2003b). These default Natural Conditions have been updated to the new IMPROVE equation by the Natural Haze Levels II Committee (Pitchford, 2006). These default Natural Conditions are used as the anchor point for the glidepaths in 2064 and are provided in Appendix D for the CENRAP Class I areas.

4.2.5 2018 URP Point

The 2018 point on the Uniform Rate of Progress (URP) glidepath is constructed by generating a linear glidepath in deciviews from the Baseline Conditions in 2004 to Natural Conditions in 2064. Where the linear glidepath crosses 2018 is the 2018 point on the URP glidepath or the 2018 URP point. Figure 4-2 displays an example linear glidepath for the Caney Creek Class I area in Arkansas. There are three years of sufficient valid IMPROVE data during the 2000-2004 Baseline (2002, 2003 and 2004) with values of 27.21, 26.52 and 25.34 dv resulting in worst 20 percent Baseline Conditions of 26.36 dv that is placed as the starting point in 2004 for the glidepath. The ending point for the glidepath is 11.58 dv which is the default Natural Conditions for the worst 20 percent days (EPA, 2003b; Pitchford, 2006). The linear glidepath crosses 2018 at 22.91 dv which becomes the 2018 URP point.

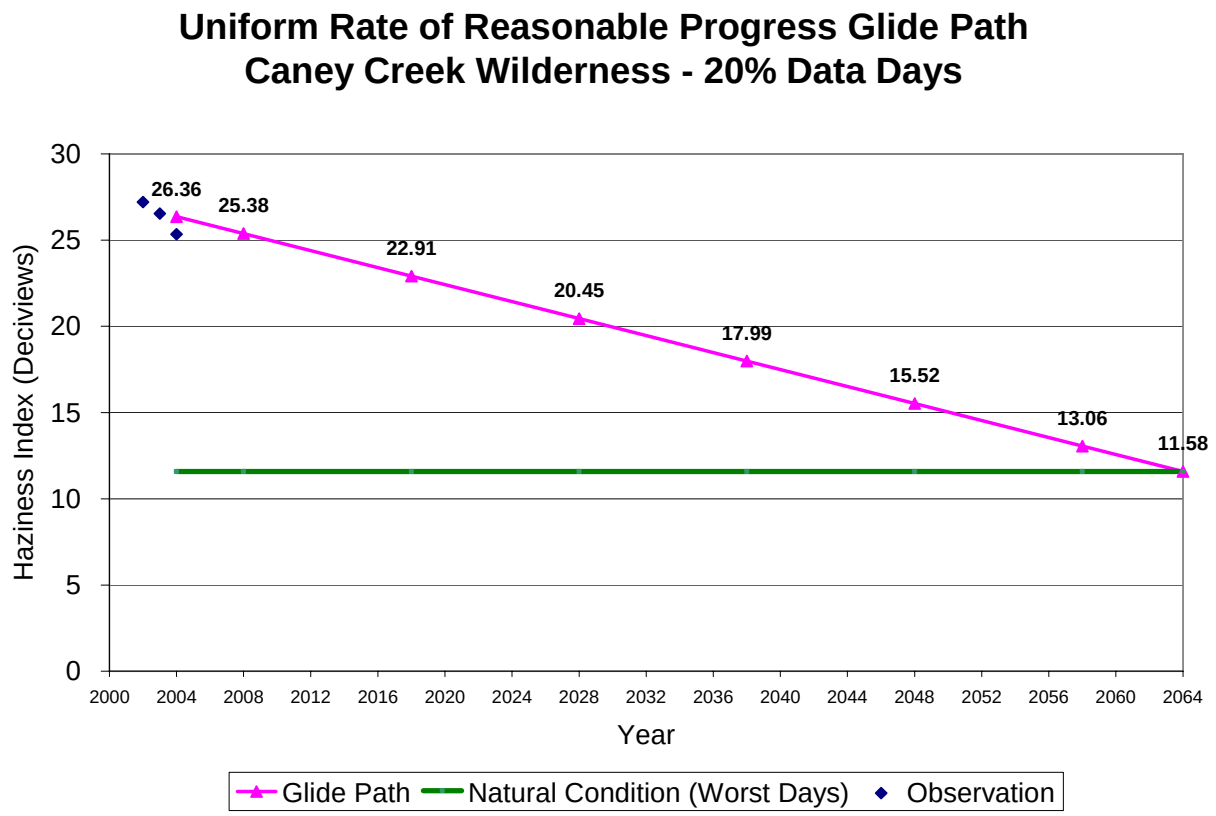


Figure 4-2. Linear Glidepath for Caney Creek (CACR), Arkansas that linearly connects the 26.36 dv Baseline Conditions in 2004 with the 11.58 dv Natural Conditions in 2064 resulting in a 22.91 dv 2018 URP Point.

4.3 EPA Default Approach to Visibility Projections

For CENRAP's model application for a single year (2002), EPA's regional haze modeling guidance recommends developing Class I area-specific and PM species-specific RRFs based on the average concentrations for the worst 20 percent days from 2002 (EPA, 2007). Thus, this is

the methodology used to project 2018 visibility estimates in this section. For example, if $SO4(2002)_i$ and $SO4(2018)_i$ are the model estimated sulfate concentrations for the 2002 worst 20 percent days (i=1…N) at a given Class I area for the 2002 and 2018 emission scenarios then the RRF for sulfate and this Class I area is given by:

$$RRF(SO4)_i = \sum SO4(2018)_i / \sum SO4(2002)_i$$

4.3.1 Mapping of Modeling Results to the IMPROVE Measurements

As noted above, to project future-year visibility at Class I areas the modeling results are used in a relative sense to scale current observed visibility for the worst 20 percent and best 20 percent visibility days using RRFs that are the ratio of modeling results for the future-year to current-year. This scaling is done separately for each of the six components of light extinction in the IMPROVE equations. The CMAQ modeled species do not necessarily exactly match up with the IMPROVE PM species, thus assumptions must be made to map the modeled species to the IMPROVE PM species for the purpose of projecting visibility improvements. For example, CMAQ explicitly simulates ammonium and sulfate may or may not be fully neutralized in the model by ammonium, whereas the IMPROVE equations assume sulfate is fully neutralized by ammonium. For the CMAQ Version 4.5 (September 15, 2005 release) model, the mapping of modeled species to IMPROVE equation PM species is listed in Table 4-2.

Table 4-2. Mapping of CMAQ V4.5 modeled species concentrations to IMPROVE PM components.

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

For the CENRAP visibility projections using the 2002 Typical and 2018 base case Base G emission scenarios, the secondary organic aerosol (SOA) module in CMAQ V4.5 was modified (SOAmods) to include additional processes related to the generation of SOA from biogenic emissions. In particular, three new species have been added that represent SOA products from biogenic emission compounds that is not included in the standard version of CMAQ V4.5 (Morris et al., 2006c):

- ASOC1 – SOA from biogenic sources (e.g., terpenes and isoprene) that has become polymerized so is no longer volatile.
- ASOC2 – SOA from biogenic sesquiterpene and higher reactivity and higher yield monoterpene emissions.
- ASOC3 – SOA from biogenic isoprene emissions.

Thus, the species mapping for Organic Mass Carbon (OMC) and the CMAQ V4.5 SOAmods version of the model used in CENRAP 2018 visibility projections is as given in Table 4-2 only with the addition of the three new biogenic SOA species to OMC as follows:

OMC = AORGAJ + AORGAI + AORGPAJ + AORGPAI + AORGBJ + AORGBI + ASOC1 + ASOC2 + ASOC3

4.3.2 Using Modeling Results to Project Changes in Visibility

Modeling results are used in a relative fashion to project future-year visibility using relative response factors (RRFs). RRFs are expressed as the ratio of the modeling results for the future-year to the results of the base year (2018/2002) and are Class I area and PM species specific. RRFs are applied to the Baseline Condition observed PM species to project future-year PM levels from which visibility can be assessed using the IMPROVE equations listed above. The following six steps are used to project future-year visibility for the worst 20 percent and best 20 percent visibility days (discussion is for worst 20 percent days but also applies to best 20 percent days):

1. For each Class I area and each monitored day, daily visibility is ranked using IMPROVE data and IMPROVE equation (either original or new IMPROVE equation) for each year from the five-year baseline period (2000-2004) to identify the worst 20 percent visibility days for each year from the five-year baseline (see Baseline Conditions discussion above).

2. Use an air quality model to simulate a base year period (ideally the five-year Baseline period of 2000-2004, but for CENRAP just the 2002 annual period was simulated) and a future-year (e.g., 2018) and use the resulting information to develop Class I area-specific RRFs for each of the six components of light extinction in the IMPROVE equation (SO4, NO3, EC, OMC, Soil and CM).

3. Multiply the RRF times the measured 24-hour PM concentration data for each day from the worst 20 percent days in each year from the five-year Baseline period to obtain projected future-year 24-hour PM concentrations for the worst 20 percent days and the five-year Baseline.

4. Compute the future-year daily extinction using the IMPROVE equation and the projected PM concentrations for each of the worst 20 percent days in the five-year baseline from Step 3.

5. For each of the worst 20 percent days within each year of the five-year baseline, convert the future-year daily extinction to deciview and average the daily deciview values within each of the five years separately to obtain five-years (or as many years with valid data in the 2000-2004 Baseline) of average deciview visibility for the worst 20 percent days.

6. Average the five-years of average deciview visibility to obtain the future-year visibility Haze Index estimate that is the future-year estimated visibility.

In calculating the RRFs, EPA draft guidance recommends selecting estimated 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. The NX x NY array of cells is grid resolution specific with EPA recommending that NX=NY=1 for 36 km grids, NX=NY=3 for 12 km grids and NX=NY=7 for 4 km grids (EPA, 2007). For the CENRAP 2002 36 km modeling, just the model estimates for the grid cell containing the monitor was used (i.e., NX=NY=1).

4.4 EPA Default 2018 Visibility at CENRAP and Nearby Class I areas and Comparisons to 2018 URP Goals

Using the EPA default visibility projection procedure described in Section 4.3 and the CENRAP 2002 Typical Base G and 2018 Base Case Base G CMAQ modeling results, 2018 visibility projections were made for CENRAP and nearby Class I areas. Appendix D details the 2018 Base G visibility projections for each Class I area in the CENRAP region using the new IMPROVE equation. Results for the Caney Creek (CACR), Arkansas Class I area are discussed in Section 4.4.1 below Displays for other CENRAP Class I areas are provided in Appendix D and summarized in Section 4.4.2

4.4.1 Example 2018 Base G Visibility Projections for Caney Creek, Arkansas

The 2018 visibility projections for the Caney Creek (CACR), Arkansas Class I area given in Figure D-1 in Appendix D are reproduced in Figure 4-3 and described below.

4.4.1.1 EPA Default 2018 Visibility Projections

The 2018 Base G visibility projection using the EPA default method (EPA, 2007a) and comparison with the 2018 URP point for the worst 20 percent days and the CACR Class I area is shown in Figure 4-3a. The 2000-2004 Baseline Conditions for CACR is 26.36 dv and the 2018 URP point is 22.91 dv so that a 3.45 dv reduction in visibility for the worst 20 percent days is needed to meet the 2018 URP point. The 2018 Base G CMAQ projected visibility is 22.48 dv so that the modeling predicts more visibility improvements (3.88 dv reduction) than required to meet the 2018 URP point (3.45 dv reduction). When looking at visibility projections across several Class I areas, it has been useful to present the 2018 visibility projections as a percentage of meeting the 2018 URP point; where 100% is meeting the point, greater than 100% surpassing the point (i.e., below the glidepath) and less than 100% means that less visibility improvement is achieved than needed to meet the 2018 URP point. For 2018 Base G CMAQ modeling at CACR, we achieve 112% of the visibility reduction needed to meet the 2018 URP point. Note that meeting the 2018 URP point is not a requirement of the RHR SIPs, rather it just serves as a benchmark to compare progress toward Natural Conditions in 2064 and is designed to help states in selecting their 2018 RPGs. As clearly stated in EPA guidance "The glidepath is not a presumptive target, and States may establish a RPG that provides for greater, lesser, or equivalent improvement as that described by the glidepath" (EPA, 2007b).

The 2018 Base G CMAQ visibility projections for the best 20 percent days and CACR is shown in Figure 4-3b. Recall the RHR goal for this visibility metric is no worsening of the visibility for the best 20 percent days. The Baseline Conditions for the best 20 percent days at CACR is 11.24 dv. The 2018 Base G projected visibility for the best 20 percent days is 10.35 dv, which represents a 0.89 dv visibility improvement for the best 20 percent days at CACR and demonstrating no worsening in visibility for the best 20 percent days.

Figure 4-3c displays "StackedBar Chart" plots of observed and model estimated extinction for each of the worst 20 percent days in 2002 and the 2002 Typical Base G CMAQ simulation and the average across the worst 20 percent days. This figure allows a comparison of how well the model is reproducing the observed extinction at CACR for the worst 20 percent days in 2002 and the breakdown of the PM components that are contributing to visibility impairment (more details on model performance were presented in Chapter 3). The 2002 worst 20 percent days at CACR are dominated by SO4 days (yellow), although during the winter there are also three days dominated by NO3 (Julian Days 80, 320 and 341). For most of the worst 20 percent days at CACR, the model reproduces the observed extinction reasonably well, although it does tend to understate SO4 on a few days and overstate NO3 on the four winter days. The observed average extinction across the 2002 worst 20 percent days at CACR is 150 Mm^{-1}, compared to a modeled value that is 23% lower (115 Mm^{-1}).

Figure 4-3d displays "Boxplots" of differences in modeled extinction for the 2002 worst 20 percent days between the 2018 Base G and 2002 Typical Base G CMAQ simulations. On most days SO4 is the largest component of the extinction that is estimated to be reduced at CACR on the worst 20 percent days. The exception to this is for the winter NO3 days where NO3 is the largest component of extinction that is reduced. The modeling results are not used directly in the visibility projections, rather they are used to develop the PM-species specific RRFs. That is, an important attribute in Figures 4-3c and 4-3d is the relative changes in the modeled PM species averaged across the worst 20 percent days that are represented by the last bar in each figure and provide insight into the RRFs used in the visibility projections. These results are summarized in Table 4-3 below. Table 4-3 compares the average extinction across the 2002 worst 20 percent days at CACR from the measured IMPROVE data, the modeled values and the modeled change in extinction between the 2018 and 2002 emissions scenarios. Although the results in Table 4-3 are not RRFs (RRFs are based on ratios of concentrations not extinction) they do show how the RRFs may magnify or deflate the importance of a modeled PM species. For example, the model estimates that approximately 23% (26.66 Mm^{-1}) of the visibility extinction average across the worst 20 percent days is due to NO3, whereas it is only 7% in the observed values (10.22 Mm^{-1}). So the modeled ~40% reduction in NO3 between the 2018 and 2002 scenarios is applied to the smaller observed NO3 value to obtain the 2018 projected NO3 value making NO3 a smaller portion of the 2018 projected visibility than the 2018 modeled visibility. On the other hand, the modeled SO4 extinction is less than observed so that its importance in the 2018 projections is much greater than in the modeled 2018 SO4 values.

Table 4-3. Observed and Modeled Extinction by Species Averaged Across the Worst 20 Percent Days in 2002 at CACR.

	2002 Average Observed W20% (Mm^{-1})	2002 Average Modeled W20% (Mm^{-1})	2018-2002 Reduction (Mm^{-1})	2018-2002 Reduction (%)
bSO4	109.50	67.90	-24.47	-36%
bNO3	10.22	26.66	-10.90	-41%
bOMC	19.65	16.68	-2.12	-13%
bEC	4.38	2.32	-0.67	-29%
bSOIL	1.43	1.04	+0.21	+20%
bCM	4.30	0.37	-0.01	-3%

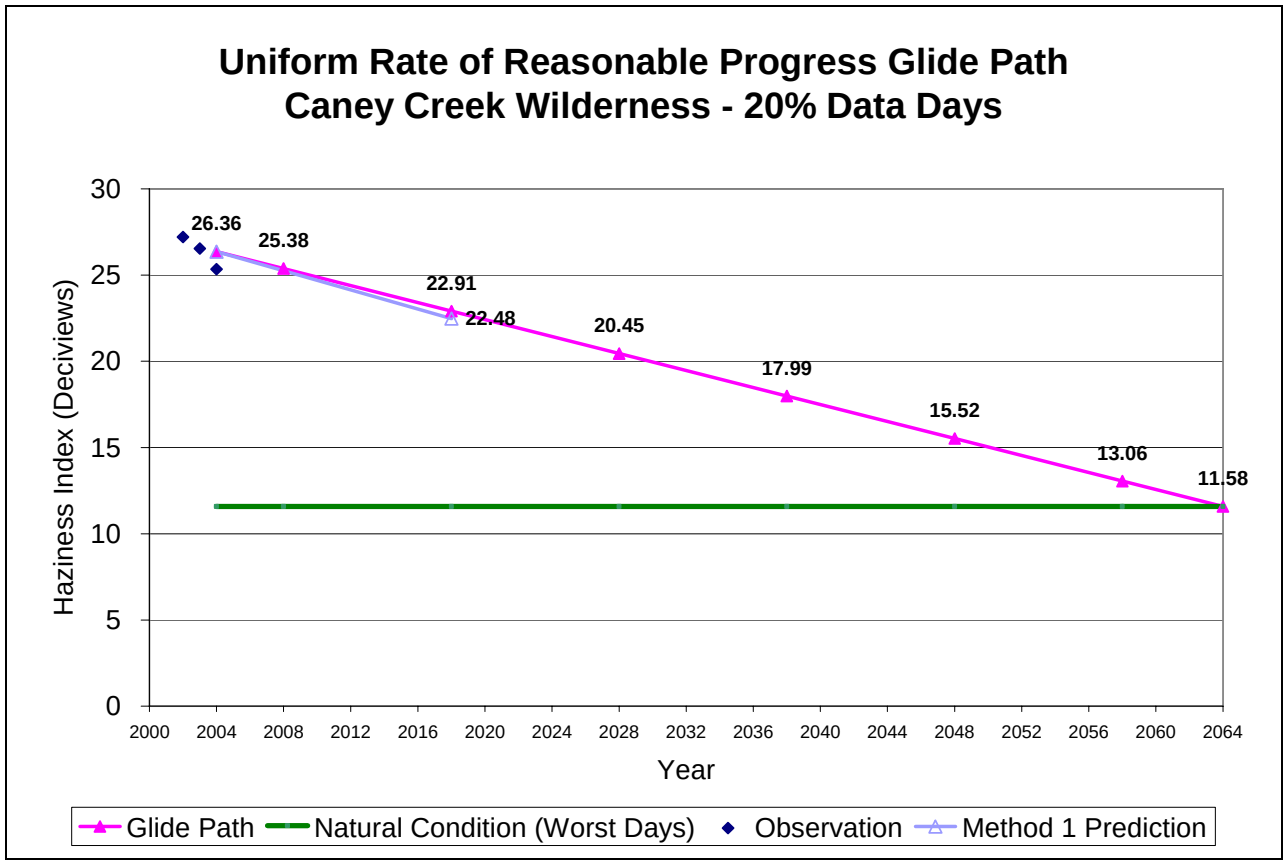


Figure 4-3a. 2018 Visibility Projections and 2018 URP Glidepaths in Deciview for Caney Creek (CACR), Arkansas and Worst 20 Percent (W20%) days Using 2002/2018 Base G CMAQ 36 km Modeling Results.

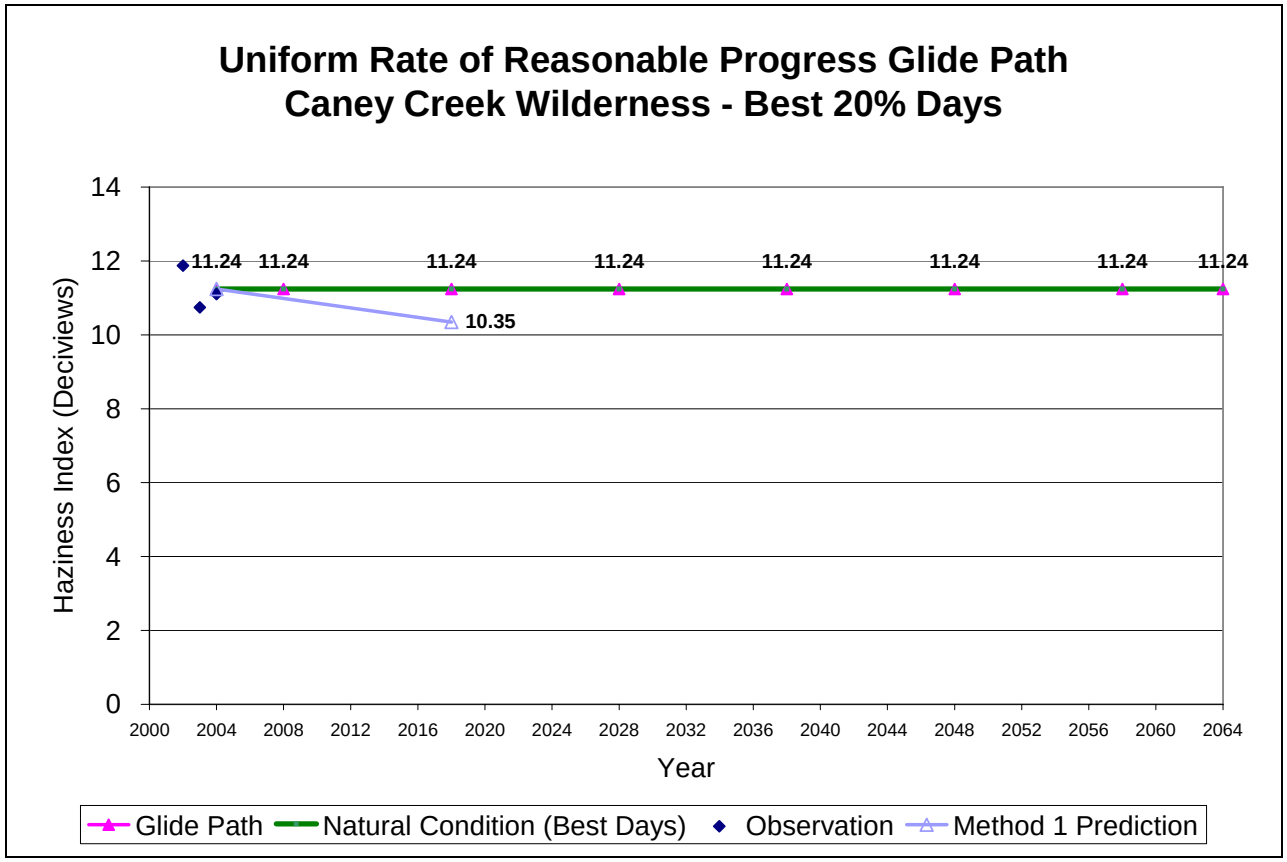


Figure 4-3b. 2018 Visibility Projections and 2018 URP Glidepaths in Deciview for CACR, Arkansas and Best 20 Percent (B20%) days Using 2002/2018 Base G CMAQ 36 m Modeling Results.

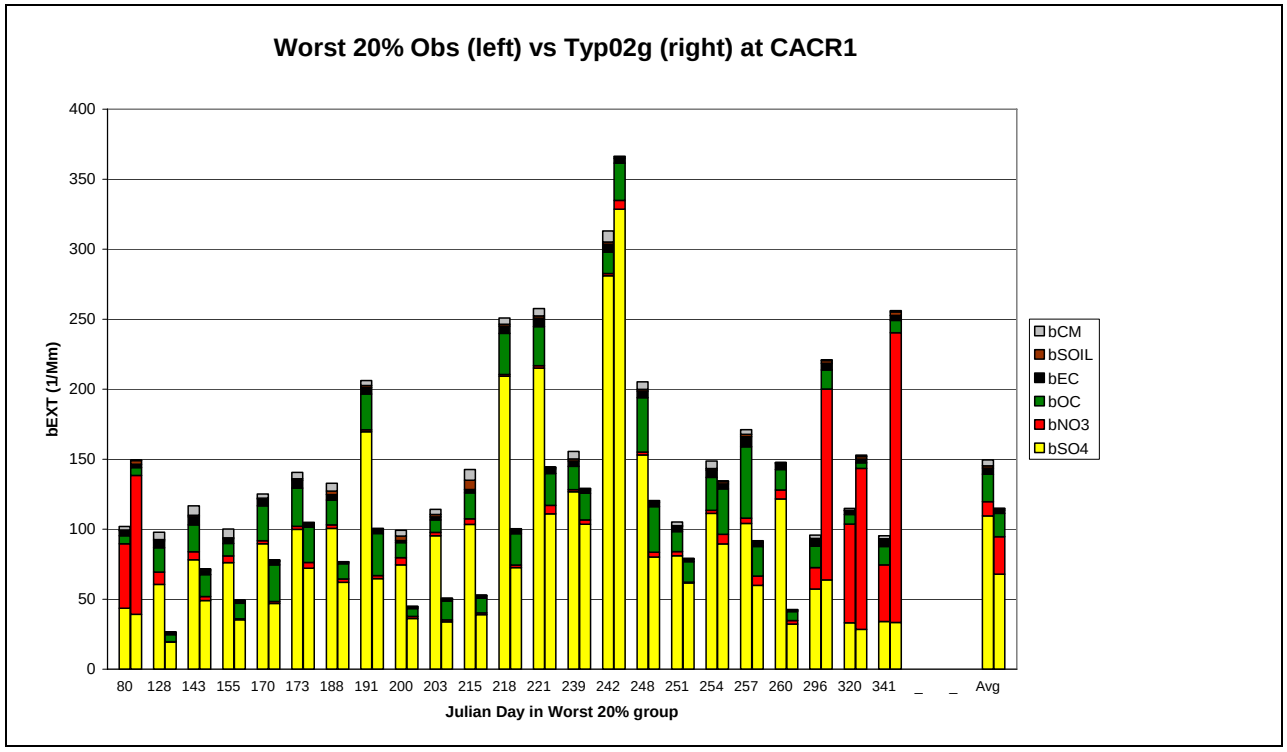


Figure 4-3c. Comparison of Observed (left) and 2002 Base G Modeled (right) Daily Extinction for Caney Creek (CACR), Arkansas and Worst 20 Percent (W20%) days in 2002.

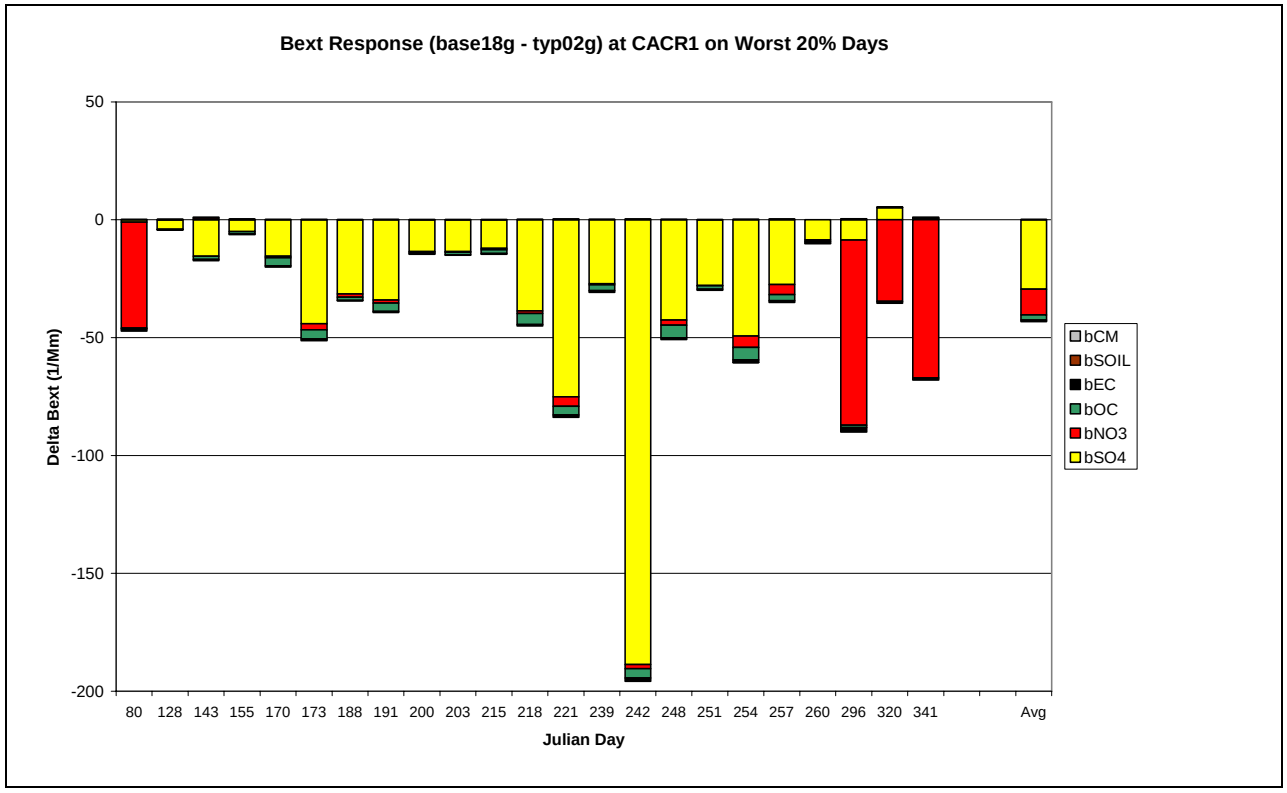


Figure 4-3d. Differences in Modeled 2002 and 2018 Base G CMAQ Results (2018-2002) Daily Extinction for Caney Creek (CACR), Arkansas and Worst 20 Percent (W20%) Days in 2002.

4.4.2 Summary 2018 Visibility Projections Across Class I Areas

Figure 4-4 displays a "DotPlot" of 2018 visibility projections using the 2002 Typical and 2018 base case Base G CMAQ 36 km modeling results. DotPlots present the 2018 visibility projections as a percentage of meeting the 2018 URP point. For example, at CACR the 2018 Base G modeling achieved 112% of the visibility reduction needed to meet the 2018 URP point so the dot under CACR is plotted at 112%. Class I areas' with dots above 100% surpass the 2018 URP point (i.e., are below the glidepath), whereas Class I areas' with dots that are under 100% fail to meet the 2018 URP point. Figure 4-4 summarizes the 2018 visibility projections using the EPA default "Regular RRF" and the two alternatives where CM is assumed to be natural (CM RRF=1) and both CM and Soil are assumed to be natural (CM&SOIL RRF=1). When CM or CM&SOIL are assumed to be natural that means that we assume the same CM or CM&SOIL occurs in the 2018 future-year as in the 2000-2004 Baseline Conditions. For the CENRAP sites, the EPA default and alternative projection, assuming CM alone or CM and Soil are natural, techniques produced similar results.

At the four eastern CENRAP Class I area sites close to the Mississippi River (CACR, UPBU, HEGL and MING), the 2018 visibility projections meet (HEGL) or surpass the 2018 URP point. Breton Island Class I area (BRET) comes up 6% short of meeting the 2018 URP point (i.e., 94% of the URP point). Wichita Mountains Class I area (WIMO) comes up approximately 40% short of the 2018 URP point. The two northern Class I areas (BOWA and VOYA) also come up about 40% short of meeting the 2018 URP point (i.e., achieve 69% and 53% of the visibility improvement needed to meet the 2018 URP point). The two Texas Class I areas only achieve

26% (BIBE) and 34% (GUMO) of the visibility improvement needed to meet the 2018 URP point for the worst 20 percent days. As discussed in more detail in Chapter 5, much of the difficulty for the Texas and some of the other CENRAP Class I areas in meeting the 2018 URP point is due to large contributions due to international transport, much of which (e.g., Mexico and global transport) is assumed to remain unchanged from 2002 to 2018.

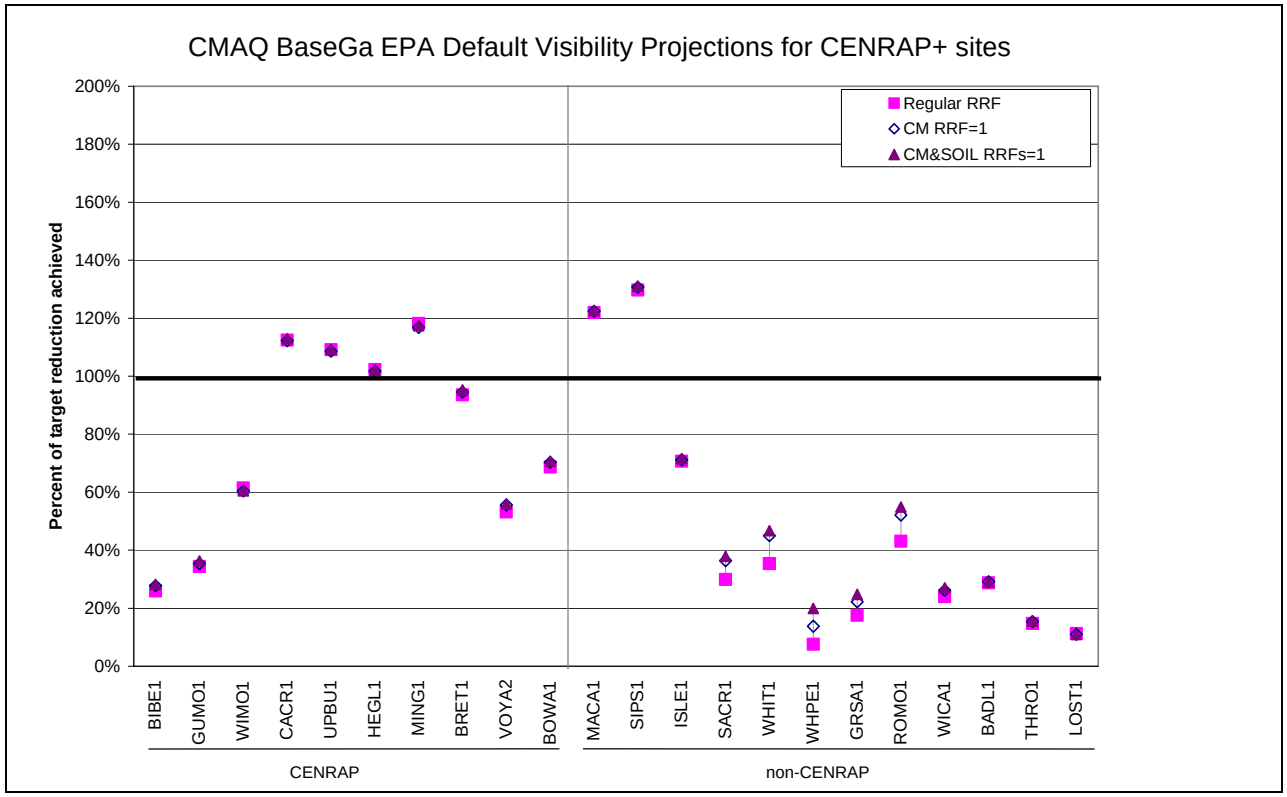
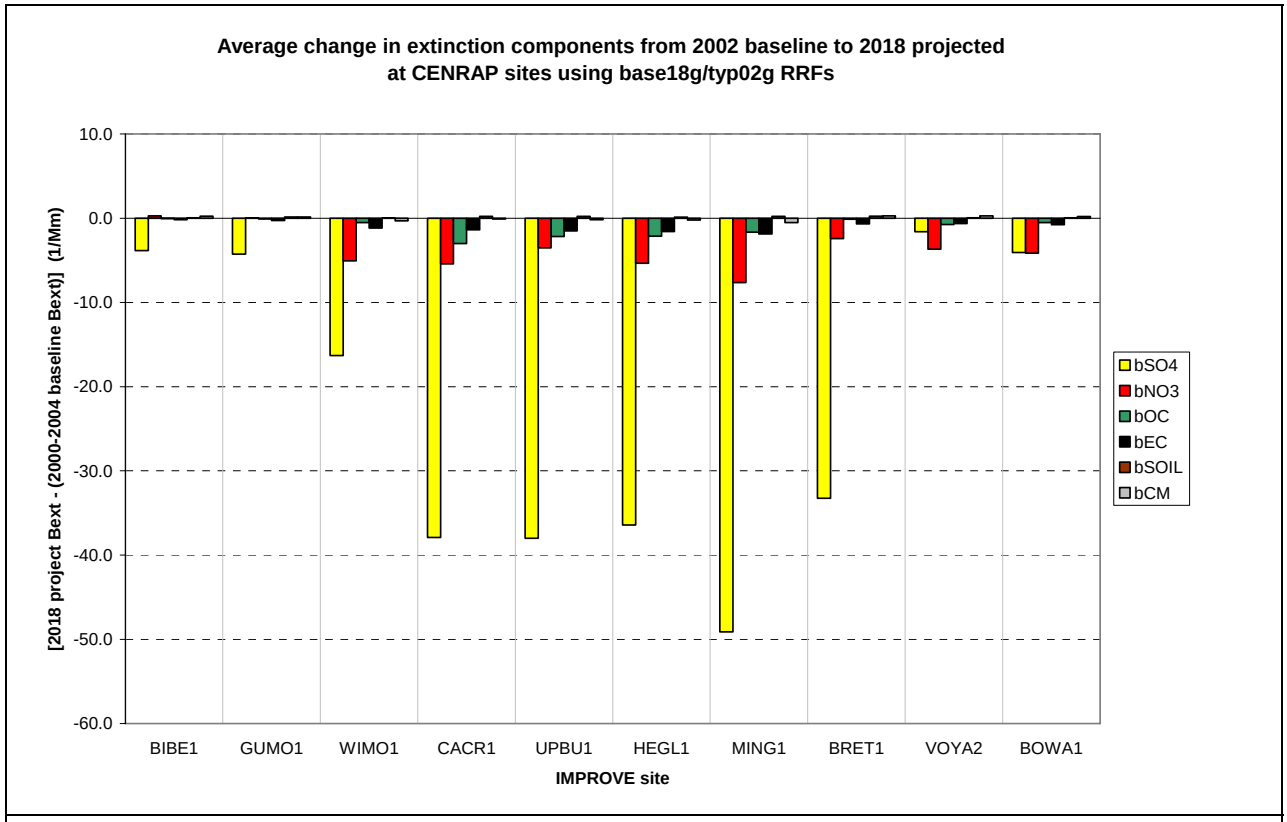


Figure 4-4. 2018 Base G CMAQ Visibility Projections for CENRAP and Nearby Class I areas Using DotPlots that Express 2018 Visibility as a Percentage of Meeting the 2018 URP Point On the Deciview Linear Glidepath.

Figure 4-5 displays the model estimated absolute change in extinction (Mm^{-1}) averaged across the 2002 worst 20 percent days at Class I areas in and near the CENRAP region. The largest modeled reductions are in SO4 extinction. Figure 4-6 displays the percent change in the projected PM extinction by PM species for each CENRAP and nearby Class I area average across the worst 20 percent days (i.e., the relative modeled change). The four CENRAP Class I areas that meet the 2018 URP point (CACR, UPBU, HEGL and MING) are characterized by large SO4, NO3 and EC extinction reductions (30-40%) with small Soil increases. At the other CENRAP Class I areas, however, there are lower levels of SO4, NO3 and EC extinction reductions and even some NO3 increases (BIBE). At the non-CENRAP Class I areas, the two VISTAS Class I areas (MACA and SIPS) have large reductions in SO4 extinction (~50%), whereas the WRAP Class I areas SO4 extinction reductions are much smaller.



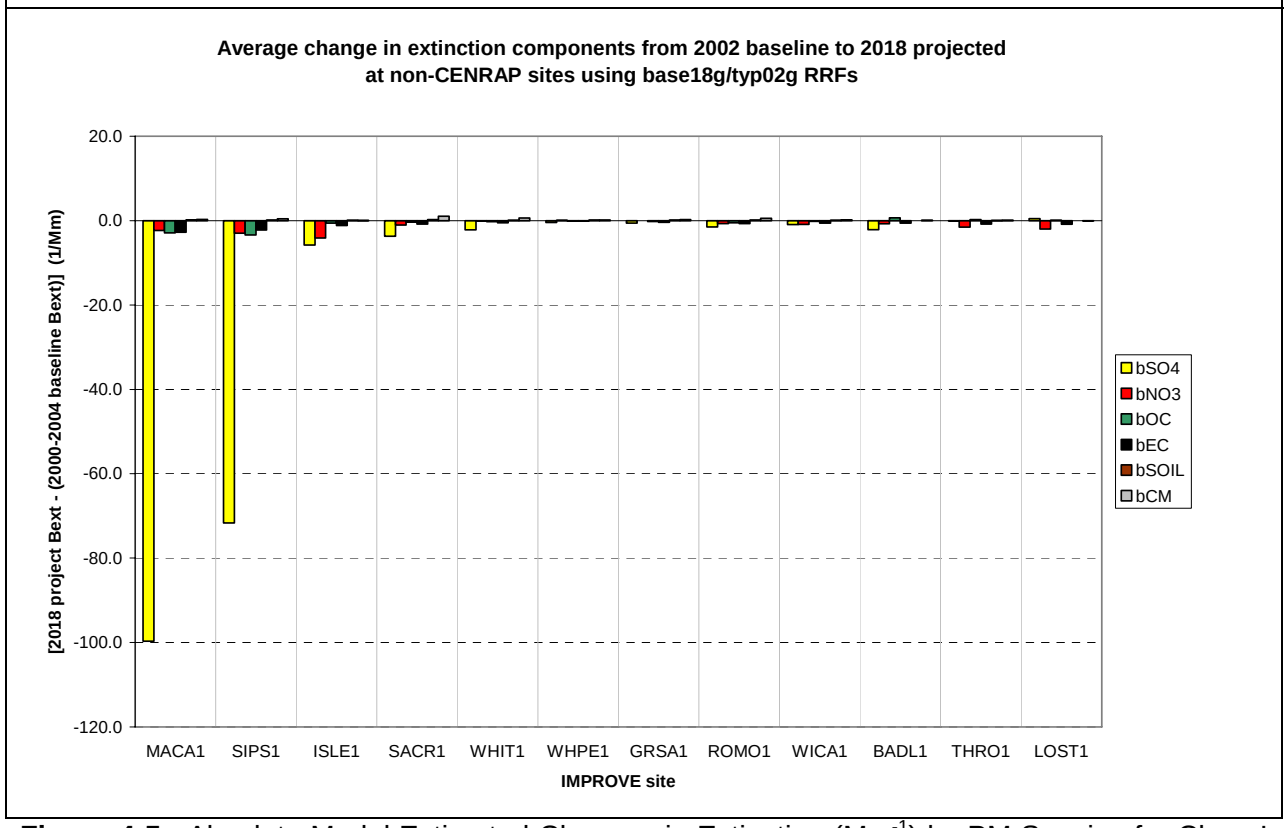


Figure 4-5. Absolute Model Estimated Changes in Extinction (Mm^{-1}) by PM Species for Class I Areas in the CENRAP region (top) and Near the CENRAP region (bottom).

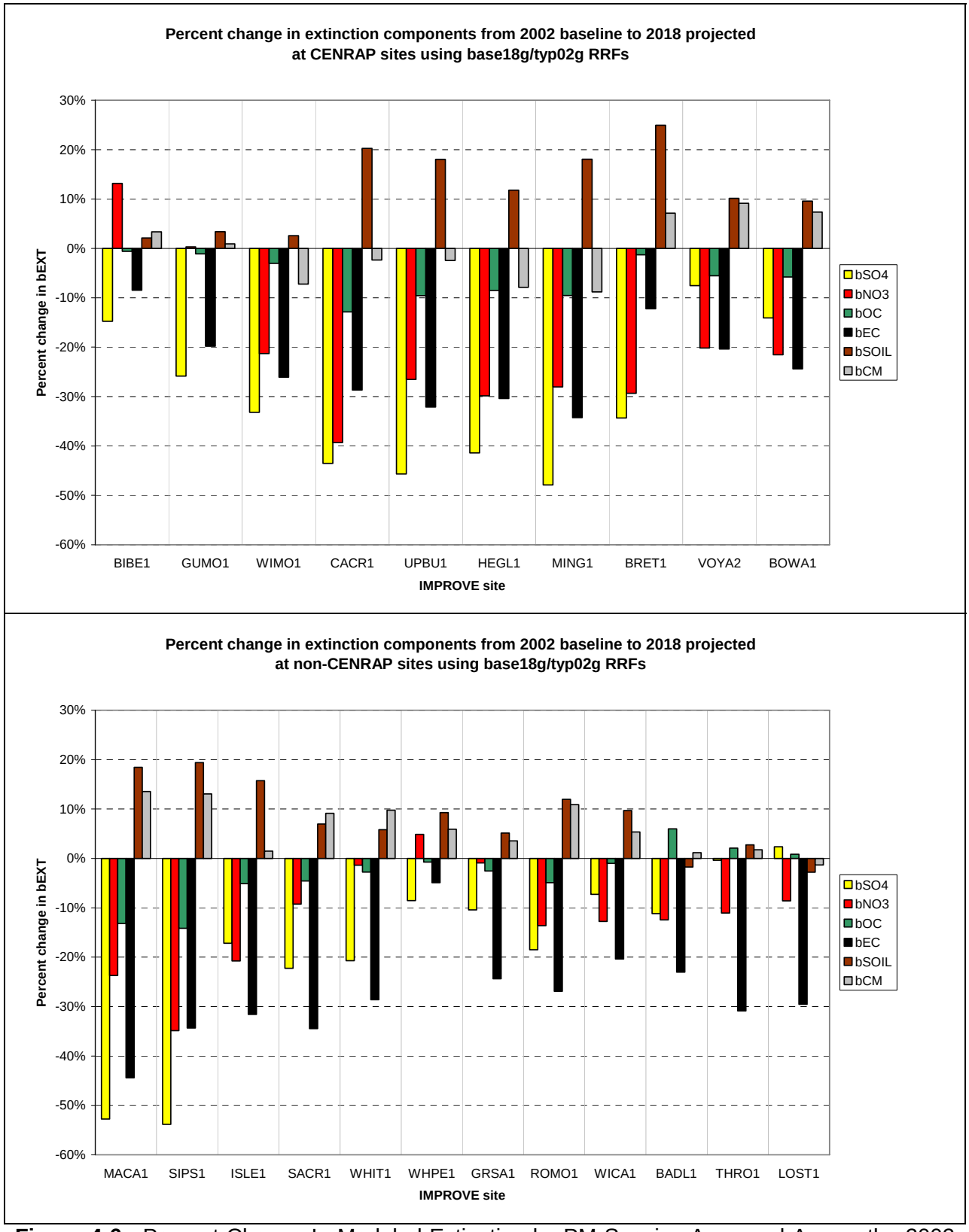


Figure 4-6. Percent Change In Modeled Extinction by PM Species Averaged Across the 2002 Worst 20 Percent Days for Class I areas in the CENRAP region (top) and Near the CENRAP region (bottom).

4.5 2018 Visibility Projections for Base G C1 Control Scenario

The 2018 visibility projections based on the CMAQ simulations for the 2018 Base G C1 Control Strategy simulations are presented in this section. The C1 Control Strategy results in reductions mainly in SO2 and NOx emissions from point sources in the CENRAP states. Consequently, PM improvements are limited to mainly SO4 and NO3 concentration reductions in the CENRAP states. Figure 4-7 displays the differences in CMAQ-estimated annual average SO4 and NO3 concentrations between the 2018 Base G base case and the 2018 Base G C1 Control Strategy case; the differences in all other PM species (with the exception of NH4) were negligible (see: http://pah.cert.ucr.edu/aqm/cenrap/cmaq.shtml#base18gc1vsbase18g). Annual average SO4 concentration reductions of over a quarter of a $\mu g/m^3$ are estimated to occur in northeast Texas, east Oklahoma, Missouri, northeast Arkansas and up into Iowa and Illinois. There are much lower reductions in NO3 that cover a similar area.

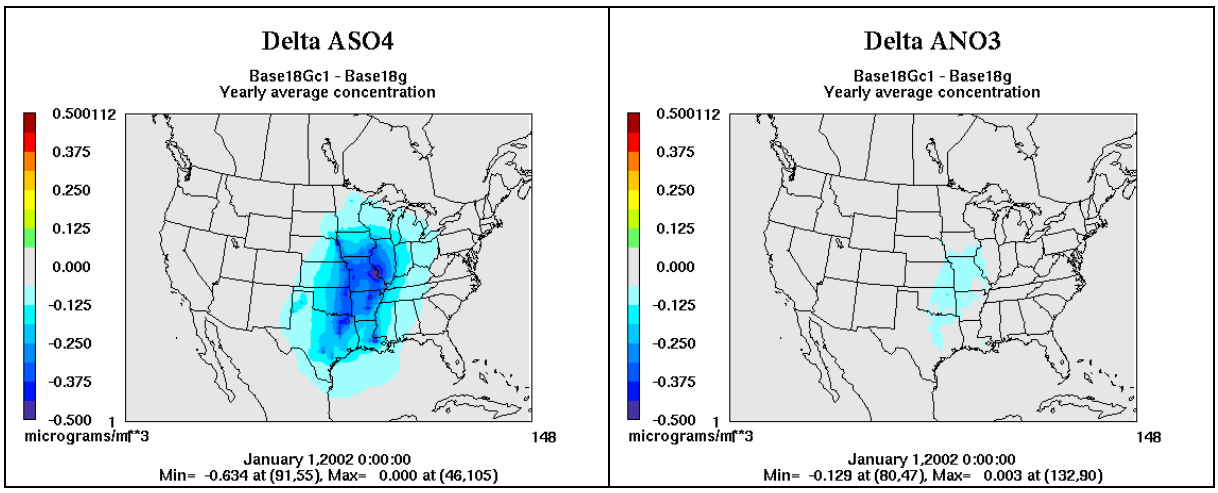


Figure 4-7. CMAQ-Estimated Reductions in Annual Average SO4 (left) and NO3 (right) Fine Particle Concentrations Between the 2018 Base G Base Case and 2018 Base G C1 Control Strategy Case.

Figure 4-8 displays the DotPlot comparisons of the 2018 visibility projections for 2018 Base G and 2018 Base G C1 Control Strategy emission scenarios. The additional controls in the C1 Control Strategy are projected to result in visibility improvements for the worst 20 percent days at Class I areas throughout and near the CENRAP region. Sites are closer to being on the glide path by 10 to 30 percent. For Breton Island this makes a difference of not meeting the 2018 URP point in 2018 Base G (94%) to surpassing the URP point in the C1 Control Strategy (106%).

Table 4-4 presents a tabular summary of the information presented in Figure 4-8, including the Baseline, 2018 URP point, and 2018 projected visibility for the Base G and C1 Control Strategy simulations.

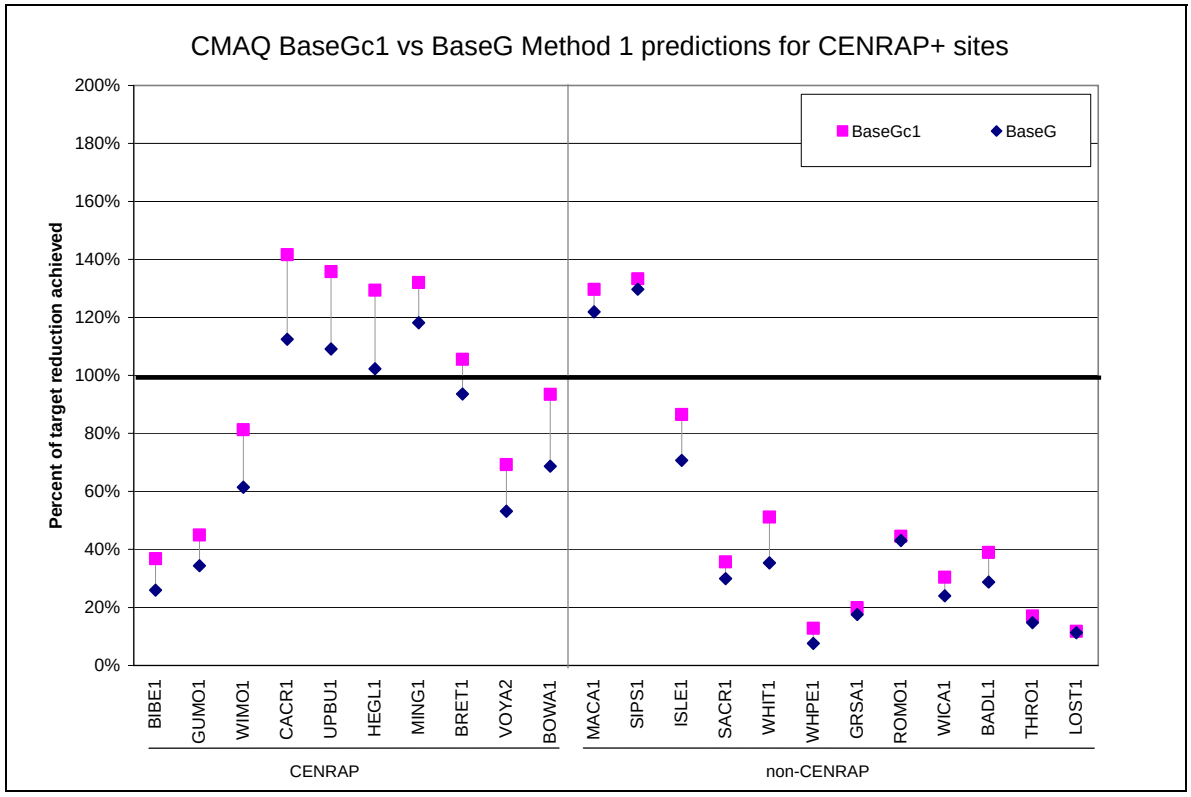


Figure 4-8. 2018 Visibility Projections as a Percentage of Meeting the 2018 URP Point (i.e., DotPlot) for the 2018 Base G and 2018 Base G C1 Control Strategy Emission Scenarios.

Table 4-4. 2000-2004 Baseline, 2018 URP Point, and Projected 2018 Visibility and Percent of Meeting the 2018 URP Point for the 2018 Base G and 2018 C1 Control Strategy CMAQ Simulations.

Class I Area Name	State	ID	Lat.	Lon.	00/04 Baseline Condit.	2018 URP Point	2018 Base G Base Case		2018 Base G C1 Control Strategy	
			(deg)	(deg)	(dv)	(dv)	(dv)	(%)	(dv)	(%)
Badlands NP	SD	BADL1	43.81	-102.36	17.14	15.02	16.53	29%	16.31	39%
Big Bend NP	TX	BIBE1	29.33	-103.31	17.30	14.93	16.69	26%	16.43	37%
Boundary Waters Canoe Area	MN	BOWA1	48.06	-91.43	19.58	17.72	18.30	69%	17.84	93%
Breton	LA	BRET1	29.87	-88.82	25.73	22.51	22.72	94%	22.34	106%
Caney Creek Wilderness	AR	CACR1	34.41	-94.08	26.36	22.91	22.48	112%	21.48	142%
Great Sand Dunes NM	CO	GRSA1	37.77	-105.57	12.78	11.35	12.53	18%	12.49	20%
Guadalupe Mountains NP	TX	GUMO1	31.91	-104.85	17.19	14.74	16.35	34%	16.09	45%
Hercules-Glades Wilderness	MO	HEGL1	36.68	-92.9	26.75	23.14	23.06	102%	22.09	129%
Isle Royale NP	MI	ISLE1	48.01	-88.83	20.74	18.78	19.36	71%	19.05	87%
Lostwood	ND	LOST1	48.59	-102.46	19.57	16.87	19.27	11%	19.26	12%
Mammoth Cave NP	KY	MACA1	37.20	-86.15	31.37	26.64	25.60	122%	25.23	130%
Mingo	MO	MING1	37.00	-90.19	28.02	24.37	23.71	118%	23.21	132%
Rocky Mountain NP	CO	ROMO1	40.35	-105.7	13.83	12.29	13.17	43%	13.14	45%
Salt Creek	NM	SACR1	33.6	-104.41	18.03	15.41	17.25	30%	17.10	36%
Sipsey Wilderness	AL	SIPS1	34.32	-87.44	29.03	24.82	23.57	130%	23.42	133%
Theodore Roosevelt NP	ND	THRO1	46.96	-103.46	17.74	15.42	17.40	15%	17.34	17%
Upper Buffalo Wilderness	AR	UPBU1	36.17	-92.41	26.27	22.84	22.52	109%	21.61	136%
Voyageurs NP	MN	VOYA2	48.47	-92.8	19.27	17.58	18.37	53%	18.10	69%
White Mountain Wilderness	NM	WHIT1	33.48	-105.85	13.70	12.11	13.14	35%	12.89	51%
Wheeler Peak Wilderness	NM	WHPE1	36.57	-105.4	10.41	9.49	10.34	8%	10.30	13%
Wind Cave NP	SD	WICA1	43.58	-103.47	15.84	13.94	15.39	24%	15.26	30%
Wichita Mountains	OK	WIMO1	34.75	-98.65	23.81	20.01	21.47	61%	20.72	81%