

CMAQ Model Performance Evaluation for 2000 in Central California

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1. Introduction:

The San Joaquin Valley (SJV) of California is currently designated as nonattainment for PM_{2.5}. Addressing this issue properly requires rigorous long-term chemical transport modeling to support the development of a plan to attain the National Ambient Air Quality Standard (NAAQS) for PM_{2.5}. These chemical transport modeling exercises serve to determine future year attainment status for the SJV given projected emissions scenarios and also the most effective emissions reduction pathways to control PM concentrations for different seasons and regions of the domain.

This document describes the performance evaluation of the United States Environmental Protection Agency (USEPA) Community Multiscale Air Quality (CMAQ) model (USEPA, 1999; CMAS, 2007) annual simulation conducted to assist the preparation of the State Implementation Plan for PM_{2.5} in the SJV. The base year for this simulation is 2000, for which a rich database of observations was collected as part of the California Regional PM₁₀/PM_{2.5} Air Quality Study.

This evaluation includes PM_{2.5} mass and its major components such as nitrate, sulfate, ammonium, organic carbon, elemental carbon, and dust. Since there are no universally accepted criteria for the evaluation of PM mass or components, we selected those proposed by Boylan and Russell (2006). Here we use the traditional statistical metrics, correlation diagrams, spatial plots, and time-history plots.

2. Regional Air Quality Methodology:

As stipulated in USEPA modeling guidance, a grid-based photochemical model is necessary to perform the modeled attainment test for PM_{2.5} (USEPA, 2007). Such models offer the best available representation of important atmospheric processes and are an essential tool in analyzing the impacts of proposed emissions controls on pollutant concentrations. The USEPA recommends guidelines for choosing a model for use in the attainment test. For example, the model source code should be free or low cost, modeling elements should have undergone rigorous scientific peer-review, and the model should have been shown to perform well in the past for similar applications.

The CMAQ model has been selected for use in the PM_{2.5} modeled attainment demonstration for the San Joaquin Valley Air Pollution Control District. CMAQ is a state-of-the-science “one-atmosphere” system that treats major atmospheric and land processes (e.g., advection, diffusion, gas phase chemistry, gas-particle mass transfer, nucleation, coagulation, wet and dry deposition, aqueous phase chemistry, etc.) and a range of species (e.g., anthropogenic and

biogenic, primary and secondary, gaseous and particulate) in a comprehensive framework (USEPA, 1999; CMAS, 2007).

CMAQ has been extensively peer-reviewed, is well-documented, and is regularly updated to reflect the latest changes in scientific understanding. CMAQ has been applied successfully in a range of environments and on many spatial and temporal scales. Given that CMAQ has also been applied successfully to episodic modeling in Central California, the CMAQ modeling system version 4.6 with California-specific updates, as described in Liang and Kaduwela (2005), was selected for use in support of the PM_{2.5} modeled attainment demonstration.

3. Chemical Mechanism:

There are a number of gas-phase chemical mechanisms readily available for application in CMAQ (e.g., CB-IV, CB-V, SAPRC-99). The user has the additional option of whether to couple the chosen gas phase mechanism with aerosol and/or aqueous phase chemical processes. In order to simulate the complex mixture of PM_{2.5} species in the San Joaquin Valley, SAPRC99 coupled with CMAQ aerosol code version 4 and aqueous phase chemistry has been chosen for this application. SAPRC-99, a complete update of SAPRC-90, is a detailed mechanism describing the gas-phase reactions of volatile organic compounds (VOCs) and oxides of nitrogen (NO_x) (Carter, 2000). AE4-AQ, the fourth-generation CMAQ aerosol code with aqueous phase chemistry, when coupled with a gas phase mechanism, represents such phenomena as gas-aerosol/aqueous phase mass transfer, chemical transformation of particulate species and their gas phase precursors, and the evolution of the aerosol size distribution.

4. Model Inputs and Setup:

4.1. Domain Structure:

Two modeling domains were used for this work. The first modeling domain, named CCAQS, covered the Central Valley and its surroundings with 63x63 lateral 12x12 km² grid cells for each vertical layer. The CCAQS domain extends from the Pacific Ocean in the west to the Mojave Desert and western Nevada in the east and runs from the northern Sacramento Valley to the Tehachapi Mountains in the south. The second domain, named SJV, is fully nested within the CCAQS domain and covers the San Joaquin Valley with 80x89 lateral 4x4 km² grid cells for each vertical layer (Figure 1). The vertical structure for both domains is composed of 15 layers of varying thickness up to the top of the meteorological domain (100 mb). The finest resolution belongs to those layers closest to the surface and is determined largely by the vertical structure of the meteorological inputs. The surface layer is approximately 30 meters thick.

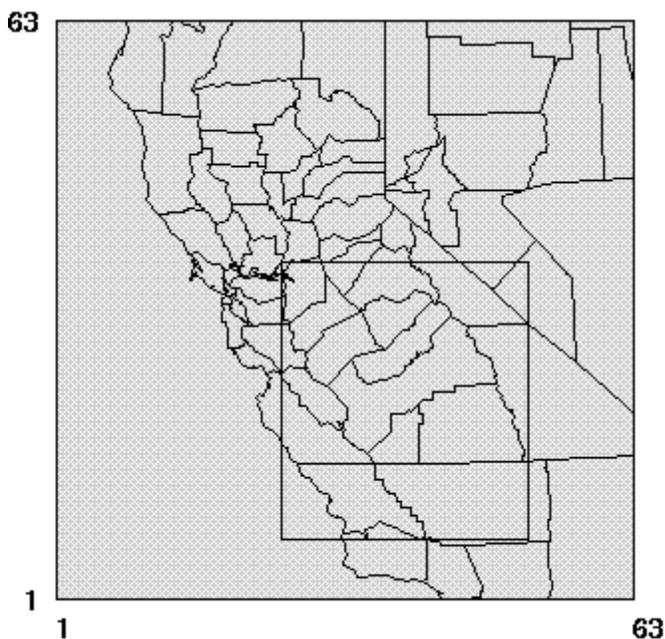


Figure 1: The CCAQS modeling domain with the SJV modeling domain inset.

4.2. Initial and Boundary Conditions:

Boundary conditions for the CCAQS domain were taken from the global chemical transport Model for Ozone And Related chemical Tracers (MOZART). Model boundary conditions for major species were extracted for the Central California modeling domain from MOZART results representative of the year 2000. In addition to VOCs and inorganic gases, boundary conditions were extracted for ammonium, nitrate, sulfate, and organic and elemental carbon. Initial conditions were estimated as an average of the extracted boundary conditions for each species. The CCAQS domain provided the initial and boundary conditions for the nested SJV domain. All species reported in the three-dimensional output fields for the simulation over the CCAQS domain were included in the initial and boundary conditions for the SJV domain. While boundary conditions for the CCAQS domain were held constant for each month, boundary conditions for the SJV domain varied for each hour. The impact of initial conditions was minimized for each domain by simulating 8-day spin up periods prior to the simulation of each month of the year.

4.3. Emissions:

A spatially, temporally, and chemically resolved emissions inventory of combined area, mobile, and point sources was generated using the California Emissions Forecasting System (CEFS) version 1.06 with offline adjustments. The inventory includes emissions estimates for gaseous and particulate species

of anthropogenic and biogenic origin. Gridded hourly emissions were developed for the CMAQ modeling domain for the years 2000, 2005, and 2014. Quality assurance checks of domain emissions totals and spatial distribution were performed at various steps in the emissions processing in order to ensure that the CMAQ emissions input files were sound. Additional information on emissions is provided separately.

4.4. Meteorological Inputs:

The meteorological input fields to CMAQ were generated with the Meteorology-Chemistry Interface Processor (MCIP) version 3.0. MCIP serves as a link between meteorological models like MM5 or WRF with CMAQ, and generates model-ready meteorological inputs like the wind and temperature fields necessary to drive the transport and chemistry calculations in CMAQ. Inputs to MCIP were generated using the PSU/NCAR Mesoscale Model (MM5) (version 3.6) (Grell et al, 1995). Planetary boundary layer and radiation characteristics were calculated in MCIP, and the Models-3 dry deposition routine (Pleim - with chlorine and mercury species) was chosen to represent dry deposition.

4.5. MM5 Simulation:

MM5 is a limited area, terrain-following sigma coordinate model on Lambert Conformal projection that was developed by Penn State and NCAR as a community mesoscale model. The model is based on non-hydrostatic, fully compressible motions that allow users to study the atmospheric motions at small scales by explicitly treating the effects of convective motions on atmospheric circulations. The MM5 model has been improved over more than two decades by contributions from a broad scientific community.

MM5 was set up for a 14 month simulation (December 1999 – January 2001) with three nested grids using (70 x 70), (133 x 133), and (94 x 85) grid points in the (x, y) or (south-north, west-east) directions with 36, 12, and 4 km horizontal resolution in each grid, respectively (Figure 2). The vertical structure of the domain was defined with 30 layers extending to 100 mb at the top of the domain. The first two coarse grids defined the atmospheric initial and boundary conditions for the area at large scale, while the innermost grid with 4 km horizontal resolution resolved the fine details of atmospheric motions within the SJV modeling domain. MM5 has several options to calculate the components of internal and external forces acting on a volume of air, such as those for radiation, convection, cloud microphysics, soil fluxes, and boundary layer physics. While many sensitivity studies were conducted using various model options to find the best agreement with observations, an effort was also made to use the same model options from one simulation to the next. The Grell (1995) cumulus parameterization scheme for coarse grids was used along with the Blackadar boundary layer scheme for calculation of fluxes (Blackadar, 1979, Grell, 1995).

The Dudhia simple ice scheme was used for the treatment of excess moisture (Dudhia, 1989) and the Dudhia cloud radiation scheme (Dudhia, 1993) was used for radiational heating and cooling of the atmosphere. The Blackadar multi-layer, force-restore method soil model (Blackadar, 1976) was used for soil physics in all grids.

Initial and boundary conditions were prepared using the analyses of observations prepared by the National Center for Environmental Prediction (NCEP) and archived at NCAR. The 14-month period (December 1999 through January 2001) was first simulated using initial and boundary conditions (IC/BCs) with the analysis nudging option on the two coarse grids. Then, IC/BCs were prepared from the 12 km grid output for the initialization of the 4 km grid. The three-dimensional (3-D) wind and temperature values simulated by the model were compared against surface observations obtained from four SJV stations (Fresno, Bakersfield, Arvin, and Parlier) to study the temporal and 3-D spatial structure of atmospheric motions as well as to evaluate the model performance within the SJV. Figure 2 shows the MM5 domains employed to generate meteorological fields for the CMAQ simulation. A detailed performance evaluation of the MM5 simulation is provided separately.

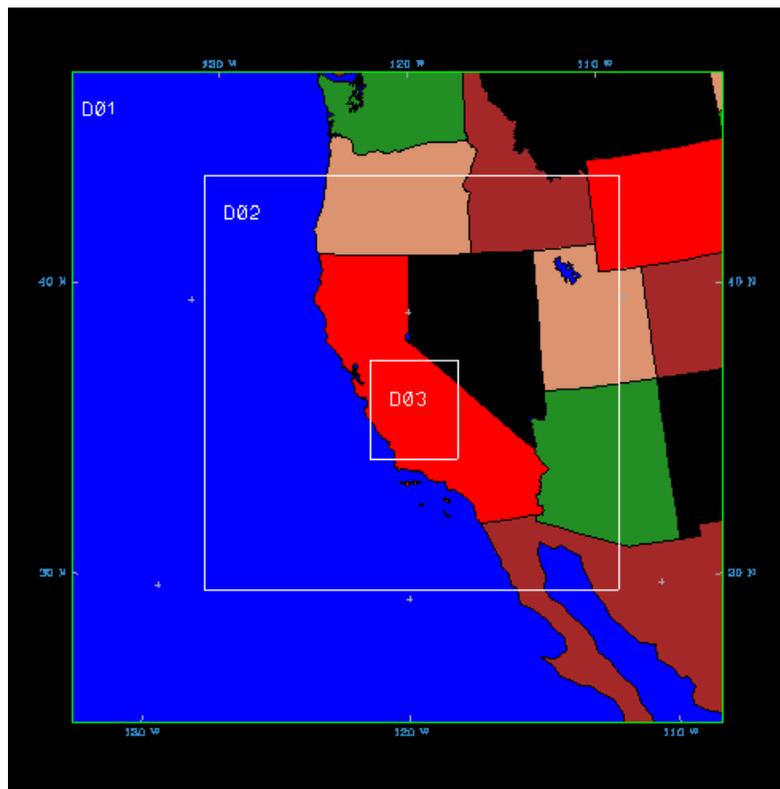


Figure 2. The location of the three nested grids adopted for numerical modeling of the SJV using MM5.

5. Model Performance Evaluation:

Methods for evaluating the performance of episodic ozone simulations are reasonably well developed and universally accepted. However, model evaluation for particulate matter (PM) simulations is still in an infant stage. Methods for performance evaluation of long-term simulations for both ozone and PM are neither reasonably developed nor universally accepted.

Thus, we employ the following approach to evaluate the annual PM simulation for 2000. First, we will examine the spatial patterns of PM_{2.5} mass and its components on an annual and quarterly basis. Second we compute fractional statistics (mean fractional error and mean fractional bias) for each measurement location. We have also computed other traditional statistics such as mean normalized error and mean normalized bias, but we present only fractional statistics here. Third, we examine time-history plots for PM_{2.5} mass and its components.

5.1. *Spatial Patterns for PM mass and components:*

Figure 3 shows the annual average spatial patterns for PM mass, nitrate, sulfate, ammonium, organic carbon, elemental carbon and dust. As expected, PM mass and components are restricted to the valley floor. The maximum mass loading for this domain is near Visalia. The major contributors to the mass are dust and ammonium nitrate, and they also peak near Visalia. The second highest mass loading is in the Bakersfield area. The sulfate concentrations are very low in the majority of the domain ($<5 \mu\text{g}/\text{m}^3$) except in the vicinity of Taft, Bakersfield, and Stockton. The concentrations of both organic and elemental carbon are relatively small on an annual basis compared to those of dust and ammonium nitrate.

Figures 4-7 show the quarterly average for PM_{2.5} mass and its major components. It is evident from these figures that nitrate formation follows the seasonal pattern expected based on seasonal temperatures and relative humidity. However, the nitrate concentrations for the third quarter appear to be excessive. The (12x12) km² simulation that provided the initial and boundary conditions for this (4x4) km² simulation does not show this behavior. Thus, the cause of this excessive nitrate is not clear at this time. It is important to note that the Federal Reference Monitor (FRM) does not retain significant amounts of nitrates for both the second and third quarters. Thus, the excess nitrate concentrations simulated here do not have a significant impact on the future year design value determination. As expected, sulfate concentrations remain relatively low for all quarters. The organic and elemental carbon concentrations are higher in the first and fourth quarters, perhaps due to enhanced wood burning which was not controlled in the 2000 base year for this simulation. Dust becomes more wide-spread in the third and fourth quarters.

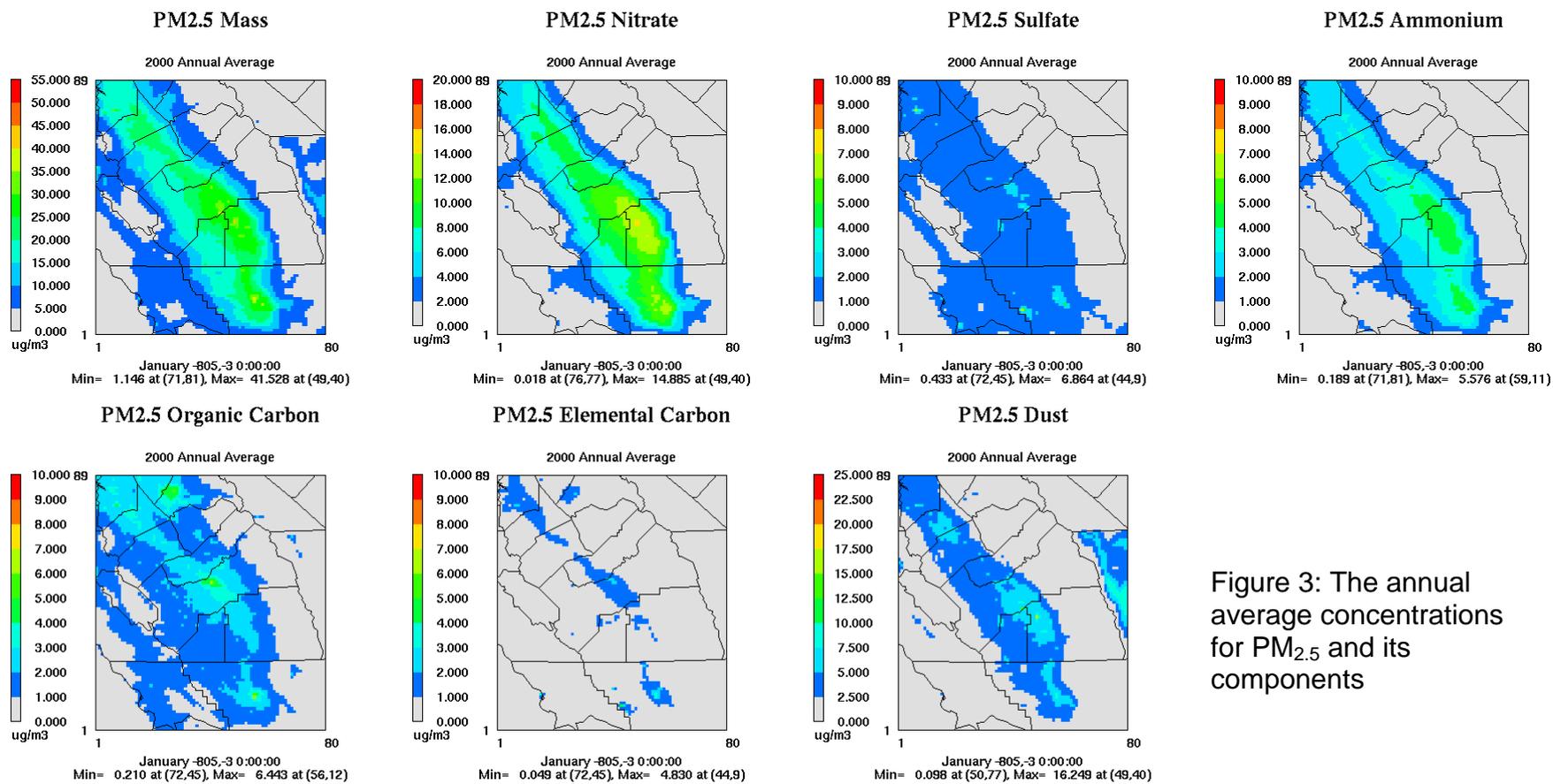


Figure 3: The annual average concentrations for PM_{2.5} and its components

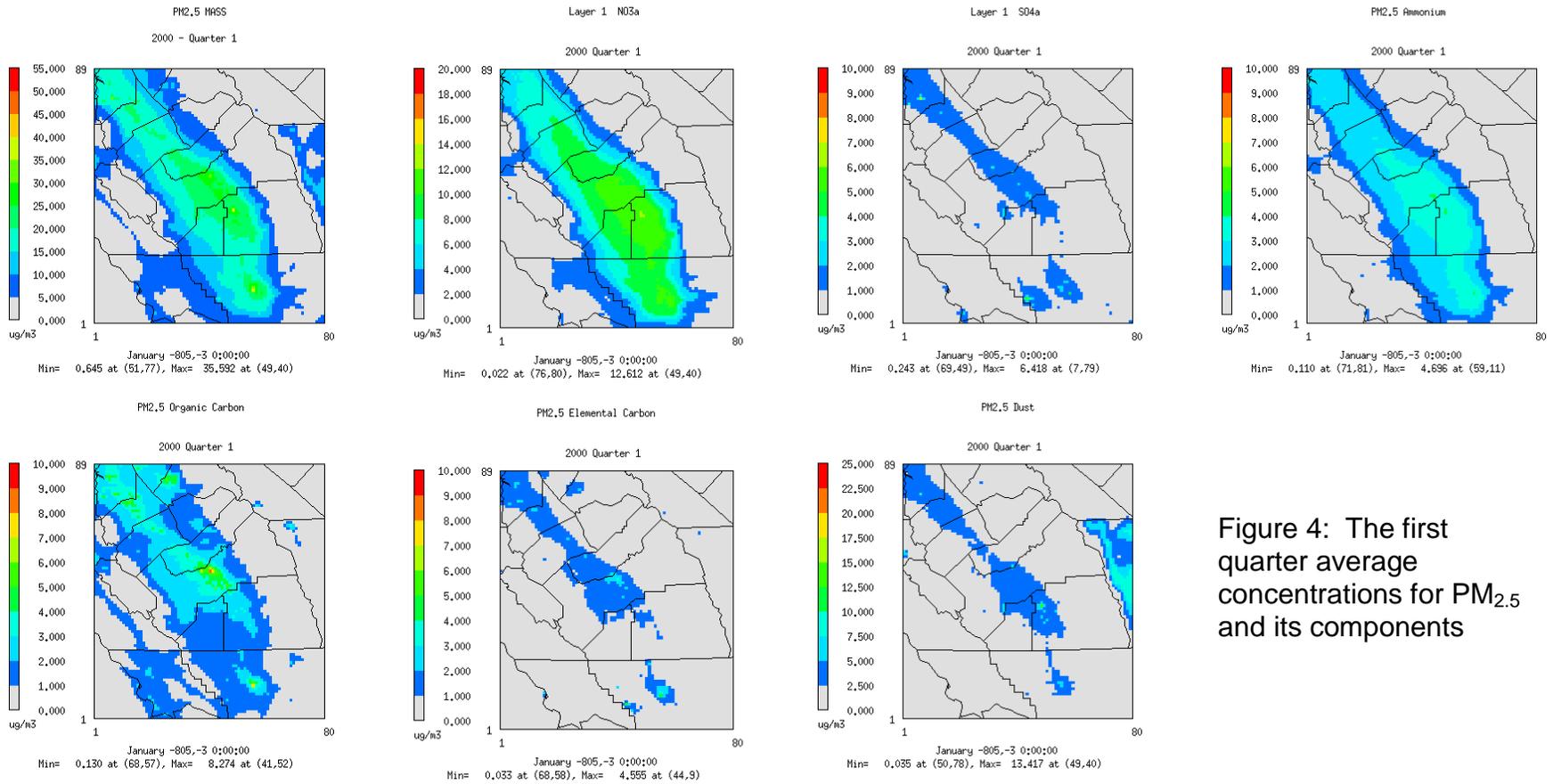


Figure 4: The first quarter average concentrations for PM_{2.5} and its components

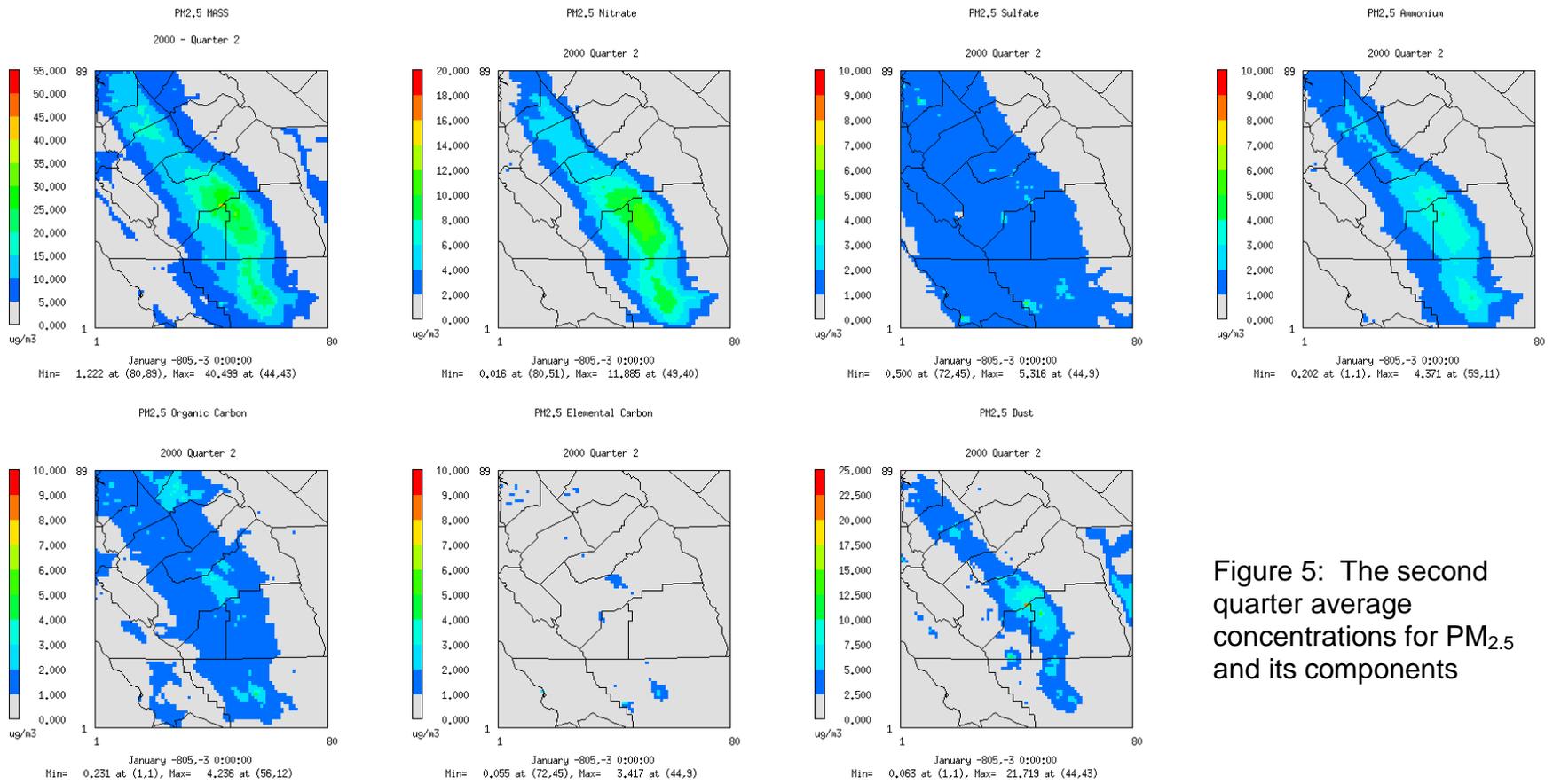


Figure 5: The second quarter average concentrations for PM_{2.5} and its components

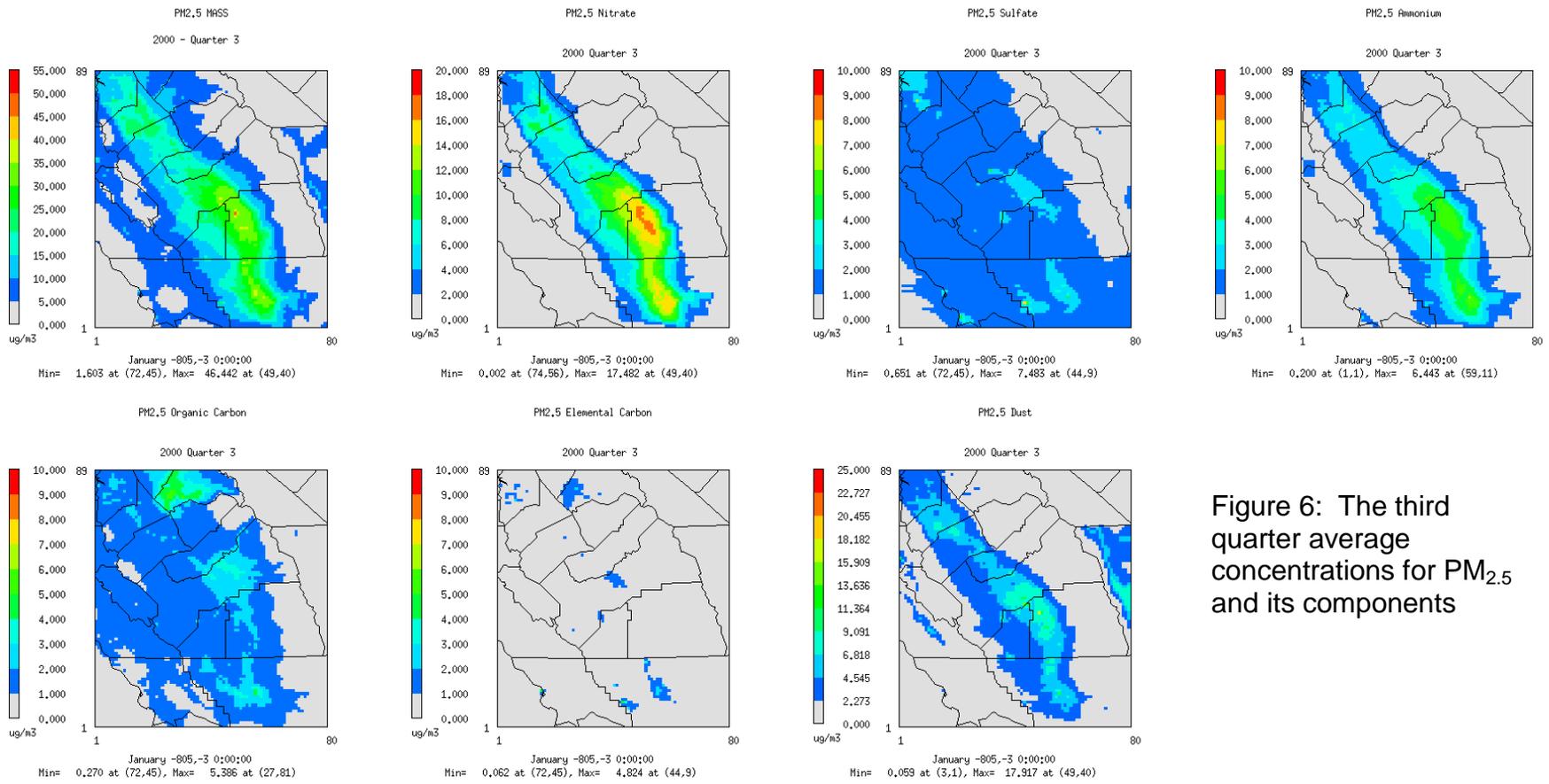


Figure 6: The third quarter average concentrations for PM_{2.5} and its components

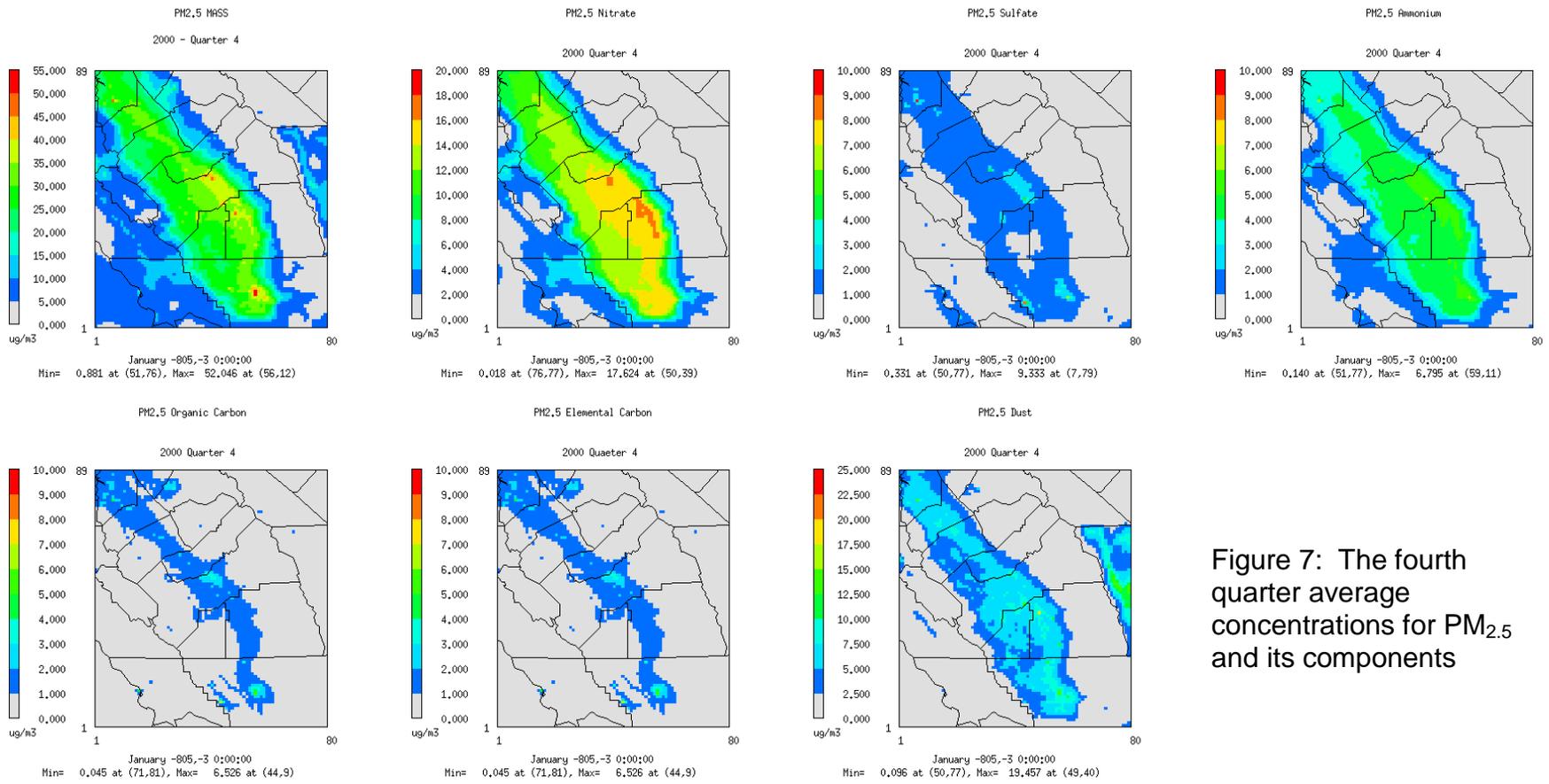


Figure 7: The fourth quarter average concentrations for PM_{2.5} and its components

5.2. Statistics for Mean Fractional Error (MFE) and Bias (MFB):

There are several statistical measures that have been used in the evaluation of episodic ozone simulations. However, their utility in the evaluation of PM models is not universally agreed upon. The general consensus among practitioners of photochemical air quality simulations is that novel concepts are needed to evaluate annual PM simulations. To that end, Boylan and Russell (2006) proposed a two-tier approach for model performance evaluation of PM. These two tiers are based on fractional statistics known as mean fractional error (MFE) and the mean fractional bias (MFB). The first tier is the model performance criteria. This is defined as “the level of accuracy that is considered to be acceptable for modeling applications.” The model performance criteria is met when both $MFE \leq +75\%$ and $MFB \leq \pm 60\%$. The second, and more restrictive, tier is the model performance goal. This is defined as the “the level of accuracy that is considered to be close to the best a model can be expected to achieve.” The model performance goal is met when both $MFE \leq +50\%$ and $MFB \leq \pm 30\%$. This method also allows for less stringent criteria/goals at lower concentrations.

The mean fractional error and mean fractional bias are defined as

$$MFE = \frac{2}{N} \sum_{i=1}^N \frac{|C_i^m - C_i^o|}{C_i^m + C_i^o},$$

and

$$MFB = \frac{2}{N} \sum_{i=1}^N \frac{C_i^m - C_i^o}{C_i^m + C_i^o},$$

where C_i^m and C_i^o are the modeled and observed concentration at a given monitor. The index i indicates an individual member of a set of N matching pairs of simulated and observed values at that monitor. These are centered statistics that give equal weights to simulated and measured values. Note here that we calculate these statistics, as shown in figure 8, for each monitoring site and each specie.

Figure 8 shows both MFE and MFB for $PM_{2.5}$ and its major components. Each point in these graphs represents an individual measurement location. We have used approximately 30 locations within the (4×4) km² domain that reported 24-hour $PM_{2.5}$ filter measurements. Chemical speciation information was used directly when available for that location. For locations where speciation information was not available, information from a nearby speciation site was used. The general procedure used to assign un-speciated monitors to speciation monitors is described elsewhere.

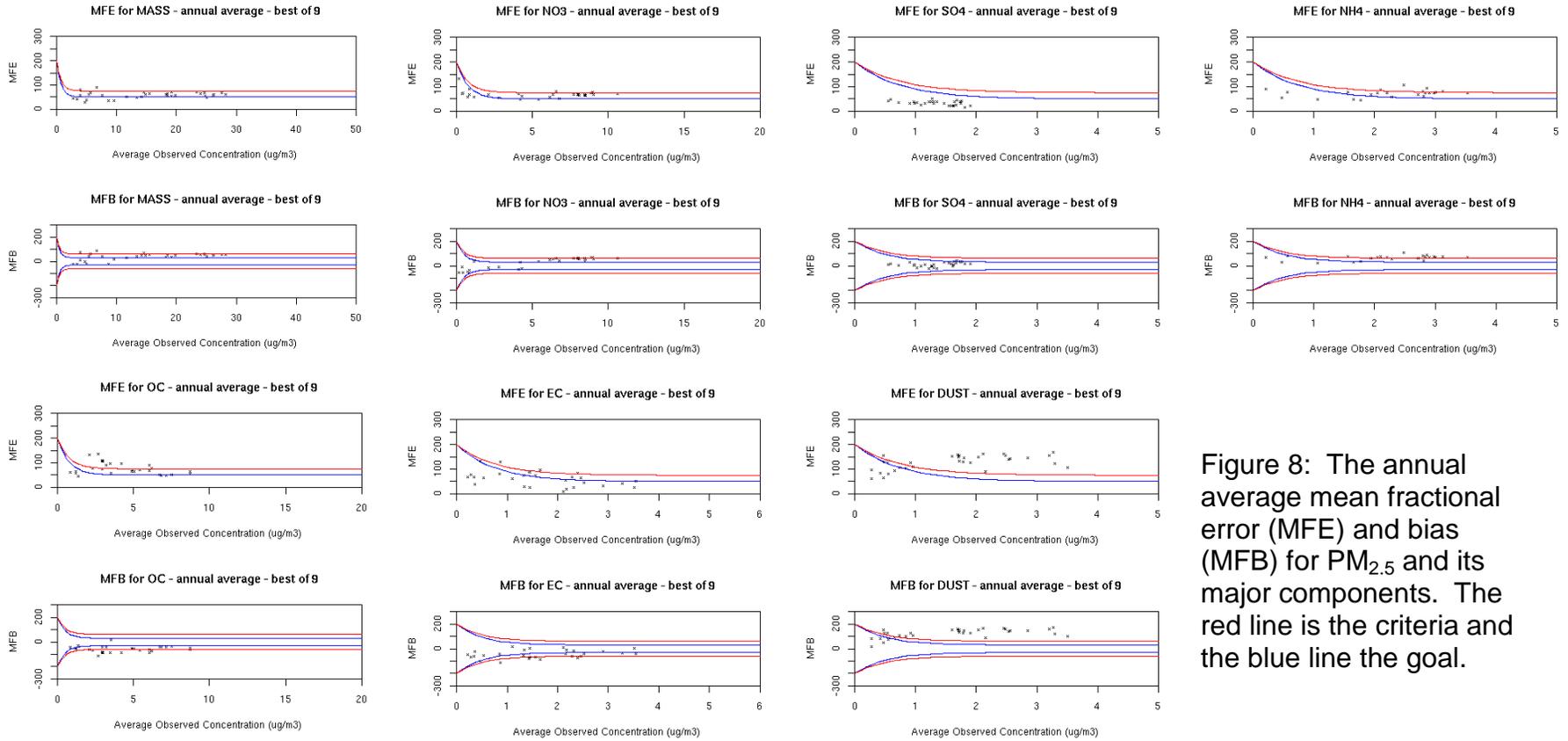


Figure 8: The annual average mean fractional error (MFE) and bias (MFB) for $\text{PM}_{2.5}$ and its major components. The red line is the criteria and the blue line the goal.

In comparing the observations with simulations, we selected the best matched simulated value within nine grid cells of the monitor. The results, not shown here, are very comparable when a nine-cell average concentration is used instead.

It is clear from figure 8 that the 2000 base simulation meets the performance criteria for both MFE and MFB for all species except for dust. The cause of overestimation of dust concentrations is not known at this time and further investigations of emissions inventories may be needed to better understand this discrepancy. It is interesting to note that the apparent overestimation of ammonium nitrate during the third quarter does not affect the model performance appreciably (despite the fact that the third quarter MFE and MFB, which are not shown here, do not meet model performance criteria).

5.3. *Time-History Plots:*

Figures 9-10 show time-history plots for $PM_{2.5}$ and its major components at the Bakersfield and Fresno monitoring stations. These two stations measured high concentrations of particulate matter. It is clear from these two figures that the air quality model is able to reproduce the seasonality of particulate matter production observed in the Central Valley of California. The overestimation of ammonium nitrate in the third quarter is obvious from these figures. The cause of this overestimation is not known at this time. But, we suspect that the simulated meteorology may be responsible for this overestimation. It is also shown that dust is overestimated throughout the year. This may be due to overestimation of dust in the emission inventory. Organic carbon, elemental carbon, and sulfate show satisfactory model performance throughout the year.

6. Conclusion:

We have conducted photochemical particulate matter modeling for the San Joaquin Valley of central California for the base year of 2000. The model performance is satisfactory based on criteria proposed by Boylan and Russell (2006). These criteria were based on an analysis of various particulate-matter modeling conducted in several areas of the United States. Our simulation overestimates ammonium nitrate concentrations for the third quarter. However, this has no significant impact on the future-year design value determination since the Federal Reference Monitor does not report significant amounts of ammonium nitrate for the third quarter. The concentration of dust is also consistently overestimated for the entire year. This may not pose a significant problem since the model results are used in a relative sense and the dust component in the measurements is not very significant. Organic carbon, elemental carbon, and sulfate show satisfactory model performance.

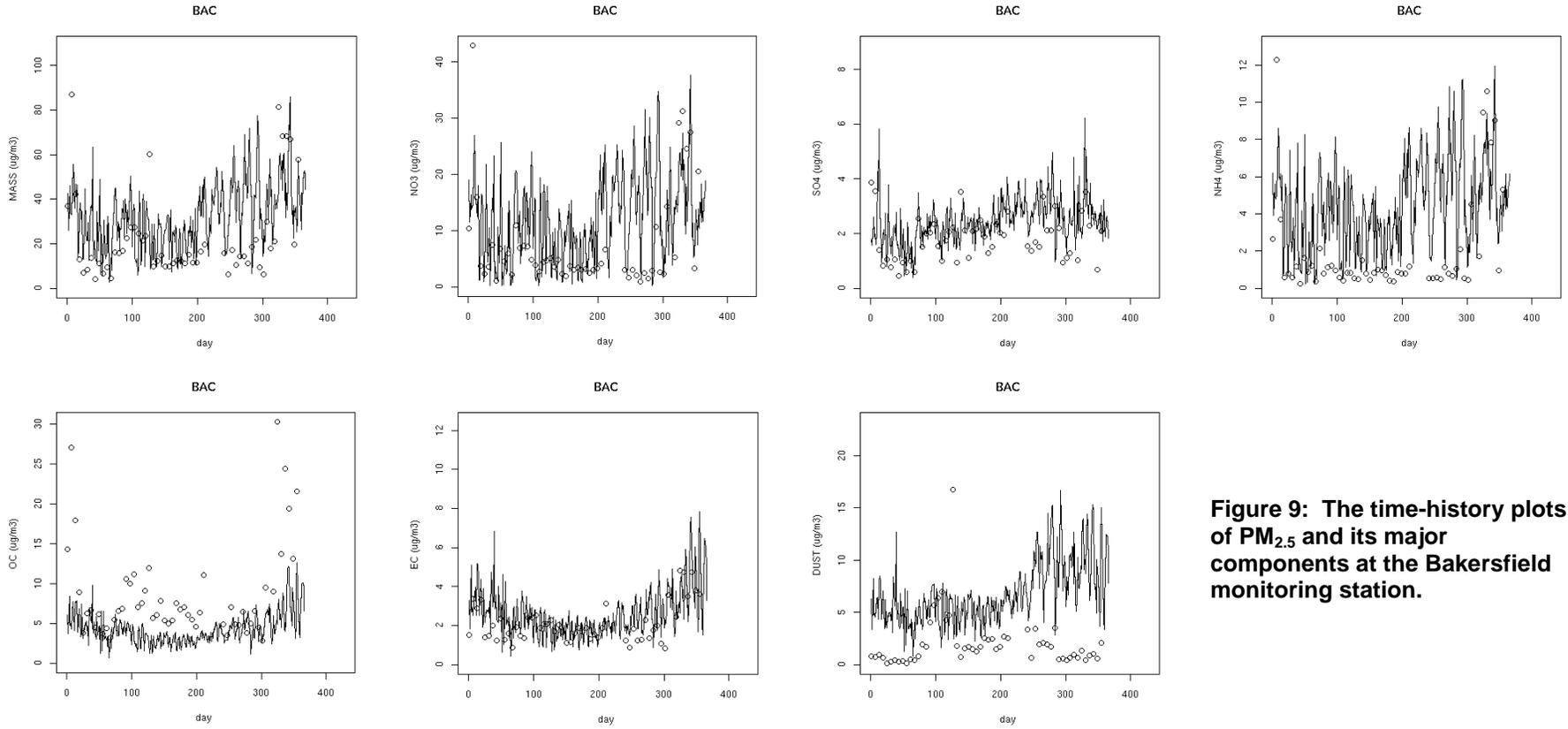


Figure 9: The time-history plots of PM_{2.5} and its major components at the Bakersfield monitoring station.

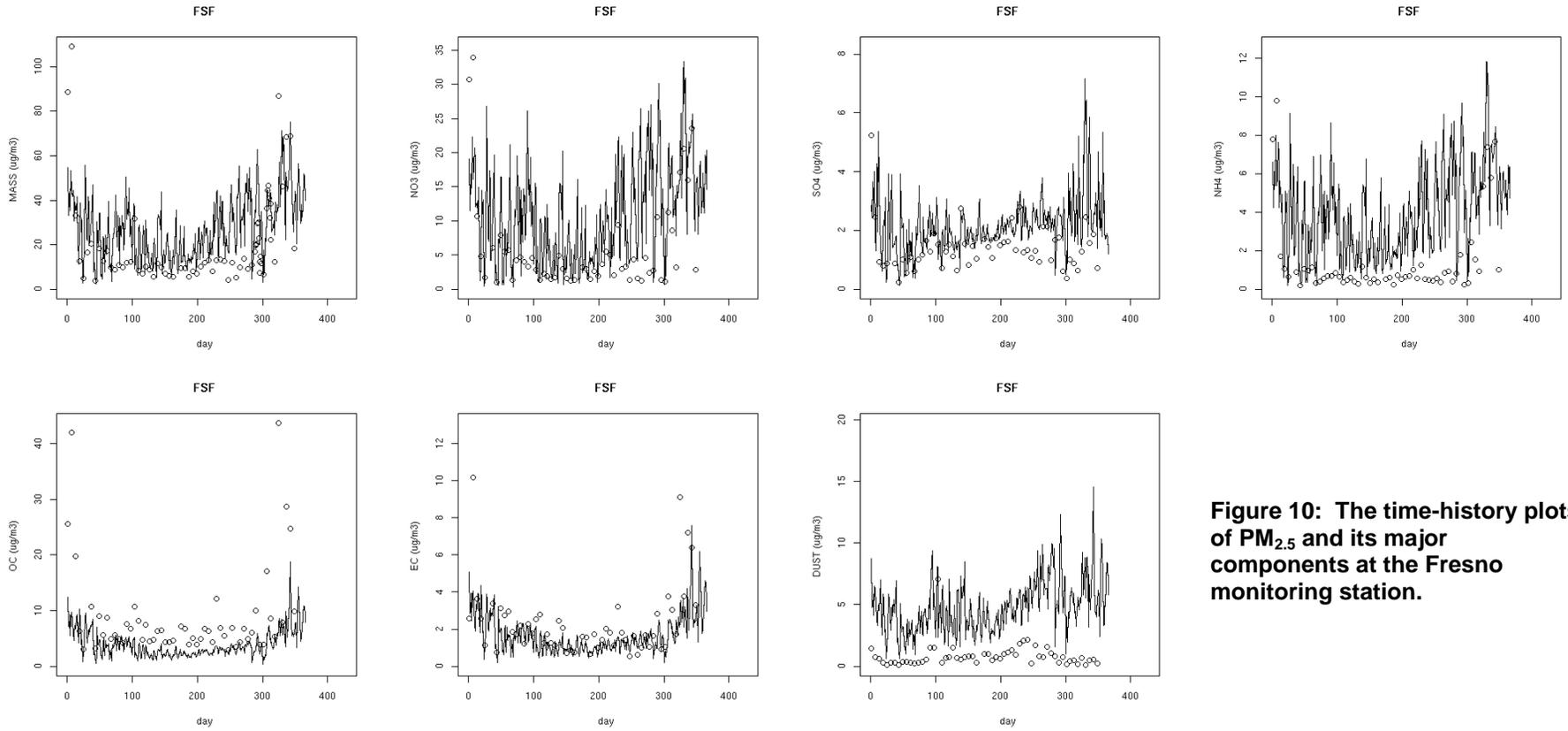


Figure 10: The time-history plots of $\text{PM}_{2.5}$ and its major components at the Fresno monitoring station.

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