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Appendix G

Regional Air Quality Modeling

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Appendix G: Regional Air Quality Modeling

Regional Air Quality Modeling and PM_{2.5} Attainment Demonstration

Introduction

The San Joaquin Valley (SJV) 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 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.

A complex interplay between meteorology and chemistry shapes the aerosol size and composition distribution. Atmospheric particulate matter is made up of both directly emitted particles, like road dust or soot, as well as secondary pollutants formed via chemical reactions with gas-phase compounds. Both primary particles and secondary particles (e.g., ammonium nitrate (NH₄NO₃) and ammonium sulfate ((NH₄)₂SO₄)) make up significant portions of the total PM_{2.5} levels in the SJV. Strong seasonal variations and many different sources, pathways, and components make PM_{2.5} in the region impossible to characterize simply. Effectively understanding the PM_{2.5} problem in the SJV therefore requires comprehensive modeling with well-characterized emissions, meteorology, and chemistry in addition to a thorough knowledge of the observed concentrations of bulk PM_{2.5} and its individual PM components. Model predictions combined with observed particulate concentrations provide the foundation for the EPA-recommended attainment demonstration for PM_{2.5}.

While model predictions represent a significant contribution to the attainment demonstration, it is recommended that models be used in a “relative” sense in conjunction with observations. Given that models may perform differently for each PM component, it may be generally assumed that models will be more successful at predicting concentration changes than absolute concentrations. To dampen the effects of varying degrees of performance amongst modeled species and the potential model bias in predicting absolute species concentrations, the EPA recommends that the models provide “relative response factors” (RRF) to quantify the effects of emissions changes between base and future years. These relative response factors in conjunction with speciated PM_{2.5} measurements form the basis of the Speciated Modeled Attainment Test (SMAT).

In the following sections, the regional air quality modeling performed for use in the Speciated Modeled Attainment Test is outlined (EPA, 2007). Following a description of the modeling methodology and inputs, the steps of the EPA-recommended Speciated Modeled Attainment Test are described in detail. Finally the

modeling results are presented alongside observational data in order to determine the future year attainment status for the San Joaquin Valley.

Regional Air Quality Methodology

As stipulated in the EPA Modeling Guidance, a grid-based photochemical model is necessary to perform the modeled attainment test for PM_{2.5} (EPA, 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 EPA 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 it should have been shown to perform well in the past for similar applications.

The Community Multiscale Air Quality Modeling System (CMAQ) 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 (EPA, 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.

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.

Model Inputs and Setup:

Domain Structure:

Two modeling domains were used for this work. The first modeling domain ("CCAQS") covers 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 ("SJV") is 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.

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 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.

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 (baseline). Quality assurance checks of domain emissions totals and spatial distribution were performed at various steps in emissions processing in order to ensure that the CMAQ emissions input files were sound.

In order to better estimate future air quality, a second 2014 emissions sensitivity scenario was generated incorporating expected reductions from future state and local controls beyond the baseline. These were applied uniformly over the domain on a percentage basis. The percentage difference between baseline and “controlled” emissions was taken from the information in Table 1.

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.

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 (x, y) or (south-north, west-east) direction 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) 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 the 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 SJV. Figure 2 shows the MM5 domains employed to generate meteorological fields for the CMAQ simulation.

Model Years:

CMAQ was run for the year 2000 to provide the basis for the model performance evaluation. It was during 2000 that the California Regional PM₁₀/PM_{2.5} Air Quality Study (CRPAQS) took place. The study resulted in a wealth of data with which to evaluate model performance. As it is necessary to execute simulations for a model reference year and a future year to perform the recommended modeled attainment demonstration, 2005 and 2014 were also simulated. Simulations for all years were driven by the meteorological inputs for 2000, while emissions varied from year to year.

Model Performance Evaluation:

To assure that the modeling system (emissions, meteorology, and air quality) is a satisfactory representation of the period modeled, the estimated emissions, meteorology, and air quality of the base-case simulation need to be compared with observations. Satisfactory performance of the model in simulating observed conditions and responses is a prerequisite for use of the modeling system to evaluate control strategies.

CRPAQS was an extensive and intensive measurement campaign designed to characterize the important chemical and physical processes involved in the formation and evolution of particulate matter in Central California (Chow et al. 2006). The CRPAQS measurement campaign extended from December 1999 through January 2001 and provided a wealth of data from diverse areas for model evaluation.

There are hourly and daily concentration data for a range of gaseous and particulate species at numerous sites available for comparison with CMAQ modeled concentrations. These data will be used to assess model performance temporally and spatially, with a focus on monthly average performance, as recommended for long-term model simulations. Appropriate goals for model performance will be based on the EPA Modeling Guidance and recommendations in the scientific literature on appropriate

measures of model performance for long term PM simulations (EPA, 2007; Boylan and Russell, 2006). A model performance analysis is forthcoming which will be provided at a later date as an appendix to this work.

Speciated Modeled Attainment Test

Regional air quality modeling only represents a portion of the attainment test. In order to perform the EPA-recommended Speciated Modeled Attainment Test, or SMAT, the relative response between the modeled reference and future years must be considered in conjunction with observations. This approach minimizes the uncertainties in predicting future year attainment that result from potential model bias in predicting absolute species concentrations. In the following sections, the Speciated Modeled Attainment Test, as described in the EPA "Guidance on the Use of Models and Other Analyses for Demonstrating Attainment of Air Quality Goals for Ozone, PM_{2.5}, and Regional Haze", is outlined in general terms. Here the recommended procedure for combining model results (relative response factors (RRFs)) with speciated and bulk observations (STN and FRM measurements) in order to determine future year attainment status is explained. This is followed by a description of the application of the SMAT procedure to the San Joaquin Valley to determine future year PM_{2.5} attainment status for the region.

General Procedure of SMAT

Step 1. Calculate the observed quarterly mean bulk PM_{2.5} concentration and composition for each measurement site. The quarterly mean species concentrations can be calculated by multiplying the observed percentage contribution of each species against the quarterly mean bulk PM_{2.5} design value. This design value is calculated from the bulk FRM concentrations averaged over a number of years (generally three but can be a weighted average spanning 5 years), one of which should be the modeled reference year. The procedure to speciate this bulk design value is described in the "SANDWICH" section below.

Step 2. Calculate the RRFs for each quarter and measurement site. Relative response factors are calculated using model results. For species *i*, site *j*, and quarter *k*, the RRF is given by the following equation:

$$RRF_{ijk} = ([C_{i, \text{quarter } k \text{ of future year}}] / [C_{i, \text{quarter } k \text{ of the base year}}]);$$

C_i represents the quarterly modeled concentration (often averaged over a number of model cells near the location of the measurement site) for the reference year and the future year attainment target. The number of model cells recommended for use in the average depends on the size of the grid cell and is justified by the long PM_{2.5} sampling times, the representative spatial scale of the monitors, and the desire to offset any potential errors stemming from the geometry of the superimposed grid system.

Step 3. Multiply the quarterly, site-specific model-based RRFs from step 2 and speciated observations from step 1 to estimate future quarterly species concentrations.

Step 4. Sum the future quarterly species concentration estimates from step 3 to estimate a future quarterly $PM_{2.5}$ estimate at each monitoring site and then average these for a projected future year annual $PM_{2.5}$ concentration for each monitoring site.

Step 5. Compare the future year annual average $PM_{2.5}$ concentrations from step 4 to the annual $PM_{2.5}$ standard of $15.0 \mu\text{g}/\text{m}^3$. If all sites have projected $PM_{2.5}$ concentrations below the standard, the attainment test is passed.

These are the basic steps of SMAT. The following sections examine the attainment test in more detail, starting with the calculation of the base year design values against which the model-based RRFs are multiplied.

Speciated Base Year Design Values

Federal Reference Method

Federal Reference Method (FRM) $PM_{2.5}$ mass measurements provide the basis for nonattainment designations. For this reason it is recommended that the FRM data also be used to project future air quality and progress towards attainment of the health-based National Ambient Air Quality Standard (NAAQS) for $PM_{2.5}$. However, given the complex physicochemical nature of $PM_{2.5}$, it is necessary to consider individual species as well. While the FRM measurements give the mass of the bulk sample, a method for apportioning this bulk mass to individual $PM_{2.5}$ components is a first step towards determining the best targets for emissions controls in order to reach NAAQS levels in a timely manner.

The FRM measurement protocol finds its roots in the past epidemiological studies of health effects associated with $PM_{2.5}$ exposure. It is upon these studies that the NAAQS is based. The protocol is sufficiently detailed so that results might be easily reproducible and involves the measurement of filter mass before and after sampling after equilibrating at narrowly defined conditions. Filters are equilibrated for more than 24 hours at a standard relative humidity between 30 and 40% and temperature between 20 and 23 °C. Due to the sampler construction and a lengthy filter equilibration period, however, FRM measurements are subjected to a number of known positive and negative artifacts. FRM measurements do not necessarily capture the $PM_{2.5}$ concentrations in the atmosphere and can differ substantially from what is measured by speciation monitors (e.g., STN). Nitrate and semi-volatile organics can be lost from the filter during the equilibration process, and particle bound water associated with hygroscopic species like sulfate provides a positive artifact. These differences present an area for careful consideration when one attempts to utilize speciated measurements to apportion the bulk FRM mass to individual species.

Given that (1) attainment status is currently dependent upon FRM measurements and (2) concentrations of individual PM_{2.5} species need to be considered in order to understand the nature of and efficient ways to ameliorate the PM_{2.5} problem in a given region, a method has been developed to speciate bulk FRM PM_{2.5} mass with known FRM limitations in mind. This method is referred to as the measured **S**ulfate, **A**adjusted **N**itrate, **D**erived **W**ater, **I**nferred **C**arbonaceous material balance approach or "SANDWICH". SANDWICH is based on speciated measurements from other (often co-located) samplers, such as those from the Speciated Trends Network (STN), and the known sampling environment of the FRM. The approach serves to provide mass closure, reconciliation between speciated and bulk mass concentration measurements, and the basis for a connection between observations, modeled PM_{2.5} concentrations, and the air quality standard.

SANDWICH

Given that the FRM is the basis for attainment status, the reconstructed PM_{2.5} mass should be based on the composition of the mass measured by the FRM. SANDWICH was developed in order to attribute portions of the bulk FRM mass to different components using STN measurements while also considering the limitations of the FRM monitor. Nitrates are often lost from the FRM filter along with semivolatile organics, and water bound to the inorganics also comprises a portion of the FRM mass. The main steps in estimating the PM_{2.5} composition are as follows:

- (1) calculate the nitrate retained on the FRM filter using hourly relative humidity and temperature alongside STN nitrate measurements,
- (2) calculate quarterly averages for retained nitrate, sulfate, elemental carbon, ammonium (or sulfate degree of neutralization, $[\text{NH}_4^+]/[\text{SO}_4^{2-}]$, if not using ammonium measurements directly),
- (3) calculate particle bound water using the concentrations of ammonium, sulfate, and nitrate, using an equilibrium model like the Aerosol Inorganic Model or a polynomial equation derived from model output, and
- (4) calculate organic carbon mass (OCM_{mb}) by difference, subtracting all inorganic species (including blank mass) from the PM_{2.5} mass.

Total PM_{2.5} mass is given by

$$\text{PM}_{2.5 \text{ FRM}} = [\text{SO}_4^{2-}] + [\text{NO}_3^-]_{\text{FRM}} + [\text{NH}_4^+]_{\text{FRM}} + [\text{EC}] + [\text{Other}] + [\text{OCM}_{\text{mb}}] + [\text{H}_2\text{O}] + [\text{blank mass} = 0.5 \mu\text{g}/\text{m}^3]$$

where all concentrations have units of $\mu\text{g}/\text{m}^3$ and

$[\text{SO}_4^{2-}]$ = measured sulfate

$[\text{NO}_3^-_{\text{FRM}}]$ = nitrate retained on the FRM filter

$[\text{NH}_4^+_{\text{FRM}}]$ = ammonium associated with the nitrate and sulfate on the FRM filter

[EC] = measured EC

Other = other inorganic mass; e.g., crustal material or sea salt

$[\text{OCM}_{\text{mb}}]$ = organic carbon mass calculated by difference by adding all inorganic species and subtracting from the FRM $\text{PM}_{2.5}$ mass. Organic carbon measurements may also be used if it seems that the OC by mass balance is clearly under or overestimated.

$[\text{H}_2\text{O}]$ = water bound to the hygroscopic species; here, calculated using a polynomial equation dependent on the concentrations of sulfate, nitrate, and ammonium or using an inorganic aerosol equilibrium model.

Blank mass represents the mass passively collected on the filter and is assumed to be held constant at a value of $0.5 \mu\text{g}/\text{m}^3$.

SANDWICH may be applied directly in areas where FRM and speciation monitors are collocated. When that is not the case, the following calculations and adjustments may still be applied using spatially interpolated speciation data or some other means to estimate the speciation. The speciation concentrations referred to in the following paragraphs can be represented, therefore, by measurements from a speciation monitor collocated with the FRM or by interpolated values for the species measured by speciation monitors in the region.

The first step in estimating the speciation of the bulk sample is to assume that, due to the stability and nonvolatility of sulfate, sulfate measured by the speciation samplers is similar to the sulfate captured in the FRM sampler. The same is assumed for [EC]. As mentioned above, a passively collected mass of $0.5 \mu\text{g}/\text{m}^3$ is assumed. Estimation of other species' contributions to the FRM mass is described in the following sections.

Adjusted Nitrate

The FRM does not retain all of the semi-volatile $\text{PM}_{2.5}$ mass, and at warmer temperatures, loss of particulate nitrate from filters has been widely observed (Chow et al., 2005). In order to estimate how much nitrate is retained on the FRM filter, simple thermodynamic equilibrium relations may be used. Necessary inputs include 24-hour average nitrate measurements and hourly temperature and relative humidity data. Frank (2006) suggests the following methodology for estimating retained nitrate:

(1) For each hour (i) of the day, calculate the dissociation constant, K_i , from ambient temperature and relative humidity.

For $RH < 61\%$: $\ln(K) = 118.87 - (24084/T) - 6.025 \ln(T)$, where T is temperature in kelvins and K is in nanobars.

For $RH \geq 61\%$, K is replaced by: $K' = [P_1 - P_2 (1-a) + P_3 (1-a)^2] \times (1-a)^{1.75} \times K$, where a is "fractional" relative humidity and

$$\ln(P_1) = -135.94 + 8763/T + 19.12\ln(T)$$

$$\ln(P_2) = -122.65 + 9969/T + 16.22\ln(T)$$

$$\ln(P_3) = -182.61 + 13875/T + 24.46\ln(T)$$

(2) From that, calculate the nitrate retained on the filter:

$$\text{Retained Nitrate} = \text{STN nitrate} - [745.7/T_R \times (\kappa-\gamma) \times 1/24 \times \sum (i=1 \text{ to } 24) (K_i)^{0.5}]$$

where T_R is the daily average temperature for the sampled air volume (K), K_i is the dissociation constant for NH_4NO_3 at ambient temperature for hour i, and $(\kappa-\gamma)$ relates to the temperature rise of the filter and vapor depletion from the inlet surface and is assumed to have a value equal to 1 (Hering and Cass, 1999). For further details, please refer to Frank (2006).

Ammonium

All nitrate on the FRM filter is assumed to be neutralized by ammonium. Ammonium associated with nitrate on the FRM filter, therefore, is given by

$$[\text{NH}_4]_{\text{NO}_3, \text{FRM}} = 0.29 \times [\text{NO}_3]_{\text{FRM}}$$

where $[\text{NO}_3]_{\text{FRM}}$ is the nitrate remaining on the FRM filter and 0.29 is the mass ratio of NH_4 to NO_3 if fully neutralized.

The form of $(\text{NH}_4)_2\text{SO}_4$, however, can vary depending on location and season. Sulfate may or may not be fully neutralized. In order to determine the amount of ammonium associated with the sulfate aerosol, the ammonium difference between the STN and FRM filter needs to be determined. Some studies point to a loss of STN NH_4 during sampling conditions where nitrate volatilization is favored. While the volatilized NO_3 will be recaptured on the basic nylon filter and reported as nitrate, the associated ammonium, not sharing the same affinity for the basic filter, may pass through. In some cases, an adjustment assuming a loss of STN NH_4 corresponds more closely with the NH_4 on the FRM filter; in other cases, the unadjusted measurement agrees better with FRM NH_4 . For the calculations for the SJV, an area rich in NH_3 , NH_4 on the filter is assumed to be the measured STN NH_4 minus any losses associated with fully neutralized nitrate (as NH_4NO_3) that may have volatilized off the FRM filter.

$$[\text{NH}_4]_{\text{FRM}} = [\text{NH}_4]_{\text{STN}} - 0.29 \times ([\text{NO}_3]_{\text{STN}} - [\text{NO}_3]_{\text{FRM}})$$

Here, $([\text{NO}_3]_{\text{STN}} - [\text{NO}_3]_{\text{FRM}})$ represents the amount of nitrate mass lost due to volatilization.

Particle Bound Water

At the FRM filter equilibration conditions, hygroscopic aerosol will retain its particle bound water (PBW) and be included in the observed FRM $\text{PM}_{2.5}$ mass. PBW can be calculated using an equilibrium model like the Aerosol Inorganics Model (AIM). AIM requires the concentrations of ammonium, nitrate, sulfate, and estimated H^+ as inputs. In addition to inorganic concentrations, the equilibration conditions are also necessary model inputs. In this case, a temperature of 294.15 K and 35% RH is recommended. For simplification, a polynomial regression equation may be constructed by fitting the calculated water concentration from an equilibrium model and the concentrations of nitrate, ammonium, and sulfate.

Other Species

Other components that may be represented on the FRM filter include elemental carbon, crustal material, sea salt, and passively collected mass. Depending on location, for example, certain species may be neglected (like sea salt for inland areas).

Carbonaceous Mass

While carbonaceous aerosol may make up a large portion of airborne aerosol, speciated measurements of carbonaceous PM are considered highly uncertain. This is due to the large number of carbon compounds in the atmosphere and the measurement uncertainties associated with samplers of different configurations. In the SANDWICH approach, organic carbonaceous mass is calculated by difference. The sum of all non-organic carbon components may be subtracted from the FRM PM_{2.5} mass as an estimate of organic carbon.

After having calculated the species concentrations as outlined above, one can calculate the percentage contribution of each species to the measured FRM mass (minus the blank concentration of 0.5 µg/m³) for each quarter of the years represented by the speciated data. One can then apply those percentages to the base year FRM design value, with the assumption that the years for which the speciation was calculated are representative of all years over which the design value is averaged. For the annual PM_{2.5} attainment demonstration, the speciated reference year FRM design value for each quarter is multiplied by the RRF for each species at each site, averaged together, and summed to get a future year PM_{2.5} concentration. Note that blank mass is kept constant at 0.5 µg/m³ between the base and future years, and future year particle bound water needs to be calculated for the future year values of nitrate, ammonium, and sulfate. A numerical example of the SMAT for the annual PM_{2.5} standard is given in the EPA modeling guidance on pp. 53-56 (U.S. EPA, 2007).

24-hour Attainment Test

The 24-hour attainment test is similar to the attainment test for the annual PM_{2.5} standard. In the case of the 24-hour test, however, the goal is to have the future 24-hour PM_{2.5} design value at or below 65 µg/m³ for all sites. The test has the following steps:

Step 1. Identify the observed 98th percentile 24-hour PM_{2.5} average concentrations for each year (e.g., of the three year period that makes up the reference year design value) and the next highest concentrations for the other quarters.

Step 2. Using the SANDWICH methodology outlined above, calculate the species percentages of the bulk FRM samples for each site, quarter, and year. These fractions should be calculated using days at the high end of the distribution (i.e., days around or above the standard).

Step 3. Calculate RRFs for each species at each site for each quarter from modeled days at the high end of the PM_{2.5} distribution (i.e., modeled days having PM_{2.5} concentrations around or above 65 µg/m³). As in the case of the annual test, for species *i*, site *j*, and quarter *k*, the RRF is given by the following equation:

$$RRF_{ijk} = ([C_{i, \text{quarter } k \text{ of future year}}]/[C_{i, \text{quarter } k \text{ of the base year}}])_j$$

Step 4. Multiply the quarterly, site-specific model-based RRFs from step 3 and speciated observations from step 2 to estimate future quarterly species concentrations.

Step 5. Sum the future quarterly species concentration estimates from step 4 to estimate a quarterly “potential” 98th percentile PM_{2.5} estimate at each monitoring site.

Step 6. Average the highest quarterly values for each year and then compare the future year design values at each site to the 24-hour PM_{2.5} standard of 65 µg/m³. If all sites are at or below the standard, the 24-hour PM_{2.5} attainment test is passed.

A numerical example of an application of the 24-hour PM_{2.5} attainment test is given on pp. 60-63 of the EPA Model Guidance (U.S. EPA, 2007).

SJV Attainment Demonstration for the Annual PM_{2.5} Standard

The SMAT procedure as outlined above was applied for FRM monitors operating in the San Joaquin Valley with minimal deviations from the recommended procedure. The 2006 design value was used as a basis from which to project forward the future year design value. Speciation data for four STN (speciation) sites was used to speciate the FRM mass for all FRM sites. For those sites not collocated with STN monitors, “surrogate” speciation sites were determined based on analysis of CRPAQS data to determine which sites had similar speciation profiles. The composition was assumed to be the same at all three Bakersfield sites (BAC, BGS, and BEP). Similarly, the percent composition at the two Fresno sites (FSF and FSH) was assumed to be the same. In addition, Stockton (SOH), Clovis (CLO), Corcoran (COP), and Modesto (MRM), were assumed to have the same speciation as one of the four speciation sites based on CRPAQS data analysis. The results of that analysis are given in Table 2. For a list of all FRM sites and their associated speciation site, see Table 3.

The steps followed in order to determine future year design values for the FRM sites of the SJV were similar to those outlined above in the generalized description of the SMAT/SANDWICH procedure. Specific points to note are that in the speciation calculations, only days with all the necessary hourly temperature and relative humidity data in addition to values for all major components (ammonium ion, nitrate ion, sulfate ion, and elemental carbon) plus FRM mass were included in the species average calculations. Temperature and relative humidity data were obtained from the ARB’s Air Quality and Meteorological Information System (AQMIS, www.arb.ca.gov/aqd/aqinfo.htm) database for each monitoring station (collocated with the STN sites or nearby if the STN site was not available) for each available hour of the years 2004-2006.

Quarterly average species concentrations were calculated at each STN site using the SANDWICH procedure described above. In addition, a blank mass average of 0.5 µg/m³ was assumed for each quarter and held constant into the future. Modeled concentrations for the reference year (2005) and future year (2014) for each component

were extracted for the FRM sites as a nine-cell average. The relative response factors (as defined above) were calculated for each component for each quarter. These calculations were performed using all modeled days, as we assumed that the selected FRM measurements provided a stable quarterly average value. Finally, particle bound water was calculated using a polynomial algorithm provided by Dr. Bong-Mann Kim of the South Coast Air Quality Management District. Organic mass was calculated by difference between the average total FRM mass and the sum of all other species and blank.

These quarterly species percentages were then multiplied against the reference year design value for 2006 (the average FRM PM_{2.5} concentrations for 2004, 2005, and 2006). The quarterly observed species concentrations were then multiplied by the RRFs and summed and averaged to get a future year PM_{2.5} design value at each FRM site. See Table 3 for the predicted baseline and controlled 2014 PM_{2.5} design values. For the “controlled” 2014 emissions sensitivity scenario described above, future annual PM_{2.5} concentrations at all FRM sites are below the annual PM_{2.5} NAAQS of 15.0 µg/m³, and, therefore, the San Joaquin Valley has passed the speciated modeled attainment test for the annual PM_{2.5} NAAQS.

SJV Attainment Demonstration for the 24-Hour PM_{2.5} Standard

A similar procedure to the attainment demonstration for the annual PM_{2.5} standard was followed for the 24-hour PM_{2.5} standard attainment demonstration. The exception was that only the top 25% of the measured and modeled days for each quarter were used instead of all available days. The top 25% of the days are expected to be more representative of the 24-hour design value than would all available days for a given quarter.

Table 4 shows the projected future year 24-hour PM_{2.5} design values for the top five 2006 design value sites for the controlled emissions sensitivity case. As shown, all sites in the SJV attained the 24-hour standard in 2006, and further emissions controls do not cause any monitors to become non-attainment.

Unmonitored peaks

EPA's modeling guidance (EPA, 2007) describes the "Unmonitored Area Analysis" as an analysis used to ensure that a proposed control strategy will be effective in reducing PM_{2.5} at locations without air quality monitors so that attainment is shown throughout a nonattainment area. The purpose of the analysis is to use a combination of model output and ambient data to identify areas that might exceed the NAAQS if monitors were located there.

This analysis has four major steps. They are:

1. Interpolation of the base year design values to create a set of spatial fields
2. Adjustment of the spatial design value fields using gridded model output gradients (base year values)
3. Application of the gridded model RRFs to the gradient adjusted spatial design value fields
4. Determination if any unmonitored areas are predicted to exceed the NAAQS in the future

We will present a complete analysis of unmonitored areas in a future version of this document. A screening analysis that is designed to assess the possibility of unmonitored violations of the annual PM_{2.5} NAAQS is presented here.

First, an annual-averaged modeled PM_{2.5} field is generated for the entire modeling domain as shown in figure 3. This field is then scrutinized to see if there will be gradients in the field that would give rise to higher values away from monitors if this field were to be used to adjust the interpolated annual-averaged design value field. As seen from figure 3, there are no areas with steep gradients that would result in higher design values than those measured at monitors. That is, for the central and southern part of the Valley where design values are high, the highest modeled concentrations occur at monitors so that there can not be higher values away from monitors.

As mentioned before, this is a simple screening analysis and a complete analysis of the unmonitored areas will be presented in the future.

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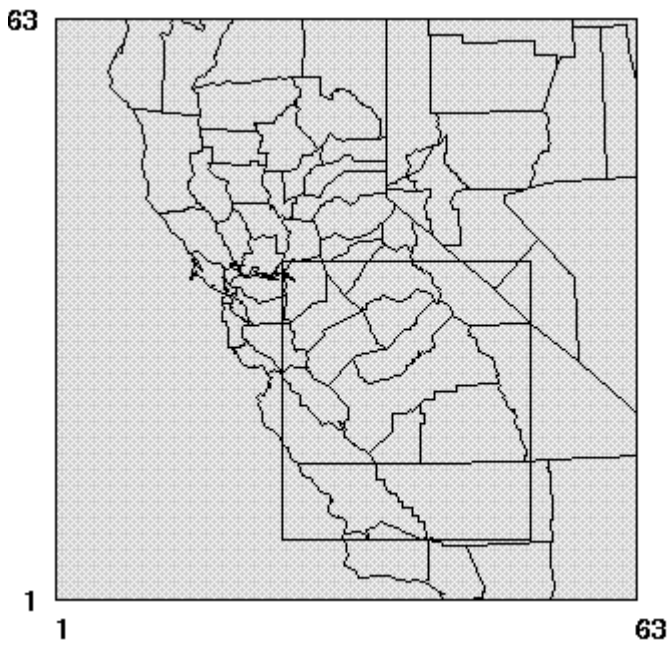


Figure 1. The CCAQS modeling domain with the SJV modeling domain inset.

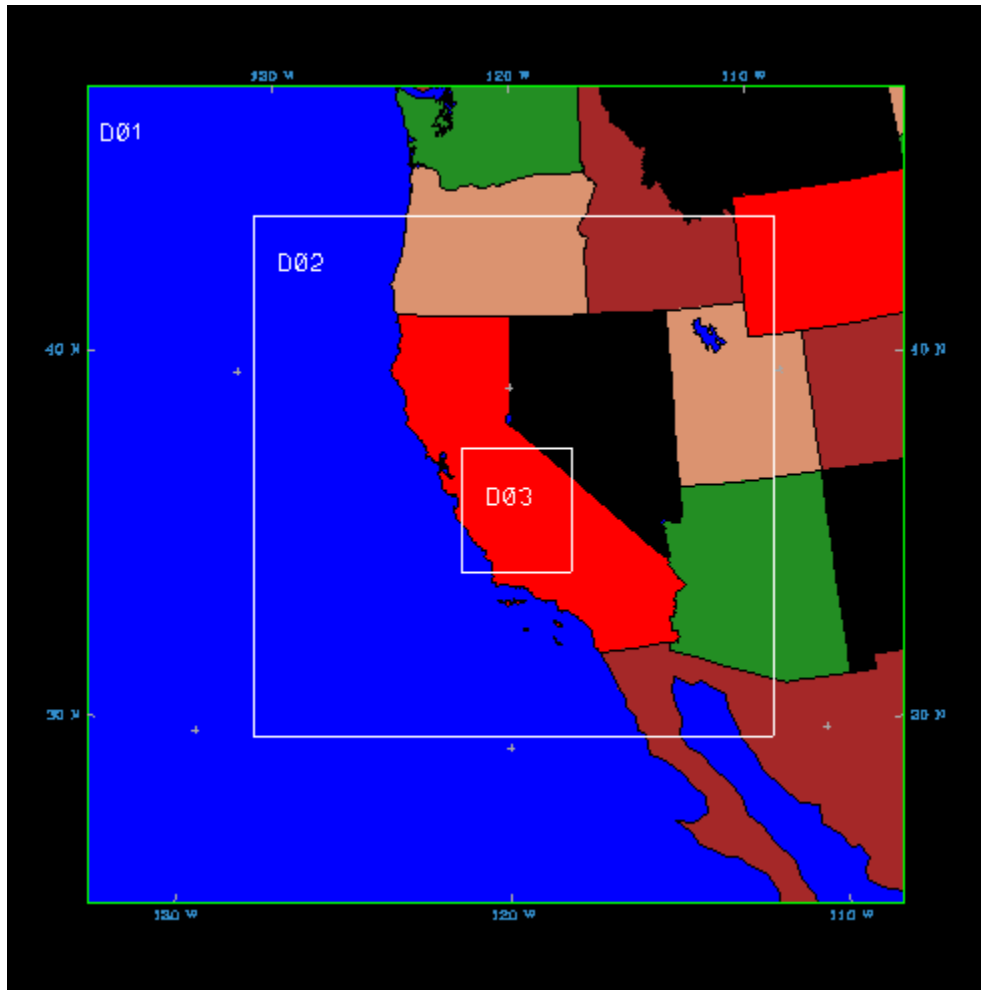


Figure 2. The location of the three nested grids adopted for the numerical modeling of SJV using MM5.

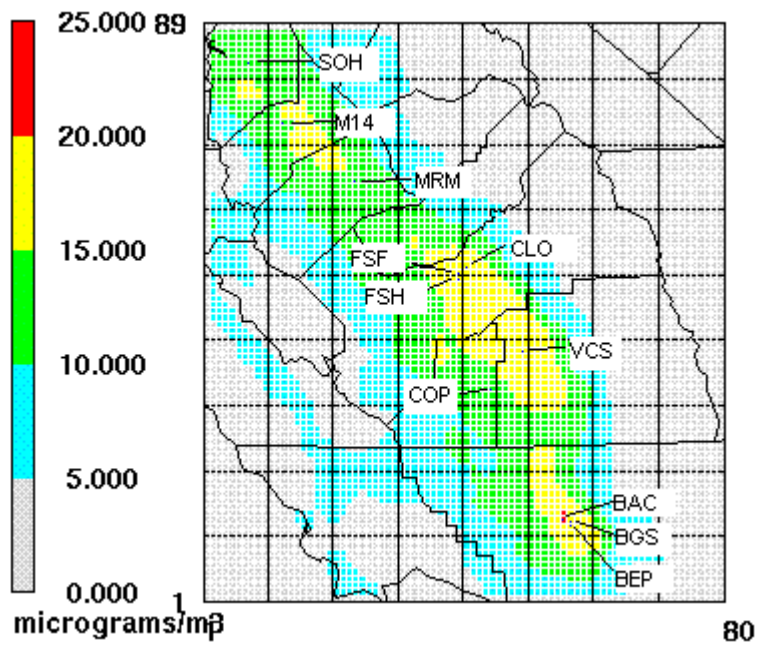


Figure 3. The annual-averaged modeled PM_{2.5} concentrations in the domain.

Table 1. Percentage reduction between 2014 baseline and controlled emissions

	NOx	PM2.5	SOx	ROG
Defined State Measures (Strategy 4/26/07)	20	5	0	6
District Rules (Dft Plan 12/11/07)	4	8	4	0
Total Reduction	24	13	4	6

Table 2. Percent Composition Ratio Based on 2000 Average CRPAQS Data

Site	AmmNitrate	AmmSulfate	EC	OC	Geological	Elements
CLO %	30.78	9.09	10.49	43.22	4.14	2.27
FSF %	26.79	10.15	7.07	49.31	4.16	2.52
CLO to FSF Ratio	1.15	0.90	1.48	0.88	1.00	0.90
COP %	36.44	9.86	8.37	37.87	5.06	2.39
VCS %	35.38	9.53	9.04	39.53	4.37	2.14
COP to VCS Ratio	1.03	1.03	0.93	0.96	1.16	1.12
MRM %	29.33	9.08	10.92	45.50	2.82	2.35
M14 %	26.39	9.84	11.43	46.35	2.71	3.27
MRM to M14 Ratio	0.90	1.08	1.05	1.02	0.96	1.39
SOH %	24.80	11.76	13.13	44.07	2.93	3.31
M14 %	26.39	9.84	11.43	46.35	2.71	3.27
SOH to M14 Ratio	0.94	1.19	1.15	0.95	1.08	1.01

Table 3. Reference and future year annual design values for SJV FRM sites

Site	Code	Speciation	2006 DV	2014 Baseline DV	2014 "Controlled" DV
<i>Bakersfield - 5558 California</i>	BAC	BAC	18.51	15.86	14.28
<i>Bakersfield - 410 E Planz Road</i>	BEP	BAC	18.86	16.26	14.70
<i>Bakersfield - Golden State</i>	BGS	BAC	18.64	15.98	14.39
<i>Clovis - N Villa Avenue</i>	CLO	FSF	16.39	14.10	12.72
<i>Corcoran - Patterson Avenue</i>	COP	VCS	17.24	14.75	13.27
<i>Fresno - 1st Street</i>	FSF	FSF	16.68	14.43	13.01
<i>Fresno - Hamilton and Winery</i>	FSH	FSF	17.16	14.93	13.47
<i>Merced - 2334 M Street</i>	MRM	M14	14.69	12.85	11.76
<i>Modesto - 14th Street</i>	M14	M14	14.10	12.52	11.44
<i>Stockton - Hazelton Street</i>	SOH	M14	12.93	11.77	10.87
<i>Visalia - N. Church Street</i>	VCS	VCS	18.20	16.05	14.47

Table 4. Reference and future year 24-hour design values for SJV FRM sites

Site	Code	Speciation	2006 DV	2014 "Controlled" DV
<i>Bakersfield - 5558 California</i>	BAC	BAC	62.4	46.2
<i>Bakersfield - 410 E Planz Road</i>	BEP	BAC	65.2	45.9
<i>Bakersfield - Golden State</i>	BGS	BAC	64.4	45.3
<i>Fresno - 1st Street</i>	FSF	FSF	58.0	41.2
<i>Fresno - Hamilton and Winery</i>	FSH	FSF	58.5	41.7