Appendix F

Modeling Protocol

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Modeling Protocol

Photochemical Modeling for the 24-Hour $PM_{2.5}$State Implementation Plan in the San Joaquin Valley

Prepared by

California Air Resources Board

San Joaquin Valley Air Pollution Control District

Prepared for

United States Environmental Protection Agency Region IX

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Acronyms:

ARB – Air Resources Board

ARCTAS-CARB – California portion of the Arctic Research of the Composition of the Troposphere from Aircraft and Satellites conducted in 2008

CalNex – Research at the Nexus of Air Quality and Climate Change conducted in 2010

CCOS - Central California Ozone Study

CMAQ Model – Community Multi-scale Air Quality Model

CIT – California Institute of Technology

CRPAQS – California Regional PM_{10}/$PM_{2.5}$ Air Quality Study

FDDA – Four-Dimensional Data Assimilation

FEM – Federal Equivalence Monitors

FRM – Federal Reference Monitors

HNO_3 – Nitric Acid

IMPROVE – Interagency Monitoring of Protected Visual Environments

IMS-95 – Integrated Monitoring Study of 1995

LIDAR – Light Detection And Ranging

MADRID – Model of Aerosol Dynamics, Reaction, Ionization, and Dissolution

MM5 – Mesoscale Meteorological Model Version 5

MOZART – Model for Ozone and Related chemical Tracers

NASA – National Aeronautics and Space Administration

NCAR – National Center for Atmospheric Research

NH_3 – Ammonia

NIOSH – National Institute for Occupational Safety and Health

NOAA - National Oceanic and Atmospheric Administration

NO_x – Oxides of nitrogen

OC – Organic Carbon

PAN – Peroxy Acetyl Nitrate

$PM_{2.5}$ – Particulate Matter with aerodynamic diameter less than 2.5 micrometers

PM_{10} – Particulate Matter with aerodynamic diameter less than 10 micrometers

RRF – Relative Response Factor

RSAC – Reactivity Scientific Advisory Committee

SANDWICH – Application of the Sulfate, Adjusted Nitrate, Derived Water, Inferred Carbonaceous Material Balance Approach

SAPRC – Statewide Air Pollution Research Center

SARMAP – SJVAQS/AUSPEX Regional Modeling Adaptation Project

SIP – State Implementation Plan

SJV – San Joaquin Valley

SJVAPCD – San Joaquin Valley Air Pollution Control District

SJVAQS/AUSPEX – San Joaquin Valley Air Quality Study/Atmospheric Utilities Signatures Predictions and Experiments

SLAMS – State and Local Air Monitoring Stations

SMAT – Application of the Speciated Modeled Attainment Test

SOA – Secondary Organic Aerosol

SO_x – Oxides of Sulfur

STN – Speciated Trend Network

UCD – University of California at Davis

U.S. EPA – United States Environmental Protection Agency

VOC – Volatile Organic Compounds

WRF Model – Weather and Research Forecast Model

1. Introduction

The purpose of this modeling protocol is to detail and formalize the procedures for conducting the 24-hour $PM_{2.5}$ State Implementation Plan photochemical modeling for the San Joaquin Valley. The protocol is intended to communicate up front how the modeling attainment test will be performed. In addition this protocol discusses additional analyses that are intended to help corroborate the modeled attainment test.

Recent History of SIPs in SJV and the Need for a 24-hour $PM_{2.5}$ SIP

Over the past decade, the San Joaquin Valley Air Pollution Control District (SJVAPCD or District) has adopted State Implementation Plans (SIPs or Plans) that set forth State and local emission reduction strategies to bring the San Joaquin Valley (SJV) into attainment for federal ozone (O_3) and particulate matter (PM) air quality standards (standards) by specified dates. In 2004, SJVAPCD adopted the 1-hour O_3 SIP. In addition, SJVAPCD adopted the 2007 Ozone Plan to address the 8-hour standard of 0.08 parts per million (ppm) set by U.S. EPA in 1997. On March 1, 2012, U.S. EPA finalized its approval this SIP (76 FR 57846).

Implementation of State and local control measures mapped out in the SJV 2003 PM_{10} Plan, resulted in the Valley reaching attainment of the PM_{10} standard ahead of schedule. In November 2008, the San Joaquin Valley was officially re-designated to attainment for PM_{10} (73 FR 66759). To ensure continued maintenance of PM_{10} attainment, SJVAPCD adopted and U.S. EPA approved the SJV 2007 PM_{10} Maintenance Plan. In 1997, U.S. EPA adopted their first $PM_{2.5}$ standard, which set two levels, an annual standard of 15 $\mu g/m^3$ and a 24-hour standard of 65 $\mu g/m^3$. The SJV 2008 $PM_{2.5}$ Plan adopted by SJVAPCD sets the course for the Valley to attain the 1997 annual standard in 2014. The plan focused on the annual standard, as in 2008, the Valley already met the 24-hour $PM_{2.5}$ standard of 65 $\mu g/m^3$. On September 30, 2011**,** U.S. EPA officially approved the SJV 2008 $PM_{2.5}$ Plan and the approval will be effective on January 9th 2012 (76 FR 69896).

In 2006, U.S. EPA tightened the 24-hour $PM_{2.5}$ standard to 35 µg/m^3, but left the annual standard unchanged. Based on 2006-2008 air quality data, U. S. EPA designated the SJV as nonattainment for the 2006 24-hour $PM_{2.5}$ standard effective December 14, 2009. Per the federal Clean Air Act (Act), the corresponding SIP is due to U.S. EPA three years after designation. Thus, the SJV SIP addressing the 2006 24-hour $PM_{2.5}$ standard is to be submitted to U.S. EPA by December 14, 2012.

1.1. Modeling Roles for the Current SIP

The Act establishes the planning requirements for those areas that routinely exceed the health-based air quality standards. As discussed above, these nonattainment areas must adopt and implement a SIP that demonstrates how they will attain the standards by specified dates. Air quality modeling is an important technical component of the SIP; it is used in combination with other technical information to project the attainment status of an area and to develop appropriate emission control strategies to achieve attainment.

For the current SIP, the SJVAPCD and ARB will jointly develop the emission inventories which are an integral part of the modeling. Working closely with the district, the ARB will perform the meteorological and air quality modeling. The SJVAPCD will then develop and adopt their local air quality plan. Upon approval by the ARB, the SIP will be submitted to U.S.EPA for approval.

1.2. Stakeholder Participation in the SIP Modeling Process

Public participation constitutes an integral part of the SIP development. It is equally important in all technical aspects of SIP development, including the modeling. As the SIP is developed, SJVAPCD and ARB will hold public workshops on the modeling and other SIP elements. Representatives from the private sector, environmental interest groups, academia, and the federal, state, and local public sectors are invited to attend and provide comments. In addition, Draft Plan documents will be available for public review and comment at various stages of plan development and at least 30 days before Plan consideration by the SJVAPCD's Governing Board and subsequently by the ARB Board. These documents will include descriptions of the technical aspects of the SIP.

Stakeholders have the choice to provide written and in-person comments at any of the Plan workshops and public Board hearings. The agencies take the comments into consideration when finalizing the Plan.

1.3. Involvement of External Scientific/Technical Experts and Their Input on the Photochemical Modeling

The California Air Resource Board (ARB) and the San Joaquin Valley Air Pollution Control District (SJVAPCD) plan to engage a group of experts on prognostic meteorological modeling and photochemical particulate matter modeling to help prepare the modeling protocol document (protocol) , which is the blueprint for the air quality modeling portion of the SIP. ARB and district staff will then carry out the work described in the protocol as part of the SIP development.

The structure of the proposed group of technical experts is:

Conveners: John DaMassa – ARB
Samir Sheikh – SJVAPCD

Members: Scott Bohning – U.S. EPA Region 9
Ajith Kaduwela – ARB
James Kelly – U.S. EPA Office of Air Quality Planning and Standards
Michael Kleeman – University of California at Davis
Jonathan Pleim – U.S. EPA Office of Research and Development
Anthony Wexler – University of California at Davis

This technical consultant group will provide technical consultations/guidance to the staffs of the ARB and SJVAPCD during the development of the protocol. This group is expected to provide technical expertise on the following components of the protocol:

- Selection of the physics and chemistry options for the prognostic meteorological and photochemical air quality models
- Selection of methods to prepare initial and boundary conditions for the air quality model

- Performance evaluations of both prognostic meteorological and photochemical air quality models. This includes statistical, diagnostic, and phenomenological evaluations of simulated results.
- Selection of emissions profiles (size and speciation) for particulate-matter emissions.
- Methods to determine of the limiting precursors for $PM_{2.5}$ formation.
- Application of the Sulfate, Adjusted Nitrate, Derived Water, Inferred Carbonaceous Material Balance Approach (SANDWICH) with potential modifications.
- Application of the Speciated Modeled Attainment Test (SMAT).
- Selection of methodologies for the determination of $PM_{2.5}$ precursor equivalency ratios.
- Preparation of Technical Support Documents.

The specific tasks for this group include:

- Attending regular meetings with ARB and SJVAPCD staff (in person or via teleconference) as needed during protocol development. These meeting are expected to take place monthly starting approximately in November 2011.

1.4. Schedule for Completion of the Plan

Final area designations kick-off the three year SIP development process. For the first two years, efforts center on updates and improvements to the Plan's technical and scientific underpinnings. These include the development of emission inventories, selection of modeling periods, model selection, model input preparation, model performance evaluation and supplemental analyses. During the last year, modeling, further supplemental analyses and control strategy development proceed in an iterative manner and the public participation process gets under way. After thorough review the District Board and subsequently the ARB Board consider the Plan. The Plan is then submitted to U.S. EPA. The table below summarizes the overall anticipated schedule for Plan completion:

Table 1-1: The Timeline for Completion of the Plan.

Timeline	Action
November 2011	Emission Inventory Completed
Summer 2012	Modeling Completed
Spring/Summer 2012	Public Workshop(s) on the Draft Plan
October 2012	San Joaquin Valley Governing Board Hearing to consider the Draft Plan
November 2012	ARB Board Hearing to consider the SJV Adopted Plan
December 14, 2012	Plan is due to U.S. EPA

2. Description of the Conceptual Model for the Nonattainment Area

2.1. History of Field Studies in the Region

The San Joaquin Valley (SJV) airshed is perhaps the second most studied airshed in the world, in terms of the number of publications in peer-reviewed international scientific/technical journals and other major reports. The Los Angeles airshed is the first. Major field studies that have taken place in the SJV and surrounding areas are listed in Table 2-1. A comprehensive listing of publications (reports and peer-reviewed journal articles) up to 2005, compiled by Professor John Watson of the Desert Research Institute, can be found at http://www.arb.ca.gov/airways/crpaqs/publications.htm.

The first major air quality study in the SJV, dubbed Project Lo-Jet, took place in 1970 and resulted in the identification of the Fresno Eddy (Lin and Jao, 1995 and references therein). The first Valley-wide study that formed the foundation for a SIP was the San Joaquin Valley Air Quality Study/Atmospheric Utilities Signatures Predictions and Experiments (SJVAQS/AUSPEX) study, also known as SARMAP (SJVAQS/AUSPEX Regional Modeling Adaptation Project). A 1-hour Extreme Ozone Attainment Demonstration Plan based on the SARMAP Study was submitted to the U.S. EPA in 2004 and was approved in 2009 (74 FR 33933; 75 FR 10420). The next major study was the Integrated Monitoring Study in 1995 (IMS-95), which was the pilot study for the subsequent California Regional $PM_{10}/PM_{2.5}$ Air Quality Study (CRPAQS) in 2000 (Solomon and Magliano, 1998). IMS-95 formed the technical basis for the 2003 PM_{10} SIP which was approved by the U.S. EPA in 2006 (71 FR 63642). The area was re-designated as attainment in 2008 (73 FR 66759). The first annual field campaign in the SJV was CRPAQS, and embedded in it was the Central California Ozone Study (CCOS) that took place during the summer of 2000 (Fujita et al., 2001). CRPAQS was a component of the technical foundation for the 2008 annual $PM_{2.5}$ SIP which was approved by the U.S. EPA in 2011 (76 FR 41338; 76 FR 69896), and CCOS was part of the technical basis for the 2007 8-hour O_3 SIP (76 FR 57846).

While CRPAQS is still very relevant to the current 24-hour $PM_{2.5}$ SIP, there are four subsequent studies that are noteworthy for several different reasons. Any of these studies would not form the technical basis for a future SIP itself, but they contributed significantly to our understanding of various atmospheric processes. The first involved NASA making airborne LIDAR measurements in the SJV in June 2003 (Rosen et al., 2006; De Yong, et al., 2006; Lewis et al., 2010). While the $PM_{2.5}$ concentrations are not high in the SJV during non-winter periods, this study demonstrated the utility of airborne LIDARs in studying $PM_{2.5}$ loadings in the SJV.

The second was the U.S. EPA Advanced Monitoring Initiative, which involved flying an aircraft fitted with a high-resolution aerosol LIDAR in the San Joaquin Valley in January 2005 (Lewis et al. 2010). NASA's B200 King Air aircraft equipped with an airborne high-spectral- resolution LIDAR (HSRL) was flown in the SJV for several days. The downward-looking HSRL measured the aerosol optical depth. These vertically-resolved measurements were very useful in determining the horizontal and vertical structure of the $PM_{2.5}$ loadings along the flight paths. This study confirmed that high aerosol loadings occur in urban areas near the surface. This study also provided a sound data set to evaluate the performance of air quality models (Ying, Jackson, and Kaduwela, 2011). Together, this study and the previous NASA study, provide the first example of the applicability of airborne LIDARs in the SJV to study $PM_{2.5}$ loadings.

The third was the California portion of the Arctic Research of the Composition of the Troposphere from Aircraft and Satellites (ARCTAS-CARB) which took place during May-July 2010 (Jacob, et al., 2010).This involved two instrumented aircraft. As Jacob et al. (2010) describe, the planning for the ARCTAS-CARB flights were based on the following questions:

- How good is our current understanding of the HO_x-NO_x-O_3-aerosol photochemical system over the Los Angeles Basin as represented in air quality models?
- How should upwind boundary conditions for simulating air quality in California be specified?

- How do ship emissions and long-range transport affect the sulfur budget in southern California?
- What are the state's emissions of VOCs and greenhouse gases from urban and industrial activities, agricultural operations, and wildfires?

The analyses of ARCTAS-CARB data are still in progress, but some of the findings could be applicable to the current 24-hour $PM_{2.5}$ SIP (Kaduwela and Cai, 2009, Huang et al., 2010; Singh et al, 2010; Pfister et al., 2011a,b; Huang et al., 2011; D'Allura et al., 2011). Note, however, that the ARCTAS-CARB field work was conducted during June-July, 2008 but the high $PM_{2.5}$ loadings in SJV occur during winter months.

The ARCTAS-CARB campaign was considered to be the pilot phase for a more comprehensive multi-platform study known as CalNex 2010 (Research at the Nexus of Air Quality and Climate Change conducted in 2010)(www.esrl.noaa.gov/csd/calnex/). This campaign was coordinated by NOAA and CARB together with researchers from several universities and national laboratories. It involved several instrumented aircraft, an instrumented ship, two surface supersites (one in Bakersfield and another in Pasadena), and networks of meteorological and ozonesonde measurements. It was designed to answer a much broader set of questions than ARCTAS-CARB did, however the data analysis phase is still in progress and only very preliminary air quality modeling has been conducted to date (Cai and Kaduwela, 2011; Kelly et al., 2011).

Table 2-1: Major Field Studies in Central California and surrounding areas.

Year	Study	Significance
1970	Project Lo-Jet	Identified summertime low-level jet and Fresno eddy
1972	Aerosol Characterization Experiment (ACHEX)	First TSP chemical composition and size distributions
1979-1980	Inhalable Particulate Network	First long-term $PM_{2.5}$ and PM_{10} mass and elemental measurements in Bay Area, Five Points
1978	Central California Aerosol and Meteorological Study	Seasonal TSP elemental composition, seasonal transport patterns
1979-1982	Westside Operators	First TSP sulfate and nitrate compositions in western Kern County
1984	Southern SJV Ozone Study	First major characterization of O_3 and meteorology in Kern County
1986-1988	California Source Characterization Study	Quantified chemical composition of source emissions
1988-1989	Valley Air Quality Study	First spatially diverse, chemical characterized, annual and 24-hour $PM_{2.5}$ and PM_{10}
Summer 1990	San Joaquin Valley Air Quality Study/Atmospheric Utilities Signatures Predictions and Experiments (SJVAQS/AUSPEX) – Also known as SARMAP (SJVAQS/AUSPEX Regional Modeling Adaptation Project)	First central California regional study of O_3 and $PM_{2.5}$
July and August 1991	California Ozone Deposition Experiment	Measurements of dry deposition velocities of O_3 using the eddy correlation technique made over a cotton field and senescent grass near Fresno
Winter 1995	Integrated Monitoring Study (IMS-95, the CRPAQS Pilot Study)	First sub-regional winter study
December	California Regional $PM_{10}/PM_{2.5}$ Air	First year-long, regional-scale effort to measure

1999-February 2001	Quality Study (CRPAQS) and Central California Ozone Study	both O_3 and $PM_{2.5}$
December 1999 to present:	Fresno Supersite	First multi-year experiment with advanced monitoring technology
July 2003	NASA high-resolution lidar flights	First high-resolution airborne lidar application in SJV in the summer
February 2007	U.S. EPA Advanced Monitoring Initiative	First high-resolution airborne lidar application in SJV in the winter
June 2008	ARCTAS - CARB	First measurement of high-time resolution (1-10s) measurements of organics and free radicals in SJV.
May-July 2010	CalNex 2010 (Research at the Nexus of Air Quality and Climate Change)	Expansion of ARCTAS-CARB type research-grade measurements to multi-platform and expanded geographical area including the ocean.

2.2. CRPAQS Relevance to SIP

As discussed in the previous section, CRPAQS has provided key technical information to support SIP development in the San Joaquin Valley. CRPAQS was a public/private partnership designed to advance our understanding of the nature of $PM_{2.5}$ in the Valley and guide development of effective control strategies. The study included monitoring at over 100 sites as well as data analysis and modeling, results of which have been published in over 60 papers and presented at national and international conferences. The field campaign was carried out between December 1999 and February 2001. The key findings remain relevant to the development of the current 24-hr $PM_{2.5}$ SIP. The Study improved our understanding of the spatial and temporal distribution of $PM_{2.5}$ in the Valley, its chemical composition, transport and transformation, and contributing sources. More details on CRPAQS can be found at the following link: http://www.arb.ca.gov/airways/ccaqs.htm

Key findings include the interplay between local and regional components and the resulting concentrations at urban versus rural sites, the sources of carbonaceous material, and identification of limiting precursors for ammonium nitrate formation. A brief description of these findings is provided in sections 2.6 and 2.7. More detailed results will be discussed in the SIP documentation.

2.3. Description of $PM_{2.5}$ Monitoring in the SJV

The San Joaquin Valley nonattainment area (the Valley) is an agricultural region encompassing approximately 64,000 km^2 and with a total population approaching four million. The majority of the population is centered in the large urban areas of Bakersfield, Fresno, Modesto, and Stockton. The nonattainment area includes seven full counties and one partial county. The full counties are San Joaquin, Stanislaus, Merced, Madera, Fresno, Kings, and Tulare. Kern is the partial county with only western Kern County included in the $PM_{2.5}$ nonattainment area. The Valley is bordered on the west by the coastal mountain ranges and on the east by the Sierra Nevada range. These ranges converge at the southern end of the basin at the Tehachapi Mountains.

There are 21 monitoring sites collecting $PM_{2.5}$ data in the San Joaquin Valley (see Table 2-1). These include seven Federal Reference Monitors (FRMs), four $PM_{2.5}$ speciation monitors, and 19 continuous monitors (eleven Federal Equivalence Monitors (FEMs) and eight non-FEMs). Several sites include multiple monitoring instruments running in parallel.

The FRM sampling frequency varies from daily to one in six days. Two monitoring sites, Bakersfield-California and Fresno-1st, collect daily FRM samples. All other FRM monitors operate on a one in three days schedule, with the exception of Corcoran and Fresno-Hamilton which operate on a one in three days schedule during the high season, but reduce frequency to one in six days during the low season.

Table 2-2: $PM_{2.5}$ monitoring sites in the San Joaquin Valley nonattainment area.

AQS SiteID	Site Name	FRM	FEM	non-FEM	Speciation
Fresno County					
060195001	Clovis-N Villa Avenue		1		
060190008	Fresno-1st Street	1		1	1
060195025	Fresno-Hamilton and Winery	1			
060192008	Huron-16875 4th Street			1	
060192009	Tranquillity		1		
Kern County					
060290016	Bakersfield-410 E Planz Road	1			
060290014	Bakersfield-5558 California Avenue	1		1	1
060292009	Lebec-Beartrap Road			1	
Kings County					
060310004	Corcoran-Patterson Avenue	1	1		
060311004	Hanford		1		
Madera County					
060392010	Madera-28261 Avenue 14		1		
Merced County					
060470003	Merced-Coffee		1		
060472510	Merced-2334 M Street	1			
Stockton County					
060772010	Manteca-530 Fishback Rd		1		
060771002	Stockton-Hazelton Street		1		
060773005	Tracy-Airport			1	
Stanislaus County					

060990005	Modesto-14th Street		1		1
060990006	Turlock-S Minaret Street		1		
Tulare County					
061072010	Porterville-1839 Newcomb Street		1	1	
061070009	Sequoia-Ash Mountain			1	
061072002	Visalia-N Church Street	1		1	1
Total		**7**	**11**	**8**	**4**

2.4. $PM_{2.5}$ Air Quality Trends

Table 2-3 lists 98th percentiles and design values for FRM and FEM sites with at least one year of data. All sites in the $PM_{2.5}$ nonattainment area exceed the 24-hour standard, with 2010 design values ranging from 41 µg/m^3 at Stockton-Hazelton to 65 µg/m^3 at Bakersfield-Planz. However, over the last ten years, the San Joaquin Valley has experienced an improvement in $PM_{2.5}$ air quality, although different rates of progress have occurred across the Valley. The biggest decreases, on the order of 25 percent to 45 percent, occurred in the northern and central Valley. The southern San Joaquin Valley, which includes the Bakersfield area, showed lesser improvement in $PM_{2.5}$ concentrations of 17 percent to 35 percent. These design values reflect a three year average of the individual year 98th percentiles. The 98th percentile values for 2010, the most recent year of data, provide a further indication of continuing progress, with values ranging from 34.5 µg/m^3 to 56.2 µg/m^3.

It is important to note that the aforementioned air-quality improvements in the SJV are not entirely due to changes in meteorology. In order to understand the effectiveness of emission control strategies and regulations on ambient air pollution levels, it is important to investigate air quality trends and link them to the impacts from meteorology versus changes in emissions. The strong linkage between meteorological conditions and air pollutant levels can obscure the effects of the change of emission levels over time. Therefore, the meteorological effects need to be removed so that the emissions-related

trends may be studied. The Classification and Regression Trees (CART) method was used to define the relationship between $PM_{2.5}$ concentrations and meteorological conditions in both the Bakersfield and Fresno areas of the San Joaquin Valley. Three years (2004-2006) were selected as base years to define these relationships. The CART model was able to explain approximately 75-80 percent of the variation in daily $PM_{2.5}$ concentrations during these years based on the local meteorological conditions. Based on the CART-defined relationships, daily $PM_{2.5}$ concentrations were predicted for all the other years using the observed meteorological data and assuming the emissions stayed constant (i.e. the predicted concentrations only represent the $PM_{2.5}$ conduciveness of meteorology). The measured $PM_{2.5}$ concentrations were then corrected for the influences of meteorology to estimate the meteorologically adjusted trends. For example, in a year with meteorology conditions that were more conducive to $PM_{2.5}$ formation, $PM_{2.5}$ concentrations were adjusted downward. Conversely, $PM_{2.5}$ concentrations were adjusted upward in years with meteorological conditions that were less conducive.

The meteorology-adjusted trend at Bakersfield indicates a greater decline than the unadjusted trend, while the two trends are generally similar at Fresno. Overall, the meteorology-adjusted trends indicate that the $PM_{2.5}$ annual averages decreased about 40-50 percent in both the Bakersfield and Fresno areas from 1999 to 2010, with an average rate of decrease of approximately 0.8 ug/m^3 per year. These meteorology-adjusted trends provide a more robust indicator of the impacts of emission reductions from on-going control programs

Table 2-3: 98th Percentiles and 24-hour Design Value.

Site Name	98th Percentiles (µg/m^3)													24-hr Design Values (µg/m^3)										
	1999	2000	2001	2002	2003	2004	2005	2006	2007	2008	2009	2010	2011	2001	2002	2003	2004	2005	2006	2007	2008	2009	2010	2011
Bakersfield-410 E Planz Road		76.5	90.6	66.8	47.5	47.6	66.4	64.7	72.2	72.3	65.5	56.2	43.2		78	68	54	54	60	68	70	70	65	55
Bakersfield-5558 California Avenue	98	92.7	94.9	73	48.3	61.5	63.2	60.5	73	64.5	66.7	53.3	65.5	95	87	72	61	58	62	66	66	68	62	62
Clovis-N Villa Avenue	59.2	72.5	71.5	53.2	48.1	52.4	63	51.3	60.9	49	49	44.3	68.5	68	66	58	51	55	56	58	54	53	47	54
Corcoran-Patterson Avenue	53	55.1	89.5	65.1	42.2	49.4	74.5	50.1	57.9	47.9	53.4	46.8		66	70	66	52	55	58	61	52	53	49	
Fresno-1st Street	120	90	75	75	56	52	71	51	67	57.4	55.8	48.8	69.5	95	80	69	61	60	58	63	58	60	54	58
Fresno-Hamilton and Winery		64.8	61.5	71.9	49.7	49.4	71.2	55	57.4	44.5	48.2	37	59.6		66	61	57	57	59	61	52	50	43	48
Merced-2334 M Street	91.9	60	49.3	55.1	44.2	43	48.3	43.8	52.7	54	45.2	35.5	35.4	67	55	50	47	45	45	48	50	51	45	39
Modesto-14th Street	100	71	69	69	47	45	55	52	57.4	53.9	54.5	38.9	54.7	80	70	62	54	49	51	55	54	55	49	49
Stockton-Hazelton Street	79	55	58	50	41	36	44	42	48	61.6	40.4	34.5	44.8	64	54	50	42	40	41	45	51	50	46	40
Turlock-S Minaret Street											53.1	39	57.4											51
Visalia-N Church Street	114	103	96	70	47	54	65	50	59.7	62.1	53.9	36.3	50.7	104	90	71	57	55	56	58	57	59	51	47

2.5. Major $PM_{2.5}$ Components

Four monitoring sites collect $PM_{2.5}$ chemical composition data in the San Joaquin Valley: Bakersfield-California, Fresno-1st, Modesto, and Visalia. The Bakersfield and Fresno speciation monitors are part of the national Speciation Trends Network (STN) while Modesto and Visalia are part of the State and Local Air Monitoring Stations (SLAMS) network. All four sites use SASS samplers (Spiral Aerosol Speciation Sampler, Met One, Grants Pass, OR.) for data collection. The STN data are analyzed by the Research Triangle Institute and the SLAMS data are analyzed by ARB. In recent years, changes were made to the carbon sampling and analysis method. The collection method changed from the MetOne SASS to the URG3000N sampler, which is very similar to the IMPROVE module C sampler. The analytical method was changed from the NIOSH-like thermal optical transmittance method to IMPROVE_A thermal optical reflectance. At Bakersfield, Modesto, and Visalia these changes were implemented in May of 2007. Consequently, these sites have over three years of data collected using the new sampling and analysis method. The Fresno site switched to the new carbon system in April of 2009, so there is less than two years of new data.

Figure 2-1 illustrates the average chemical composition on exceedance days at each of the four speciation sites. Widespread ammonium nitrate is the major contributor to wintertime $PM_{2.5}$ episodes, accounting for 50 percent to 67 percent of $PM_{2.5}$ mass on a typical exceedance day. Carbonaceous aerosol contributions range from 16 percent at Bakersfield to 33 percent at Fresno. Ammonium sulfate, geological material, and elements are smaller components of $PM_{2.5}$.

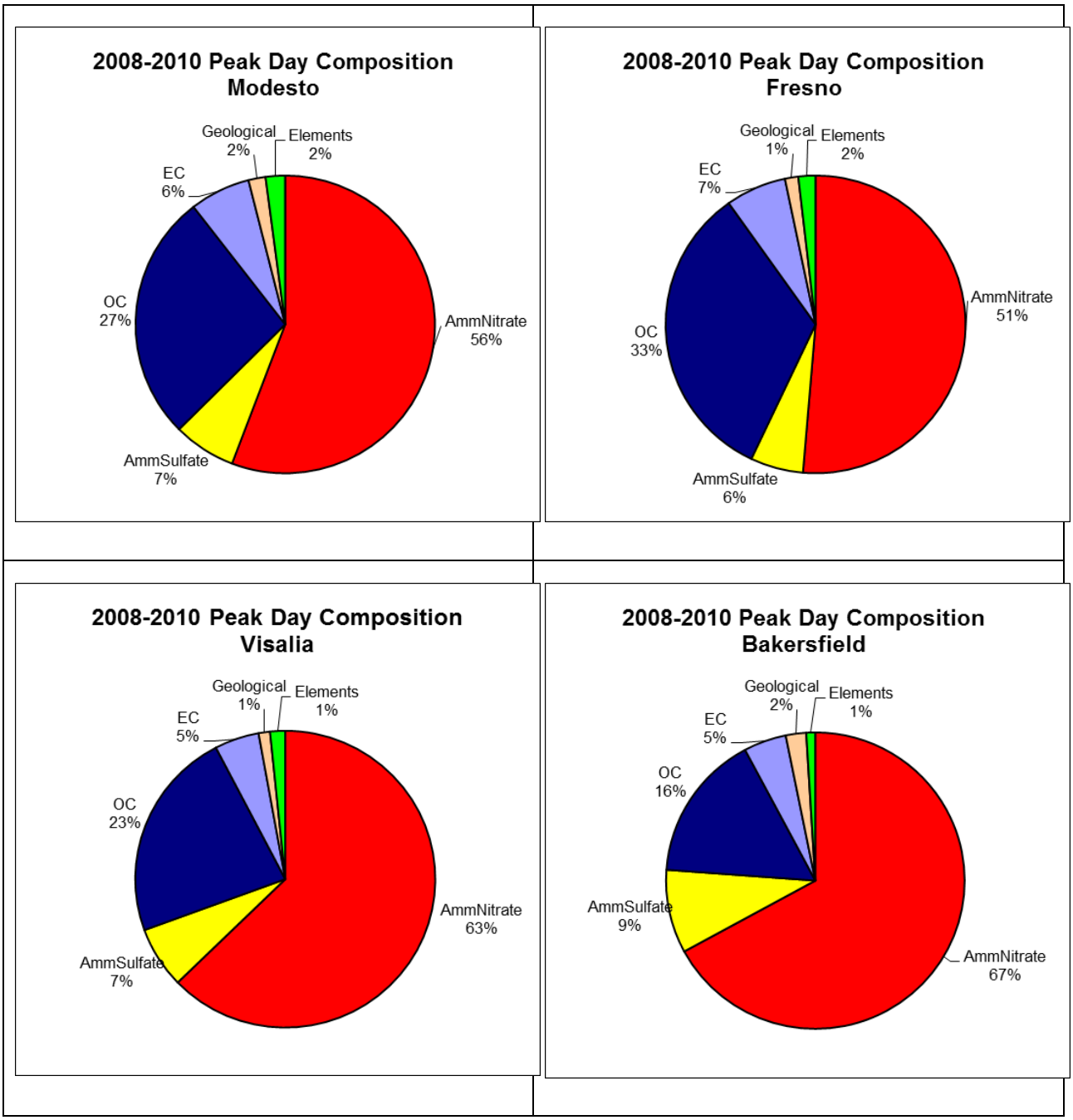


Figure 2-1: PM2.5 composition on an average exceedance day

2.6. Conditions Leading to $PM_{2.5}$ Exceedances

$PM_{2.5}$ concentrations in the San Joaquin Valley exhibit a strong seasonal variability, with highest concentrations during the months of November through February. The highest

$PM_{2.5}$ concentrations occur almost exclusively during multiday pollution episodes under stagnant winter weather when a high pressure system (the Great Basin High) reduces the ventilation in the Valley (Ferreria et al., 2005). These stagnation events, sandwiched between two weather systems, are characterized by low wind speeds, moderate temperatures, vertical atmospheric stability, and high relative humidity. This stable atmosphere prevents precursor gases and primary (or directly emitted) $PM_{2.5}$ released at the surface in the Valley from rapidly dispersing. The moderate temperatures and high relative humidity also enhance the formation of secondary particulate matter, especially ammonium nitrate and sulfate.

$PM_{2.5}$ episodes can last for many days, resulting in multiple exceedances of the 24-hour $PM_{2.5}$ standard. At the beginning of an episode, concentrations are low but increase daily because of both the accumulation of primary pollutants and formation of secondary pollutants (Watson et al, 2002). Concentrations continue to build until there is a change in the weather significant enough to wash out particles through rainfall or increased ventilation of the Valley. The two main episodes captured during CRPAQS had up to 18 days with $PM_{2.5}$ concentrations exceeding 65 $\mu g/m^3$ (Turkiewicz et al., 2006). During episodes, urban sites recorded elevated concentrations earlier than rural sites, and as a consequence, had a greater number of days with high concentrations. However, due to the buildup of $PM_{2.5}$ concentrations, rural sites can achieve concentrations of similar magnitude as urban sites by the end of an episode.

$PM_{2.5}$ particles can be either directly emitted (known as primary particulate matter) or formed via atmospheric reactions (known as secondary particulate matter). Ammonium nitrate, the dominant $PM_{2.5}$ component throughout the Valley, is formed in the atmosphere as a result of chemical reactions between precursor pollutants such as NO_x, VOC, and ammonia. Carbonaceous aerosol, the second most abundant component, is mostly directly emitted, and is the result of contributions from wood combustion, mobile sources, and cooking.

As shown earlier in Figure 2-1, carbonaceous aerosols and ammonium nitrate together comprise approximately 85 to 90 percent of the $PM_{2.5}$ mass during an episode. Each

episode has a local component (primarily carbonaceous aerosols) and regional component (primarily ammonium nitrate). The relative proportions between ammonium nitrate and carbonaceous material differ among urban and rural sites. Since most of the carbonaceous aerosol is emitted into the atmosphere as directly emitted particles, its transport is much more limited compared to gaseous precursors of ammonium nitrate. Concentrations of carbonaceous material are two to three times higher at urban sites than at rural, corresponding to the higher emission density of primary carbon sources in urban areas (Turkiewicz et al., 2006). Ammonium nitrate can be formed both at the surface and aloft. Concentrations of ammonium nitrate, which result from more regional-scale secondary formation and mixing of emissions, can be fairly uniform across urban and rural sites. The spatial homogeneity of ammonium nitrate is influenced by higher wind speeds aloft (which allow more efficient transport), and the diurnal variation in mixing heights (which allow entrainment of ammonium nitrate down to the surface).

Ammonium nitrate is also formed via both daytime and nighttime chemistry. The amount of ammonium nitrate produced will be limited by the relative abundance of its precursors in the atmosphere. In the San Joaquin Valley, the nighttime formation is considered to be the most important pathway (Lurmann et al., 2006). The nighttime pathway involves gas-phase oxidation of NO_2, followed by reaction with ammonia to form ammonium nitrate. Since ammonia is abundant in the Valley in the winter, NO_x is considered to be the limiting precursor. In contrast, the daytime pathway also involves VOCs. Modeling studies that investigated winter episodes in the Valley estimated that reductions in VOC emissions have a small impact on nitrate concentrations only at very high $PM_{2.5}$ concentrations (Pun, Balmori, and Seigneur, 2009). However, at current $PM_{2.5}$ levels the impact was very limited, and in some cases VOC reductions lead to an increase in $PM_{2.5}$ concentrations (Kleeman, et al., 2005). The results of these studies are discussed in greater detail in the following section.

2.7. Past Modeling Efforts and Results

The first peer-reviewed journal article on photochemical simulation in the SJV was conducted using a photochemical box model to study conversion of NO_x to nitrate (Stockwell et al., 2000). That study found that about 33% of emitted moles of NO_x were converted to nitrate. The study also found that about 80% of the nitric acid (HNO_3) produced was in the particle phase, suggesting an ammonia rich environment. These observations were found to be in reasonable agreement with observations. Stockwell et al., (2000) also reported that while increasing NO_x emissions led to increased production of particle nitrate, the reduction of VOC had no appreciable effect on nitrate production. However, increases in VOC emissions led to reduction in nitrates. Taken together, these three observations suggest that the PM nitrate in the SJV is NO_x limited. Pun and Seigneur (2001) also employed a photochemical box model that covered urban Fresno, and determined that VOC controls would be more effective than NO_x controls in reducing $PM_{2.5}$ nitrate. This finding is in conflict with that of Stockwell et al., (2000). However, box modeling approaches have a number of limitations, including lack of transport in/out of the box, robust vertical transport, and use of older chemical mechanisms. In addition, in the work done by Pun and Seigneur (2001), the VOC emissions were increased by a factor of two to improve model performance. As such the box modeling does not fully represent the complete scope of atmospheric variations and has limited usefulness in assessing the responsiveness to VOC controls.

The first published application of a full-scale photochemical grid model with diagnostic meteorological data to simulate PM concentrations in the SJV, which was also the first study outside of the Los Angeles area to include complete PM model performance statistics, was conducted by Held et al. (2004). In this study, the source-oriented external mixture CIT-UCD model was applied during the January 4-6, 1996 episode of the IMS-95 (Solomon and Magliano, 1998). As Held et al., (2004) reported, the CIT-UCD model was able to capture many key air quality features of the January 4–6, 1996 episode including (1) regional ozone, (2) regional PM mass, (3) chemically speciated mass at core stations, and (4) the size distribution of major PM species. Given the robust model agreement with both gas and condensed phase measurements, it

appeared that the CIT-UCD model adequately captured the fundamental chemistry and transport in the IMS-95 domain, suggesting that this model could be used to explore various control scenarios designed to improve the air quality in the SJV. The results reported in this publication also confirmed previous unpublished findings based on the application of UAM-Aero to the same IMS-95 episode (Kaduwela, 2003). These findings were a part of the SJV's 2003 PM_{10} SIP. In a follow-up analysis, Held et al. (2005) compared the source apportionment $PM_{2.5}$ obtained using the CIT-UCD model with that obtained using the Chemical Mass Balance method and concluded that the model was able to predict source contributions to airborne particulate matter at all locations and times throughout the study domain.

Investigation of precursor limitations for the January 4-6, 2006 IMS-95 episode using the CIT-UCD model revealed that NO_x controls were the most effective control strategy to reduce $PM_{2.5}$ concentrations (Kleeman, Ying, and Kaduwela, 2005). A 50 percent reduction in NO_x in the SJV resulted in a 25 percent reduction in total nitrate, while a 50 percent reduction in VOCs resulted in a 17.5 percent reduction. A 50 percent reduction in ammonia resulted in a 10 percent reduction in total nitrate. However, to evaluate the significance and effectiveness of VOC controls in the context of control strategy design, the study's isopleths of $PM_{2.5}$ nitrate response to combined NO_x/VOC emission reductions provide more in-depth information. Modeled isopleths show that, based on the shapes of the graphs, NO_x controls are the most effective approach to reduce $PM_{2.5}$ nitrate concentrations at Fresno and the location of the highest modeled $PM_{2.5}$ nitrate concentration. Once NO_x controls are taken into consideration, VOC emission reductions produce essentially no benefit, and in some instances, may actually lead to an increase in $PM_{2.5}$ nitrate formation. Nitrogen-containing molecules such as PAN can act as temporary sinks for NO_2. When VOCs are controlled, the reduced availability of certain radicals which are generated from VOCs reduces the amount of NO_2 that is sequestered, thereby increasing the availability of NO_2 and enhancing ammonium nitrate formation (Meng et al., 1997). This may be generally true not only for PAN, but also for organic nitrates which can lead to increases in NO_x and ozone

concentrations if emissions of specific VOC compounds are controlled (Farmer et al., 2011).

It was also revealed in a subsequent analysis of the same episode that approximately 45-57 percent of the $PM_{2.5}$ nitrate and 34-40 percent of the $PM_{2.5}$ ammonium ion in the SJV were formed from precursor gaseous species released from sources upwind of the modeling domain (Ying and Kleeman, 2006). However, it is important to note that the modeling domain did not include the entire Valley, with the domain starting just north of Fresno.

Longer periods were simulated as a part of CRPAQS (Solomon and Magliano, 1998) using the Community Multi-scale Air Quality (CMAQ) model (Liang and Kaduwela, 2005; Liang et al., 2006; Fahey et al., 2006; Livingstone et al., 2009), CMAQ-UCD model (Zhang et al., 2005), UCD/CIT model (Ying et al., 2008a,b; Ying et al., 2009a,b; Ying, 2011), and the CMAQ-MADRID model (Pun, Balmori, and Seigneur, 2009; Zhang et al., 2010). The UCD/CIT model is an improved version of the CIT-UCD model with significant modifications made at the University of California at Davis.

The first group of simulations for the December 2000-January 2001 episode of CRPAQS were focused on revisions to the CMAQ model (Liang and Kaduwela, 2005), comparison of the standard and UC Davis versions of the CMAQ model (Zhang et al., 2005), and a detailed CMAQ model performance analysis (Liang et al., 2006). This was followed by an annual simulation of the CRPAQS period using the CMAQ model (Fahey et al., 2006). These simulations established the ability of the CMAQ model to satisfactorily simulate the $PM_{2.5}$ concentrations in the SJV, and the results were used in the 2008 annual $PM_{2.5}$ SIP (76 FR 41338; 76 FR 69896).

The first published $PM_{2.5}$ modeling in the SJV using the UCD/CIT model at 4 km horizontal grid spacing (Ying et al., 2008a) found general agreement between simulated and observed concentrations for both gaseous and PM species. The UCD/CIT model was able to simulate the major observed features of this 22 day severe particulate pollution event. The over-prediction of $PM_{2.5}$ at the rural site of Angiola was due to excessive emissions of fugitive dust. The model was able to reproduce the observed

PM nitrate during the first half of the episode, but the performance degraded during the second half due to issues with the meteorological fields.

The source apportionment of primary $PM_{2.5}$ in the SJV (Ying et al., 2008b) found elemental and organic carbon (EC and OC) to be the two major components. Higher concentrations of these two pollutants occur in urban areas and the concentrations were lower in rural areas. Wood burning and emissions from diesel engines were the two major sources of EC and OC. The source apportionment of secondary $PM_{2.5}$ revealed that diesel engines are the largest contributor to PM nitrate, while catalyst equipped gasoline engines also contributed significantly. The major ammonia source that contributed to the ammonium ion concentrations was agriculture. Sharp gradients of $PM_{2.5}$ concentrations were observed in urban areas.

The apportionment of PM OC to primary and secondary components is a very active area of current research. The oxidation of emitted organic compounds make gaseous, semi-volatile, and non-volatile products depending on the vapor pressure of the products. Using the UCD/CIT model, the apportionment of PM OC was investigated for the same 22 day period that was discussed above (Chen et al., 2010). It was found that, of the total predicted PM OC at Fresno, Angiola, and Bakersfield, 6 percent, 37 percent, and 4 percent were secondary in nature, respectively. On a SJV-wide basis ~20 percent of the total PM OC was secondary. The major precursors of secondary organic aerosol (SOA) were long-chain alkanes followed by aromatic compounds. The sources of these precursors were solvent use, catalyst gasoline engines, wood smoke, non-catalyst gasoline engines, and other anthropogenic sources, in that order.

In contrast, air quality modeling exercises conducted as part of the San Joaquin Valley 2008 $PM_{2.5}$ SIP using the CMAQ model showed that primary $PM_{2.5}$ emissions are the main contributor to organic aerosols and SOA contribute to only a small extent. Furthermore, SOA are primarily formed during the summertime, when total $PM_{2.5}$ concentrations are low, and are mainly derived from biogenic emission sources. Simulations of the CRPAQS wintertime episode conducted using CMAQ-MADRID (Pun et al., 2009) a model with an enhanced secondary organic aerosol formation

mechanism, also found that organic aerosol concentrations were dominated by directly emitted $PM_{2.5}$. Because of the dominance of directly emitted $PM_{2.5}$ organic matter, overall a 50 percent reduction in anthropogenic VOC emissions had limited effects on the modeled $PM_{2.5}$ organic matter concentrations.

The transport of gaseous precursors and $PM_{2.5}$ from upwind areas has to be taken into account when developing effective control strategies for a given region. The UCD/CIT model was employed to investigate such transport in the SJV during the 22-day CRPAQS modeling period (Ying and Kleeman, 2009b). It was found that transport distances for $PM_{2.5}$ diminish as the air mass moves from north to south in the SJV due to diminishing wind speeds. The gaseous precursors transport longer distances compared to directly emitted $PM_{2.5}$, but the rate of active nitrogen partitioning into the particle phase increases as the air masses move towards the central and southern portions of the SJV. This is mainly due to the increased availability of ammonia in the central and southern SJV. Thus, the transported $PM_{2.5}$ impacts are the least in the southern SJV where the design values are the highest. For example, nearly 70 percent of the ammonium nitrate in the most polluted areas of the SJV is of local origin.

The CRPAQS winter period was also simulated using the CMAQ-MADRID model (Pun, Balmori, and Seigneur, 2009). Their main finding was that NO_x controls were the most effective strategy, followed by VOC and ammonia. This finding was consistent with that for the 1995 IMS-95 episode (Kleeman, Ying, and Kaduwela, 2005). They also found that VOC controls tend to reduce the oxidant concentrations, but had a relatively small effect on PM nitrate concentrations, indicating that background oxidant concentrations were sufficient to sustain the PM nitrate production. They observed that NO_x reductions can, in some cases, increase the night-time PM nitrate concentrations. This was due to the fact that reduced NO_x would lead to increased O_3 at the end of the day enhancing the N_2O_5 formation leading to increased PM nitrate formation. But, in general a 50 percent NO_x reduction resulted in ~30-50 percent reduction in PM nitrate.

Pun, Balmori, and Seigneur (2009) also found VOC and ammonia controls to be beneficial at some locations at certain times. However, the response of $PM_{2.5}$ nitrate to

a 50 percent reduction in VOC emissions increased as $PM_{2.5}$ levels rose during the episode. The difference in the VOC response on the days with the higher $PM_{2.5}$ concentrations as compared to those days with lower concentrations may be due to a difference in the chemical formation regime for nitrate. In general, there is sufficient background ozone to generate enough free radicals to initiate and propagate the chemistry of nitrate formation (Ying et al., 2009). However, on days with high $PM_{2.5}$ concentrations, the daytime photochemistry may have contributed to a rapid increase in nitrate, resulting in higher VOC and NO_x sensitivity. It does not appear that VOCs contributed significantly to the free radical budget on the simulated days, mainly because rapid increases in ozone were not observed. The effect of VOC levels on nitrate formation may also have a diurnal pattern since the hydroxyl and hydroperoxyl radical levels are high during the daytime and negligible at night. In addition, more reactive VOCs react quickly during the day and there is a minimal carryover to the next day. Therefore it is reasonable to assume that the higher response to VOC and NO_x at higher concentrations may be due to the nitrate formation mechanisms rather than the $PM_{2.5}$ accumulation due to the length of the episode. Overall, nitrate was only responsive to a 50 percent reduction in VOCs at $PM_{2.5}$ concentration levels that are no longer reached in the San Joaquin Valley.

Pun at al., 2009 also shared Ying et al.'s (2008a) concern regarding the need for improved meteorological fields by stating that "… misprediction in the timing and coverage of the meteorological phenomenon can put a stop to PM accumulation in key areas of the SJV. Therefore, weaknesses in the meteorological models for simulating calm wintertime conditions would necessarily translate into performance issues pertaining to the air quality simulation."

The issues related to meteorological fields were further investigated by developing three alternative meteorological fields (Hu et al, 2010). In this study the Weather and Research Forecast (WRF) model was used to generate two meteorological fields, with and without four dimensional data assimilation. The third field was generated using a diagnostic wind model. After using all three models to simulate air quality with the UCD/CIT model, it was concluded that the "diagnostic wind fields based on a dense

measurement network are the preferred choice for air quality model studies during stagnant periods in locations with complex topography." This finding is also consistent with that of a previous investigation of O_3 production in the SJV (Jackson et al., 2006). However, at this time, there is no preprocessor to process diagnostic wind fields for the CMAQ model and the diagnostic wind fields do not have all the quantities required by the CMAQ model. Therefore, we will continue to use the prognostic meteorological fields developed using both the MM5 and WRF models for this SIP.

For a shorter CRPAQS period (December 25-31, 2000) $PM_{2.5}$ mass, number, and size distributions were simulated using CMAQ-MADRID model (Zhang et al., 2010). While the model was able to reproduce the observed 24-hour $PM_{2.5}$ mass well, the prediction of component mass and time evolutions needed improvements. This study also highlighted the difficulties in simulating particle numbers and size distributions due to inaccuracies in model inputs and uncertainties in model formulations.

Recently, the UCD/CIT model was updated to include a process analyses scheme (Ying, 2011). Application of this updated UCD/CIT model to the same 22-day CRPAQS period indicated that, during the day, PM nitrate is photochemically formed within a few hundred meters above ground. This formation is more pronounced in urban areas where NO_x concentrations are higher relative to rural areas. During the early afternoon, the temperatures may be high enough to evaporate some of the PM nitrate. During the night, PM nitrate is formed via the N_2O_5 pathway within a few hundred meters above the surface. This formation is enhanced in the rural areas due to relatively higher O_3. During stagnant days, in which PM nitrate concentrations are generally higher, the PM nitrate concentrations build up aloft and lead to rapid increases in surface PM nitrate concentrations due to vertical diffusion.

The post-2000 applications of photochemical models in the SJV include the February 10-18, 2007 U.S. EPA Advanced Monitoring Initiative to measure the aerosol optical depth in the SJV (Rosen et al., 2006; Lewis et al., 2010; Ying, Jackson, and Kaduwela, 2011), the California portion of the Arctic Research of the Composition of the Troposphere from Aircraft and Satellites (ARCTAS-CARB) which took place during

May-July 2008 (Kaduwela and Cai, 2009; Jacob, et al., 2010; Huang et al., 2010; Singh et al, 2010; Pfister et al., 2011a,b; Huang et al., 2011; D'Allura et al., 2011), and CalNex 2010 (Research at the Nexus of Air Quality and Climate Change conducted in 2010,http://www.arb.ca.gov/research/calnex2010/calnex2010.htm, www.esrl.noaa.gov/csd/calnex/) for which only very preliminary air quality modeling has been conducted to date (Cai and Kaduwela, 2011; Kelly et al., 2011).

3. Selection of the Modeling Periods

3.1. Reference Year Selection and Justification

From an air quality perspective, ARB and the District have selected 2007 baseline design values for the modeled attainment test. These baseline concentrations values will serve as the anchor point for estimating future year projected concentrations. The selection of 2007 is based on the following considerations:

- The extensive wild fires that occurred in the San Joaquin Valley and throughout Northern California during 2008, adversely impacted air quality and the resulting $PM_{2.5}$ design values from 2008 through 2010. Therefore, this period is not suitable for air quality modeling purposes due to the atypical conditions;
- The design values recorded in 2007 were some of the highest in recent years. Analysis of the impacts of meteorology on $PM_{2.5}$ levels in the Valley over the last ten years indicate that the 2007 meteorology was one of the most conducive to $PM_{2.5}$ formation. Thus, the selection of 2007 represents a conservative approach to the attainment demonstration modeling.

Thus, 2007 will be used as both the base case and baseline year. A 2007 base case inventory will be used, together with 2007 meteorology fields, for model performance evaluation. The same emissions, without day-specific information, will then be projected to the future year for the calculation of Relative Response Factors (RRF).

3.2. Future years and justifications

As specific U.S. EPA guidance for the implementation of the 2006 $PM_{2.5}$ standard is not yet available, we have used the framework set forth in the original $PM_{2.5}$ Implementation Rule to determine appropriate deadlines for attainment. The $PM_{2.5}$ Implementation Rule requires areas to achieve attainment within five years from the date of designation, with the potential for up to a five year extension. The Valley was designated nonattainment on December 14, 2009. For the 2006 $PM_{2.5}$ standard, these dates would be December

14, 2014 and December 14, 2019. Given the severity of the San Joaquin Valley's $PM_{2.5}$ problem, initial modeling will be focused on evaluating attainment in the ten year timeframe.

December 14th is for all practical purposes the end of the year; we will conduct the attainment year modeling for the calendar year January 1, 2019 through December 31, 2019. This is consistent with U.S. EPA guidance published on March 2, 2012.

3.3. Justification for Quarterly Modeling instead of Several Episodes

One of the key observations made in the revised modeled attainment test for 24-hour $PM_{2.5}$ is that the temporal distribution of high days in the base and future periods will not remain the same (Fox, 2011). This requires that we simulate at least eight high $PM_{2.5}$ days per quarter for each year we simulate. It is possible that these eight high days will not come from a single episode and, thus, more than one, and perhaps several, episodes would need to be simulated. If that is the case, it is simpler to simulate the whole quarter in one attempt than to keep track of simulations for several episodes. It is possible, however, that there will be no high $PM_{2.5}$ days in quarters other than winter months for the San Joaquin Valley. In that case, modeling the 4th and 1st quarters (that include winter months) would suffice. In fact, preliminary modeling has verified that this is the case. Therefore, we propose to simulate only the first and fourth quarters instead of all four quarters, since this will not affect the attainment modeling outcome.

3.4. Identification of Exceptional Events to be excluded from Base/Reference/Future Year Modeling

Exceptional events are unusual or natural events that can overwhelm existing control strategies for man-made pollution. If such an event occurs, U.S. EPA allows states to exclude these values from use in SIP air quality modeling since these events cannot be controlled. Projecting these events into the future is not representative of an area's ability to attain the $PM_{2.5}$ standard. ARB and the district will review the data proposed for use in the modeling and identify exceptional events. Examples of exceptional events

that will be evaluated include (but are not limited to): wildfires, high winds and dust, and fireworks. For each event identified, documentation will be included justifying exclusion.

4. Development of Emissions Inventories

In support of the various SIPs across California to meet the federal 24-hour $PM_{2.5}$ standard, emission inputs for modeling (commonly and interchangeably referred to as 'modeling inventories' or 'gridded inventories') have been developed by ARB and district staff. The following sections of this document describe how base case and future year emissions estimates for modeling were prepared.

A document that provides a more detailed description of the emission inventory will be prepared separately and submitted to U.S. EPA as a part of the SIP documentation.

4.1. $PM_{2.5}$ Emissions Inventory Development

In support of emissions inventory development, the Air Resources Board convened two inventory coordination groups:

- The $PM_{2.5}$ SIP Emission Inventory Working Group. This group was focused on annual average emission estimates for each county, air basin, and district. ARB maintains an electronic database of emissions and other useful information for these aggregate emission estimates, which provide a foundation for the development of a more refined (hourly, grid-cell specific) set of emission inputs that are required by air quality models. ARB's database is called the California Emission Inventory Development and Reporting System (CEIDARS). This group was focused on improving ARB-District emission estimates in ARB's CEIDARS database. Participants included district staff from the Bay Area, Imperial, Sacramento, San Joaquin, Butte, South Coast, El Dorado, Yolo-Solano, Shasta, Northern Sierra, Feather River and Placer regions. The purpose of this group was to update the 2005 CEIDARS inventory (emissions and other needed data) in preparation for the SIPs.

- The SIP Gridded Inventory Coordination Group (SIP-GICG). This group was focused on more refined emissions estimates to be used in air quality modeling

(e.g. for a specific grid cell and hour). The purpose of the SIP-GICG is to conduct quality assurance of the associated data, and to distribute and coordinate the development of emission inputs for SIP modeling. Local air districts that participated included San Joaquin Valley Unified APCD, Bay Area AQMD, Sacramento Metropolitan AQMD, South Coast AQMD, Ventura County APCD, San Diego County APCD, Imperial County APCD, Mojave Desert AQMD, Northern Sierra AQMD, Yolo/Solano AQMD, Placer County APCD, El Dorado County APCD, San Luis Obispo County APCD, and Santa Barbara County APCD.

In addition to the two coordination groups described above, a great deal of work preceded this modeling effort through the Central California Air Quality Studies (CCAQS). CCAQS consists of two studies: 1) the Central California Ozone Study (CCOS); and 2) the California Regional PM_{10}/$PM_{2.5}$ Air Quality Study (CRPAQS).

The sections below provide details as to how the emissions inputs required by air quality modeling are created.

4.1.1. Background

In order to understand how the modeling inventories are developed, it is necessary to understand the basics of how an annual average emission inventory is developed. California's emission inventory is an estimate of the amounts and types of pollutants emitted from thousands of industrial facilities, millions of motor vehicles, and of hundreds of millions of applications of other products such as paint and consumer products. The development and maintenance of the inventory is a multi-agency effort involving the ARB, 35 local air pollution control and air quality management districts (Districts), regional transportation planning agencies (RTPAs), and the California Department of Transportation (Caltrans). The ARB is responsible for the compilation of the final, statewide emission inventory, and maintains this information in a complex electronic database. Each emission inventory reflects the best information available at the time.

To produce regulatory, countywide emissions estimates, the basic principle for estimating emissions is to multiply an estimated, per-unit emission factor by an estimate of typical usage or activity. For example, on-road motor vehicle emission factors are estimated for a specific vehicle type and model year based on dynamometer tests of a small sample of that vehicle type and applied to all applicable vehicles. The usage of those vehicles is based on an estimate of such activities as a typical driving pattern, number of vehicle starts, typical miles driven, and ambient temperature. It is assumed that all vehicles of this type in each region of the state are driven under similar conditions.

Developing emission estimates for stationary sources involves the use of per unit emission factors and activity levels. Under ideal conditions, facility-specific emission factors are determined from emission tests for a particular process at a facility. More commonly, a generic emission factor is developed by averaging the results of emission tests from similar processes at several different facilities. This generic factor is then used to estimate emissions from similar types of processes when a facility-specific emission factor is not available. Activity levels from point sources are measured in such terms as the amount of product produced, solvent used, or fuel used.

ARB maintains an electronic database of emissions and other useful information. Annual average emissions are stored for each county, air basin, and district. The database is CEIDARS. Emissions are stored in CEIDARS for criteria and toxic pollutants. The criteria pollutants are total organic gases (TOG), carbon monoxide (CO), oxides of nitrogen (NO_x), oxides of sulfur (SO_x), and total particulate matter (PM). Emissions may also be reported for reactive organic gases (ROG), particulate matter 10 microns in diameter and smaller (PM_{10}) and particulate matter 2.5 microns in diameter and smaller ($PM_{2.5}$) in CEIDARS. However, for modeling inventories, ROG, PM_{10} and $PM_{2.5}$ are calculated from TOG and PM, respectively. Modeling inventories require speciated emissions that are calculated from total organics or total particulate matter. Ammonia emissions are also estimated for some sources. Following are more details on how emissions are estimated for point and area sources, on-road motor vehicles,

and biogenic sources. Additional information on emission inventories can be found at: http://www.arb.ca.gov/ei/ei.htm

4.1.2. Terminology

Emission Source Type Terminology: The terms "point sources" and "area sources" are often confused. Traditionally, these terms have had different meanings to the developers of emissions inventories and the developers of modeling inventories. Table 4-1 summarizes the difference in the terms. Both sets of terms are used in this document. In modeling terminology, "point sources" refers to elevated emission sources that exit from a stack and have a potential plume rise. "Area sources" refers collectively to area-wide sources, stationary-aggregated sources, and other mobile sources (including aircraft, trains, ships, and all off-road vehicles and equipment). That is, "area sources" are low-level sources from a modeling perspective. In the development of the $PM_{2.5}$ inventories, all point sources were treated as possible elevated sources. Processing of the inventory for the air quality model will determine which vertical layer the emissions from a process will be placed into. So, for the modeling inventories, the use of the term "point sources" is the same whether using the modeling or emission inventory definition.

Table 4-1: Inventory Terms for Emission Source Types

Modeling Term	Emission Inventory Term	Examples
Point	Stationary – Point Facilities	Stacks at Individual Facilities
Area	Off-Road Mobile	Industrial Equipment, Construction Equipment, Vessels, Trains
Area	Area-wide	Fugitive Dust,, Wood Stoves/Fireplaces, Farming Operations, Consumer Products
Area	Stationary - Aggregated	Industrial Fuel Use
On-Road Motor Vehicles	On-Road Mobile	Cars and Trucks
Biogenic	Biogenic	Trees

Emissions Scenarios and the Modeled Attainment Test: Since emission changes have a significant influence on the calculation of the relative response factor (RRF), it's important that the emission inventory scenarios used in modeling are consistent with modeling guidance and that the terms used for the emission inventory scenarios are clearly defined.

- **Base Case Modeling Inventory (2007)**: Base case modeling is only intended to demonstrate confidence in the capability of the modeling system that is used for the modeled attainment test; however, it is not used as part of the modeled attainment test itself. Since model performance is assessed relative to how well model-simulated concentrations match actual measured concentrations, the modeling inputs are developed to represent (as best as possible) actual, day-specific conditions. Thus, for use in assessing model performance, a day-specific base case modeling inventory for 2007 will be developed. This will include, for instance, actual SJVAPCD-reported point source emissions information for 2007 as well as other available day-specific activities and emission adjustments. The year 2007 was selected to coincide with the year selected for baseline design values (described below). The U.S. EPA modeling guidance states that once the model has been shown to perform adequately, the use of day-specific emissions is no longer needed. In preparation for SIP development, both ARB and the SJVAPCD began a comprehensive review and update of the emission inventory several years ago. At that time, the 2005 emissions inventory was the most recent inventory required to be submitted to the U.S. EPA. Therefore, 2005 was selected as the emission inventory base year for the SJVAPCD's 24-hour $PM_{2.5}$ SIP. As a result, where day-specific 2007 emissions information is not available for certain categories, the 2005 base year emission inventory will be projected to 2007.

- **Reference Year (or Baseline) Modeling Inventory (2007):** Unlike the base case modeling inventory for 2007described previously, the reference year inventory is not developed to capture day-specific emission characteristics.

Rather, per U.S. EPA guidance, the reference year inventory is intended to be a representation of emission patterns occurring through the baseline design value period (described above) and the emission patterns expected in the future year. U.S. EPA modeling guidance describes the reference year modeling inventory as "a common starting point" that represents average or "typical" conditions that are consistent with the baseline design value period. U.S. EPA guidance also states "using a 'typical' or average year reference year inventory provides an appropriate platform for comparisons between the base year and future years." The 2007 reference year inventory represents typical, average conditions and emission patterns through the 2007 design value period; and it will exclude day-specific information other than temperature, humidity, and solar insolation effects and District-reported point source emissions information for 2007.

- **Future Year Modeling Inventory (2019)**: As described previously, future year modeling inventories along with the reference year modeling inventory are used in the model-derived RRF calculation. These inventories maintain the "typical", average patterns of the 2007 Reference Year modeling inventory. The 2019 inventory will include temperature, humidity, and solar insolation effects from reference year (2007) meteorology. Future year point source emissions will be projected from the 2007 District-reported point source emissions used in the 2007 Reference Year Modeling Inventory.

In summary and based on the terminology above, the following modeling emission inventories will be developed:

- **2007 Base Case Modeling Inventory**: This day-specific inventory will be used for the model performance evaluation.
- **2007 Reference Year (Baseline) Modeling Inventory**: This 2007 reference year inventory will be used to determine site-specific RRFs in the modeled attainment test. It is <u>not</u> a day-specific inventory. Rather, the 2007 reference year modeling inventory represents typical, average conditions and emission patterns over the baseline design value period, excluding day-specific

information other than 2007 meteorological effects and District-reported point source emissions information for 2007.

- **Future Year Modeling Inventories for 2019**: These typical, average-day inventories will be used to determine year and site-specific RRFs in the modeled attainment test. Consistent with the 2007 Reference Year Modeling Inventory, the 2019 inventory includes 2007 meteorological effects.

4.2. Point and Area Source Emissions

4.2.1. Development of Base-Year Emission Inventory

The stationary source component of the emission inventory is comprised of nearly 20,000 individual facilities, called “point sources”, and about 160 categories of “aggregated point sources”. Aggregated point sources are groupings of many small point sources that are reported as a single source category (gas stations, dry cleaners, and print shops are some examples). These emission estimates are based mostly on area source methodologies or emission models. Thus, the aggregated point sources include emissions data for the entire category of point sources, not each specific facility. All districts report as point sources any facility with criteria pollutant emissions of 10 tons per year and greater. Most districts choose a cutoff smaller than 10 tons per year for reporting facilities as point sources. Any remaining sources not captured in the point source inventory are reported as aggregated point sources.

The area-wide source component includes several hundred source categories and is made up of sources of pollution mainly linked to the activity of people. Examples of these categories are emissions from paved and unpaved road dust; wood stoves and fireplaces; farming operations, and consumer products. The emissions for these categories are located mostly within major population centers. Some of the emissions in these categories come from agricultural centers and construction sites.

The other mobile source inventory is based on the population, activity, and emissions estimates of the varied types of off-road equipment. Major categories includes engines and vehicles used in industrial, agricultural, construction, airport ground support, and

lawn and garden activities, from hedge trimmers to cranes. Other sources include ocean-going vessels, locomotives, aircraft and recreational boats and vehicles. Emissions are estimated by fuel type, such as gasoline, diesel, compressed natural gas, and liquefied petroleum gas. Emissions are estimated for about 2,000 separate categories. Carrying this level of detail allows for more accurate application of control measures as well as more specific assignments of speciation and spatial distribution. For more information, see: http://www.arb.ca.gov/msei/offroad/offroad.htm.

Local air districts estimate emissions from point sources. The districts provide point source information to ARB to update the annual average CEIDARS database. Estimating emissions from area sources is a cooperative effort between ARB and air district staffs. Updating the emission inventory is a continual process, as new information becomes available.

4.2.2. Quality Assurance of Base Year Emissions

In order to prepare the best inventory possible for use in modeling, ARB and district staff devoted considerable time and effort to conduct quality assurance (QA) of the inventory. Staffs from local air districts conducted extensive quality assurance to provide an accurate and complete inventory.

In particular, facility location, stack data, and temporal data were closely checked. This information is critical whenever air quality modeling is conducted, such as during SIP preparation or special studies such as CCAQS. However, these data are not always of sufficient quality in the inventory database since this information is not needed in the actual calculation of emissions and resources are limited. ARB ran several types of QA reports on the inventory to assist the districts in locating errors or incomplete information. This QA process began with the 1999 CEIDARS database, and continued with the 2002 CEIDARS database that was used for previous $PM_{2.5}$ and ozone inventory preparation. The QA process has continued with the 2005 and subsequent CEIDARS databases. The 2005 CEIDARS database is the basis for the modeling inventories developed for the 24-hour $PM_{2.5}$ SIPs in northern California. Staff of the

South Coast AQMD is using the 2008 CEIDARS database for their modeling effort covering southern California (approximately the Tehachapi Mountains southward).

- Stack data – The report checks for missing or incorrect stack data. The report lists missing stack data and also checks the data for reasonable stack height, diameter, temperature, and stack velocity. Additionally, the report compares the reported stack flow rate with the computed theoretical flow rate (calculated using the diameter and stack velocity).

- Location data – The report checks for missing or wrong Universal Transverse Mercator) UTM coordinates. The report lists missing UTM coordinates for both facilities and stacks. UTM coordinates are also checked to ensure that they are in the range for a given county. Another report is also run that shows the UTM coordinates for a facility grouped by the city in which the facility is located. This allows staff to look for outliers that may indicate facilities whose locations are in the county, but not in the correct location. Additionally, ARB staff reviewed location coordinates for accuracy and completeness. Comparisons were made using address or zip code mapping.

- Temporal data – The report checks for missing or invalid temporal information. Temporal codes used to describe the hours per day, days per week, and weeks per year are checked for completeness, accuracy, and validity. The relative monthly throughput, which assigns a relative amount of activity to each month of the year, is checked to ensure the sum is 100%.

- Code Assignments – Source Classification Codes (SCC) and Standard Industrial Classification Codes (SIC) were reviewed for accuracy. The SCC is used to determine the speciation profile assigned (speciation is discussed in another section of this document). The SIC and SCC combined determine which emission control rules may apply for forecasting emissions (see Section 4.3) along with the categorization of emissions for reporting purposes.

4.3. Future Year (Forecasted) Emissions

Air pollution programs have always depended on predictive models for gaining a better understanding of what the emissions will be in the future—these predictions are based on expectations of future economic conditions, population growth, and emission controls.

ARB's model to forecast or backcast emissions is known as the California Emission Projection Analysis Model (CEPAM). One module of CEPAM is the California Emission Forecasting System (CEFS) that has been used for many years to project emissions. CEPAM is designed to generate year-specific emissions estimates for each county/air basin/district combination taking into account two factors: 1) the effects of growth and 2) the effects of adopted emission control rules. It does this by linking these growth and control factors directly to emission categories for a particular base year. A key component of the model is the Rule Tracking Subsystem (RTS). The RTS was developed to link year-specific implementation of emission control rules to the emission process level. The emission process level is identified in one of two ways. For facilities, the Source Classification Code (SCC) and Standard Industrial Classification (SIC) are used. For all other sources, the Emission Inventory Code (EIC) is used. In total, the emission process level comprises more than 30,000 possible emission categories statewide.

4.3.1. Growth Factors

Growth factors are derived from county-specific economic activity profiles, population forecasts, and other socio/demographic activity. These data are obtained from a number of sources, such as:

- Districts and local regional transportation planning agencies (RTPAs) when they are available;
- Economic activity studies contracted by the ARB; and

- Demographic data, such as population survey data from the California Department of Finance (DOF) and Vehicle Miles Traveled (VMT) data from the California Department of Transportation (Caltrans).

Growth profiles are typically associated with the type of industry and secondarily to the type of emission process. For point sources, economic output profiles by industrial sector are linked to the emission sources via industrial sector classification, such as SIC or NAICS codes. For area-wide and aggregated point sources, other growth parameters such as population, dwelling units and fuel usage may be used. Growth factors are developed from the latest and best available data sources with input from stakeholders.

4.3.2. Control Factors

Control factors are derived from adopted State and Federal regulations and local district rules that impose emission reductions or a technological change on a particular emission process. These data are provided by the agencies responsible for overseeing the regulatory action for the particular emission categories affected. For example, the ARB staff develops the control factors for sectors regulated by the ARB, such as consumer products and clean fuels. The districts develop control factors for locally enforceable stationary source regulations that affect emissions from such equipment as internal combustion engines or power plant boilers. The Department of Pesticide Regulation (DPR) supplies control data for pesticides. In general, control factors account for three variables:

- Control Efficiency which estimates the technological efficiency of the abatement strategy
- Rule Effectiveness which estimates the “real-world” application of the strategy taking into account factors such as operational variations and upsets
- Rule Penetration which estimates the degree a control strategy will penetrate a certain regulated sector taking into account such things as equipment exemptions.

Control factors are closely linked to the type of emission process and secondarily to the type of industry. Control levels are assigned to emission categories, which are targeted by the rules via emission inventory codes (SCC/SIC, EIC etc.) that are used in CEIDARS.

4.4. Day-Specific Emissions

Day-specific data were used for preparing base case inventories when data were available. In previous studies, day-specific data were gathered for large point sources, unusual events (e.g. breakdowns), shipping, prescribed burns, and wildfires. Those previous studies focused on an episode lasting a few days. In this current work, inventories have been created for multiple years. The gathering of day- or hour-specific data from certain kinds of sources, such as large facilities or ship activity, becomes very resource intensive. However, ARB and district staffs were able to gather hourly/daily emission information for 1) wildfires and prescribed burns 2) paved and unpaved road dust and 3) agricultural burns in the San Joaquin Valley and Sacramento County. Additionally, a special model developed for ocean-going vessels was used.

4.4.1. Wildfires and Prescribed Burns

Day-specific, base case estimates of emissions from wildfires and prescribed fires were developed in a two part process. The first part consists of estimating micro-scale, fire-specific emissions (i.e. at the fire polygon scale, which can be at a smaller spatial scale than the grid cells used in air quality modeling). The second part consists of several steps of post-processing fire polygon emission estimates into gridded, hourly emission estimates that are formatted for use in air quality modeling.

4.4.2. Paved Road Dust

Statewide emissions from paved road dust were adjusted for each day of the year 2007. The adjustment reduced emissions by 25% from paved road dust on days when precipitation occurred.

Paved road dust emissions are calculated using the method described in AP-42, Fifth Edition, Volume I, Chapter 13: Miscellaneous Sources, Section 13.2.1 Paved Road, January 2011, (http://www.epa.gov/ttn/chief/ap42/ch13/final/c13s0201.pdf). This methodology includes equations that adjust emissions based on average precipitation in a month; these precipitation-adjusted emissions were placed in the CEIDARS databases. Since daily precipitation totals are readily available, ARB and district staff agreed that paved road dust emissions should be estimated for each day rather than by month. The emissions from CEIDARS were replaced with day-specific data for the appropriate years. A description of the steps used to calculate day-specific emissions is as follows:

1) Daily uncontrolled emissions for each county/air basin are estimated from the AP-42 methodology [Equation (1) on page 13.2.1-4]. No monthly precipitation adjustments are incorporated into the equation to estimate emissions.
2) To adjust for precipitation, daily precipitation data for 2005 and 2007 from ARB's meteorological database (http://www.arb.ca.gov/aqmis2/metselect.php) are used. The specific data sources for these data include: Remote Automated Weather Stations (RAWS), AIRS, and California Irrigation Management Information System (CIMIS) networks. Precipitation data are not available from ARB's meteorological database for San Francisco County and the Lake Tahoe Air Basin portion of Placer County (Placer/LT). Precipitation at the San Francisco International Airport in San Mateo County is used to determine precipitation in San Francisco County. Likewise, precipitation measured at stations in the Lake Tahoe Air Basin portion of El Dorado County is used to determine precipitation in Placer/LT.
3) The emissions from item 1 are adjusted using the precipitation data from item 2. If the precipitation is greater than or equal to 0.01 inches (measured anywhere in a county or county/air basin piece on a particular day), then the uncontrolled emissions are reduced by 25% for that day only. This reduction of emissions follows the recommendation in AP-42 as referenced above.

4) Replace the annual average emissions with day-specific emissions for every day in the corresponding emission inventory dataset.

4.4.3. Unpaved Road Dust

Statewide emissions from unpaved road dust were adjusted for rainfall suppression for each day of the year. The adjustment reduced countywide emissions by 100% (total suppression) from unpaved road dust on days when precipitation greater than 0.01" occurred in a county.

Dust emissions from unpaved roads were calculated using an emission factor (EF) derived from tests conducted by the University of California, Davis, (UCD) and the Desert Research Institute (DRI). Unpaved road vehicle miles traveled (VMT) were based on county-specific road mileage estimates. Emissions were assumed to be suppressed for each day with rainfall of 0.01 inch or greater using the method described in AP-42, Fifth Edition, Volume I, Chapter 13: Miscellaneous Sources, Section 13.2.2 Unpaved Road, November 2006, (http://www.epa.gov/ttn/chief/ap42/ch13/final/c13s0202.pdf). Equation (2) adjusts emissions based on annual precipitation; these precipitation-adjusted emissions were placed in the CEIDARS database. Similar to paved road dust, ARB and district staff agreed that unpaved road dust emissions should be estimated for each day. The emissions from CEIDARS were replaced with day-specific data for the appropriate years. Following is a description of the steps that were taken to calculate day-specific emissions.

1) Start with the daily uncontrolled emissions for each county/air basin as estimated from ARB's methodology. In other words, no precipitation adjustments have been incorporated in the emission estimates.
2) Use daily precipitation data from ARB's meteorological database (http://www.arb.ca.gov/aqmis2/metselect.php). Data sources come from outside sources, including Remote Automated Weather Stations (RAWS), AIRS, and California Irrigation Management Information System (CIMIS) networks. Convert from millimeters to inches.

3) If the precipitation is greater than or equal to 0.01 inches measured anywhere in a county or county/air basin portion on a particular day, then the emissions are removed for that day only.
4) Replace the annual average emissions with day-specific emissions for every day.
5) Precipitation data are not available from ARB's meteorological database for San Francisco County and the Lake Tahoe Air Basin portion of Placer County (Placer/LT). Precipitation at the San Francisco International Airport in San Mateo County is used to determine precipitation in San Francisco County. Likewise, precipitation measured at stations in the Lake Tahoe Air Basin portion of El Dorado County is used to determine precipitation in Placer/Lake Tahoe.

4.4.4. Agricultural Burn Data for San Joaquin Valley

The San Joaquin Valley Air Pollution Control District estimated emissions for each day during 2005 through 2010 when agricultural burning occurred. Emissions were estimated for the burning of prunings, field crops, weed abatement and other solid fuels. Information needed to estimate emissions came from the district's Smoke Management System, which stores information on burn permits issued by the district. In order to obtain a daily burn authorization, the person requesting the burn provides information to the district, including the acres and type of material to be burned, the specific location of the burn and the date of the burn. Acres are converted to tons of fuel burned using a fuel loading factor based on the specific crop to be burned. Emissions are calculated by multiplying the tons of fuel burned by a crop-specific emission factor. More information is available at: http://www.arb.ca.gov/ei/areasrc/distmiscprocwstburndis.htm

To determine the location of the burn, district staff created spatial allocation factors for each 4 kilometer grid cell used in modeling. These factors were developed for "burn zones" in the San Joaquin Valley based on the agricultural land coverage. Daily emissions in each "agricultural burn zone" were then distributed across the zone/grid cell combinations using the spatial allocation factors. Emissions were summarized by grid cell and day.

Burning was assumed to occur over three hours from 10:00 a.m. to 1:00 p.m., except for two categories. Orchard removals were assumed to burn over eight hours from 10:00 a.m. to 6:00 p.m. Vineyard removals were assumed to burn over five hours from 10:00 a.m. to 3:00 p.m.

4.4.5. Ocean-Going Vessels

The emissions for ocean-going vessels were generated with version 2-3H of the ARB Marine Model. The model uses a power-based methodology to estimate emissions. Inputs to the model include vessel call data obtained from the California Lands Commission; vessel specifications and power ratings from Lloyds-Fairplay, vessel berthing statistics from port authorities, and vessel routing based upon the Ship Transportation Energy and Economic Model (STEEM) developed by the University of Delaware under contract with the Air Resources Board. Emissions were calculated by estimating ship emissions on a ship by ship and a port call by port call basis, using actual ship engine power estimates, speeds, and actual ship hoteling times where possible.

Emission control measures included in the inventory include the South Coast 20/40 nautical-mile voluntary vessel speed reduction program, the 2007 Shore Power regulation, the 2005 auxiliary engine regulation (while in effect) and the subsequent 2008 low sulfur fuel regulation, IMO tier 1 NOx engine standards, and the IMO North American Environmental Control Area which includes the IMO tier 3 NOx engine standards.

4.5. Temporally and Spatially Resolved Emissions

Emission inventories that are temporally and spatially resolved are needed for modeling purposes, for both the base year and future years. Annual average emissions for point and area sources were used as input to version 2.6 of SMOKE (Sparse Matrix Object Kernel Emission). The SMOKE processor was developed by the MCNC-North Carolina Supercomputing Center, Environmental Sciences Division, with U.S. EPA cooperation and support. Temporal information is input into SMOKE. Adjustments are made for

variations in months, day of week and hour of day. Emissions are estimated for each county, air basin, and district combination for each day of the year. The SMOKE processor also distributes emissions to each grid cell. The spatial allocation of emissions is discussed in Section 4.9.

The emission inventories for $PM_{2.5}$ modeling in northern California were developed from the 2005 annual average CEIDARS database for TOG, NO_x, SO_x, CO, PM, and ammonia. Inventories for point and area sources were developed for each day for a variety of years between 2005 and 2020 as needed for input to air quality models.

4.6. Surface Temperature and Relative Humidity Fields

The calculation of gridded emissions for some categories of the emissions inventory is dependent on meteorological variables. More specifically, biogenic emissions are sensitive to air temperatures and solar radiation while emissions from on-road mobile sources are sensitive to air temperature and relative humidity. As a result, estimates of air temperature (T), relative humidity (RH), and solar radiation are needed for each grid cell in the modeling domain in order to take into account the effects of these meteorological variables on mobile source and biogenic emissions in each grid cell.

Gridded temperature, humidity, and radiation fields are readily available from prognostic meteorological models such as MM5, which is used to prepare meteorological inputs for the air quality model. However, it is widely recognized that diagnostic (i.e. observation-based) models provide more accurate local-scale estimates of ground surface temperature and humidity. As a result, the CALMET diagnostic meteorological model is used to generate a gridded temperature field and an objective analysis scheme is used to generate a gridded humidity field. The solar radiation fields needed for biogenic emission inventory calculations were taken from the MM5 prognostic model, which is also used to generate meteorology for the air quality model.

The principal steps involved in generating a gridded, surface-level temperature field using CALMET include the following:

1) Compute the relative weights of each surface observation station to each grid cell (the weight is inversely proportional to the distance between the surface observation station and grid cell center).
2) Adjust all surface temperatures to sea level. In this step, a lapse rate of -0.0049 ^{o}C/m is used (this lapse rate is based on private communication with Gary Moore of Earth Tech, Inc., Concord, MA). This lapse rate (=2.7 F/1000 feet) is based on observational data.
3) Use the weights to compute a spatially-averaged sea-level temperature in each grid cell.
4) Correct all sea-level temperatures back to 10 m height above ground level (i.e. the standard height of surface temperature measurement) using the lapse rate of -0.0049 ^{o}C/m again.

The current version of CALMET does not generate estimates of relative humidity. As a result, a post-processing program was used to produce gridded, hourly relative humidity estimates from observed relative humidity data. The major steps needed to generate gridded, surface-level relative humidity are described as follows:

1) Calculate actual vapor pressure from observed relative humidity and temperature at all meteorological stations. The McRae (1980) method is used to calculate the saturated vapor pressure from temperature;
2) Compute the relative weights of each surface observation station to each grid in question, exactly as done by CALMET to compute the temperature field;
3) Use the weights from step 2 to compute a spatially-averaged estimate of actual vapor pressure in each grid cell;
4) For each grid cell, calculate relative humidity from values for actual vapor pressure and temperature for the same grid cell.

4.7. On-Road Mobile Source Emissions

As described in the prior sections, air quality models require gridded, hourly emission inputs. However, California's official on-road motor vehicle emission inventory model, EMFAC, is designed to produce *county-level, average-day* estimates. As a result,

emission estimates from EMFAC must be disaggregated spatially and temporally from county-level, average-day estimates into gridded, hourly estimates. The general methodology that ARB has used to disaggregate EMFAC emission estimates in the past is described below and will be used again. Basically, it involves using the Direct Travel Impact Model (DTIM) (Systems Applications, Inc. 2001) to produce gridded, hourly emission estimates, and then uses these estimates as a gridded hourly spatial surrogate to distribute EMFAC emissions. The methodology has been peer reviewed by the Institute of Transportation Studies department at the University of California, Irvine, under a CCOS contract.

The most recent version of EMFAC, EMFAC2011, is comprised of two separate emission model components: EMFAC2011-LD and EMFAC2011-HD. The LD model generates emissions for light- and medium- duty gasoline vehicles, heavy-duty gasoline vehicles, and light- and medium-duty diesel vehicles. The HD model generates emissions for heavy-duty diesel vehicles. The general methodology described below will be performed three times: the first time for light duty gasoline vehicle emissions from EMFAC2011-LD; a second time for heavy duty gasoline vehicle emission estimates from EMFAC2011-LD; and a third time for heavy duty diesel vehicle emissions from EMFAC2011-HD. Methodological details are currently being updated where necessary to work with the new version of EMFAC.

4.7.1. General Methodology

Mobile source emissions are sensitive to ambient temperature and humidity. Both EMFAC and DTIM account for meteorological effects using day-specific inputs (the gridded, hourly meteorological data used are described under the prior section titled “Surface Temperature and Relative Humidity Fields”). For EMFAC, hourly gridded temperature and humidity fields are averaged by county using a gridded VMT weighted average (i.e. weighted proportional to the VMT per grid cell in a county). DTIM accepts gridded, hourly data directly.

EMFAC provides vehicle-class-specific emissions estimates for exhaust emissions, evaporative emissions, tire wear emissions and brake wear emissions. EMFAC also

produces estimates of fuel consumption, vehicle miles traveled (VMT), and the number of vehicles in use. More information on EMFAC is available at the following link. http://www.arb.ca.gov/msei/modeling.htm

Temporal Adjustment (Day-of-Week adjustments to EMFAC daily totals): Day-of-Week (DOW) adjustments are made to the total daily emissions estimated by EMFAC for Friday, Saturday, Sunday, and Monday days of the week. The logic behind this is that EMFAC produces emission estimates for an *average day of the week*. It is assumed that EMFAC's average day of week emissions generally represents Tuesday, Wednesday, and Thursday. Day of week adjustment factors were developed using Automatic Vehicle Classifier (AVC) count data from the California Department of Transportation (Caltrans). These data were collected at 139 sites in the state during the summer of 2004 (specifically, data for the months of June, July and August were used, excluding data from July 2-5 to remove unusual traffic patterns around the July 4th holiday). Three Caltrans factors were developed: (1) passenger cars (LD), (2) light and medium duty trucks (LM), and (3) heavy-heavy duty trucks (HHDT). An example of the prior assignment of these factors to EMFAC2007 classifications is summarized below.

Caltrans' Factor for EMFAC2007 Class*	Description	Day-of-Week (DOW)
1	LDA	LD
2	LDT1	LD
3	LDT2	LD
4	MDV	LD
5	LHDT1	LM
6	LHDT2	LM
7	MHDT	LM
8	HHDT	HHDT
9	Other Bus	LM
10	School Bus	Unadjusted on weekdays, zeroed on

		weekend days
11	Urban Bus	LD
12	Motorhomes	LD
13	Motorcycles	LD

* Vehicle classes are being updated for use with EMFAC2011

Separate factors were developed for each Caltrans District. All counties within each Caltrans district use the same adjustment. So, the day of week adjustment process consists of applying four Caltrans day of week (DOW) factors to EMFAC daily total emission estimates (i.e. which represent Tuesday, Wednesday, and Thursday): one each for Friday, Saturday, Sunday, and Monday.

Temporal Adjustment (Hour-of-Day re-distribution of hourly travel network volumes): The travel networks provided by local government agencies and used for DTIM represent an average day hourly distribution. Like for EMFAC, it is assumed that these average day of week hourly distributions represent hourly mid-week activities (i.e. for Tuesday, Wednesday, and Thursday). As such, they lack the day-of-week temporal variations that are known to occur on other days of the week. To rectify this, hour-of-day profiles for Friday through Monday were developed using Caltrans data. These are used to re-allocate the hourly travel network distributions used in DTIM to Friday through Monday.

Spatial Adjustment: The spatial allocation of countywide EMFAC emissions is accomplished using gridded, hourly emission estimates from DTIM normalized by county. DTIM uses emission rates from EMFAC along with activity data, digitized roadway segments (links) and traffic analysis zone centroids to calculate gridded, hourly emissions for travel and trip ends. DTIM considers fewer vehicle categories than EMFAC outputs, so a mapping between EMFAC and DTIM vehicle categories is necessary (this is being updated to work with EMFAC2011). DTIM's 40 emission categories are presented in the table below. The categories are represented by the listed source classification codes (SCC) and depend on vehicle type, technology, and

whether the vehicle is catalyst, non-catalyst, or diesel. Light- and medium-duty vehicles are separated from heavy-duty vehicles to allow for separate reporting and control strategy applications.

Table 4-2: **DTIM Emission Categories**

SCC for Light-duty and Medium-duty Vehicles	SCC for Heavy-Duty Vehicles	Description
202	302	Catalyst Start Exhaust
203	303	Catalyst Running Exhaust
204	304	Non-catalyst Start Exhaust
205	305	Non-catalyst Running Exhaust
206	306	Hot Soak
207	307	Diurnal Evaporatives
208	308	Diesel Exhaust
209	309	Running Evaporatives
210	310	Resting Evaporatives
211	311	Multi-Day Resting
212	312	Multi-Day Diurnal
213	313	PM Tire Wear
214	314	PM Brake Wear
215	315	Catalyst Buses
216	316	Non-catalyst Buses
217	317	Diesel Bus
218	318	Catalyst Idle
219	319	Non-catalyst Idle
220	320	Diesel Idle
221	321	PM Road Dust

Summary of On-road Emissions Processing Steps: Five general steps are used to spatially and temporally allocate EMFAC emissions by hour and grid cell:

Step 1 (DTIM T & RH inputs). Gridded, hourly temperature (T) and relative humidity (RH) fields for each day are prepared as inputs to DTIM.

Step 2 (DTIM emission factor inputs). EMFAC is run in default mode (i.e. without day-specific temperature and relative humidity) to generate a look-up table of on-road mobile source emission factors by speed, temperature, and relative humidity for each county.

Step 3 (Day-specific EMFAC runs to yield daily and hourly estimates). EMFAC is run using episode-specific T and RH data to provide countywide on-road mobile source emission estimates by day and hour for EMFAC categories. The episode-specific meteorological inputs for EMFAC are generated via averaging (VMT-weighted) the gridded, hourly meteorology from Step1 by county and hour.

Step 4 (DTIM inputs – redistribute roadway network hourly volumes using Caltrans DOW factors)

- 4a. Sum the hourly volumes by vehicle type and county on the roadway network into daily totals.
- 4b. Tuesday through Thursday. No DOW adjustment. For hour of day, redistribute heavy-duty volumes by county using Caltrans hourly profiles. No change to light duty hourly volumes.
- 4c. Friday, Saturday, Sunday, and Monday. Adjust total daily volumes by county using Caltrans DOW factor. Use Caltrans hourly profiles by county to redistribute DOW-adjusted total volumes using Caltrans hourly profiles for all vehicles.

Step 5 (Run DTIM and spatially/temporally distribute EMFAC emissions)

- 5a. Run DTIM with revised roadway network activity from Step 4.
- 5b. Sum DTIM emissions by county and SCC.
- 5c. Distribute EMFAC emissions. EMFAC daily, countywide emissions (adjusted for weekend days, if needed), are disaggregated by category into grid-cells for each hour of the day using the DTIM output as a spatial and temporal surrogate. The disaggregation follows the equation:

$$E_{P,ijhr,cat} = \frac{EF_{P,cat} \times DTIM_{P,ijhr,cat}}{DTIM_{P,daily,cat,cnty}}$$

where:

E = grid cell emissions

EF = EMFAC emissions

DTIM = DTIM emissions

P = pollutant

ij = grid cell

hr = hourly emissions

cat = Emission Category

daily = daily emissions

cnty = county

Future Year On-road Emissions: Forecasted on-road modeling inventories are developed using the same methodology, where future year emissions are based on running EMFAC for the associated future year.

4.8. Biogenic Emissions

Development of a comprehensive emissions inventory requires estimation of both man-made and biogenic emissions. These biogenic volatile organic compounds (BVOCs) include compounds such as isoprene and monoterpenes. Due to the heterogeneity of vegetation land cover, species composition, and leaf mass distribution in California, quantifying BVOC emissions in this domain requires an emission inventory model with region-specific input databases and a high degree of spatial and temporal resolution. In response to this need, the California Air Resources Board (CARB) developed a Geographic Information System (GIS)-based model for estimating BVOC emissions, called BEIGIS (Scott and Benjamin, 2003), which uses California-specific input databases with a minimum spatial resolution of 1 km^2 and an hourly temporal resolution. To take advantage of recent scientific advances in biogenic emissions modeling, CARB has recently transitioned from the BEIGIS model to the Model of Emissions of Gases

and Aerosols from Nature (MEGAN) version 2.04 (Guenther et al., 2006). MEGAN is a state-of-the-science biogenic emissions model, which represents an evolution of the Biogenic Emissions Inventory System (BEIS), and is being integrated into the Community Multi-scale Air Quality (CMAQ) modeling system by U.S. EPA scientists.

MEGAN estimates biogenic emissions as a function of normalized emission rates (i.e., emission rates at standard conditions), which are adjusted to reflect variations in temperature, light, leaf area index (LAI), and leaf age (estimated from changes in LAI). MEGAN requires input datasets of Emission Factors (EF; at standard conditions: temperature = 303 ˚K, LAI = 5, photosynthetically active radiation ~ 1500 µmol $m^{-2}s^{-1}$), Plant Functional Type (PFT), and hourly surface temperature and insolation. The default MEGAN input databases for EFs, PFTs, and LAI are not used in the application of MEGAN in California. Instead, California-specific emission factor and PFT databases were translated from those used in BEIGIS to improve emission estimates and to maintain consistency with previous California biogenic emission inventories. LAI data is derived from the MODIS 8-day LAI satellite product. Hourly surface temperatures are from observations gridded with the CALMET meteorological model and insolation (light reaching the surface) data is provided by the MM5 meteorological model. Emissions of isoprene, monoterpenes, and methylbutenol are estimated from California-specific gridded emission factor data, while emissions of sesquiterpenes, methanol, and other volatile organic compounds are estimated from California-specific PFT data and PFT derived emission rates. For urban areas, land use/vegetation land cover databases were developed from regional planning agency data and botanical surveys (Horie et al. 1990; Nowak 1991; Sidawi and Horie 1992; Benjamin et al. 1996, 1997; McPherson et al. 1998). Natural areas are represented using the GAP vegetation database (also satellite-derived and air photo interpreted) developed by the U.S.G.S. Gap Analysis Program (Davis et al. 1995). Agricultural areas are represented using crop land cover databases developed by the California Department of Water Resources (*http://www.waterplan.water.ca.gov*).

Future-year specific biogenic emissions are not estimated because future inputs to BEIGIS, such as changes in climate and land use/land cover, are highly uncertain.

Photochemical modeling for future years uses the biogenic emissions developed for the base year.

4.9. Spatial Allocation

Once the base year or future year inventories are developed, as described in the previous sections, the next step of modeling inventory development is to spatially allocate the emissions. Air quality modeling attempts to replicate the physical and chemical processes that occur in an inventory domain. Therefore, it is important that the physical location of emissions be specified as accurately as possible. Ideally, the actual location of all emissions would be known exactly. In reality, however, some categories of emissions would be virtually impossible to determine – for example, the actual amount and location of consumer products used every day. Therefore, the spatial allocation of emissions in a modeling inventory only approximates the actual location of emissions.

Before any spatial allocation can be performed, the modeling grid domain must be defined. A modeling grid domain is a rectangular area that is sufficient in size to contain all emission sources that could affect modeling results. The definition of the modeling domain for this SIP is described below.

Once a grid is defined, the spatial allocation of emissions can be performed. Each area source category is assigned a spatial surrogate that is used to allocate emissions to a grid cell. Examples of surrogates include population, land use, and other data with known geographic distributions for allocating emissions to grid cells. The sections below discuss in detail the spatial surrogates developed for the SJV $PM_{2.5}$ SIP modeling.

Point sources are allocated to grid cells using the UTM coordinates reported for each stack. If there are no stack UTM coordinates, the facility UTM coordinates are used. When location data are not reported, the county centroid is used.

Emissions are also distributed vertically into their proper layer in the air quality model. The vertical layer is determined from the calculation of buoyancy for those emissions

that are released from an elevated height with a significant upward velocity and/or buoyancy. Most vertical allocation is from significant point sources with stacks. In most modeling exercises, low-level point sources are screened out at this point and placed with the area sources. However, in this modeling exercise, all point sources from the inventory were kept as possible elevated sources. The air quality model will then place the point sources in the appropriate layer of the model. Additionally in this modeling exercise, day-specific wildfire emissions were also distributed vertically.

The spatial treatment of area and point sources has been described above. The spatial allocation of on-road motor vehicles is based on DTIM as described previously. For biogenic emissions, the spatial allocation is built “from the ground up” since MEGAN estimates emissions using a Geographic Information System (GIS) at a minimum resolution of one square kilometer.

4.9.1. Grid Definition

The ARB emissions inventory domain is defined to match the MM5 model domain, which is used to generate the meteorological parameter fields used for air quality modeling. MM5 uses a Lambert projection and assumes a spherical Earth. The emission grid is defined in a similar way to match as closely as possible.

The emission inventory grid uses a Lambert Conical Projection with two parallels. The Parallels are at 30° and 60° N latitude, with a central meridian at 120.5° W longitude. The coordinate system origin is offset to 37° N latitude. The emissions inventory uses a grid with a spatial resolution of 4 km x 4 km.

The domain extends entirely over California and 100 nautical miles west over the Pacific Ocean. A smaller subdomain is often used when modeling is being done for the San Joaquin Valley. It has the same grid definitions and resolution as the main domain, but has a smaller area offset to cover central and northern California.

The specifications of the emissions inventory domain and CCOS subdomain are:

MAP PROJECTION

Lambert Conformal Conic

Datum: NONE (Clarke 1866 spheroid)

1st Standard Parallel: 30.0° N

2nd Standard Parallel: 60.0° N

Central Meridian: -120.5° W

Latitude of Projection Origin: 37.0° N

COORDINATE SYSTEM

Units: Meters

Semi-major Axis: 6370 km

Semi-minor Axis: 6370 km

DEFINITION OF GRID

321 x 291 cells (4 km x 4 km)

Lambert Origin @ (-684,000 m, -564,000 m)

Geographic Origin @ -120.5° Latitude and 37.0° Longitude

DEFINITION OF SUBGRID (CCOS)

192 x 192 cells (4 km x 4 km)

Lambert Origin @ (-384,000 m, -300,000 m)

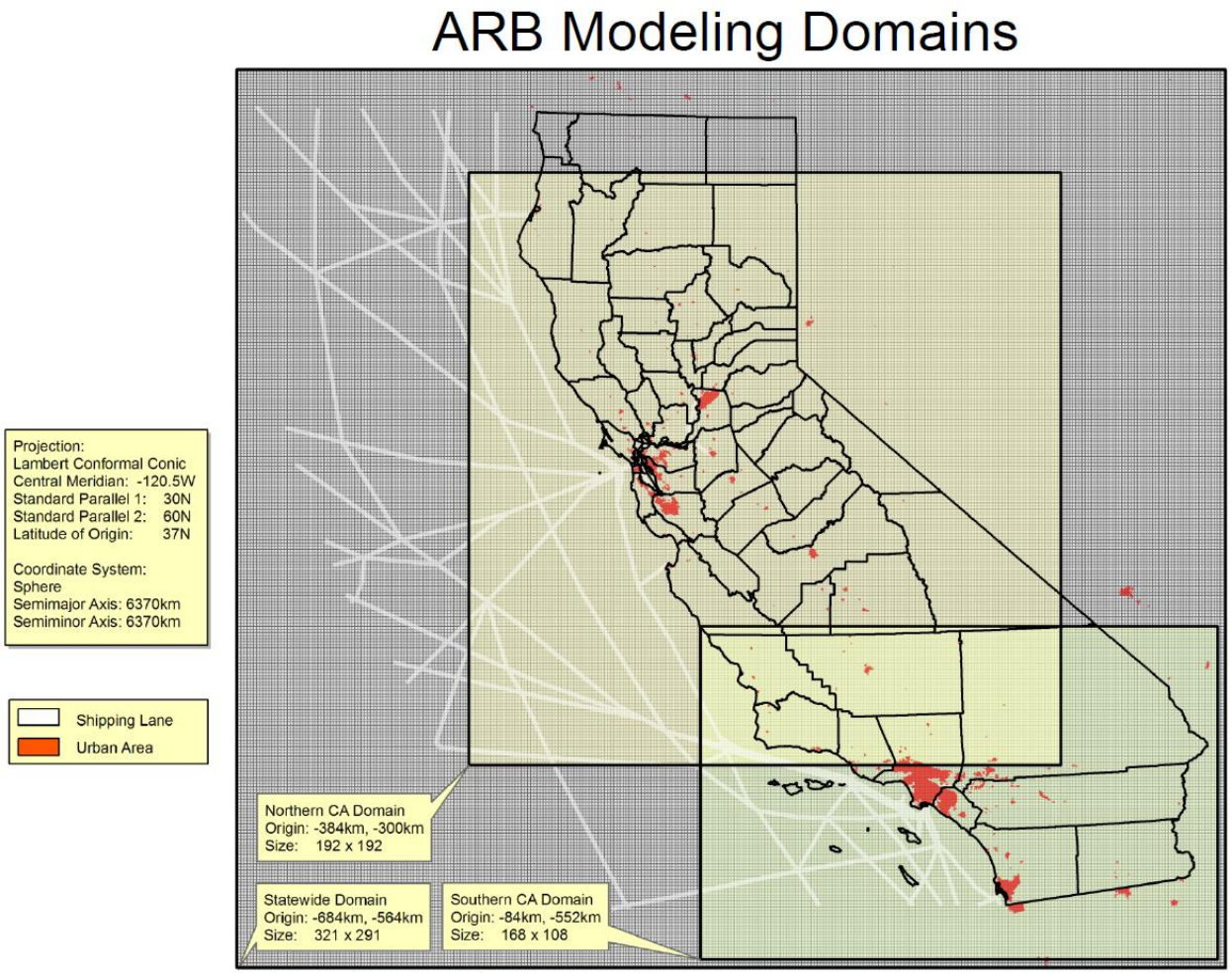
Geographic Origin @ -120.5° Latitude and 37.0° Longitude

4.9.2. Spatial Surrogates

Spatial surrogates are processed into spatial allocation factors for use in geographically distributing countywide area source emissions to individual grid cells. Spatial surrogates are developed based on economic, demographic, and land cover data which exhibit patterns that vary geographically. As has previously been discussed, point source emissions are allocated to grid cells using the location of the emission source. On-road motor vehicle emissions are spatially allocated by DTIM. Biogenic emissions are allocated by the MEGAN emissions model.

In support of CRPAQS and CCOS, Sonoma Technology, Inc. (Funk et al. 2001) developed gridded spatial allocation factors for a 2000 base-year and three future years

(2005, 2010, and 2020) for the entire state of California. STI's work was based on the statewide 4-kilometer (km) grid cell domain defined by the ARB. The definition and extent of the 4-km grid were used to create a 2-km nested grid for which spatial allocation factors were developed. In 2007, STI was contracted by CCOS again to update the spatial allocation factors. STI updated the underlying spatial data and updated the spatial surrogate cross-reference file to account for new emission source categories (Reid et al., 2006). STI then updated spatial allocation factors for ARB's statewide modeling domain for a base year of 2000 and future years of 2010, 2015, and 2020. This task was completed in March 2008.



In preparation for modeling for the $PM_{2.5}$ SIPs, ARB staff reviewed the STI spatial surrogates associated with the highest emissions to see which surrogates were candidates for update. ARB staff searched for more recent or improved sources of data, since the underlying data used by STI were pre-recession, then updated 15 of the surrogates using more recent data. A total of 61 unique surrogates are available for use. A summary of the spatial surrogates for which spatial allocation factors were developed is listed in the table below.

Three basic types of surrogate data were used to develop the spatial allocation factors: land use and land cover; facility location; and demographic and socioeconomic data. Land use and land cover data are associated with specific land uses, such as agricultural tilling or recreational boats. Facility locations are used for sources such as gas stations and dry cleaners. Demographic and socioeconomic data, such as population and housing, are associated with residential, industrial, and commercial activity (e.g. residential fuel combustion). To develop spatial allocation factors of high quality and resolution, local socioeconomic and demographic data were used where available; for rural regions, for which local data were not available, data from the Caltrans Statewide Transportation Model were used.

Table 4-3: Summary of spatial surrogates

Spatial Surrogate	Description
Airports	Spatial locations of all airports
All_PavedRds	Spatial distribution of road network (all paved roads)
AutobodyShops	Locations of autobody repair and refinishing shops
Cemeteries	Spatial locations of cemeteries
Comm_Airports	Spatial locations of commercial airports
Devplnd_HiDensity	Spatial distribution of high-density developed land
Devplnd_LoDensity	Spatial distribution of low-density developed land
Drycleaners	Locations of drycleaning facilities
DryLakeBeds	Locations of Dry lake beds
Elev5000ft	Elevation over 5000 feet developed from topological contours
Employ_Roads	Spatial distribution of total employment and road density (all paved roads)
Forestland	Spatial distribution of forest land
Fugitive_Dust	Spatial distribution of undeveloped, open land
GasStations	Locations of gasoline service stations
GasWells	Locations of gas wells
GolfCourses	Spatial locations of golf courses
HE_Sqft	Computed surrogate based on housing and employment (est. ft2 / person)
Hospitals	Spatial locations of hospitals
Housing	Spatial distribution of total housing
Housing_Autobody	Spatial distribution of housing and autobody refinishing
Housing_Com_Emp	Spatial distribution of total housing and commercial employment
Housing_Restaurants	Spatial distribution of total housing and
IndusEmploy_Autobody	Spatial distribution of industrial employment and autobody/refinishing shops
Industrial_Emp	Spatial distribution of industrial employment
InlandShippingLanes	Spatial distribution of major shipping lanes within bays and inland areas
Irr_Cropland	Spatial location of agricultural cropland
Lakes_Coastline	Locations of lakes, reservoirs, and coastline
Landfills	Locations of landfills
LiveStock	Spatial distribution of cattle ranches, feedlots, dairies, and poultry farms
Metrolink_Lines	Spatial distribution of metrolink network
MiltaryAirBases	Location of military air bases
MiltaryBases	Locations of military bases
NonIrr_Pastureland	Spatial location of non-irrigated pasture land
NonRes_Chg	Computed surrogate based on the change in spatial distribution of non-residential areas

Table 4-3. Summary of spatial surrogates (continued)

Spatial Surrogate	Description
OffShore_OilWells	Locations of off-shore oil wells
OilWells	Locations of oil wells
Pop_ComEmp_Hos	Spatial distribution of hospitals, population and commercial employment
Population	Spatial distribution of population
Ports	Locations of shipping ports
POTWs	Coordinate locations of Publically Owned Treatment
PrimaryRoads	Spatial distribution of road network (primary roads)
Raillines	Spatial distribution of railroad network
RailYards	Locations of rail yards
Rds_HE	Calculated surrogate based on road densities and housing/employment (est. ft2 / person)
RefineriesTankFarms	Coordinate locations of refineries and tank farms
Res_NonRes_Chg	Computed surrogate based on the change in spatial distribution of residential and non-residential areas
ResGasHeating	Spatial distribution of gas heating population
Residential_Chg	Computed surrogate based on the change in spatial distribution of residential areas
ResNonResChg_IndEmp	Spatial distribution of industrial employment and residential/ non-residential change
Restaurants	Locations of bakeries and restaurants
ResWoodHeating	Spatial distribution of wood heating population
SandandGravelMines	Locations of sand/gravel excavation and mining
Schools	Spatial locations of schools
SecondaryPavedRds	Spatial distribution of road network (secondary roads)
Ser_ComEmp_Sch_GolfC_Cem	Spatial distribution of service and commercial employment, schools, cemeteries, and golf courses
Service_Com_Emp	Spatial distribution of service and commercial employment
Service_Emp	Spatial distribution of service employment
Shiplanes	Spatial distribution of major shipping lanes
SingleHousingUnits	Spatial distribution of single dwelling units
UnpavedRds	Spatial distribution of road network (unpaved roads)
Wineries	Locations of wineries

4.10. Speciation

The ARB's emission inventory and photochemical air quality models both quantify organic compounds as Total Organic Gases (TOG). Photochemical models simulate the physical and chemical processes in the lower atmosphere, and include all emissions of the important compounds involved in photochemistry. Organic gases are one of the most important classes of chemicals involved in photochemistry. Organic gases emitted to the atmosphere are referred to as total organic gases (TOG). ARB's chemical speciation profiles (CARB 2006) are applied to characterize the chemical composition of the TOG emitted from each source type.

TOG includes compounds of carbon, excluding carbon monoxide, carbon dioxide, carbonic acid, metallic carbides or carbonates, and ammonium carbonate. TOG includes all organic gas compounds emitted to the atmosphere, including the low reactivity, or exempt, VOC compounds (e.g., methane, ethane, various chlorinated fluorocarbons, acetone, perchloroethylene, volatile methyl siloxanes, etc.). TOG also includes low volatility or low vapor pressure (LVP) organic compounds (e.g., some petroleum distillate mixtures). TOG includes all organic compounds that can become airborne (through evaporation, sublimation, as aerosols, etc.), excluding carbon monoxide, carbon dioxide, carbonic acid, metallic carbides or carbonates, and ammonium carbonate.

Total Organic Gas (TOG) emissions are reported in the ARB's emission inventory and are the basis for deriving the Reactive Organic Gas (ROG) emission components, which are also reported in the inventory. ROG is defined as TOG minus ARB's "exempt" compounds (e.g., methane, ethane, CFCs, etc.). ROG is nearly identical to U.S. EPA's term "VOC", which is based on U.S. EPA's exempt list. For all practical purposes, use of the terms ROG and VOC are interchangeable. Also, various regulatory uses of the term "VOC", such as that for consumer products exclude specific, additional compounds from particular control requirements.

4.10.1. Speciation Profiles

Speciation profiles are used to estimate the amounts of various organic compounds that make up TOG. A speciation profile contains a list of organic compounds and the weight fraction that each compound comprises of the TOG emissions from a particular source type. Each process or product category is keyed to one of several hundred currently available speciation profiles. The speciation profiles are applied to TOG to develop both the photochemical model inputs and the emission inventory for ROG.

It should be noted that districts are allowed to report their own reactive fraction of TOG that is used to calculate ROG rather than use the information from the assigned organic profiles. These district-reported fractions are not used in developing modeling inventories because the information needed to calculate the amount of each organic compound is not available.

To the extent possible (i.e. given available data), ARB's organic gas speciation profiles contain all emitted organic species that can be identified (ideally, detected to very low levels). This includes reactive compounds, unreactive and exempt compounds, and to the extent the data are available, low vapor pressure compounds. Research studies are conducted regularly to improve ARB's species profiles. These profiles support ozone modeling studies but are also designed to be used for aerosol and regional toxics modeling. The profiles are also used to support other health or welfare related modeling studies where the compounds of interest cannot always be anticipated. Therefore, organic gas emission profiles should be as complete and accurate as possible.

The speciation profiles used in the emission inventory are available for download from the ARB's web site at: http://www.arb.ca.gov/ei/speciate/speciate.htm.

The Organic Speciation Profiles (ORGPROF) file contains the weight fraction data (expressed as percent for ease of display) of each chemical in each profile. Each chemical fraction is multiplied by the Total Organic Gas (TOG) emissions for a source category to get the amount of each specific constituent chemical. In addition to the

chemical name for each chemical constituent, the file also shows the chemical code (a 5-digit internal identifier) and the Chemical Abstracts Service (CAS) number, which is a unique identifying code (up to 9 digits) assigned to chemicals by the CAS Registry Service.

Also available for download from ARB's web site is a cross-reference file that indicates which Organic Gas profile is assigned to each source category in the inventory. The inventory source categories are represented by an 8-digit Source Classification Code (SCC) for point sources, or a 14-digit Emission Inventory Code (EIC) for area and mobile sources. This file also contains the fraction of reactive organic gas (FROG) values for organic profiles. Some of the Organic Gas Speciation Profiles related to motor vehicles and fuel evaporative sources vary by the inventory year of interest, due to changes in fuel composition and vehicle fleet composition over time.

ARB has an ongoing effort to update speciation profiles as data become available, such as through testing of emission sources or surveys of product formulations. New speciation data generally undergo technical and peer review, and updating of the profiles is coordinated with users of the data. Several recent changes to ARB's speciation profiles were for: 1) consumer products, 2) aerosol coatings, 3) architectural coatings, 4) pesticides and 5) hot soak from gasoline-powered vehicles.

The particulate matter emissions are size fractionated by using PM size profiles, which contain the total weight fraction for $PM_{2.5}$ and PM_{10} out of total PM. The fine and coarse PM chemical compositions are characterized by applying the PM chemical speciation profiles for each source type, which contain the weight fractions of each chemical species for $PM_{2.5}$, PM_{10} and total PM. PM size profiles and speciation profiles are typically generated based on source testing data. In most previous source testing studies aimed at determining PM chemical composition, filter-based sampling techniques are used to collect PM samples for chemical analyses. Recently, the Micro-Orifice Uniform Deposit Impactor (MOUDI) has been used to collect PM samples for size resolved chemical composition analysis.

4.10.2. Chemical Mechanisms

Airshed models are essential for the development of effective control strategies for reducing photochemical air pollution because they provide the only available scientific basis for making quantitative estimates of changes in air quality resulting from changes in emissions. The chemical mechanism is the portion of the model that represents the processes by which emitted primary pollutants, such as TOG, carbon monoxide (CO), and oxides of nitrogen (NO_x), react in the gas phase to form secondary pollutants such as ozone (O_3) and other oxidants.

For State Implementation Plan (SIP) attainment demonstrations and evaluations, the U.S. EPA has approved the California Air Resources Board's photochemical air quality models. The air quality models used by the ARB for SIP attainment demonstrations use the SAPRC photochemical mechanism. This mechanism is based on extensive scientific research and is documented in the scientific literature (Carter 2000). Table 4-4 shows modeled ROG species (or species categories) for the SAPRC-99 chemical mechanism. Table 4-5 shows modeled species for NOx.

Table 4-4: ARB's SAPRC-99 Emitted Organic Model Species

Model Species Name	Description
HCHO	Formaldehyde
CCHO	Acetaldehyde
RCHO	Lumped C3+ Aldehydes
ACET	Acetone
MEK	Ketones and other non-aldehyde oxygenated products
PROD	
RNO3	Lumped Organic Nitrates
PAN	Peroxy Acetyl Nitrate

PAN2	PPN and other higher alkyl PAN analogues
BALD	Aromatic aldehydes (e.g., benzaldehyde)
PBZN	PAN analogues formed from Aromatic Aldehydes
PHEN	Phenol
CRES	Cresols
NPHE	Nitrophenols
GLY	Glyoxal
MGLY	Methyl Glyoxal
MVK	Methyl Vinyl Ketone
MEOH	Methanol
HC2H	Formic Acid
CH4	Methane
ETHE	Ethene
ISOP	Isoprene
TERP	Terpenes
MTBE	Methyl Tertiary Butyl Ether
ETOH	Ethanol
NROG	Non-reactive
LOST	Lost carbon
ALK1	Alkanes and other non-aromatic compounds that react only with OH, and have kOH < 5 x 10^2 ppm-1 min-1. (Primarily ethane)
ALK2	Alkanes and other non-aromatic compounds that react only with OH, and have kOH between 5 x 10^2 and 2.5 x 10^3 ppm-1 min-1. (Primarily propane and acetylene)
ALK3	Alkanes and other non-aromatic compounds that react only with OH, and have kOH between 2.5 x 10^3 and 5 x 10^3 ppm-1 min-1.
ALK4	Alkanes and other non-aromatic compounds that react only with OH, and have kOH between 5 x 10^3 and 1 x 10^4 ppm-1 min-1.
ALK5	Alkanes and other non-aromatic compounds that react only with

	OH, and have kOH greater than 1 x 10^4 ppm-1 min-1.
ARO1	Aromatics with kOH < 2x10^4 ppm-1 min-1.
ARO2	Aromatics with kOH > 2x10^4 ppm-1 min-1.
OLE1	Alkenes (other than ethene) with kOH < 7x10^4 ppm-1 min-1.
OLE2	Alkenes with kOH > 7x10^4 ppm-1 min-1.

Table 4-5: Model Species for NOx

Model Species Name	Description
HONO	Nitrous Acid
NO	Nitric Oxide
NO2	Nitrogen Dioxide

Both U.S. EPA's and ARB's models require estimates of total organic gases, which include the "exempt VOCs", and, to the extent data are available, any low vapor pressure compounds that become airborne. Model results for ozone non-attainment areas have demonstrated that even compounds with low photochemical reactivity or low vapor pressure can contribute to photochemical ozone formation. For example, even an "exempt VOC" like ethane has been shown to have a contribution to ozone formation. If all exempt compounds and low vapor pressure compounds were omitted from photochemical model simulations, the ozone attainment demonstration would be compromised. The model takes into account that, individually, compounds with low reactivity or that are present in small amounts have a small impact on ozone formation. However, the cumulative effect of several low reactive compounds or many low emission compounds can be a significant contributor to photochemical ozone formation.

4.11. Quality Assurance

To facilitate thorough quality assurance (QA), a variety of standardized emission summary reports for the periods simulated will be produced. Some examples of the standardized reports are contained in the sections below.

As indicated in the prior section, day-specific and external baseline adjustments were applied to baseline emission estimates. For the purpose of checking adjustment levels for accuracy, “baseline” and “adjusted” emission summary reports will be generated.

Inventory corrections will be prioritized based on emissions magnitude, schedule, and potential impact on air quality modeling results. As gridded emissions are processed and quality assured, suspect or unresolvable issues that may impact air quality model performance will be summarized and reported.

4.11.1. Examples of Standard Tabular Summaries

This section contains examples of tabular summaries that will be provided for review.

Domain Totals by Pollutant and Time Period for Baseline and Adjusted Emissions

CO	NOx	SOx	TOG	PM	NH3	ROG	PM_{10}	$PM_{2.5}$
17,939.63	4,308.18	285.01	7,334.56	4,109.78	762.98	3,620.07	2,472.03	810.70

Totals by Major Category, Pollutant, and Time Period for Baseline and Adjusted Emissions

EIC1	DESCRIPTION	CO	NOx	SOx	TOG	PM	NH3	ROG	PM_{10}	$PM_{2.5}$
0	FUEL COMBUSTION	384.18	406.63	48.20	148.62	45.55	5.49	34.17	40.08	37.24
1	WASTE DISPOSAL	2.18	3.02	0.67	1,245.77	1.62	42.56	14.86	0.83	0.73
EIC1	**DESCRIPTION**	**CO**	**NOx**	**SOx**	**TOG**	**PM**	**NH3**	**ROG**	**PM_{10}**	**$PM_{2.5}$**
2	CLEANING AND SURFACE COATINGS	0.15	0.40	0.04	381.17	0.39	2.13	279.20	0.38	0.36
3	PETROLEUM PROD AND MARKETING	10.08	13.97	58.60	536.56	4.90	1.85	219.60	3.05	2.26
4	INDUSTRIAL PROCESSES	53.52	96.16	31.57	95.55	174.20	9.22	79.44	100.22	51.50
5	SOLVENT EVAPORATION	0.00	0.00	0.00	475.95	0.03	37.45	419.42	0.03	0.03
6	MISCELLANEOUS PROCESSES	2,545.81	156.27	9.64	1,811.66	3,726.68	538.27	300.23	2,173.18	586.03
7	ON-ROAD MOTOR VEHICLES	12,726.85	2,315.33	11.27	1,343.71	74.73	75.25	1,233.16	74.09	57.91
8	OTHER MOBILE SOURCES	2,216.86	1,316.41	125.03	484.40	81.69	0.00	431.80	80.18	74.65
9	NATURAL SOURCES	0.00	0.00	0.00	811.17	0.00	50.76	608.19	0.00	0.00

Totals by Summary Category, Pollutant, and Time Period for Baseline and Adjusted Emissions

EIC3	DESCRIPTION	CO	NOX	SOX	TOG	PM	NH3	ROG	PM_{10}	$PM_{2.5}$
010	ELECTRIC UTILITIES	56.74	51.52	4.76	30.97	6.82	2.35	4.97	6.35	5.89
020	COGENERATION	49.01	30.87	1.87	17.27	4.43	0.18	4.04	4.03	3.72
030	OIL AND GAS PRODUCTION (COMBUSTION)	22.66	45.18	7.44	26.59	2.09	0.10	4.15	2.08	2.08
040	PETROLEUM REFINING (COMBUSTION)	10.22	46.03	12.75	3.52	4.26	0.61	1.79	4.06	3.98
050	MANUFACTURING AND INDUSTRIAL	52.77	86.07	14.52	20.28	5.92	1.63	3.96	5.71	5.45
052	FOOD AND AGRICULTURAL PROCESSING	111.24	22.60	2.69	7.72	3.02	0.10	6.06	2.94	2.89
060	SERVICE AND COMMERCIAL	71.00	104.86	3.66	35.62	8.31	0.40	6.90	8.24	8.19
099	OTHER (FUEL COMBUSTION)	10.55	19.50	0.50	6.65	10.70	0.11	2.31	6.68	5.05
110	SEWAGE TREATMENT	0.25	0.39	0.28	1.29	0.03	0.25	0.70	0.02	0.02
120	LANDFILLS	0.85	0.67	0.21	1,182.55	0.89	9.78	7.92	0.40	0.35
130	INCINERATORS	1.01	1.77	0.14	0.94	0.23	0.09	0.16	0.11	0.10
140	SOIL REMEDIATION	0.06	0.09	0.03	0.49	0.11	0.00	0.34	0.04	0.03
199	OTHER (WASTE DISPOSAL)	0.01	0.10	0.00	60.49	0.36	32.42	5.74	0.25	0.25
210	LAUNDERING	0.00	0.00	0.00	8.60	0.00	0.00	0.84	0.00	0.00
EIC3	**DESCRIPTION**	**CO**	**NOX**	**SOX**	**TOG**	**PM**	**NH3**	**ROG**	**PM_{10}**	**$PM_{2.5}$**
220	DEGREASING	0.00	0.00	0.00	178.79	0.00	0.00	99.87	0.00	0.00
230	COATINGS AND RELATED PROCESS SOLVENTS	0.11	0.16	0.04	122.45	0.32	0.03	114.08	0.30	0.29
240	PRINTING	0.01	0.05	0.00	25.31	0.05	0.04	25.31	0.05	0.04
250	ADHESIVES AND SEALANTS	0.00	0.00	0.00	35.84	0.01	0.00	31.80	0.01	0.01
299	OTHER (CLEANING AND SURFACE COATINGS)	0.03	0.19	0.00	10.17	0.02	2.06	7.30	0.02	0.02
310	OIL AND GAS PRODUCTION	1.91	3.32	0.53	104.11	0.10	0.00	53.90	0.08	0.08
320	PETROLEUM REFINING	6.03	9.85	58.06	49.04	3.99	1.85	38.43	2.54	2.08
330	PETROLEUM MARKETING	2.14	0.80	0.00	382.93	0.81	0.00	126.85	0.43	0.10
399	OTHER (PETROLEUM PROD AND MARKETING)	0.00	0.00	0.00	0.47	0.00	0.00	0.42	0.00	0.00
410	CHEMICAL	0.44	1.82	2.69	34.07	5.99	0.25	27.38	5.09	4.71

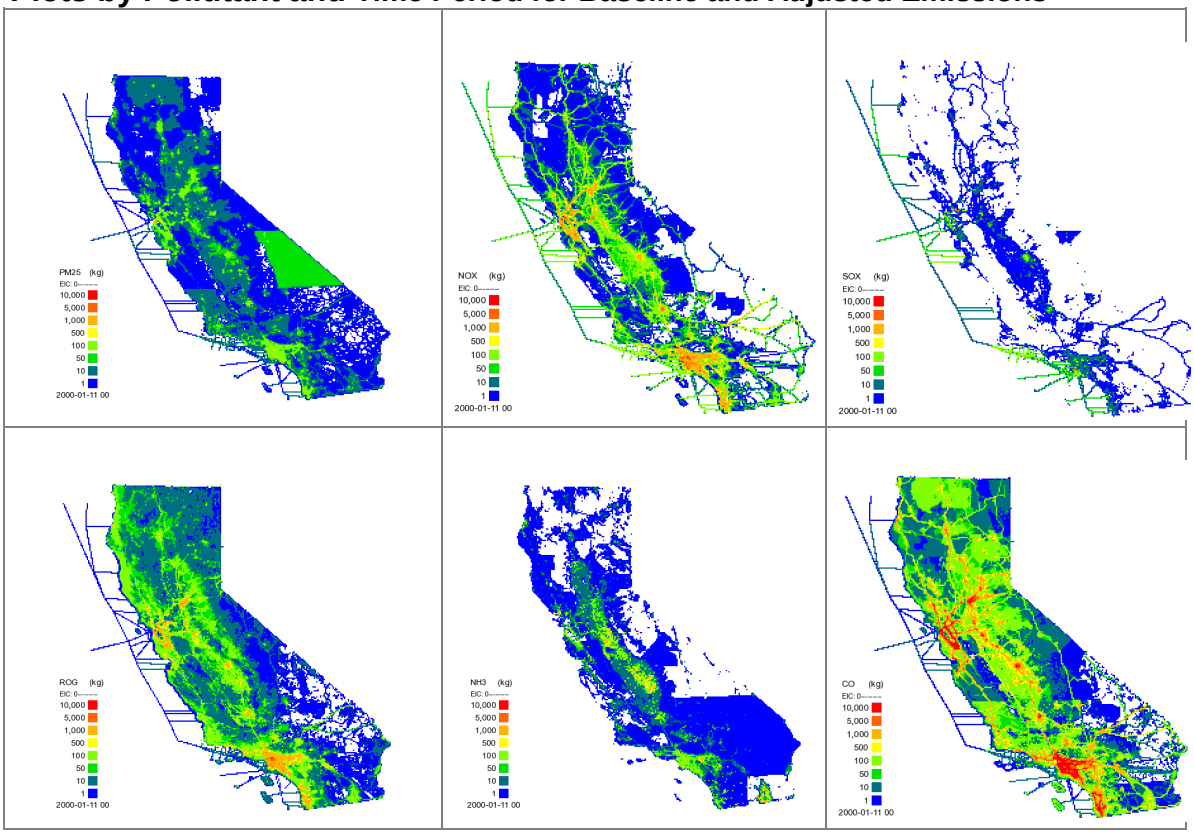
420	FOOD AND AGRICULTURE (Note: Skipping some categories from here to fit on page…)	2.71	9.60	2.52	23.33	29.67	0.07	21.15	12.05	2.79
499	OTHER (INDUSTRIAL PROCESSES)	10.37	9.31	0.85	22.72	18.20	8.82	18.42	11.70	7.86
510	CONSUMER PRODUCTS	0.00	0.00	0.00	305.34	0.00	0.00	259.30	0.00	0.00
520	ARCHITECTURAL COATINGS AND SOLVENTS	0.00	0.00	0.00	111.39	0.00	0.00	108.74	0.00	0.00
530	PESTICIDES/FERTILIZERS	0.00	0.00	0.00	39.41	0.00	37.45	32.38	0.00	0.00
540	ASPHALT PAVING / ROOFING	0.00	0.00	0.00	19.82	0.03	0.00	19.01	0.03	0.03
610	RESIDENTIAL FUEL COMBUSTION	1,741.05	129.11	8.59	274.46	270.85	12.36	120.38	253.79	244.63
620	FARMING OPERATIONS	0.00	0.00	0.00	1,419.61	147.04	467.32	113.57	72.64	17.07
630	CONSTRUCTION AND DEMOLITION	0.00	0.00	0.00	0.00	415.08	0.00	0.00	203.10	20.30
640	PAVED ROAD DUST	0.00	0.00	0.00	0.00	810.83	0.00	0.00	370.71	55.62
645	UNPAVED ROAD DUST	0.00	0.00	0.00	0.00	235.99	0.00	0.00	140.25	14.02
650	FUGITIVE WINDBLOWN DUST	0.00	0.00	0.00	0.00	1,718.35	0.00	0.00	1,016.94	135.06
660	FIRES	10.14	0.24	0.00	1.01	1.17	0.00	0.71	1.15	1.08
670	WASTE BURNING AND DISPOSAL	793.31	26.85	1.05	107.70	92.67	4.64	59.38	90.31	83.67
690	COOKING	0.16	0.00	0.00	8.77	33.40	0.00	6.13	23.38	14.03
699	OTHER (MISCELLANEOUS PROCESSES)	1.15	0.07	0.00	0.10	1.31	53.95	0.07	0.92	0.55
EIC3	**DESCRIPTION**	**CO**	**NOX**	**SOX**	**TOG**	**PM**	**NH3**	**ROG**	**PM_{10}**	**$PM_{2.5}$**
700	On-Road Motor Vehicles	12,726.85	2,315.33	11.27	1,343.71	74.73	0.00	1,233.16	74.09	57.91
710	LIGHT DUTY PASSENGER (LDA)	0.00	0.00	0.00	0.00	0.00	41.86	0.00	0.00	0.00
722	LIGHT DUTY TRUCKS - 1 (LDT1)	0.00	0.00	0.00	0.00	0.00	9.32	0.00	0.00	0.00
723	LIGHT DUTY TRUCKS - 2 (LDT2)	0.00	0.00	0.00	0.00	0.00	15.73	0.00	0.00	0.00
724	MEDIUM DUTY TRUCKS (MDV)	0.00	0.00	0.00	0.00	0.00	5.82	0.00	0.00	0.00
732	LIGHT HEAVY DUTY GAS TRUCKS - 1 (LHDV1)	0.00	0.00	0.00	0.00	0.00	1.20	0.00	0.00	0.00
733	LIGHT HEAVY DUTY GAS TRUCKS - 2 (LHDV2)	0.00	0.00	0.00	0.00	0.00	0.38	0.00	0.00	0.00
734	MEDIUM HEAVY DUTY GAS TRUCKS (MHDV)	0.00	0.00	0.00	0.00	0.00	0.26	0.00	0.00	0.00
736	HEAVY HEAVY DUTY GAS TRUCKS (HHDV)	0.00	0.00	0.00	0.00	0.00	0.14	0.00	0.00	0.00

742	LT HEAVY DUTY DIESEL TRUCKS - 1 (LHDV1)	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
743	LT HEAVY DUTY DIESEL TRUCKS - 2 (LHDV2)	0.00	0.00	0.00	0.00	0.00	0.01	0.00	0.00	0.00
744	MED HEAVY DUTY DIESEL TRUCKS (MHDV)	0.00	0.00	0.00	0.00	0.00	0.03	0.00	0.00	0.00
746	HEAVY HEAVY DUTY DIESEL TRUCKS (HHDV)	0.00	0.00	0.00	0.00	0.00	0.09	0.00	0.00	0.00
750	MOTORCYCLES (MCY)	0.00	0.00	0.00	0.00	0.00	0.05	0.00	0.00	0.00
760	HEAVY DUTY DIESEL URBAN BUSES (UB)	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
762	HEAVY DUTY GAS URBAN BUSES (UB)	0.00	0.00	0.00	0.00	0.00	0.02	0.00	0.00	0.00
770	SCHOOL BUSES (SB)	0.00	0.00	0.00	0.00	0.00	0.01	0.00	0.00	0.00
776	OTHER DIESEL BUSES	0.00	0.00	0.00	0.00	0.00	0.04	0.00	0.00	0.00
780	MOTOR HOMES (MH)	0.00	0.00	0.00	0.00	0.00	0.26	0.00	0.00	0.00
810	AIRCRAFT	249.71	54.02	2.81	40.28	9.03	0.00	35.91	8.81	8.72
820	TRAINS	28.90	194.16	8.05	13.29	4.40	0.00	11.12	4.40	4.05
830	SHIPS AND COMMERCIAL BOATS	38.84	276.79	109.70	17.62	20.28	0.00	14.77	19.62	18.94
840	RECREATIONAL BOATS	126.38	3.82	0.01	36.92	1.39	0.00	34.86	1.25	0.95
EIC3	**DESCRIPTION**	**CO**	**NOX**	**SOX**	**TOG**	**PM**	**NH3**	**ROG**	**PM_{10}**	**$PM_{2.5}$**
850	OFF-ROAD RECREATIONAL VEHICLES	135.10	1.08	0.25	41.00	0.80	0.00	38.28	0.72	0.54
860	OFF-ROAD EQUIPMENT	1,536.69	680.34	3.49	259.95	39.32	0.00	225.28	38.92	35.52
870	FARM EQUIPMENT	101.24	106.20	0.72	24.87	6.47	0.00	21.29	6.46	5.93
890	FUEL STORAGE AND HANDLING	0.00	0.00	0.00	50.46	0.00	0.00	50.28	0.00	0.00
910	BIOGENIC SOURCES	0.00	0.00	0.00	709.42	0.00	14.54	578.69	0.00	0.00
920	GEOGENIC SOURCES	0.00	0.00	0.00	101.75	0.00	36.22	29.50	0.00	0.00

4.11.2. Spatial Plots

Spatial plots are useful to ensure that emissions are distributed correctly into each grid cell.

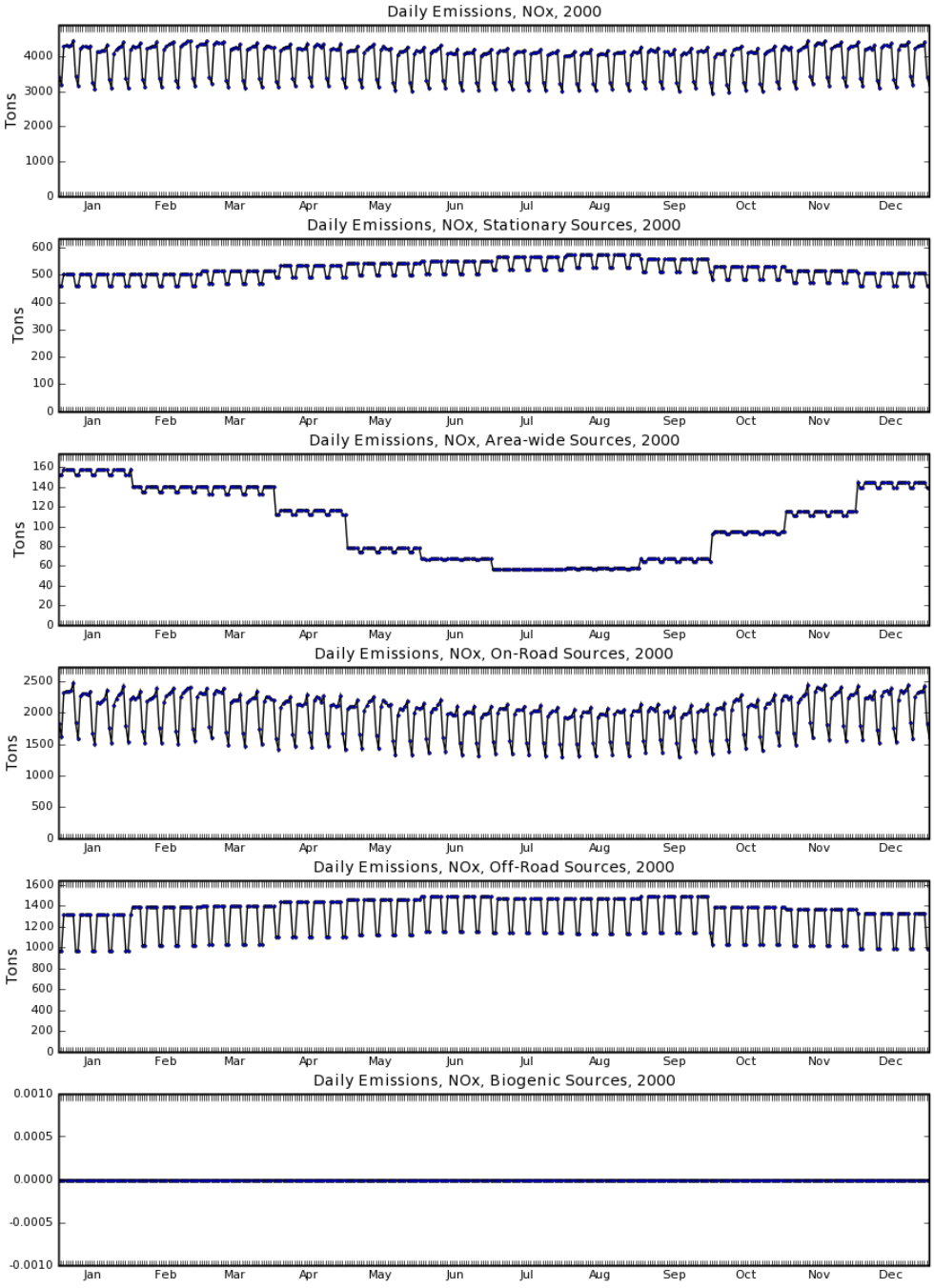
Plots by Pollutant and Time Period for Baseline and Adjusted Emissions



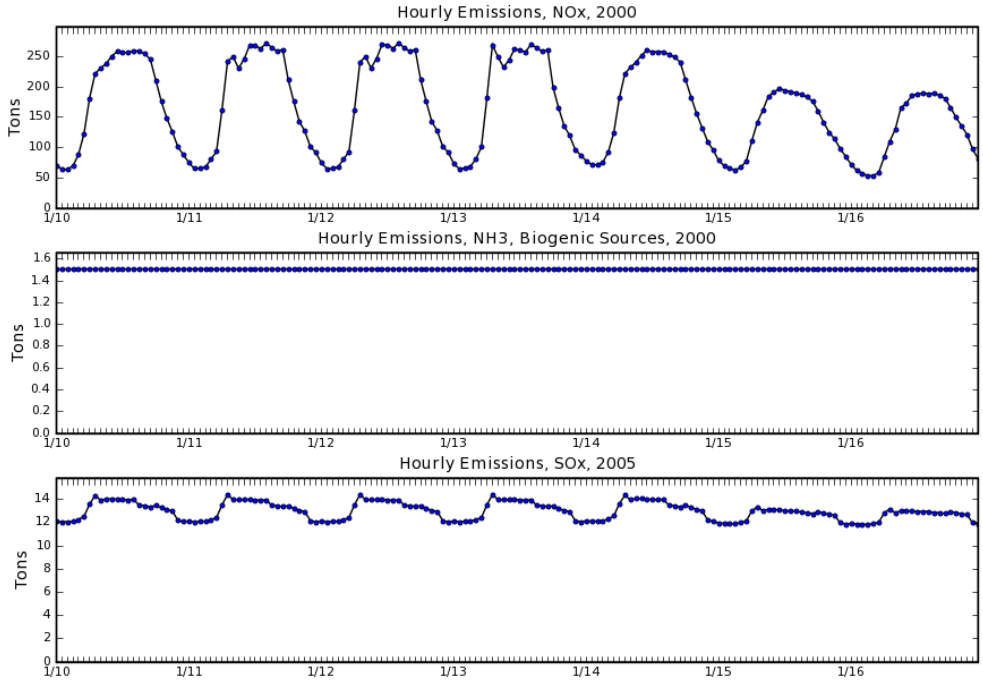
4.11.3. Time Series Plots

Time series plots are useful to ensure that emissions are distributed correctly in time across the modeling period.

Weekly Time-Series Plots of Emissions by Year



Hourly Time-Series Plots of Emissions by Week



5. Models and Inputs

5.1. Rationale for the Selection of Models

5.1.1. Meteorology Model

Meteorological model selection is based on a need to accurately simulate the synoptic and mesoscale meteorological features exhibited during the selected episodic periods. The main difficulties in accomplishing this are California's extremely complex terrain and its diverse climate. It is desirable that atmospheric modeling adequately represent essential meteorological features, such as wind flows, ambient temperature variation, evolution of the boundary layer, etc., to properly characterize the meteorological component of photochemical modeling.

In the past, the ARB has applied prognostic, diagnostic, and objective models to prepare meteorological fields for photochemical modeling. There are various numerical models that are used by the scientific community to study the meteorological characteristics of an air pollution episode. For this SIP, the models under consideration for meteorological modeling are:

- Mesoscale Meteorological Model Version 5 (MM5) (Grell et al, 1994), and
- Weather and Research Forecasting Model (WRF) (Skamarock et al, 2005).

MM5 is a mesoscale, limited area, non-hydrostatic numerical model developed by Penn State and the National Center for Atmospheric Research (NCAR). It uses a terrain-following, Lambert Conformal, sigma coordinate system. MM5 allows users to study the atmospheric motions at small scales by explicitly treating the effects of convective motions on atmospheric circulations. It has been improved on an ongoing basis over the last two decades by contributions from a broad scientific community and has been maintained by NCAR along with necessary meteorological and geographical input data. Based on the complexity of terrain in northern and central California, the MM5 model represents an appropriate tool for resolving dynamics and thermodynamics using nesting capabilities. The ARB has also been using the MM5 model over the last two

decades, since it has been widely used and tested for various meteorological regimes over the world and has been supported by NCAR. NCAR terminated model development for MM5 in October 2006 and the code was frozen at the minor version of V3-7-4.

Since then NCAR has devoted its resources to the development of the WRF model, which was designed to be the replacement for MM5. The WRF model is being continually updated, but ARB's experience with the model is limited compared to that with MM5. The preliminary WRF fields produced by ARB have not shown any significant improvement over those from MM5.

Based on the long history of using MM5 by ARB and stakeholder groups in California in regulatory modeling, the MM5 numerical model was chosen to generate meteorological fields for SIP modeling. A more detailed description of prognostic meteorology models and their known limitations in the complex terrain of California, see Section 6.1.

ARB will continue to evaluate the WRF model for future SIP modeling and potentially as a corroborative tool to MM5 for this SIP. More details on this effort are provided in Section 9.3.

5.1.2. Air Quality Model

U.S. EPA guidance requires several factors to be considered as criteria for choosing a qualifying air quality model to support the attainment demonstration. These criteria include: (1) documentation and past track record of candidate models in similar applications; (2) advanced science and technical features available in the model and/or modeling system; (3) experience of staff and available contractors; (4) required time and resources versus available time and resources; and (5) in the case of regional applications, consistency with regional models applied in adjacent regions (U.S. EPA, 2007). For the $PM_{2.5}$ modeled attainment test, a grid-based photochemical model is necessary to offer the best available representation of important atmospheric processes and the ability to analyze the impacts of proposed emission controls on $PM_{2.5}$ concentrations.

The Community Multiscale Air Quality (CMAQ) Modeling System has been selected for modeling $PM_{2.5}$ in the SJV. The CMAQ model, a state-of-the-science "one-atmosphere" modeling system developed by U.S. EPA, was designed for applications ranging from regulatory and policy analysis to understanding of the atmospheric chemistry and physics. It is a three-dimensional Eulerian modeling system that simulates ozone, particulate matter, toxic air pollutants, visibility, and acidic pollutant species throughout the troposphere (UNC, 2010). The CMAQ model has undergone peer review every few years and was found to be state of the science (Aiyyer et al., 2007). The CMAQ model is regularly updated to incorporate new mechanisms, algorithms, and data as they become available in the scientific literature (e.g., Foley, et al., 2010). In addition, the CMAQ model is well documented in terms of its underlying scientific algorithms as well as guidance on operational uses (e.g., Binkowski and Roselle, 2003; Byun and Ching, 1999; Byun and Schere, 2006; Carlton et al., 2010; Foley et al., 2010; Kelly, et al., 2010a; UNC, 2010).

The CMAQ model was the regional air quality model used for the 2008 SJV annual $PM_{2.5}$ SIP. A number of previous studies have also used the CMAQ model to study ozone and $PM_{2.5}$ in the SJV (e.g., Jin et al., 2008, 2010; Kelly et al., 2010b; Liang and Kaduwela, 2005; Livingstone, et al., 2009; Pun et al, 2009; Tonse et al., 2008; Vijayaraghavan et al., 2006; Zhang et al., 2010). The CMAQ model has also been used for regulatory analysis for many of U.S. EPA's rules, such as the Clean Air Interstate Rule (U.S. EPA, 2005) and Light-duty and Heavy-duty Greenhouse Gas Emissions Standards (U.S. EPA, 2010, 2011a). There are numerous applications of the CMAQ model in the U.S. and in the world (e.g., Appel, et al., 2007, 2008; Civerolo et al., 2010; Eder and Yu, 2006; Hogrefe et al., 2004; Lin et al., 2008, 2009; Marmur et al., 2006; O'Neill, et al., 2006; Philips and Finkelstein, 2006; Sokhi et al., 2006; Smyth et al., 2006; Tong et al., 2006; Wilczak et al., 2009; Zhang et al., 2004, 2006). Staff at CARB has developed expertise in applying the CMAQ model, since it has been used at CARB for over a decade. In addition, technical support for the CMAQ model is available from the

Community Modeling and Analysis System (CMAS) Center (http://www.cmascenter.org/) established by the U.S. EPA.

The most recent version, CMAQv4.7.1 (Foley et al., 2010) will be used. While U.S. EPA released the CMAQ version 5.0 in October 2011, that release came too late for current modeling efforts.

5.2. Model Setup and Inputs

5.2.1. Meteorology Model (modeling domains, horizontal and vertical resolution, physics options, regional reanalysis data, etc.)

The MM5 meteorological modeling domain consists of three nested grids, of 36 km, 12 km and 4 km uniform, horizontal grid spacing (illustrated in Figure 5.1). The purpose of the coarse, 36 km grid (D01) is to provide synoptic-scale conditions to all three grids, while the purpose of the 12 km grid (D02) is to provide input data to the 4 km grid (D03). The D01 grid is centered at 37 N x 120.5 W while the two inner grids, D02 and D03, are placed within the coarser grid such that they are not too close to the lateral boundaries. The D01 grid consists of 70 x 70 grid cells. The D02 grid consists of 132 x 132 grid cells and the D03 grid consists of 327 x 297 grid cells having an origin at -696 km x -576 km (Lambert Conformal projection). The first two coarse grids were run simultaneously, and the D03 grid was run independently using the output of its coarser, parent D02 grid as input. The D03 grid is intended to resolve the fine details of atmospheric motion and is used to feed the air quality modeling simulations. The vertical layer structure has 30 layers, as shown in Table 5.1. The physics options are shown in Table 5.2.

The initial and boundary conditions (IC/BC) for MM5 were prepared based on 3-D analyses of the NCEP/NCAR Reanalysis Project (NNRP) that is archived at NCAR. These data are archived from global simulations and have a 209 km horizontal resolution. Initial conditions to MM5 were updated at 6-hour intervals for the 36 and 12 km grids. In addition, surface and upper air synoptic observations obtained from NCEP are also used to further refine the IC/BCs.

The MM5 model was nudged toward observed meteorological conditions by using the analysis nudging option of the Four Dimensional Data Analysis (FDDA) for the 36 and 12 km grids only. Input conditions for the 4 km grid were obtained from the output of the 12 km grid, and the observational nudging option of FDDA was used to enhance these input conditions. Only wind measurements were used for observational nudging.

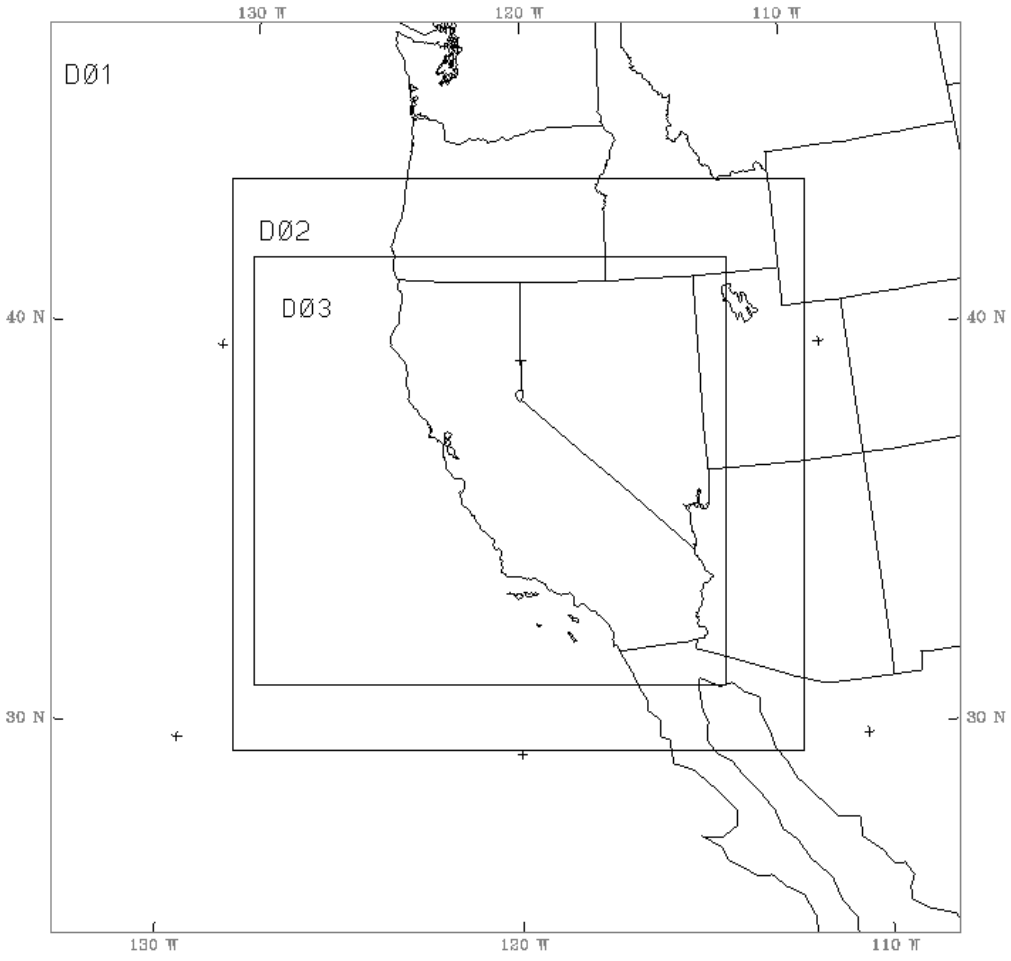


Figure 5-1: The three nested grids for the MM5 model (D01 36km; D02 12km; and D03 4km).

Table 5-1: MM5 30 Vertical Layer Configuration.

Layer No.	Height (m)	Layer Thickness (m)
30	15674	998
29	14676	982
28	13694	976
27	12718	970
26	11748	972
25	10776	973
24	9803	979
23	8824	983
22	7841	994
21	6847	1002
20	5845	972
19	4873	818
18	4055	687
17	3368	577
16	2791	484
15	2307	407
14	1900	339
13	1561	285
12	1276	238
11	1038	199
10	839	166
9	673	139
8	534	115
7	419	97
6	322	81

5	241	67
4	174	56
3	118	47
2	71	39
1	32	32
0	0	0

Table 5-2: MM5 Physics Options.

Physics Option	D01	D02	D03
Cumulus Parameterization	Grell	Grell	None
Planetary Boundary Layer Scheme	Gayno-Seaman	Gayno-Seaman	Gayno-Seaman
Explicit Moisture Scheme	Dudhia Simple Ice	Dudhia Simple Ice	Dudhia Simple Ice
Radiation Scheme	RRTM	RRTM	RRTM
Soil Temperature Model	5-layer soil slab	5-layer soil slab	5-layer soil slab

5.2.2. Air Quality Model (modeling domains, horizontal and vertical resolution, chemical mechanisms, PM routines, initial and boundary conditions, etc.)

The principle determinants of the extent of the modeling domain are the nature of the $PM_{2.5}$ problem and the scale of the emissions that impact the nonattainment area. Isolated nonattainment areas that are not impacted by regional transport and its precursors may be able to use a relatively small domain (U.S. EPA, 2007). Figure 5.2 shows modeling domains used by ARB. The two modeling domains that are proposed for this work are shown in blue (12 km coarse domain) and magenta (4 km nested domain). The coarse domain (blue) includes 107x97 lateral 12 km grid cells for each

vertical layer. This domain extends from the Pacific Ocean in the west to the Eastern Nevada in the east and runs from the U.S.-Mexico border in the south to the California-Oregon border in the north. The nested domain (magenta) covers Central California with 192x192 lateral 4 km grid cells. The domain is based on the Lambert Conformal Conic projection with reference longitude at -120.5°W, reference longitude at 37°N, and two standard parallels at 30°N and 60°N, respectively.

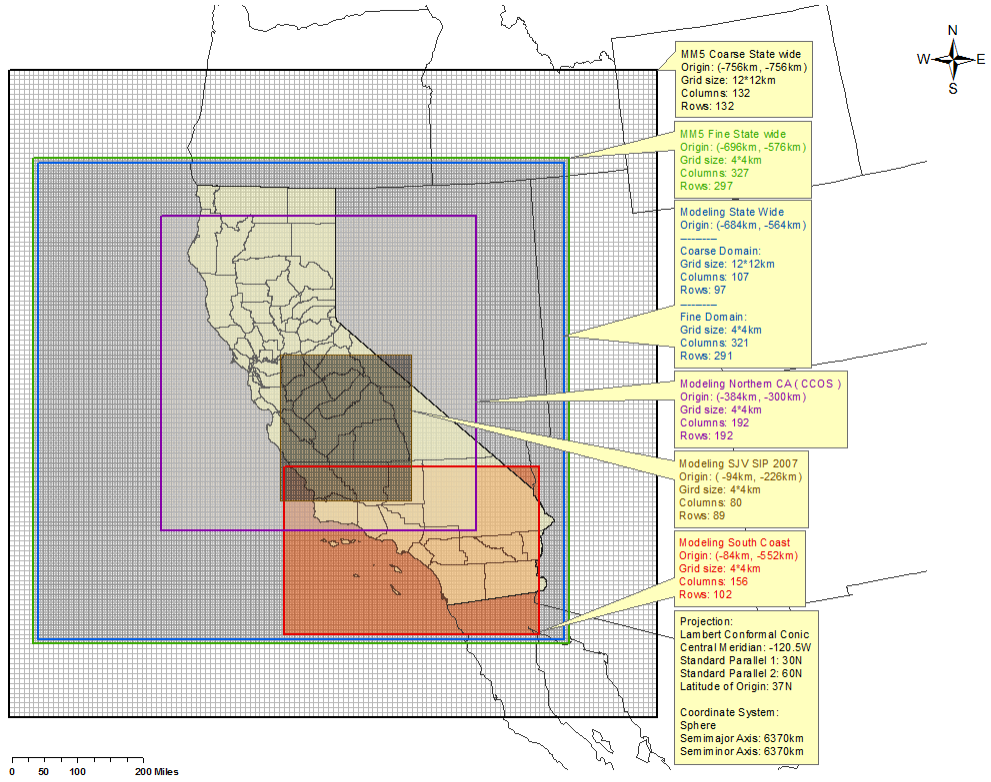


Figure 5-2: Modeling domains used by ARB

For the coarse portions of nested regional grids, U.S. EPA guidance suggests a grid cell size of 12 km if feasible but not larger than 36 km. For the fine scale portions of nested regional grids, it is desirable to use grid cells about 4 km (U.S. EPA, 2007). Our selection of modeling domains is consistent with the guidance. U.S. EPA guidance does not require a minimum number of vertical layers for an attainment demonstration, although typical applications of “one- atmosphere” models (with the model top at

100 mb) employ 12 to 21 vertical layers. For the present SIP, 15 vertical layers will be used in the CMAQ model, extending from the surface to 100 mb, consistent with the number of vertical layers used for the 2008 SJV $PM_{2.5}$ SIP. The vertical structure is based on the sigma-pressure coordinate, with the layers separated at 1.0, 0.9958, 0.9907, 0.9846, 0.9774, 0.9688, 0.9585, 0.9463, 0.9319, 0.9148, 0.8946, 0.7733, 0.6254, 0.293, 0.0788, and 0.0. This ensures that the majority of the layers are in the planetary boundary layer.

The small black domain in the center of Figure 5-2 is the air quality modeling domain used for the previous annual $PM_{2.5}$ SIP which is now approved by the U.S. EPA (76 FR 41338; 76 FR 69896). The originally proposed 4 km domain is ~5 times larger than the previously used 4 km domain. However, preliminary modeling for the current SIP, in combination with the anticipated number of modeling runs that will be necessary to complete the SIP modeling, have demonstrated the infeasiblity of using the larger 4 km (magenta) domain with available resources. Therefore, we will use the small 4 km (black) domain which has already been approved by the U.S. EPA (76 FR 41338; 76 FR 69896).

Table 5.3 shows the CMAQv4.7.1 configuration that will be used to model $PM_{2.5}$ in the SJV. The same configuration will be used for all simulations for the base, reference, and future years. CMAQv4.7.1 will be compiled using the Portland Group FORTRAN Compiler version 10.9.

Table 5-3: CMAQv4.7.1 Schemes used for Current Simulations.

Processes	Scheme
Horizontal advection	PPM (piecewise parabolic method)
Vertical advection	PPM (piecewise parabolic method)
Horizontal diffusion	Multi-scale
Vertical diffusion	Eddy
Gas-phase chemical mechanism	SAPRC99
Chemical solver	EBI

Aerosol module	Aero5
Cloud module	ACM_AE5
Photolysis rate	Table Generated by the JPROC program

In order to simulate the complex mixture of $PM_{2.5}$ species in the SJV, the SAPRC99 mechanism coupled with the CMAQ model aerosol code version 5 and aqueous phase chemistry (AE5-AQ) has been chosen for this application. SAPRC99, developed by Dr. William Carter at the University of California, Riverside, is a detailed mechanism describing the gas-phase reactions of volatile organic compounds (VOCs) and oxides of nitrogen (NOx) (Carter, 2000). It is a well-known chemical mechanism and has been used widely in California and the U.S. (e.g., Hakami, et al., 2004a, 2004b; Liang and Kaduwela, 2005; Lin et al., 2005; Jackson, et al., 2006; Napelenok, 2006; Dennis et al., 2008; Jin et al., 2008, 2010; Lane et al., 2008; Tonse et al., 2008; Ying et al., 2008; Livingstone et al., 2009; Pun et al., 2009; Kelly, et al., 2010b; Zhang et al., 2010; Zhang and Ying, 2011).

CARB established the Reactivity Scientific Advisory Committee (RSAC) in April 1996. RSAC is a group of independent scientists who make non-binding recommendations on the science related to the reactivity of VOCs. RSAC consists of the following members: Drs. John Seinfeld (Chair, California Institute of Technology), Roger Atkinson (University of California at Riverside), Jack Calvert (National Center for Atmospheric Research), Harvey Jeffries (University of North Carolina at Chapel Hill), Jana Milford (University of Colorado at Boulder), and Armistead Russell (Georgia Institute of Technology). In 1998, RSAC recommended that the SAPRC99 mechanism undergo a scientific review. Following RSAC's recommendation, CARB contracted Dr. William R. Stockwell in 1999 to conduct a review of the SAPRC99 mechanism, its documentation, and the Maximum Incremental Reactivity scale derived from SAPRC99. Stockwell (1999) compared the chemical kinetic data used in the SAPRC99 mechanism with values from standard kinetic databases (e.g., Atkinson et al., 1994, 1997; DeMore et al., 1997) and the most recent literature available at the time. The kinetic parameters

checked included the reactions, rate constants, product yields, and lumping methods. Stockwell's (1999) comments led to the revision of the mechanism and identification of outstanding issues to be resolved with further experimental studies. Stockwell (1999) concluded that SAPRC99 reflected the best available science at its completion date, and RSAC approved both the SAPRC99 peer review and the mechanism in October 1999. They also recommended that the SAPRC family of mechanisms be used for regulatory photochemical modeling activities in California.

The 2008 SJV $PM_{2.5}$ SIP also used the SAPRC99 mechanism. While a newer version, SAPRC07 (Azzi et al., 2010; Carter, 2010a,b; Derwent et al., 2010;Mollner et al., 2010; Cai et al., 2011a,b), will be incorporated into CMAQv5.0, the timeline of the official release of SAPRC07 and CMAQv5.0 is not consistent with the current modeling effort.

AE5-AQ, the newest aerosol and aqueous-phase chemistry code in CMAQv4.7.1, when coupled with a gas phase mechanism, simulates the formation and evaporation of aerosol and the evolution of the aerosol size distribution (Foley et al., 2010). AE5 includes a comprehensive yet computationally efficient inorganic thermodynamic model ISORROPIA to simulate the physical state and chemical composition of inorganic atmospheric aerosols (Nenes, et al., 1998). ISORROPIA has been proven to be the model of choice for many three-dimensional air quality models (Yu et al., 2005). AE5 also features an improved secondary organic aerosol (SOA) module with up-to-date scientific information (Carlton et al., 2010). In addition to SOA formation from more traditional aromatic compounds and biogenic monoterpene species, the SOA module in AE5 incorporates SOA formation from benzene, isoprene, and sequiterpenes, in-cloud SOA production from glyoxal and methylglyoxal, particle-phase oligomerization, acid enhancement of isoprene SOA, and NOx dependent aromatic SOA yields (Carlton et al., 2010).

CMAQv4.7.1 offers two advection schemes: the piecewise parabolic method (PPM) and the Yamartino scheme. PPM is based on the finite-volume subgrid definition of the advected scalar. It is implemented in a global mass-conserving scheme in the CMAQ model (UNC, 2010). We chose the PPM scheme because the Yamartino scheme leads

to unrealistic O_3 mixing ratio predictions in the mountainous areas of Central California during winter. For example, Figure 5-3 shows an example of 1-hour O_3 mixing ratio predictions during January 2007 simulated by CMAQv4.7.1 with the Yamartino advection scheme. 1-hour O_3 mixing ratios greater than 100 ppb were predicted for some mountainous areas. This is not supported by observed O_3 mixing ratios, which only range up to 50 ppb in Yosemite and Sequoia National Parks in January 2007. The excessive O_3 prediction is due to the advection scheme that brings the upper troposphere O_3 down to the surface levels. $PM_{2.5}$ predictions from the PPM and the Yamartino schemes are comparable. For example, Figure 5-4 shows that the difference in monthly average $PM_{2.5}$ predictions for January 2007 using CMAQv4.7.1 with the PPM and Yamartino schemes is between -0.4 to 1.0 $\mu g/m^3$.

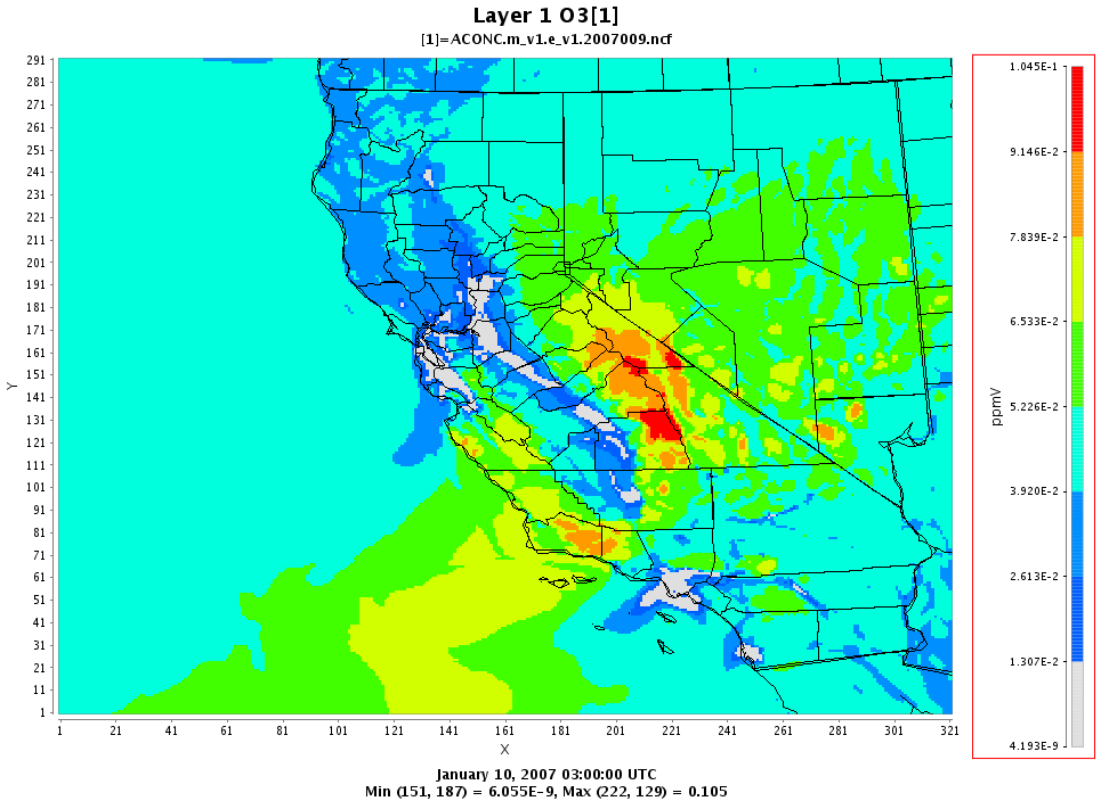


Figure 5-3: 1-hour O_3 mixing ratio at 3 am of Jan 10, 2007 (UTC) predicted by CMAQv4.7.1 with the Yamartino advection scheme.

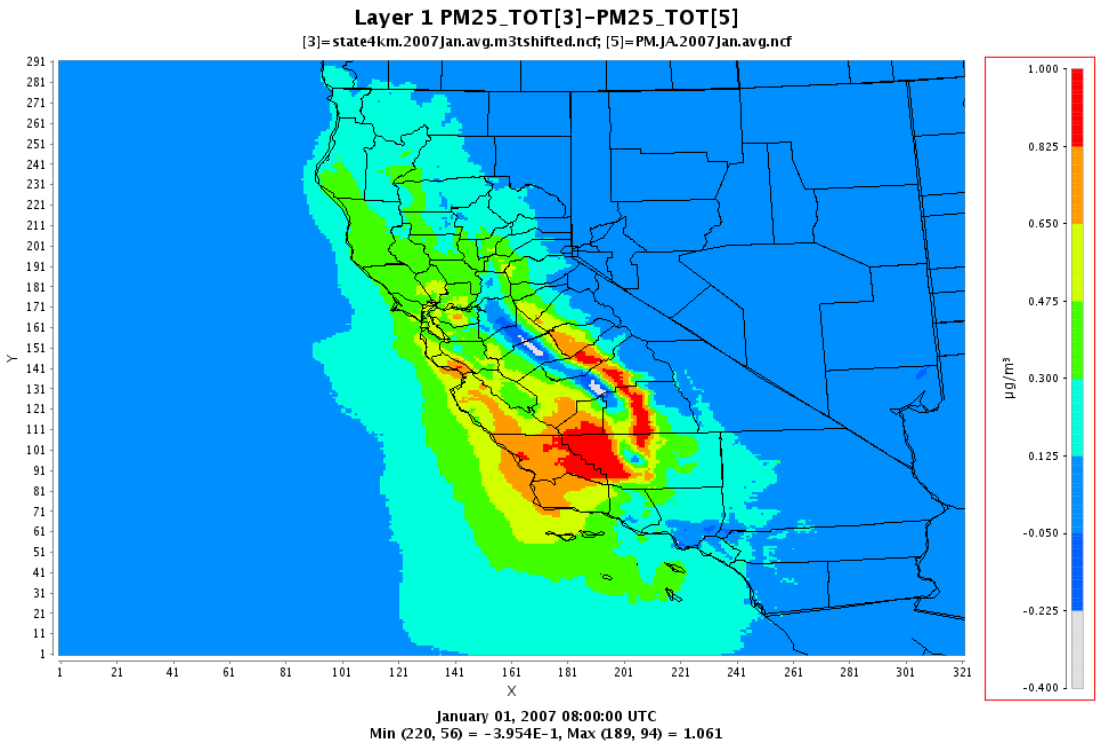


Figure 5-4: Difference in monthly average $PM_{2.5}$ predictions for January 2007 simulated using CMAQv4.7.1 with the PPM and Yamartino schemes.

U.S. EPA guidance recommends using a "ramp-up" period by beginning a simulation 5-10 days prior to the period of interest for modeling $PM_{2.5}$ (U.S. EPA, 2007). Instead of running the CMAQ model sequentially from the beginning to the end of the simulation year, we simulate each month in parallel. For each month, we run seven spin-up days prior to the beginning of each month to generate the initial conditions for the coarse domain. We then use the output from the coarse modeling domain to specify the initial conditions for the nested domain because the nested domain simulation starts after the beginning of the simulation for the outer grid, consistent with U.S. EPA guidance.

In recent years, the use of global chemical transport model (CTM) outputs as boundary conditions (BCs) in regional CTM applications has become increasingly common (Hogrefe et al., 2011; Chen et al., 2008; Lin et al., 2010; Lam and Fu, 2009; Lee et al., 2011), and has been shown to improve model performance in many cases (Tong and

Mauzerall, 2006; Tang et al., 2007; Tang et al., 2009; Borge et al., 2010; Appel et al., 2007). The advantage of using global CTM model outputs as opposed to fixed climatological-average BCs is that the global CTM derived BCs capture spatial, diurnal, and seasonal variability, as well as provide a set of chemically consistent pollutant concentrations. The Model for Ozone And Related chemical Tracers (MOZART; Emmons et al., 2010a) is a global CTM that has been widely used for such applications. MOZART has been extensively peer-reviewed and applied in a range of studies including global change impacts on air quality (e.g., Wiedinmyer et al., 2006; Brasseur et al., 2006; Huang et al., 2008; Avise et al., 2009), long-range transport of pollution (e.g., Liu et al., 2005; Liu an Mauzerall, 2007; Pfister et al., 2010), and atmospheric chemistry/air quality studies (e.g., Emmons et al., 2010b; Pfister et al., 2008; Apel et al., 2010; Fiore et al., 2005).

The MOZART model is a comprehensive global model for simulating atmospheric composition including both gases and bulk aerosols (Emmons et al., 2010a). It was developed by the National Center for Atmospheric Research, the Max-Planck-Institute for Meteorology (in Germany), and the Geophysical Fluid Dynamics Laboratory of the National Oceanic and Atmospheric Administration, and is widely used in the scientific community. In addition to inorganic gases and VOCs, boundary conditions were extracted for aerosol species including elemental carbon, organic matter, sulfate, soil and nitrate.

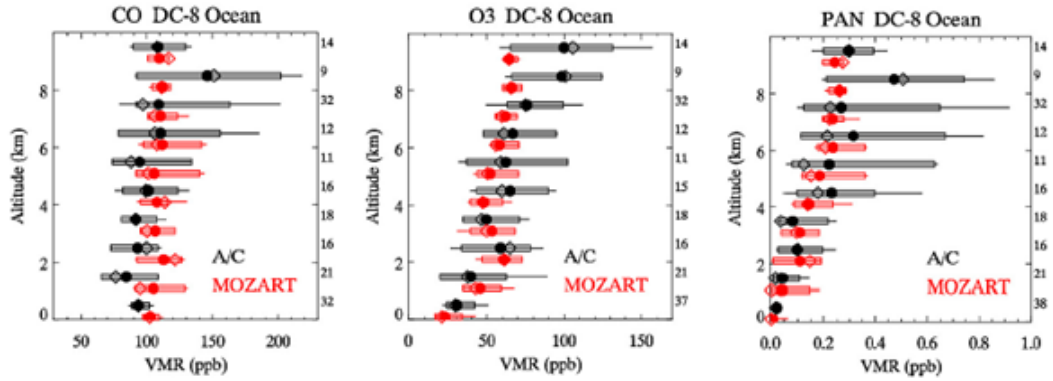


Figure 5-5: Comparison of MOZART (red) simulated CO (left), ozone (center), and PAN (right) to observations (black) along the DC-8 flight track. Shown are mean (filled

symbol), median (open symbols), 10th and 90th percentiles (bars) and extremes (lines). The number of data points per 1-km wide altitude bin is shown next to the graphs. Adapted from Figure 2 in Pfister et al. (2011).

In particular, MOZART version 4 (MOZART-4) was recently used in a study characterizing summertime air masses entering California from the Pacific Ocean (Pfister et al., 2011). In their work, Pfister et al. (2011) compared MOZART-4 simulation results to measurements of CO, ozone, and PAN made off the California coast during the ARCTAS-CARB airborne field campaign (Jacob et al., 2010) and showed good agreement between the observations and model results (see Figure 5-5).

Boundary conditions for the outer 12-km modeling domain were derived from MOZART4-GEOS5 simulations by Louisa Emmons (NCAR) for the year 2007; available for download at http://www.acd.ucar.edu/wrf-chem/mozart.shtml. These simulations are similar to those of Emmons et al. (2010), but with updated meteorological fields. Boundary condition data was extracted from the MOZART-4 output and processed to CMAQ model ready format using computer code developed by ARB staff, which has been used to generate BCs for previous air quality studies (Chen et al., 2008; Avise et al., 2009; Chen et al., 2009a,b; Cai et al., 2011; Kelly et al., 2011). The final BCs represent day-specific concentrations, which vary in both space (horizontal and vertical) and time (every six hours).

The boundary conditions for the nested 4 km domain were extracted from the output for the coarse 12 km domain simulation using the BCON program in the CMAQ modeling system. The boundary conditions for the coarse domain for the reference year will be used for future years as well, consistent with U.S. EPA guidance.

Overall, using a 4 km nested domain within the 12 km coarse domain will reduce the computational burden without compromising the accuracy of the modeling results when compared to a simulation using a 4 km grid for the entire outer domain. Figure 5-6 shows the difference in average $PM_{2.5}$ prediction for January 2007 between a simulation

with the nested domain and a simulation using a 4km grid for the entire outer domain. The discrepancy in monthly average $PM_{2.5}$ predictions is extremely small (± 0.1 µg/m^3) for the areas of interest.

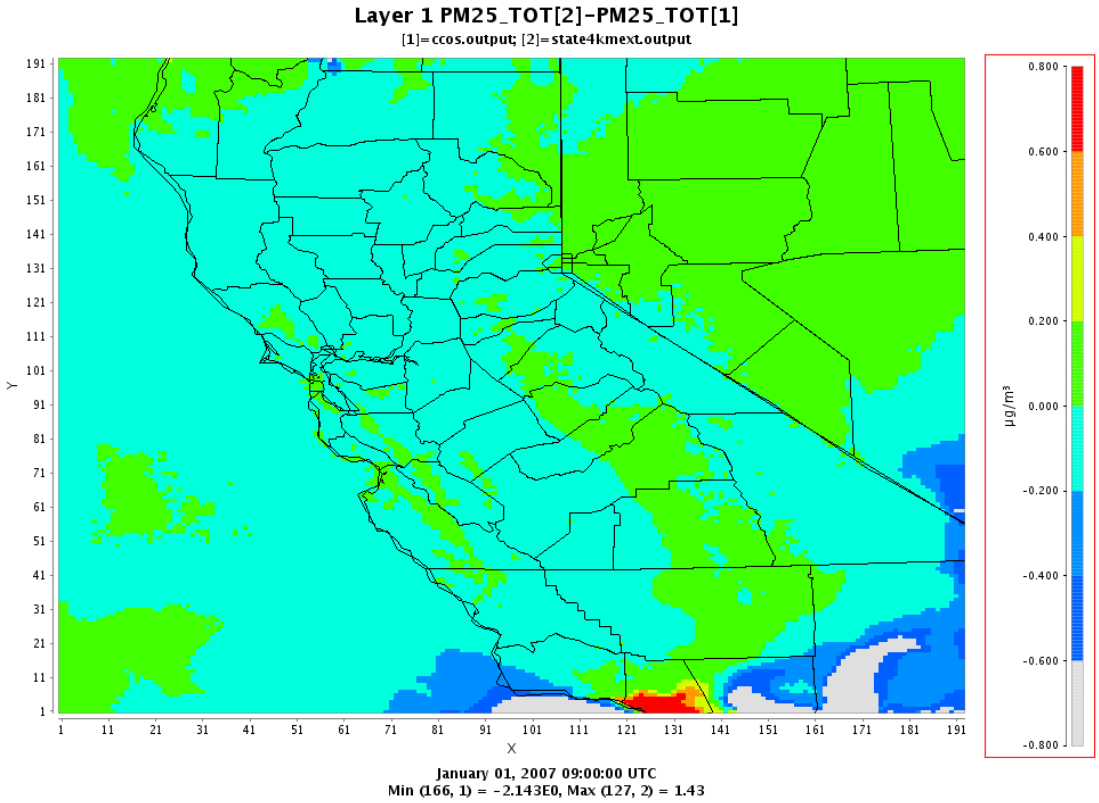


Figure 5-6: Difference in average $PM_{2.5}$ prediction for January 2007 between simulation with the nested domain and simulation using 4km grid for the entire coarse domain.

The dry and wet deposition (also known as lost processes) of pollutants (both gaseous and particulate) is explicitly included in the continuity equation solved by the CMAQ model. The time-varying species-dependent dry deposition velocities are calculated in the Meteorology-Chemistry Interface Processor (MCIP) and are passed along to the CAMQ model for the calculation of dry deposition fluxes. The wet deposition fluxes due to rainfall are calculated in the cloud module of the CMAQ model. Dry and wet deposition estimates are then saved in separate output files.

5.2.3. Construction of the Simulated $PM_{2.5}$ Mass

The CMAQ model does not output $PM_{2.5}$ total mass concentrations. Instead, it outputs concentrations for individual aerosol components in each aerosol mode (e.g., sulfate in the accumulation mode, nitrate in the coarse mode, etc.). These outputs require additional processing to generate predictions for $PM_{2.5}$ mass. For this effort, we choose to use the hourly average model species concentrations saved in the ACONC file as modeled concentrations (UNC, 2010). We will use the "combine" program in the CMAQ modeling system to generate the predictions for total $PM_{2.5}$ mass as well as $PM_{2.5}$ components that can be compared with observations.

5.2.4. Quality Assurance of Model Inputs

In developing the IC/BCs and FDDA datasets, quality control is performed on all associated meteorological data. Generally, all surface and upper air data are plotted in space and time to identify extreme values that are suspected to be "outliers". Data points are also compared to other, similar surrounding data points to determine whether there are any large relative discrepancies. If a scientifically plausible reason for the occurrence of suspected outliers is not known, the outlier data points are flagged as invalid and not used in the modeling analyses.

6. Meteorological Model Performance Evaluation

6.1. Known Performance Issues of Meteorological Models in the Complex Terrain of California and Current Attempts to Improve Performance

The San Joaquin Valley is bordered on the west by the Coastal Mountain Range and on the east by the Sierra Nevada range. These ranges converge at the southern end of the basin at the Tehachapi Mountains. West of the Coastal Mountain Range is the Pacific Ocean. The SJV is considered to be the most fertile desert in the world. The ocean-land interface, mountain-valley topography, and the drastic temperature changes make the SJV one of the most challenging areas in the country to simulate using meteorological models.

One can generate meteorological fields using two different methods. The first is known as the diagnostic method where observed fields are interpolated. These fields represent the actual meteorological state of the atmosphere where the measurements were made. However, such measurements are sparse and often made at the surface level. Some monitors may have limited spatial representation due to their locations (e.g., in canyons). These diagnostic meteorological fields do not have dynamic consistency among variables (Seaman, 2000) and may not have all the variables required by modern air quality models. However, they have been shown to provide better air-quality model performance during the summer (Jackson et al., 2006) and winter (Hu et al., 2010) in SJV. This may be due to their ability to better represent the wind speeds and temperatures.

When a dense network of representative meteorological measurements are not available, one can use a set of non-linear partial differential equations, known as governing equations, which describe the time evolution of the atmospheric system through space and time. The governing equations are comprised of the equations of conservation of mass, motion, heat, and water (Pielke, 1984). Meteorological models that integrate the set of governing equations through space-time are known as

prognostic models. There is a long history of prognostic meteorological model applications in the SJV (Seaman, Stauffer, and Lario-Gibbs, 1995; Stauffer et al., 2000; Tanrikulu et al., 2000; Jackson et al., 2006; Bao et al., 2008; Livingstone et al., 2009; Michelson et al., 2010; Jin et al., 2010; Hu at al., 2010).

The integration of the governing equations requires simplifying assumptions that lend them to numerical integrations methods. These simplifying assumptions can lead to two undesirable consequences. First, they may cause the simulated solution to stray from the ideal solution. To minimize this, four-dimensional data assimilation (FDDA) techniques were developed. While FDDA is known to steer the simulated solution towards the measured fields, the momentum redistribution within the model causes spurious features where no measurements are available. While FDDA is not considered to be a panacea, it is an operational necessity to develop meteorological fields that are accurate enough for the operation of air quality models.

The second undesirable consequence is due to the complex terrain of California itself. The centered finite difference scheme used in prognostic models works well when the terrain features are smooth and continuous. However, the SJV is bounded by three steep and rugged mountain ranges. The elevation can change by tens to hundreds of meters in one 4 km grid cell. The Coastal Range on the west is near the ocean-land interface which is also difficult to simulate. This makes the terrain in California complex compared to other parts of the country where the application of prognostic models have been more successful. To overcome this difficulty, the grid sizes were reduced from 4 km to 1.33 km as a test. The minor improvements in the fine-scale meteorological fields did not justify the nine fold increase in the computational time. Another option is to investigate the effect of using different model options, especially those related to sub-grid-scale processes. This is being done now in collaboration with Professor Robert Fovell of the University of California at Los Angeles with funding from the San Joaquin Valley Study Agency.

Figure 6-1: Terrain height changes along with counties and major rivers and lakes in California (http://geology.com/state-map/california.shtml).

6.2. Ambient Data Base and Quality of Data

The Air Quality and Meteorological Information System (AQMIS) is a web-based source for real-time and official air quality and meteorological data

(www.arb.ca.gov/airqualitytoday/). This database contains 1969-2011 meteorological data (partial months for 2011). The data until the end of 2010 are quality assured and deemed official. The air quality data from 1980 to 2009 are also available on a DVD and at http://www.arb.ca.gov/aqd/aqdcd/aqdcd.htm. In addition ARB also has quality-assured upper-air meteorological data obtained using balloons, aircraft, and profilers.

6.3. Model Performance Evaluation Procedures and Metrics

While there are several U.S. EPA approved meteorological models that can be used for SIP applications, the MM5 and WRF models have been used most frequently. For the reasons provided in Section 5.1.1, the MM5 model will be used here to demonstrate model performance for the year 2007. A comparison between MM5 and WRF will be provided for the months of July and December to demonstrate the model performance differences between the two models.

6.3.1. Statistical Evaluation

Statistical analyses will be performed to evaluate how well the MM5 model captured the overall structure of the observed atmosphere during the 12-month simulation period, using wind speed, wind direction, and temperature. Since observed moisture data are very scarce, relative humidity or mixing ratio will not be used in these comparisons. It is quite common to see, especially in such a long numerical simulation period, that observed statistical characteristics of atmospheric flow may be captured well by the model during a certain time period and/or within some sub-domain while the agreement between the model and observations may not be reasonably good at other times and/or locations. As a result, the very first sign that we look for in model results is whether the model can capture the overall characteristics of the atmosphere in a statistical sense during the entire simulated period and within the entire domain. Then, the same statistical calculations will be repeated within each subregion to find out in which subregions model predictions are good or acceptable and which subregions predictions are not acceptable, so that the reason for weak model performance issues in a subregion can be investigated.

For this purpose, the performance of the MM5 model against observations will be evaluated using the METSTAT analysis tool (Emery et al, 2001). The model output and observations for all 12 months in 2007 will be read, and data points at each observational site for wind speed, wind direction, temperature, and moisture data will be extracted. Then, the following values will be calculated: Mean values of observations and model estimates, bias error (BE), gross error (GE), normalized mean bias (NMB), root mean square error (RMSE), and the index of agreement (IOA) when applicable.

The mathematical expressions for these quantities are:

$$BE = \frac{\sum_{1}^{N}(Model - Obs)}{N},$$

$$GE = \frac{\sum_{1}^{N}|Model - Obs|}{N},$$

$$NMB = \frac{\sum_{1}^{N}(Model - Obs)}{\sum_{1}^{N}Obs} \times 100\%,$$

$$RMSE = \left(\frac{\sum_{1}^{N}(Model - Obs)^2}{N} \right)^{1/2},$$

$$IOA = 1 - \frac{\sum_{1}^{N}(Model - Obs)^2}{\sum_{1}^{N}\left[(Model - Obs) + (Model + Obs)\right]^2},$$

where, “Model” is the simulated concentrations, “Obs” is the observed value, and N is the number of observations. The model performance expectations are:

Wind Speed	RMSE Bias IOA	≤ 2 m/s < ±0.5 m/s ±0.6
Wind Direction	Gross Error: Bias	≤30 deg ≤ ±10 deg
Temperature	Gross Error Bias IOA	≤ 2 K ≤ ±0.5 K ±0.8
Humidity	Gross Error Bias IOA	≤ 2 g/kg < ±1 g/kg ±0.6

These values will be tabulated and plotted for the entire domain as well as eight subregions (the Mountain Counties; North Central Coast; South Central Coast; San Francisco Bay Area; north, central, and southern San Joaquin Valley; and the Sacramento Valley) to obtain an overall understanding of model performance within each subregion. Then, model results of the u and v-components of the wind and temperature will be plotted against observations at each station to see the degree of agreement visually, as well.

Another way to quantify the agreement between the simulated and observed quantities is to examine their frequency distributions. Model results and observations of u and v-components of the wind and temperature will be accumulated into several bins and a frequency distribution of each variable will be plotted. The observed and predicted frequency distribution indicates the dominant bins or categories of a particular variable and how the model prediction compares to the observed frequency distribution.

Time-history plots reveal information that is not readily apparent from the aforementioned analyses. Thus, a direct comparison of model results using temporal variation of wind speed, wind direction, and temperature at each station, hour-by-hour,

for each week in every month will be conducted to study the model performance much more closely than can be done using statistical analyses. Due to the limited availability of continuous hourly relative humidity measurements compared to other meteorological variables, hourly comparison of relative humidity will not be performed. Based on our previous experience with meteorological simulations in California, we expect the analysis to show that wind speed is overestimated at some stations while the difference is small at others. The diurnal variations of temperature and wind direction at most stations would be captured reasonably well. However, we expect the model to underestimate the larger magnitudes of temperature during the day and smaller magnitudes at night.

6.3.2. Phenomenological Evaluation

One possible performance evaluation technique is to examine the meteorological observations in relation to ambient air quality values, to determine the relationships between air quality and key meteorological variables. As indicated above, we will examine the simulated results to see if these relationships are also evident in simulated meteorological variables and air quality. This analysis will be conducted at the station/region level.

Another possibility is to generate the geopotential height charts at 500 and 850 mb using the simulated results and to compare them to the standard charts. This will reveal if the large-scale weather systems at those pressure levels were adequately simulated by the regional prognostic meteorology model.

Another similar approach is to identify the larger-scale meteorological conditions associated with air quality events using the NCEP Reanalysis dataset. We plan to examine the simulated meteorological fields to see if those large-scale meteorological conditions were accurately simulated. We will then examine if the relationships observed in the NCEP reanalysis were present in the simulated data sets.

Trajectory analyses can be used estimate the area of influence of a monitor using both simulated and observed wind data. In the SJV, the high $PM_{2.5}$ values are observed

during winter months when the air is stagnant. Under such conditions, back trajectories constructed using observed winds would be concentrated in the area of observations. We expect to see very similar back trajectory patterns with simulated winds as well.

Spectral analysis may also be used to separate various time-scales (e.g., seasonal, synoptic, inter- and intra-day) in the $PM_{2.5}$ time-series to determine which time-scales contribute most to peak 24-hr $PM_{2.5}$ concentrations. For example, the synoptic scale $PM_{2.5}$ concentration leading up to an exceedance may contribute more to the exceedance than the intra-day contribution. This would likely mean that synoptic scale meteorological model performance is more important than performance based on hourly statistics. We will explore the possibility of using spectral analysis to separate various time scales in the SJV.

CMAQ also has process analyses capabilities. Depending on available time and resources, we may explore the possibility of using process analyses as a part of our phenomenological evaluation.

7. Air Quality Model Performance Evaluation

7.1. Ambient Data Base and Quality of Data

Air quality observations are routinely made at state and local monitoring stations. Gas species and PM species are measured on various time scales (e.g., hourly, daily, weekly). Quality controlled air quality observations for 2007 will be used for model evaluation. The U.S. EPA guidance recommends model performance evaluations for the following gaseous pollutants: ozone (O_3), nitric acid (HNO_3), nitric oxide (NO), nitrogen dioxide (NO_2), peroxyacetyl nitrate (PAN), volatile organic compounds (VOCs), ammonia (NH_3), NO_y (sum of NOx and other oxidized compounds), sulfur dioxide (SO_2), carbon monoxide (CO), and hydrogen peroxide (H_2O_2). The U.S. EPA recognizes that not all of these species are routinely measured (U.S. EPA, 2007) and therefore may not be available for evaluating every model application. Recognizing that $PM_{2.5}$ is a mixture, U.S. EPA recommends model performance evaluation for the following individual $PM_{2.5}$ species: sulfate (SO_4^{2-}), nitrate (NO_3^-), ammonium (NH_4^+), elemental carbon (EC), organic carbon (OC) or organic mass (OM), crustal, and other primary $PM_{2.5}$ (U.S. EPA, 2007).

Table 7-1: Observations for evaluating model performance.

Species	Sampling frequency	# of sites-2007
O_3	1 hour	
NO	1 hour	
NO_2	1 hour	
NO_x	1 hour	
CO	1 hour	
SO_2	1 hour	
Selected VOCs from the PAMS	3 hours (not every day)	

measurement		
$PM_{2.5}$ measured using FRM[1]	24 hours (daily to one in six days)	
$PM_{2.5}$ Speciation sites	24 hours (not every day)	
Sulfate ion	24 hours (not every day)	
Nitrate ion	24 hours (not every day)	
Ammonium ion	24 hours (not every day)	
Organic carbon	24 hours (not every day)	
Elemental carbon	24 hours (not every day)	
Other primary particulate matter	24 hours (not every day)	

[1] Direct comparison between modeled and FRM $PM_{2.5}$ may not be appropriate because of various positive and negative biases associated with FRM measurement procedures.

Table 7-1 lists the species for which observations are available in the SJV for 2007. They will be used for the model performance evaluation. All observational data will be obtained from the official California ambient air quality database (http://www.arb.ca.gov/aqd/aqdcd/aqdcd.htm). The $PM_{2.5}$ speciation data was originally obtained from the U.S. EPA's Air Quality System (http://www.epa.gov/ttn/airs/airsaqs/). Quality assurance information on ambient air quality monitoring data in California can be found in http://www.arb.ca.gov/aaqm/qa/qa.htm.

These species cover the majority of pollutants of interest for model performance evaluations as recommended by the U.S. EPA. Other species such as H_2O_2, HNO_3, NH_3, and PAN are not routinely measured. Observations of these species are not available in the SJV for 2007 and are therefore not available for model evaluations. However, Zhang et al. (2010) have evaluated the CMAQ model (with the SAPRC99 mechanism) performance for NH_3 and PAN in the SJV during the winter episode of CRPAQS. In addition, the CMAQ model performance for species such as H_2O_2 and HNO_3 has been carried out in other studies and was found to be favorable (e.g., Yu et al., 2007; 2010).

7.2. Model Performance Evaluation Procedures and Metrics

As recommended by U.S. EPA, we will use a number of metrics to evaluate the model performance for $PM_{2.5}$ mass as well as $PM_{2.5}$ components. These metrics include mean fractional bias (MFB), mean fractional error (MFE), normalized mean bias (NMB), and normalized mean error (NME). The formulae for estimating these metrics are given below (U.S. EPA, 2007).

$$MFB = \frac{2}{N}\sum_{1}^{N}\left(\frac{Model - Obs}{Model + Obs}\right) \times 100\%,$$

$$MFE = \frac{2}{N}\sum_{1}^{N}\left(\frac{|Model - Obs|}{Model + Obs}\right) \times 100\%,$$

$$NMB = \frac{\sum_{1}^{N}(Model - Obs)}{\sum_{1}^{N} Obs} \times 100\%,$$

$$NME = \frac{\sum_{1}^{N}|Model - Obs|}{\sum_{1}^{N} Obs} \times 100\%,$$

where, "Model" is the simulated concentration, "Obs" is the observed value, and N is the number of observations.

For evaluating O_3, we will also use mean normalized bias (MNB) and mean normalized gross error (MNGE). Their definitions are given below.

$$MNB = \frac{1}{N}\sum_{1}^{N}\left(\frac{Model - Obs}{Obs}\right) \times 100\%,$$

$$MNGE = \frac{1}{N}\sum_{1}^{N}\left(\frac{|Model - Obs|}{Obs}\right) \times 100\%.$$

In addition, we will also calculate other statistics such as mean bias, mean error, and the correlation coefficient whenever they provide meaningful information.

In terms of averaging time, both daily and seasonally averaged simulated and observed values will be compared for $PM_{2.5}$ mass and $PM_{2.5}$ components, consistent with U.S. EPA's Guidance. The FRM and STN measurements are averaged daily, so a detailed comparison of daily pairs is helpful for assessing model performance. Typically, gaseous pollutants are measured on an hourly basis, so hourly comparisons between simulated and observed values will be made.

In addition, various forms of graphics will be created to visually examine comparison of the model predictions to observations. As recommended by U.S. EPA, time series plots are useful in the examination of temporal comparisons of predictions and observations. Tile plots are useful in examining spatial comparisons. Scatter plots, on the other hand, are useful in understanding the comparisons of magnitudes. However, the frequency distributions of observed and simulated variables are not readily visible on scatter plots. Thus, we will either present scatter plots together with their frequency distribution plots or combine them so that scatter and frequency would be visible on the same plot. All these plots will be created for the pairs of observations and predictions over time scales dictated by the averaging frequencies of observations (i.e., hourly, daily, monthly, seasonally) for the species of interest. They will provide a comprehensive view of model performance during different time periods, in different sub-regions, and over different concentrations levels.

Model performance goals will be based on U.S. EPA guidance as well as performance recommendations proposed in peer-reviewed journal articles (e.g., Boylan and Russell, 2006; U.S. EPA, 2007). For example, for $PM_{2.5}$ and its components, we will create the so-called "bugle plots" that were recommended by Boyland and Russell (2006), which show the model performance criteria as goal lines together with actual model performance. An example of a "bugle plot" from Boylan and Russell (2006) is shown in Figure 7-1. We will also create the so-called "soccer plots." The soccer plot visualizes model performance by showing both the model bias and error (e.g., MFB and MFE, or

NMB and NME) on a single plot with various performance "goals" shown as dashed lines. An example of a "soccer plot" from Tesche (2006) is also given in Figure 7-2.

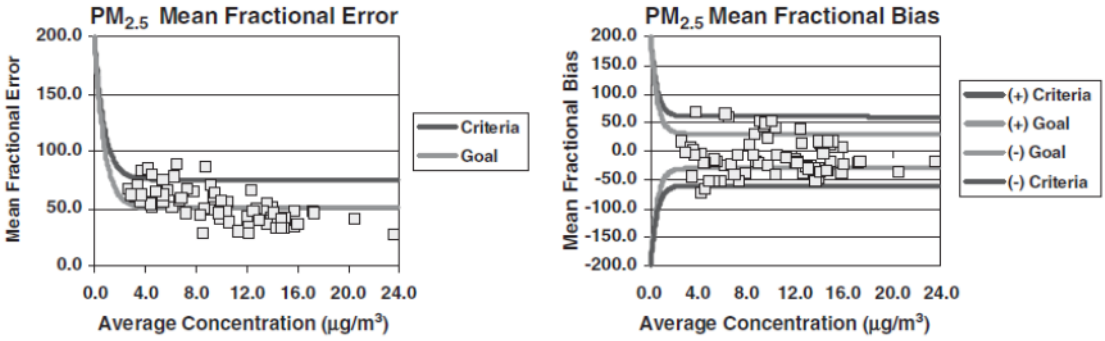


Figure 7-1: Example of "bugle plots" showing $PM_{2.5}$ actual model performance as compared to model performance criteria and goals (from Boylan and Russell, 2006).

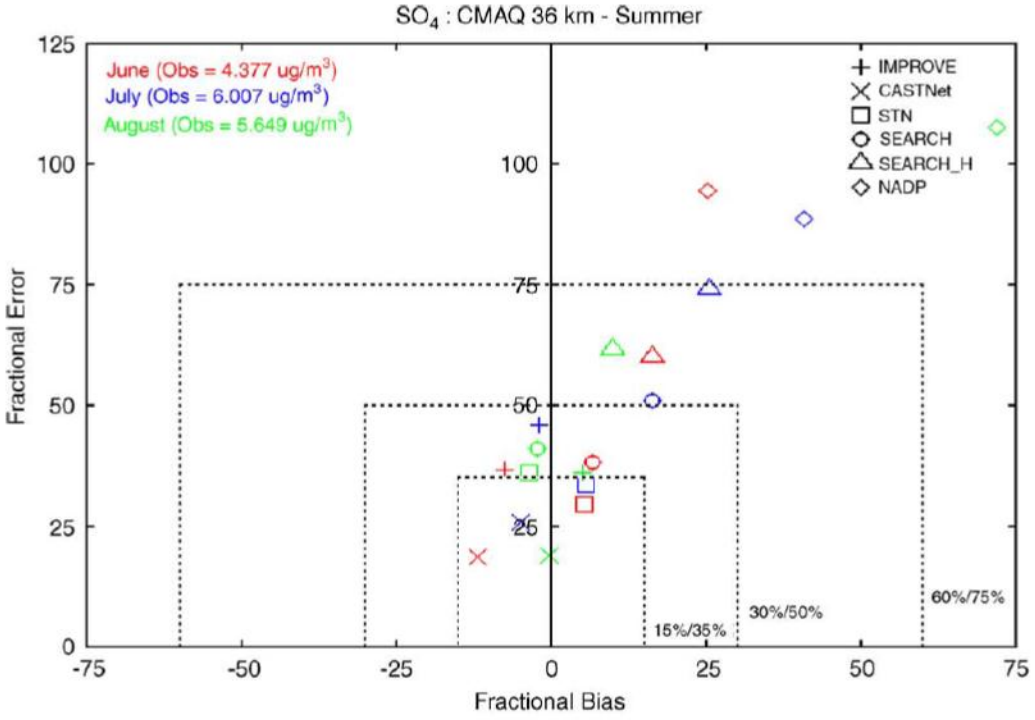


Figure 7-2: Example of a "soccer plot" showing $PM_{2.5}$ fractional bias and error (from Tesche et al., 2006).

Another convenient way to summarize the comparison between a simulated and an observed field is to use a Taylor diagram (Taylor, 2001). These diagrams can provide a concise statistical summary of how well two patterns match each other in terms of their correlation, root-mean-square difference, and ratio of their variances. These three quantities are interrelated with only two independent quantities and, thus, we are able to plot all three on a two dimensional diagram. Figure 7-3 shows an example of a Taylor diagram. Here, the radial distances from the origin to the points are proportional to the standard deviations for the test patterns (e.g., simulations) with that for the reference field (e.g., observations) indicated as REF on the x-axis. The azimuthal positions give the correlation coefficient between the reference and test fields. The dotted lines, representing circular arches centered on the standard deviation of the reference field (REF on the x-axis) indicate the root-mean-square error.

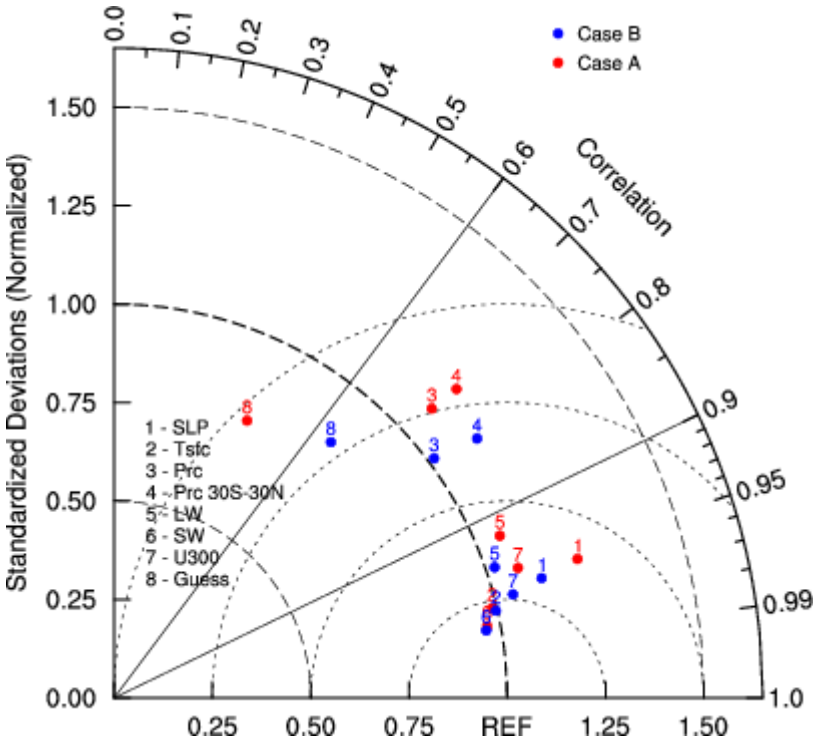


Figure 7-3: An example of a Taylor diagram.

When the metrics are normalized to the variance of the observed field (as shown in Figure 7-3), the comparison of several simulated and observed fields can be plotted on the same diagram. For example, these diagrams may be useful in displaying the model's skill at simulating $PM_{2.5}$ and its components on one diagram. We will explore the applicability and the feasibility of using Taylor diagrams in the model performance evaluation.

7.3. Diagnostic Testing

Possible Diagnostic Testing that could be used to Improve Model Performance is discussed in this section. Throughout the modeling process, many sensitivity analysis runs will be performed to improve the model performance and to find out the best set of model combinations and configurations. Examples of these analyses include different meteorological models (i.e., WRF or MM5), different meteorological model inputs and physics options, different algorithms/schemes in the CMAQ model, different setup of modeling domain and resolutions, etc. The best combinations of configurations/schemes will be used along with the consideration of computational burden.

Receptor models such as Positive Matrix Factorization can also be performed to complement the grid-based photochemical models. These models do not use emissions and meteorological data. Instead, they only rely on the chemical compositions to identify and quantify the contributions to the ambient $PM_{2.5}$ from various source types.

Furthermore, other techniques such as decoupled direct method (DDM), dynamic, or probabilistic model evaluations (Dennis et al., 2010) could also be explored as part of a broader ongoing model performance evaluation and improvement project.

8. Attainment Plan

8.1. Calculation of Relative Response Factors

According to new U.S. EPA guidance (U.S. EPA, 2011b), for the 24-hour $PM_{2.5}$ attainment test, for each quarter, the relative response factor (RRF) is calculated as the ratio of future year to reference year modeled predictions for sulfate, nitrate, elemental carbon, organic carbon, salt, and other primary $PM_{2.5}$ for the top 10% of modeled $PM_{2.5}$ days based on predicted concentrations of 24-hour average $PM_{2.5}$ for each quarter. Since we are modeling each day of the year, the top 10% of simulated $PM_{2.5}$ days would be equal to nine days per quarter. The RRF for component j at a site i is given by:

$$RRF_{ij} = \left(\frac{C_{j,future}}{C_{j,reference}} \right)_i ,$$

where $C_{j,reference}$ is the reference year mean species concentrations (for the nine high modeled $PM_{2.5}$ days for each quarter) predicted at the grid cell containing the monitoring site i; and $C_{j,future}$ is the future year mean species concentrations (for the high nine modeled $PM_{2.5}$ days for each quarter) predicted at the grid cell containing the monitoring site i.

8.2. Sulfate, Adjusted Nitrate, DerivedWater, Inferred Carbonaceous Material Balance Approach (SANDWICH) and Potential Modifications

Federal Reference Method (FRM) $PM_{2.5}$ mass measurements provide the basis for the attainment/nonattainment designations. For this reason it is recommended that the FRM data be used to project future air quality and progress towards attainment. However, given the complex physicochemical nature of $PM_{2.5}$, it is necessary to consider individual $PM_{2.5}$ 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 the first step towards determining the best emissions controls strategies 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 together with 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 ºC. Due to the sampler construction and a lengthy filter equilibration period, 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 including the Speciation Trends Network (STN) monitors (see http://www.epa.gov/ttnamti1/specgen.html for more details). Nitrate and semi-volatile organic mass 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**djusted **N**itrate, **D**erived **W**ater, **I**nferred **C**arbonaceous material balance approach or "SANDWICH" (Frank, 2006). SANDWICH is based on speciated measurements from other (often co-located) samplers, such as those from STN, and the known sampling artifacts of the FRM. The approach strives 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.

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 together with the STN nitrate measurements,

(2) Calculate quarterly averages for retained nitrate, sulfate, elemental carbon, sea salt, and ammonium[1],

(3) Calculate particle bound water using the concentrations of ammonium, sulfate, and nitrate, using an equilibrium model like the Aerosol Inorganic Model (AIM) or a polynomial equation derived from model output[2],

(4) Add 0.5 µg/m^3 as blank mass, and

(5) Calculate organic carbon mass (OCMmb) by difference, subtracting all inorganic species (including blank mass) from the $PM_{2.5}$ mass.

The FRM does not retain all of the semi-volatile $PM_{2.5}$ mass, and at warmer temperatures, loss of particulate nitrate from filters has been commonly 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. For each hour *i* of the day, calculate the dissociation constant, K_i, from ambient temperature and relative humidity (RH).

For RH < 61%:

$$\ln(K_i) = 118.87 - (24084/T_i) - 6.025 \times \ln(T_i),$$

[1] Ammonium mass will be calculated assuming complete neutralization of retained nitrate and sulfate. As we described in the supporting documentation for the 2008 Annual $PM_{2.5}$ SIP approval, the abundance of ammonia in the San Joaquin Valley makes both nitrate and sulfate fully neutralized. This will also make the calculation of ammonium mass consistent for both reference and future years.

[2] We will use the polynomial regression equation used during the preparation of the 2008 Annual $PM_{2.5}$ SIP.

where, T_i is the hourly temperature in Kelvins and K_i is in nanobars.

For RH ≥ 61%, K_i is replaced by:

$$K_i^{'} = [P_1 - P_2(1-a_i) + P_3(1-a_i)^2] \times (1-a_i)^{1.75} \times K_i ,$$

where, a_i is "fractional" relative humidity and

$$\ln(P_1) = -135.94 + 8763/T_i + 19.12 \times \ln(T_i) ,$$

$$\ln(P_2) = -122.65 + 9969/T_i + 16.22 \times \ln(T_i) ,$$

$$\ln(P_3) = -182.61 + 13875/T_i + 24.46 \times \ln(T_i) .$$

Using this information, calculate the nitrate retained on the filter as:

$$\text{Retained Nitrate} = \text{STN nitrate} - 745.7/T_R \times (\kappa - \gamma) \times \frac{1}{24} \sum_{i=1}^{24} \sqrt{K_i} ,$$

where, T_R is the daily average temperature for the sampled air volume in Kelvin, 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 one (Hering and Cass, 1999).

Under the FRM filter equilibration conditions, hygroscopic aerosol will retain its particle bound water (PBW) and be included in the observed FRM $PM_{2.5}$ 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. Here, we will use the polynomial regression equation used during the preparation of the 2008 Annual $PM_{2.5}$ SIP.

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

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 nonorganic carbon components will be subtracted from the FRM $PM_{2.5}$ mass to estimate the mass of organic carbon.

After having calculated the species concentrations as outlined above, we will calculate the percentage contribution of each species to the measured FRM mass (minus the blank concentration of 0.5 $\mu g/m^3$) for each quarter of the years represented by the speciated data. Note that blank mass is kept constant at 0.5 $\mu g/m^3$ 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.

8.3. Estimation of Species Concentrations at Federal Reference Method (FRM) Monitors that Lack Speciation Data

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 both Bakersfield sites (BAC and BEP). Similarly, the percent composition at the three Fresno sites (CLO, FSF and FSH) was assumed to be the same. Stockton (SOH), Corcoran (COP), and Modesto (MRM) were assumed to have the same speciation as one of the four speciation sites based on CRPAQS data analysis. For a list of all FRM sites and their associated speciation site, see Table 8.1.

Table 8-1: The FRM sites in SJV and their companion speciation sites.

Site Name	Code	Speciation
Bakersfield-410 E Planz Road	BEP	BAC
Bakersfield-5558 California Avenue	BAC	BAC
Clovis-N Villa Avenue	CLO	FSF
Corcoran-Patterson Avenue	COP	VCS
Fresno-1st Street	FSF	FSF
Fresno-Hamilton and Winery	FSH	FSF
Merced-2334 M Street	MRM	M14
Modesto-14th Street	M14	M14
Stockton-Hazelton Street	SOH	M14
Visalia-N Church Street	VCS	VCS

8.4. Speciated Modeled Attainment Test (SMAT)

Following U.S. EPA's latest guidance (U.S. EPA, 2011b), the modeled attainment test will be performed with the following steps.

Step 1: Determine the eight highest observed 24-hour $PM_{2.5}$ concentrations days in each quarter for each year at each FRM site (32 days per year), and determine the day rank of the observed 98^{th} percentile value for each year based on the number of collected ambient samples.

Step 2: Calculate quarterly ambient species fractions on "high" $PM_{2.5}$ days for each of the major component species of $PM_{2.5}$ (i.e., sulfate, nitrate, ammonium,

elemental carbon, organic carbon, particle bound water, salt, and blank mass). The "high" days are the top 10% of days in each quarter. Depending on the sampling frequency, the top 10% of days would range from three to nine. The species fractions of $PM_{2.5}$ are calculated using the "SANDWICH" approach which was described previously. These quarter-specific fractions along with the FRM $PM_{2.5}$ concentrations are then used to calculate species concentrations for each of the 32 days per year determined in step 1.

Step 3: Apply the component and quarter specific RRF, described in Section 8.1, to observed daily species concentrations from step 2 to obtain future year concentrations for sulfate, nitrate, elemental carbon, organic carbon, salt, and other primary $PM_{2.5}$.

Step 4: Calculate the future year concentrations for the remaining $PM_{2.5}$ components (i.e., ammonium, particle bound water, and blank mass). The future year ammonium is calculated based on the calculated future year sulfate and nitrate, using a constant value for the degree of neutralization of sulfate from the ambient data. The future year particle bound water is calculated from an empirical formula derived from the AIM model.

Step 5: Add the concentrations of species components to produce total $PM_{2.5}$ concentrations for each of the 32 days per year at each site. Then the 32 days for each site for each year are sorted by total $PM_{2.5}$ concentrations. For each site and year, the monitored 98^{th} percentile rank is used to determine the 98^{th} percentile rank for each year.

Step 6: Average the future-year 98^{th} percentile values to obtain the future-year design value. Compare the future-year 24-hour design values to the NAAQS. The 24-hour $PM_{2.5}$ design values are truncated after the first decimal place. Any value that is less than 35.5 $\mu g/m^3$ is compliant with the NAAQS.

8.5. Sensitivity Analyses

The effectiveness of reducing $PM_{2.5}$ precursors, such as NO_x, SO_x, VOCs, and NH_3, as compared to reducing direct $PM_{2.5}$ emissions is quantified using inter-pollutant equivalency ratios. Sensitivity analysis will be performed for five cases involving 10% reductions of primary $PM_{2.5}$, NO_x, SO_x, VOCs, and NH_3 emissions separately. The changes in simulated $PM_{2.5}$ concentrations compared to the base case without the 10% emission reductions will be quantified at a given FRM monitor. The effectiveness of reducing emissions, or the change in concentrations per unit emissions change, will then be determined by dividing the change in the 24-hour $PM_{2.5}$ design value by the amount of emission reductions corresponding to the 10% reduction. The equivalency ratios between $PM_{2.5}$ precursors (i.e., NO_x, SO_x, VOCs, and NH_3) and primary $PM_{2.5}$ will be determined by dividing primary $PM_{2.5}$ effectiveness by the precursors' effectiveness (i.e., the effectiveness of NO_x, SO_x, VOCs, and NH_3).

This analysis will be conducted for the FRM sites in the Bakersfield and Fresno areas in the future year using only anthropogenic emissions changes. The emissions changes will be implemented only in and around these two urban areas. We will determine the area of influence for these monitors depending on the season in which the 98^{th} percentile value occurs. Past experience dictates that, in the San Joaquin Valley, the 98^{th} percentile value will occur in the winter and it has been shown previously that, during the winter, monitors in these areas are impacted predominantly by local emissions (Ying et al., 2009b).

In addition, carrying capacity diagrams for pairs of precursors will also be developed. These pairs will include NO_x vs. primary $PM_{2.5}$, NO_x vs. VOC, NO_x vs. NH_3, and NO_x vs. SO_x. These diagrams will be used to assess significant precursors.

8.6. Unmonitored Area Analysis

The unmonitored area analysis ensures that a control strategy leads to reductions in $PM_{2.5}$ at other locations which could have baseline or future design values exceeding the NAAQS if a monitor was located there (U.S. EPA, 2007). U.S. EPA recommends

combining interpolated spatial fields and modeled gradients to generate the gradient adjusted spatial fields for $PM_{2.5}$. Future year estimates for unmonitored grids are created by applying the grid specific RRFs to the gradient adjusted spatial fields. The general procedures are as given below:

Step 1: Interpolate base year ambient $PM_{2.5}$ to create a set of spatial fields. For 24-hour $PM_{2.5}$, U.S. EPA recommends interpolating the $PM_{2.5}$ concentrations in each quarter which is equal to or less than the 98th percentile value of the year. For the $PM_{2.5}$ component species, U.S. EPA recommends interpolating the high $PM_{2.5}$ days in each quarter.

Step 2: Adjust the spatial fields using gridded model output gradients for the base year. For 24-hour $PM_{2.5}$, the gradient adjusted fields can be created from the high end of the distribution of daily averages in each quarter.

Step 3: Apply the gridded model RRFs to the gradient adjusted spatial fields created in step 2 to obtain the future year concentrations. For $PM_{2.5}$, the RRFs for each of the species in each quarter are multiplied by the gradient adjusted spatial fields for each species and each quarter.

We do not know at this time if we will use the U.S. EPA software (MAPS), since complete source code is not available, or will develop in-house software for this task.

9. Supplemental Analyses

9.1. Additional Analyses to be completed to corroborate the Modeling

The Weight of Evidence (WOE) analysis provides a corroborative set of analyses supplementing the SIP required modeling that provides confidence that the correct pollutants are being controlled and the attainment demonstration is appropriate. These analyses can include consideration of measured air quality, emissions, and meteorological data, evaluation of other air quality indicators, and additional air quality modeling. Each analysis is weighted based on its ability to quantitatively assess the ability of the proposed control measures to yield attainment.

For the San Joaquin Valley, the $PM_{2.5}$ WOE analysis will include an evaluation of air quality trends, emission trends, observational models, indicator species, meteorological trends, and air quality modeling results to demonstrate attainment of the 35 $\mu g/m^3$ $PM_{2.5}$ standard. The air quality trends will include data from the official Federal Reference Monitor and chemical composition networks and other types of $PM_{2.5}$ monitoring data. ARB will analyze the data to examine the yearly, seasonal, and spatial trends. In addition, ARB will discuss the yearly meteorological conditions and the impact of these conditions on the measured $PM_{2.5}$ air quality. The met-adjusted trends can also be used in conjunction with emissions trends to review the impacts of emission reductions. Two complementary observational models, chemical mass balance (CMB) and positive matrix factorization (PMF) will be used to identify the sources contributing to the San Joaquin Valley $PM_{2.5}$ problem. ARB will use the latest version of CMB and PMF and appropriate input data for California. In addition, ARB will compare these PMF and CMB results with other published results on the sources of $PM_{2.5}$ in the San Joaquin Valley.

The speciated rollback technique (NRC, 1993) can also be applied to study the changes in ambient concentrations due to changes in emissions. A fundamental assumption here is that the changes in ambient concentration of a pollutant is linear with changes in its precursors. While this assumption may be sound for directly-emitted pollutants (such

as primary $PM_{2.5}$), the response of secondary pollutants to changes in their precursors is known to be non-linear. Fully allowing for such non-linearity is not possible within the speciated rollback technique.

ARB will explore the possibility of using an indicator species approach to investigate the effectiveness of precursor controls on secondary species such as ammonium nitrate. This approach would incorporate air quality data, a review of San Joaquin Valley specific published papers, and air quality modeling sensitivity runs to identify the limiting precursors for ammonium nitrate formation in the context of the 24-hour $PM_{2.5}$ standard. Finally, ARB will evaluate the grid-based modeling results in the context of the corroborative analyses to provide confidence that $PM_{2.5}$ attainment is reached as expeditiously as practicable in the San Joaquin Valley.

9.2. Base Case Air-Quality Modeling with Meteorological Fields Generated with the Weather and Research Forecast (WRF) Model

The prognostic meteorological model that will be used to generate meteorology will be MM5 for the reasons outlined in Section 5.1.1.

A base year CMAQ model simulation will also be performed using meteorological fields generated with the WRF model (Skamarock et al., 2008). The primary objective is to study how $PM_{2.5}$ predictions in the San Joaquin Valley differ when the meteorological fields from WRF instead of MM5 are used to drive the CMAQ model. Traditionally, MM5 has been used to provide meteorological data for air quality simulations (Appel et al., 2009). With the emergence of WRF, many air quality model simulations started to use WRF to provide the meteorological fields for air quality models (e.g., Appel et al., 2009; de Meji, 2009; Eder et al., 2009; Hu, et al., 2010; Lin et al., 2010; Shimadera, 2011).

The WRF model version 3.3 will be used. Detailed configuration of the WRF model can be found in the meteorological modeling sections. The WRF model output will be processed by the Meteorology-Chemistry Interface Processor (MCIP, Otte and Pleim, 2010) of the CMAQ modeling system. The MCIP version 3.6 in the CMAQv4.7 modeling system will be used. Compared to the base year simulation using MM5

meteorological fields (MM5-CMAQ), all modeling inputs and configurations for the CMAQ model will be the same except that the meteorological fields are generated by the WRF model (WRF-CMAQ). This will ensure that the difference in the CMAQ model output is only attributed to the different meteorological fields.

WRF-CMAQ model output in terms of $PM_{2.5}$ total mass and individual $PM_{2.5}$ components (i.e., nitrate, sulfate, ammonium, elemental and organic carbon, other primary $PM_{2.5}$ components) will be compared to the MM5-CMAQ model outputs. WRF-CMAQ model outputs will also be evaluated against the ambient air quality data using the same modeling performance procedures and metrics used for the MM5-CMAQ model outputs. Model performance metrics such as mean fractional bias (MFB), mean fractional error (MFE), normalized mean bias (NMB), and normalized mean error (NME) will be calculated and will be compared to the performance metrics of the MM5-CMAQ model outputs.

10. Procedural Requirements

10.1. How Modeling and other Analyses will be Archived, Documented, and Disseminated

The air quality modeling system covers the central portion of California with 4x4 km^2 grids. In total there are approximately half a million grid cells in each simulation (192 x 192 cells in the lateral direction and 15 levels in the vertical). The meteorological modeling system has roughly double the number of grid cells since it has 30 vertical layers. Archiving of all the inputs and outputs takes several terabytes (TB) of computer disk space (for comparison, one single-layer DVD can hold roughly 5 gigabytes (GB) of data and it would take ~200 DVDs to hold one TB). Please note that this estimate is for simulated surface-level pollutant concentrations only. If three-dimensional pollutant concentrations are needed, it would add a few more TB. Therefore, transferring the modeling inputs/outputs over the internet using file transfer protocol (FTP) is not practical. Interested parties may send a request for model inputs/outputs to Mr. John DaMassa, Chief of the Modeling and Meteorology Branch at the following address.

John DaMassa, Chief
Modeling and Meteorology Branch
Planning and Technical Support Division
Air Resources Board
California Environmental Protection Agency
P.O. Box 2815
Sacramento, CA 95814, USA

The requesting party will need to send an external disk drive(s) to facilitate the data transfer. The requesting party should also specify what input/output files are requested so that ARB can determine the capacity of the external disk drive(s) that the requester should send.

10.2. Specific Deliverables to U.S. EPA

The following is a list of modeling-related documents that will be provided to the U.S. EPA.

- The modeling protocol
- Emissions preparation and results
- Meteorology
    - Preparation of model inputs
    - Model performance evaluation
- Air Quality
    - Preparation of model inputs
    - Model performance evaluation
- Documentation of corroborative and weight-of-evidence analyses
- Predicted Future 24-hour $PM_{2.5}$ Design Value Calculations using SANDWICH, RRF, and SMAT
- Unmonitored area analysis
- Access to input data and simulated results

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