

Appendix I

Modeling Protocol

Appendix I: Modeling Protocol

[This Appendix is provided by the California Air Resources Board]

PHOTOCHEMICAL MODELING PROTOCOL

Photochemical Modeling for the 8-Hour Ozone 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

BEARPEX – Biosphere Effects on Aerosols and Photochemistry Experiment in 2007 and 2009

BCs – Boundary Conditions

CABERNET – California Airborne BVOC Emission Research in Natural Ecosystem Transects in 2011

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

CARES – Carbonaceous Aerosols and Radiative Effects Study in 2010

CCOS - Central California Ozone Study

CMAQ Model – Community Multi-scale Air Quality Model

CIT – California Institute of Technology

CRPAQS – California Regional PM₁₀/PM_{2.5} Air Quality Study

CSJV – Central San Joaquin Valley

DISCOVER-AQ - Deriving Information on Surface Conditions from Column and Vertically Resolved Observations Relevant to Air Quality

DV – Design Value

FDDA – Four-Dimensional Data Assimilation

HNO₃ – Nitric Acid

ICs – Initial Conditions

IMS-95 – Integrated Monitoring Study of 1995

LIDAR – Light Detection And Ranging

MDA – Maximum Daily Average

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

NCEP – National Centers for Environmental Prediction

NARR - North American Regional Reanalysis

NOAA - National Oceanic and Atmospheric Administration

NO_x – Oxides of nitrogen

NSJV – Northern San Joaquin Valley

OFP - Ozone Forming Potential

PAMS – Photochemical Assessment Monitoring Stations

PAN – Peroxy Acetyl Nitrate

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

PM₁₀ – Particulate Matter with aerodynamic diameter less than 10 micrometers

RH – Relative Humidity

ROG – Reactive Organic Gases

RRF – Relative Response Factor

RSAC – Reactivity Scientific Advisory Committee

SAPRC – Statewide Air Pollution Research Center

SARMAP – SJVAQS/AUSPEX Regional Modeling Adaptation Project

SIP – State Implementation Plan

SJV – San Joaquin Valley

SJVAB – San Joaquin Valley Air Basin (SJVAB)

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

SOA – Secondary Organic Aerosol

SoCAB – Southern California Air Basin

SSJV – Southern San Joaquin Valley

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 photochemical modeling that forms the basis of the attainment demonstration in the 8-hr Ozone State Implementation Plan (SIP) for the San Joaquin Valley (SJV). 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.

1.1 Recent History of Ozone SIPs in SJV and the Need for the Current 8-hr Ozone 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 of federal ozone (O₃) and particulate matter (PM) air quality standards by specified dates.

In 1997, the U.S. EPA adopted the first 8-hour ozone standard of 0.08 ppm, which became effective in June 2004. In April 2007, the District adopted its first 8-hour Ozone Plan to address the 0.08 ppm standard. The 2007 Plan predicted attainment of the 0.08 ppm standard by 2023 with a NO_x carrying capacity (the level of emissions that needs to be achieved to meet the standard) of ~160 tons per day valley-wide, which was approved by U.S. EPA on March 1, 2012 (76 FR 57846). In 2008, the U.S. EPA adopted a more stringent 8-hour ozone standard of 0.075 ppm, which became effective in 2010. This protocol addresses the modeling to be used in the attainment demonstration for the SJV 0.075 ppm 8-hour ozone SIP.

1.2 Modeling roles for the current SIP

The Clean Air Act (Act) establishes the planning requirements for those areas that routinely exceed the health-based air quality standards. 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, as 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.

1.3 Stakeholder participation

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.

1.4 Involvement of external scientific/technical experts and their input on the photochemical modeling

During the development of the modeling protocol for the 2012 SJV 24-hour PM_{2.5} SIP, ARB and the SJVAPCD engaged a group of experts on prognostic meteorological modeling and photochemical/aerosol modeling to help prepare the modeling protocol document.

The structure of the technical expert group was as follows:

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

The technical consultant group provided technical consultations/guidance to the staff at ARB and SJVAPCD during the development of the protocol. Specifically, the group provided technical expertise on the following components of the protocol (only those comments specifically related to ozone modeling are shown):

- 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.
- Preparation of Technical Support Documents.

The current approach to regional air quality modeling has not changed significantly since the 2012 SJV 24-hour PM_{2.5} SIP, so the expertise provided on the above components to the protocol remain highly relevant. In addition, since regional air quality modeling simulates ozone chemistry and PM chemistry/formation simultaneously, there is generally no difference in how the models are configured and simulations conducted for ozone vs. PM. Therefore, development of the current ozone modeling protocol will rely heavily on the recommendations made by this group of technical experts, as well as recently published work in peer-review journals related to regional air quality modeling for ozone.

1.5 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. Timeline for Completion of the Plan

Timeline	Action
Fall 2015	Emission Inventory Completed
Winter 2015/Spring 2016	Modeling Completed
Winter 2015/Spring 2016	Public Workshop(s) on the Draft Plan
June 2016	San Joaquin Valley Governing Board Hearing to consider the Draft Plan
July 2016	ARB Board Hearing to consider the SJV Adopted Plan
July 16, 2016	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 (SVJ) air basin is perhaps the second most studied air basin in the world, in terms of the number of publications in peer-reviewed international scientific/technical journals and other major reports, with the Los Angeles air basin being the first. Major field studies that have taken place in the SVJ and surrounding areas are listed in Table 2-1.

The first major air quality study in the SVJ, 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 (SVJQAQS/AUSPEX) study, also known as SARMAP (SVJQAQS/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 PM₁₀/PM_{2.5} Air Quality Study (CRPAQS) in 2000 (Solomon and Magliano, 1998). IMS-95 formed the technical basis for the 2003 PM₁₀ 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 SVJ 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 O₃ SIP (76 FR 57846). While CCOS is still very relevant to the current 8-hr O₃ SIP, there are five subsequent studies with relevance to ozone formation in the Valley and surrounding regions: 1) ARCTAS-CARB 2008, 2) CalNex 2010, 3) CARES 2010, 4) BEARPEX 2007 & 2009, 5) CABERNET 2011. Each of these studies has contributed significantly to our understanding of various atmospheric processes in the Valley.

The ARCTAS-CARB aircraft field campaign was a joint research effort by NASA and CARB and took place from June 18 to 24, 2008. During the study, DC-8 aircraft performed two flights over southern California on June 18 and 24 with a focus on the Southern California Air Basin (SoCAB), one flight over northern California with a focus on the San Joaquin Valley Air Basin (SVJAB) on June 20, and one flight off shore on

June 22 to quantify the pollutant levels in the air masses entering California from the Pacific Ocean. During the campaign, large wildfires occurred in California, particularly in the north. The DC-8 aircraft encountered many of the fire plumes, which allowed for the study of fire emissions and their chemical composition, as well as evaluation of the simulated fire impacts. The ARCTAS-CARB campaign provided a unique dataset for evaluating the impacts of wildfires on ozone levels through photochemical modeling studies and for evaluating the distribution of reactive nitrogen species in California (Huang et al., 2011; Cai et al., 2016).

The CalNex May-July 2010 field campaign was organized by NOAA (NOAA, 2014) and CARB. The focus of this field study included airborne measurements using the NOAA WP-3D aircraft and the Twin Otter Remote Sensing aircraft, and surface measurements using the R/V *Atlantis* mobile platform as well as two stationary ground supersites, one of which was located in Bakersfield. Analysis of the data collected during CalNex has shown that photochemical ozone production in the southern and central portions of the Valley is transitioning to a NO_x-limited chemistry regime, where further NO_x reductions are expected to lead to a more rapid reduction in ozone than what was observed over the past decade or more (Pusede and Cohen, 2012). Studies have also shown that there is evidence for an unidentified temperature-dependent VOC emissions source on the hottest days (Pusede and Cohen, 2012; Pusede et al., 2014) and large sources of hydrocarbon compounds from petroleum extraction/processing, dairy (and other cattle) operations, and agricultural crops in SJV (Gentner et al., 2014a,b).

The CARES field campaign took place in the central California region, to the northeast of Sacramento in June 2010. Comprehensive data sets of trace gases and aerosols were taken from the daily evolving Sacramento urban plume under relatively well-defined and regular meteorological conditions using multiple suites of ground-based and airborne instruments onboard the Gulfstream (G-1) research aircraft. The ground-based measurements were conducted at two sites: one within the Sacramento urban source area and the other in a downwind area about 70 km to the northeast in Cool, CA. A combination of measurement and model data during CARES (Fast et al., 2012) shows that emissions from the San Francisco Bay area transported by intrusions of marine air contributed a large fraction of the carbon monoxide in the vicinity of Sacramento. The study also showed that mountain venting processes contributed to aged pollutants aloft in the valley atmosphere that are then entrained into the growing boundary layer the following day. Although the CARES study did not take place within the SJV itself, it remains relevant to the SJV for two reasons: 1) CARES took place within the delta region north of the SJV, which can influence air quality in the northern SJV (see Section 2.4), and 2) the improved scientific understanding of the interaction between urban

emissions and downwind biogenic emissions gained during CARES is applicable to the SJV, which experiences a similar confluence of anthropogenic and biogenic emissions.

BEARPEX was conducted at the University of California's Blodgett Forest Research Station during June-July 2007 and September-October 2009. Blodgett Forest is located 65 miles northeast of Sacramento. The project was designed to study chemistry downwind of urban areas where there is high VOC reactivity (due to biogenic emissions sources) and low NO_x, to understand the full oxidation sequence and subsequent fate of biogenic VOC and the processes leading to formation and removal of biogenic secondary organic aerosol (SOA) and the associated chemical and optical properties of SOA. A study by Bouvier-Brown et al., (2009) suggests that reactive and semi-volatile compounds, especially sesquiterpenes, significantly impact the gas- and particle-phase chemistry of the atmosphere at Blodgett Forest. An analysis of absolute PANs mixing ratios by Lafranchi et al. (2009) reveals a missing PANs sink that can be resolved by increasing the peroxy acetyl radicals + RO₂ rate constant by a factor of 3. At the BEARPEX field site, the sum of the individual biogenically derived nitrates account for two-thirds of the organic nitrate, confirming the importance of biogenic nitrates to the NO_y budget (Beaver et al., 2012).

The CABERNET field campaign was conducted in June 2011 in California. The objectives were to develop and evaluate new approaches for regional scale measurements of biogenic VOC emissions, quantify the response of biogenic VOC emissions to land cover change, investigate the vertical transport of isoprene and oxidation products, and evaluate biogenic emission models. Isoprene fluxes were measured on board the Center for Interdisciplinary Remotely-Piloted Aircraft Studies (CIRPAS) Twin Otter (<http://www.cirpas.org/twinOtter.html>) using the virtual disjunct eddy covariance method (Karl et al. 2012). Isoprene flux measurements from CABERNET have formed the basis for evaluating the biogenic emissions inventory used in California's SIP modeling (Misztal et al., 2016).

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 1999 – February 2001	California Regional PM ₁₀ /PM _{2.5} Air Quality Study (CRPAQS) and Central California Ozone Study	First year-long, regional-scale effort to measure 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
August-October 2007; June-July 2009	BEARPEX (Biosphere Effects on Aerosols and Photochemistry Experiment)	Research-grade measurements to study the interaction of the Sacramento urban plume with downwind biogenic emissions
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.
June 2010	CARES (Carbonaceous Aerosols and Radiative Effects Study)	Research-grade measurements of trace gases and aerosols within the Sacramento urban plume to investigate SOA formation
June 2011	CABERNET (California Airborne BVOC Emission Research in Natural Ecosystem Transects)	Provided the first ever airborne flux measurements of isoprene in California
January- February 2013	DISCOVER-AQ (Deriving Information of Surface Conditions from Column and Vertically Resolved Observations Relevant to Air Quality)	Research-grade measurements of trace gases and aerosols during two PM _{2.5} pollution episodes in the SJV

2.2 Description of the Ambient Monitoring Network

The San Joaquin Valley covers an area of 23,490 square miles and is home to approximately 4 million residents. 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. 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 (San Joaquin, Stanislaus, Merced, Madera, Fresno, Kings, and Tulare) and one partial county Kern (only the western portion of Kern County, which lies in the jurisdiction of the SJVAPCD is included).

The Valley can be divided into three regions that are characterized by distinct geography, meteorology, and air quality: 1) northern SJV (San Joaquin, Stanislaus, and Merced counties), 2) central SJV (Madera, Fresno, and King counties), and 3) southern SJV (Tulare and Western Kern counties). A third of the Valley population lives in the northern SJV. This lowland area is bordered by the Sacramento Valley and Delta lowland to the north, the central portion of the SJV to the south, and mountain ranges to the east and west. Because of the marine influence, which extends into this area through gaps in the coastal mountains to the west, the northern SJV experiences a more temperate climate than the rest of the Basin. These cooler temperatures and the predominant air flow patterns generally favor better air quality. Similar to the northern SJV, the central and southern SJV are also low lying areas, flanked by mountains on their west and east sides. The worst air quality within the Valley occurs in these two regions, where the population is primarily clustered around the Fresno and Bakersfield urban areas. In these regions the interaction between geography, climate, and a mix of natural (biogenic) and anthropogenic emissions pose significant challenges to air quality progress. The southern SJV represents the terminus of the Valley and is flanked by mountains on the south, as well. The surrounding mountains in both areas act as barriers to air flow, and combined with recirculation patterns and stable air to trap emissions and pollutants near the valley floor. The higher temperatures and more stagnant conditions in these two regions lead to a build-up of ozone and overall poorer air quality. In addition to the urban air quality problems, emissions and pollutants from these areas are transported downwind, resulting in poor air quality in downwind areas.

As discussed above, the Valley's diverse area includes several major metropolitan areas, vast expanses of agricultural land, industrial sources, and highways, all of which pose many issues to air quality. The San Joaquin Valley Air Pollution Control District (SJVAPCD or District), the California Air Resources Board (CARB), and the National Park Service work together and operate an extensive network of air quality monitors throughout the Valley to help improve and protect public health. The data collected from

the Valley air monitoring network is used to generate daily air quality forecasts, issue health advisories as needed, support compliance with various ambient air quality standards and serves as the basis for developing long-term attainment strategies and tracking progress towards health-based air quality standards.

Figure 2-1 shows the spatial distribution of the ozone, NO_x, and PAMS (Photochemical Assessment Monitoring Stations) monitors in the Valley (see Table 2-2 for longitude/latitude information for each monitor). The monitors are located throughout the Valley floor, higher elevation locations, and within higher population density urban areas, and have been shown to sufficiently capture the highest ozone mixing ratios and the corresponding precursors under various weather conditions and in all major population centers. A detailed discussion about the monitoring network and its adequacy can be found in the Valley's 2015 Air Monitoring Network Plan (<http://www.valleyair.org/aqinfo/Docs/2015-Air-Monitoring-Network-Plan.pdf>) and 2014 California Infrastructure SIP (<http://www.arb.ca.gov/planning/sip/infrasip/docs/i-sip.pdf>).

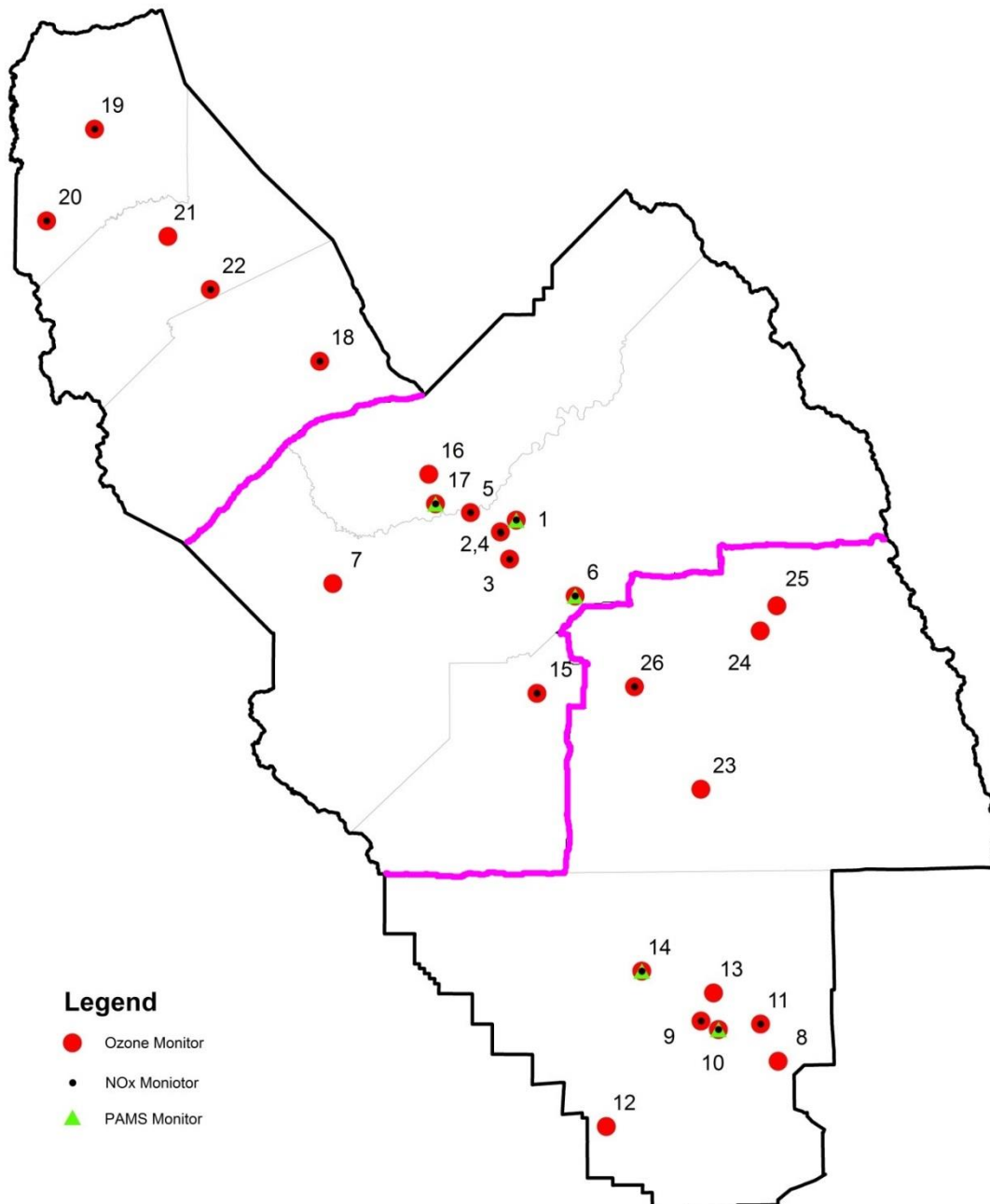


Figure 2-1. Map of the Monitoring Sites in the San Joaquin Valley. The red and black circle markers denote the location of ozone and NO_x monitors while the green triangle markers denote the PAMS monitors. The magenta lines denote the regional boundaries of the northern, central and southern SJV sub-regions that are used for evaluating the meteorological and photochemical modeling performance.

Table 2-2. 2012-2015 San Joaquin Valley Ozone, NO_x, and PAMS Sites

#	County	Sub Region	Site	NO _x	Ozone	PAMS	Latitude	Longitude
1	Fresno	Central SJV	Clovis-N Villa Avenue	X	X	X	36.8194	-119.7164
2	Fresno	Central SJV	Fresno-1st Street	X	X		36.7819	-119.7731
3	Fresno	Central SJV	Fresno-Drummond Street	X	X		36.7053	-119.7413
4	Fresno	Central SJV	Fresno-Garland	X	X		36.7853	-119.7742
5	Fresno	Central SJV	Fresno-Sierra Skypark #2	X	X		36.8417	-119.8828
6	Fresno	Central SJV	Parlier	X	X	X	36.5974	-119.5039
7	Fresno	Central SJV	Tranquility-32650 West Adams Avenue		X		36.6342	-120.3823
8	Kern	Southern SJV	Arvin-Di Giorgio		X		35.2367	-118.7894
9	Kern	Southern SJV	Bakersfield-5558 California Avenue	X	X		35.3567	-119.0628
10*	Kern	Southern SJV	Bakersfield-Municipal Airport	X	X	X	35.3313	-119.001
11	Kern	Southern SJV	Edison	X	X		35.3458	-118.8506
12	Kern	Southern SJV	Maricopa-Stanislaus Street		X		35.0514	-119.4028
13	Kern	Southern SJV	Oildale-3311 Manor Street		X		35.4381	-119.0167
14	Kern	Southern SJV	Shafter-Walker Street	X	X	X	35.5033	-119.2728
15	Kings	Central SJV	Hanford-S Irwin Street	X	X		36.3147	-119.6436
16	Madera	Central SJV	Madera-28261		X		36.9533	-120.0342

			Avenue 14					
17	Madera	Central SJV	Madera-Pump Yard	X	X	X	36.8672	-120.01
18	Merced	Northern SJV	Merced-S Coffee Avenue	X	X		37.2817	-120.4336
19	San Joaquin	Northern SJV	Stockton-Hazelton Street	X	X		37.9517	-121.2689
20	San Joaquin	Northern SJV	Tracy-Airport	X	X		37.6825	-121.4406
21	Stanislaus	Northern SJV	Modesto-14th Street		X		37.6419	-120.9942
22	Stanislaus	Northern SJV	Turlock-S Minaret Street	X	X		37.4882	-120.8359
23	Tulare	Southern SJV	Porterville-1839 Newcomb Street		X		36.0318	-119.055
24	Tulare	Southern SJV	Sequoia and Kings Canyon Natl Park		X		36.4911	-118.8342
25	Tulare	Southern SJV	Sequoia Natl Park-Lower Kaweah		X		36.564	-118.773
26	Tulare	Southern SJV	Visalia-N Church Street	X	X		36.3325	-119.2908

* As the Bakersfield municipal airport site in Kern County became operational in June 2012, the measurements were not available for calculating 8-hr ozone design values in 2012 and 2013. Hence this site was excluded from the current SIP attainment demonstration.

2.3 Ozone Trends and Sensitivity to Emissions Reductions

The San Joaquin Valley is one of the most severely polluted air basins in the U.S., and is designated as an extreme ozone nonattainment area for the U.S. EPA 2008 0.075 ppm 8-hour ozone standard. Anthropogenic sources of the oxides of nitrogen (NO_x) and reactive organic gases (ROG) are the major precursors that lead to ozone formation in the valley. Biogenic hydrocarbons are also important contributors to ozone precursors in the region, and are projected to play an even more important role in the future as emission controls reduce anthropogenic ROG. Since the 1980's, the Valley's

emission control programs have substantially reduced the amounts of both anthropogenic NO_x and ROG throughout the valley. As these control programs have led to changes in the relative levels of NO_x and ROG in the valley over time, the control programs have also adapted so as to reduce ozone levels as rapidly as possible. This adaptation within the control programs is necessary because ozone formation responds differently to NO_x and ROG controls as the relative levels of NO_x and ROG in the atmosphere change.

Specifically, ozone formation exhibits a nonlinear dependence to NO_x and ROG precursors in the atmosphere. In general terms, under ambient conditions of high-NO_x and low-ROG (NO_x-disbenefit region in Figure 2-2), ozone formation tends to exhibit a disbenefit to reductions in NO_x emissions (i.e., ozone increases with decreases in NO_x) and a benefit to reductions in ROG emissions (i.e., ozone decreases with decreases in ROG). In contrast, under ambient conditions of low-NO_x and high-ROG (NO_x-limited region in Figure 2-2), ozone formation shows a benefit to reductions in NO_x emissions, while changes in ROG emissions result in only minor decreases in ozone. These two distinct “ozone chemical regimes” are illustrated in Figure 2-2 along with a transitional regime that can exhibit characteristics of both the NO_x-disbenefit and NO_x-limited regimes. Note that Figure 2-2 is shown for illustrative purposes only, and does not represent the actual ozone sensitivity within the SJV for a given combination of NO_x and VOC (ROG) emissions.

During the 1980's in the SJV, when NO_x emissions were high relative to ROG and the region exhibited a NO_x-disbenefit towards ozone formation, ROG emission controls outpaced NO_x controls. During the 1990's, emission controls slowly shifted to a more balanced approach between ROG and NO_x, and by the 2000's NO_x reductions began to outpace ROG reductions. For much of the 1980's through the mid-2000's, the Valley was in a NO_x-disbenefit or transitional chemical regime and it's only been within the past decade (mid- to late-2000's) where the Valley began transitioning to a NO_x-limited chemical regime. This transition from a NO_x -disbenefit to a NO_x -limited chemical regime can be analyzed through the year-to-year variability in biogenic ROG emissions, which during the summer ozone season can be many times greater than anthropogenic ROG emissions in the Valley, as well as through the so called “weekend effect” which shows an increase in ozone on the weekend under NO_x -disbenefit conditions (and a decrease under NO_x -limited conditions).

Basin-wide summer emission trends from 2000 to 2014 for the SJV are shown in Figure 2-3 (top) for anthropogenic NO_x and ROG, as well as biogenic ROG (biogenic trends are for 2001 to 2014). Figure 2-3 clearly shows large decrease in both anthropogenic NO_x (from 627 tpd to 340 tpd) and ROG (from 503 tpd to 337 tpd) emissions from 2000

to 2012. Over the same time period, biogenic ROG emissions exhibited large year-to-year variability, ranging from ~1000 tpd in 2005 to ~2000 tpd in 2006 and 2010. However, even at its lowest levels, biogenic ROG is estimated to be three times as high as the anthropogenic ROG inventory in 2012 and upwards of seven times as high during peak biogenic years.

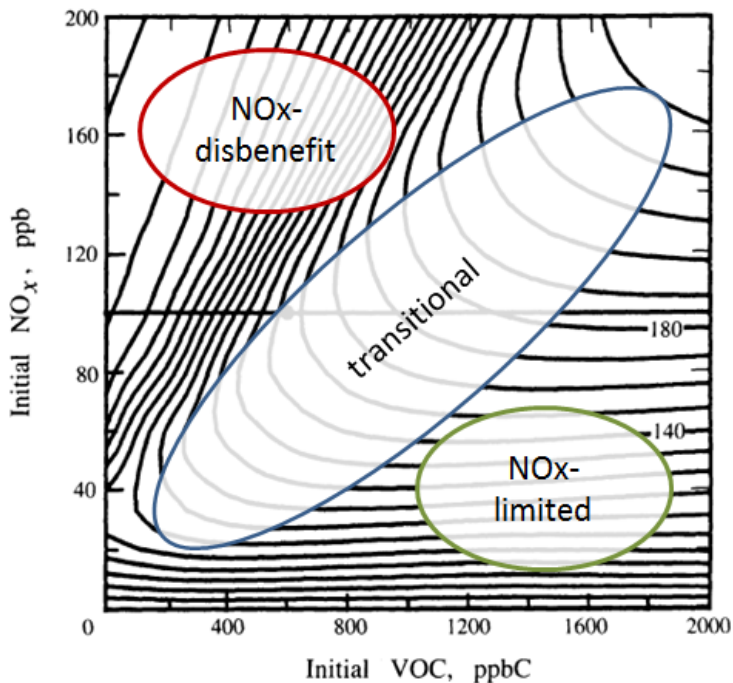


Figure 2-2. Illustrates a typical ozone isopleth plot, where each line represents ozone mixing ratio, in 10 ppb increments, as a function of initial NO_x and VOC (or ROG) mixing ratio (adapted from Seinfeld and Pandis, 1998, Figure 5.15). General chemical regimes for ozone formation are shown as NO_x-disbenefit (red circle), transitional (blue circle), and NO_x-limited (green circle).

Over the same 2000 to 2014 time period, the ozone design value and days above the ozone standard (exceedance days) within the SJV declined steadily (Figure 2-3 middle and bottom, respectively), but did also exhibit a fair amount of variability due to year-to-year variability in meteorology and the associated changes in biogenic emissions. Overall, the basin-wide design values have declined from 111 ppb in 2000 to 95 ppb in 2014. However, these DVs are still substantially higher than the current 75 ppb standard.

Since the basin-wide DV is focused on the highest ozone values and the location of these peaks can change from year-to-year, the exceedance days, a measure of overall

air quality and the frequency of ozone exposure, may be a better metric for evaluating changes in ozone chemistry when viewed in the context of changing biogenic ROG emissions. Exceedance days in the Valley have substantially decreased over time from 144 in 2000 to 86 in 2014 (40% lower with respect to 2000) indicating significant improvements in ozone air quality across the entire valley. The decline in weekend exceedance days was slightly higher (44% decrease from 43 to 24) than the corresponding decline in weekday exceedance days (~38% decrease from 101 to 62) between the years 2000 and 2014. Comparing the year-to-year variability in exceedance days to similar variability in the biogenic ROG emissions, shows that from 2001-2007 the two were strongly correlated (i.e., when biogenic ROG emissions increased, so did the number of exceedance days). This is consistent with valley being primarily in a NO_x -disbenefit regime, where increases in ROG emissions result in enhanced ozone formation. From 2008 onwards, this correlation no longer exists and the two are actually anti-correlated for all years except 2009. Although other factors beyond chemistry, such as meteorology, play a large role in the year-to-year variability in ozone, this suggests a shift from a NO_x -disbenefit regime to a transitional or NO_x -limited regime around the 2008 timeframe.

Investigating the “weekend effect” and how it has changed over time is also a useful metric for evaluating the ozone chemistry regime in the SJV. The weekend effect is a well-known phenomenon in some major urbanized areas where emissions of ozone precursors are substantially lower on weekends than on weekdays, but measured levels of ozone are higher on weekends than on weekdays. There are several hypotheses to explain the higher frequency of elevated O_3 on weekends but the reduced NO_x emissions during weekends is a key contributor (Swamy et al., 2012). The basic premise here is that a strong weekend effect would be an indication of a NO_x disbenefit regime (Heuss et al., 2003). The excess NO_x in this regime not only titrates the O_3 but also mutes the VOC reactivity by using peroxy radicals to terminate NO_2 as NO_3 radicals and subsequently HNO_3 . The reduction of NO_x during the weekend (mainly due to the reduced motor vehicle and diesel truck activity) would lessen the titration and increase the VOC reactivity. The final result is elevated O_3 mixing ratios occurring disproportionately on weekends. A lack of a weekend effect (i.e., no pronounced high O_3 occurrences during weekends) would suggest that the region is in a transition regime. The reversed weekend effect (i.e., lower O_3 during weekends) would suggest that the region is in a NO_x -limited regime.

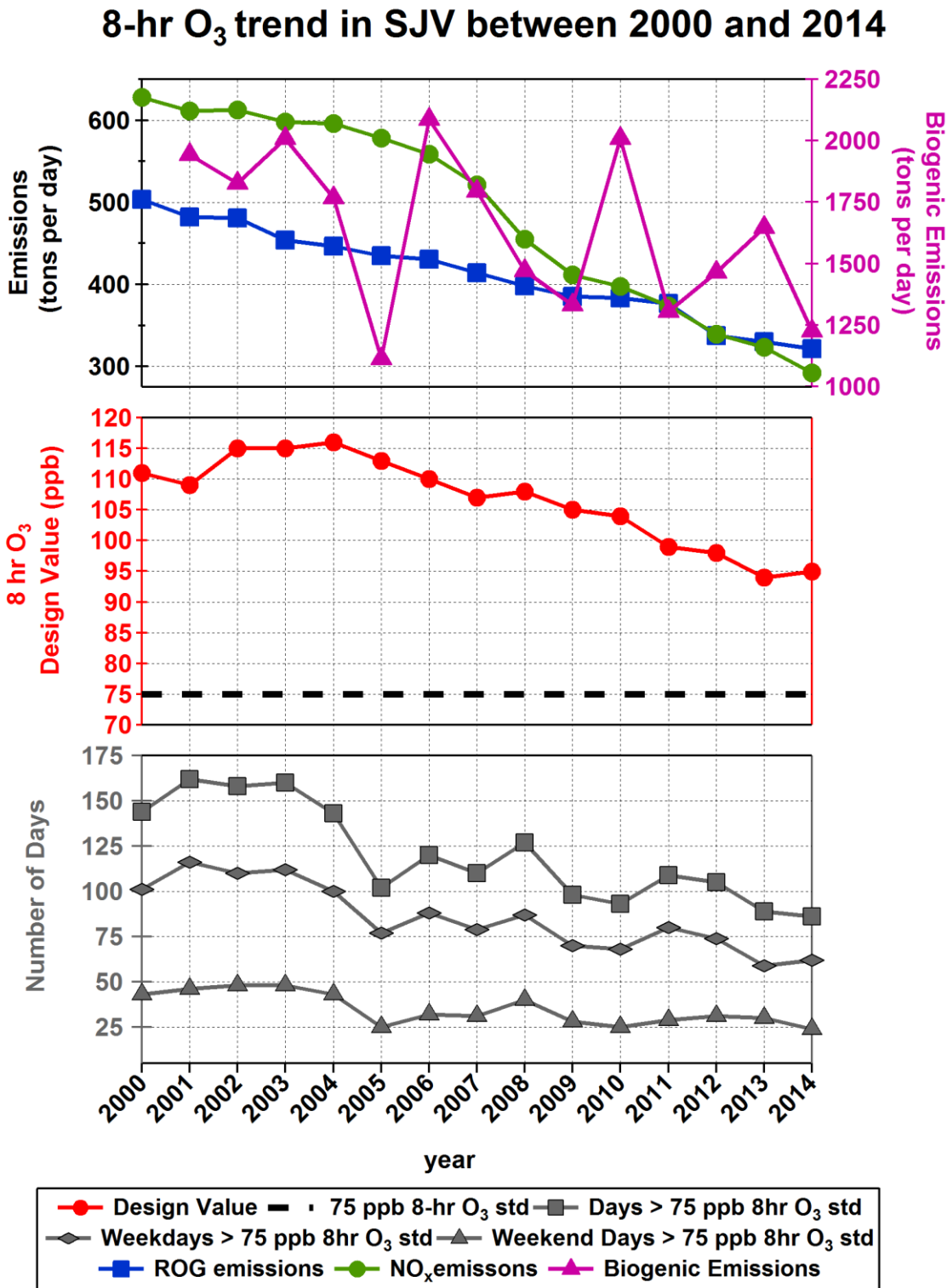


Figure 2-3. Trends in SJV air basin emissions (top), 8-hour ozone design value (middle), and number of days above the 8-hour ozone standard.

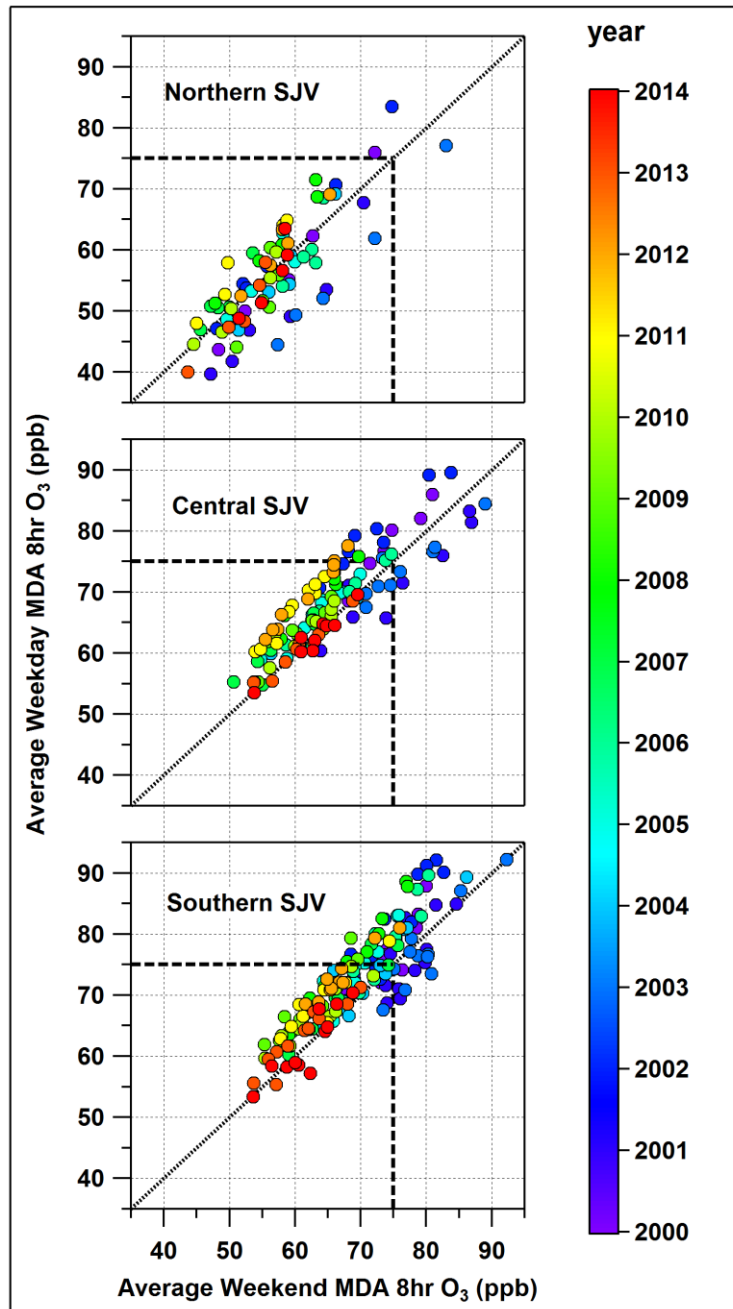


Figure 2-4. Site-specific average weekday and weekend maximum daily average 8-hour ozone for each year from 2000 to 2014 for the Northern SJV (top), Central SJV (middle), and Southern SJV (bottom). Points falling below the 1:1 dashed line represent a NO_x-disbenefit regime, those on the 1:1 dashed line represent a transitional regime, and those above the 1:1 dashed line represent a NO_x-limited regime.

The trend in day-of-week dependence of the Valley's sub-regional observed ozone levels between 2000 and 2014 is shown in Figure 2-4. The three-panel scatter plot shown in Figure 2-4 compares the average site-specific weekday (Wednesday and Thursday) and weekend (Sunday) observed summertime (June through September) maximum daily average (MDA) 8-hr ozone value by year (2000 to 2014), separated into three sub-regions: Northern SJV (top), Central SJV (middle), and Southern SJV (bottom). Different definitions of weekday and weekend days were also investigated and did not show appreciable differences from the Wednesday/Thursday and Sunday definitions.

From Figure 2-4 it can be seen that ozone levels are highest in the southern (i.e. Bakersfield area) and central (i.e. Fresno area) SJV regions, with the lowest levels seen in the northern SJV region. A key observation in Figure 2-4 is that the summertime average weekday and weekend ozone levels have steadily declined between 2000 and 2014, consistent with the decline in the basin-wide DV and exceedance days shown in Figure 2-3. Along with the declining ozone, there is a pattern shift in the weekday and weekend ozone between 2000 and 2014. In the early 2000's, the central and southern regions of the SJV exhibited roughly the same number of sites with weekend ozone greater than weekday ozone as sites with weekday ozone greater than weekend ozone, which suggests that the regions may have been in the transitional chemical regime for ozone formation. By the mid-2000's, the majority of the sites were showing weekday ozone greater than weekend ozone, which is consistent with a shift into complete NO_x -limited chemistry. By 2014, however, some of the sites had shifted back towards a more equal distribution between weekday and weekend ozone. This shift though, is expected due to the relatively low level of biogenic emissions in 2014 (Figure 2-3), which could cause a shift from a NO_x -limited environment to a more transitional chemistry environment (Figure 2-2). In contrast to the central and southern portions of the SJV, the northern region clearly experienced a greater NO_x -disbenefit in the early 2000's and then moved into a transitional chemical regime in the mid-2000's and has yet to move fully into the NO_x -limited regime.

These findings are consistent with an independent analysis by UC Berkeley researchers on the observed response of ozone from 1995 to 2010 in the SJV to emission reductions in NO_x and VOC reactivity. This study concluded that NO_x emission reductions have been effective at reducing ozone levels and have successfully transitioned the southern and central portions of the SJV into a NO_x -limited chemistry regime, while the northern portion of the SJV is currently in the process of transitioning to the same chemical regime (Pusede et al. 2012).

2.4 Meteorological Conditions Leading to Ozone Exceedances

Figure 2-5 illustrates the topography, air basin and county boundaries in California. The San Joaquin Valley (highlighted in pink) is a region of highly complex terrain, and is surrounded by the Sierra Nevada Mountains on the east, coastal mountain ranges to the west, and the Tehachapi Mountains to the south. Weather conditions during much of the summer ozone season are dominated by an area of high pressure, known as the East Pacific Ridge, which creates a broad region of warm, descending air over Central California. Weather conditions and summertime ozone levels in Central California have been shown to be strongly influenced by the strength and positioning of this ridge (Lehrman et al., 2004; Pun et al., 2008).



Figure 2-5. California topography, air basins, and counties.

Synoptic forcing under the East Pacific Ridge is typically weak, with wind flows above the planetary boundary layer from the northwest, resulting in wind flows in Central California that are primarily thermally driven and strongly influenced by orographic effects (Zhong et al., 2004). Thermal gradients between the eastern Pacific Ocean and inland in the Valley result in a strong daytime sea breeze which follows the terrain and can extend well inland through the Carquinez Strait and to a lesser extent the

Altamont, Pacheco, and Cholame Passes. When meteorological conditions are favorable, polluted air masses from the Bay Area traveling through the Carquinez Straight bifurcate over the Delta region, with one branch flowing to the northeast into the southern Sacramento Valley and the other branch flowing southeast into the northern San Joaquin Valley (Figure 2-6).

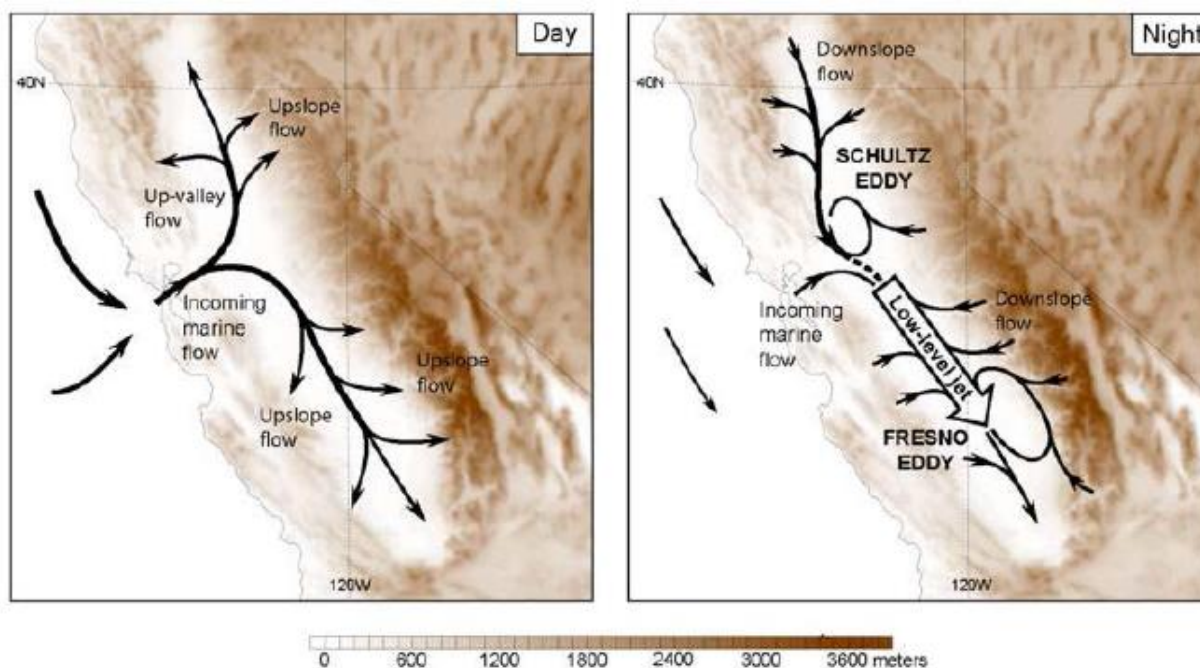


Figure 2-6. Conceptual low-level wind patterns in Central California during the day (left panel) and night (right panel) for typical ozone episode conditions (adapted from Bao et al., 2006).

At night, the sea breeze gradually weakens and can even reverse in some cases, but up-valley flow off of the Delta usually persists. Nighttime surface wind flow in the Central Valley is dominated by downslope flows off of the mountain ranges on all sides (Figure 2-6) and when combined with the continued up-valley flows from the Delta, result in low-level eddies such as the Schultz eddy in the southern Sacramento Valley and the Fresno eddy in the SJV (Lehrman et al., 2004). At night, winds aloft become decoupled from the surface and can form a low-level nocturnal jet (Zhong et al., 2004), which has been shown to be an important nighttime pollutant transport mechanism within the Valley (Lehrman et al., 2001). The conditions that promote the formation of this nocturnal jet within the Valley may also limit ventilation of the Valley, resulting in a buildup of pollution over multiple days.

Clustering and classification techniques have been utilized on both observed meteorology (Lehrman et al., 2001; Blanchard et al., 2008; Beaver and Palazoglu, 2009) and observed and modeled ozone (Fujita et al., 1999; Jin et al., 2011) in the Valley and the surrounding region to better understand the relationship between meteorology and elevated ozone. These various studies reveal that the position and strength of the Pacific High has a dominant influence on ozone levels throughout the Central Valley, along with the height of the marine inversion and strength of the low-level on-shore flow. Synoptic flows that weaken or break down the Pacific High result in lower ozone throughout the Central Valley, while a strong sea breeze with a deep marine boundary layer results in lower ozone levels within the Bay Area, but also an enhanced transport of polluted air masses into the Delta region. Under such conditions, elevated ozone can occur in the Sacramento and San Joaquin Valleys if the synoptic forcing is sufficiently weak so that vertical mixing is reduced and recirculation is enhanced. The highest ozone levels in the Valley occur as the thermal gradient between off-shore and inland weakens and the high pressure system strengthens, resulting in reduced transport of polluted air masses from the Bay Area inland to the Delta, which is accompanied by a rise in temperatures inland. As the sea breeze weakens even further, conditions stagnate within the Valley and ozone levels peak. Ozone levels will remain elevated until a synoptic system moves through the area and breaks down the Pacific High.

3. SELECTION OF MODELING PERIODS

3.1 Reference Year Selection and Justification

From an air quality and emissions perspective, ARB and the District have selected 2012 as the base year for design value calculation and for the modeled attainment test. These baseline values will serve as the anchor point for estimating future year projected design values.

The selection of 2012 is based on the following two considerations:

- Most complete and up to date emissions inventory, which reduces the uncertainty associated with future emissions projections.
- Analysis of the ozone forming potential (OFP) for recent years, as well as the frequency of meteorological conditions that are known to be associated with ozone exceedance events.

Details on these analyses can be found in the Weight of Evidence Appendix to this SIP.

3.2 Future Year Selection and Justification

The future year modeled is determined by the year for which attainment must be demonstrated. The extreme nonattainment designation for the SJV requires that attainment of the 2008 8-hour ozone standard be demonstrated by 2031. Therefore, 2031 will be the future year modeled in this attainment demonstration.

3.3 Justification for Seasonal Modeling Rather than Episodic Modeling

Recent ozone based studies, which focused on model performance evaluation for regulatory assessment, have recommended the use of modeling results covering the full synoptic cycles and full ozone seasons (Hogrefe et al., 2000; Vizuite et al., 2011). This enables a more complete assessment of ozone response to emission controls under a wide range of meteorological conditions.

The four highest ozone mixing ratios for a given year at any monitor within the Valley generally occur between June and September. This is important because it's the 4th highest ozone mixing ratio that is used in the Design Value (DV) calculation. In some cases, these top four days may all come from a single episode, but it is more likely that they occur during different episodes throughout the ozone season. Furthermore, based on the work of Foley et al. (2015), the revised U.S. EPA modeling guidance requires the model attainment demonstration to utilize the top ten modeled days when projecting Design Values (DVs) to the future. Rather than modeling many different episodes in an attempt to capture the top ten modeled days over the 2012 ozone season, we propose to model the entire ozone season (May – September) to ensure that all of the top days are modeled.

4. DEVELOPMENT OF EMISSION INVENTORIES

For a detailed description of the emissions inventory, updates to the inventory, and how it was processed from the planning totals to a gridded inventory for modeling, see the Modeling Emissions Inventory Appendix.

5. MODELS AND INPUTS

5.1 Meteorological Model

Meteorological model selection is based on a need to accurately simulate the synoptic and mesoscale meteorological features observed during the selected modeling period. 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 fields such as wind flows, ambient temperature variation, evolution of the boundary layer, and atmospheric moisture content to properly characterize the meteorological component of photochemical modeling.

In the past, the ARB has applied prognostic, diagnostic, and hybrid 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, we will use the Weather and Research Forecasting (WRF) model (Skaramock et al, 2005) to develop the meteorological fields that drive the photochemical modeling. The U.S. EPA (2014) recommends the use of a well-supported grid-based mesoscale meteorological model for generating meteorological inputs. The WRF model is a community-based mesoscale prediction model, which represents the state-of-the-science and has a large community of model users and developers who frequently update the model as new science becomes available. In recent years, WRF has been applied in California to generate meteorological fields for numerous air quality studies (e.g., Angevine, et al., 2012; Baker et al., 2015; Ensberg et al., 2013; Fast et al., 2014; Hu et al., 2014a, 2014b; Huang et al., 2010; Kelly et al., 2014; Lu et al., 2012; Mahmud et al., 2010), and has been shown to reasonably reproduce the observed meteorology in California.

5.1.1 Meteorological Modeling Domain

The WRF 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 12 km grid (D02) is used to provide finer resolution data that feeds into the 4 km grid (D03). The D01 grid is centered at 37 °N and 120.5 °W and was chosen so that the inner two grids, D02 and D03, would nest inside of D03 and be sufficiently far away from the boundaries to minimize boundary influences. The D01 grid consists of 90 x 90 grid cells, while the D02 and D03 grids encompass 192 x 192 and 327 x 297 grid cells, respectively, with an origin at -696 km x -576 km (Lambert Conformal projection). WRF

will be run for the three nested domains simultaneously with two-way feedback between the parent and the nest grids. The D01 and D02 grids are meant to resolve the larger scale synoptic weather systems, while the D03 grid is intended to resolve the finer details of the atmospheric conditions and will be used to drive the air quality model simulations. All three domains will utilize 30 vertical sigma layers (defined in Table 5-1), as well as the various physics options listed in Table 5-2 for each domain.

The initial and boundary conditions (IC/BCs) for WRF will be prepared based on 3-D North American Regional Reanalysis (NARR) data that are archived at the National Center for Atmospheric Research (NCAR). These data have a 32km horizontal resolution. Boundary conditions to WRF are updated at 6-hour intervals for the 36km grid (D01). In addition, surface and upper air observations obtained from NCAR will be used to further refine the analysis data that are used to generate the IC/BCs. Analysis nudging will be employed in the outer 36km grid (D01) to ensure that the simulated meteorological fields are constrained and do not deviate from the observed meteorology.

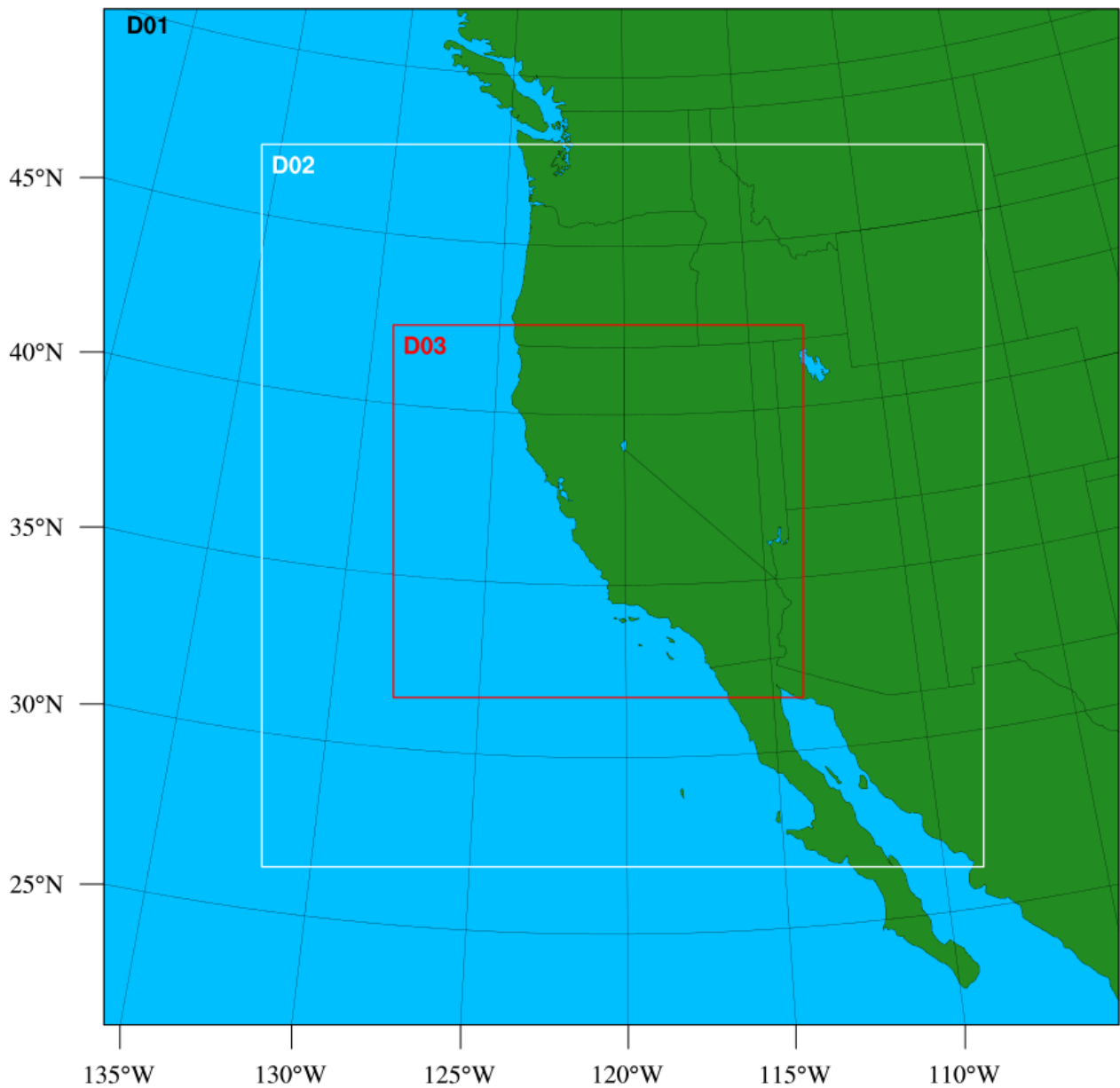


Figure 5-1. The three nested grids for the WRF model (D01 36km; D02 12km; and D03 4km).

Table 5-1. Proposed WRF vertical layer structure.

Layer Number	Height (m)	Layer Thickness (m)	Layer Number	Height (m)	Layer Thickness (m)
30	16082	1192	14	1859	334
29	14890	1134	13	1525	279
28	13756	1081	12	1246	233
27	12675	1032	11	1013	194
26	11643	996	10	819	162
25	10647	970	9	657	135
24	9677	959	8	522	113
23	8719	961	7	409	94
22	7757	978	6	315	79
21	6779	993	5	236	66
20	5786	967	4	170	55
19	4819	815	3	115	46
18	4004	685	2	69	38
17	3319	575	1	31	31
16	2744	482	0	0	0
15	2262	403			

Note: Shaded layers denote the subset of vertical layers to be used in the CMAQ photochemical model simulations. Further details on the CMAQ model configuration and settings can be found in subsequent sections.

Table 5-2. WRF Physics Options.

Physics Option	Domain		
	D01 (36 km)	D02 (12 km)	D03 (4 km)
Microphysics	WSM 6-class graupel scheme	WSM 6-class graupel scheme	WSM 6-class graupel scheme
Longwave radiation	RRTM	RRTM	RRTM
Shortwave radiation	Dudhia scheme	Dudhia scheme	Dudhia scheme
Surface layer	Revised MM5 Monin-Obukhov	Revised MM5 Monin-Obukhov	Revised MM5 Monin-Obukhov
Land surface	Pleim-Xiu LSM	Pleim-Xiu LSM	Pleim-Xiu LSM
Planetary Boundary Layer	YSU	YSU	YSU
Cumulus Parameterization	Kain-Fritsch scheme	Kain-Fritsch scheme	None

5.2 Photochemical Model

U.S. EPA guidance (U.S. EPA, 2014) requires several factors to be considered as criteria for choosing a qualifying air quality model to support the attainment demonstration. These criteria include: (1) It should have received a scientific peer review; (2) It should be appropriate for the specific application on a theoretical basis; (3) It should be used with databases which are available and adequate to support its application; (4) It should be shown to have performed well in past modeling applications; and (5). It should be applied consistently with an established protocol on methods and procedures (U.S. EPA, 2014). In addition, it should be well documented with a user's guide as well as technical descriptions. For the ozone 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 ozone mixing ratios. The Community Multiscale Air Quality (CMAQ) Modeling System has been selected for modeling ozone 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 investigating the atmospheric chemistry and physics that contribute to air pollution. CMAQ 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 model has undergone peer review every few years and represents the state-of-the-science (Brown et al., 2011). The CMAQ

model is regularly updated to incorporate new chemical and aerosol mechanisms, algorithms, and data as they become available in the scientific literature (e.g., Appel et al., 2013; Foley, et al., 2010; Pye and Pouliot, 2012;). In addition, the CMAQ model is well documented in terms of its underlying scientific algorithms as well as guidance on operational uses (e.g., Appel et al., 2013; Binkowski and Roselle, 2003; Byun and Ching, 1999; Byun and Schere, 2006; Carlton et al., 2010; Foley et al., 2010; Kelly, et al., 2010a; Pye and Pouliot, 2012; UNC, 2010).

The CMAQ model was the regional air quality model used for the 2008 SJV annual PM_{2.5} SIP, the 2012 SJV 24-hour PM_{2.5} SIP and the 2013 1-hr ozone SIP for the SJV. A number of previous studies have also used the CMAQ model to study ozone and PM_{2.5} formation in the SJV (e.g., Jin et al., 2008, 2010b; 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 have been numerous applications of the CMAQ model within the U.S. and abroad (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), which have shown it to be suitable as a regulatory and scientific tool for investigating air quality. Staff at the 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 readily available from the Community Modeling and Analysis System (CMAS) Center (<http://www.cmascenter.org/>) established by the U.S. EPA.

Version 5.0.2 of the CMAQ model, released in May 2014, will be used in this SIP (http://www.airqualitymodeling.org/cmaqwiki/index.php?title=CMAQ_version_5.0.2_%28April_2014_release%29_Technical_Documentation). Compared to the previous version CMAQv4.7.1, which was used for the 2013 1-hour SIP, CMAQ version 5 and above incorporated substantial new features and enhancements to topics such as gas-phase chemistry, aerosol algorithms, and structure of the numerical code (http://www.airqualitymodeling.org/cmaqwiki/index.php?title=CMAQ_version_5.0_%28February_2012_release%29_Technical_Documentation#RELEASE_NOTES_for_CMAQ_v5.0_.C2.A0February_2012).

5.2.1 Photochemical Modeling Domain

Figure 5-2 shows the photochemical modeling domains used by ARB for this work. The larger domain, covering all of California, has a horizontal grid resolution of 12 km and extends from the Pacific Ocean in the west to Eastern Nevada in the east and runs from south of the U.S.-Mexico border in the south to north of the California-Oregon border in the north. The smaller domain nested within the outer 12 km domain covers most of northern and central California and incorporates a finer scale 4 km grid resolution to better reflect the finer scale details of meteorology, topography, and emissions. Consistent with the WRF modeling, the 12 km and 4 km CMAQ domains are based on a Lambert Conformal Conic projection with reference longitude at -120.5°W , reference latitude at 37°N , and two standard parallels at 30°N and 60°N . The 30 vertical layers from WRF were mapped onto 18 vertical layers for CMAQ, extending from the surface to 100 mb such that the majority of the vertical layers fall within the planetary boundary layer. This vertical layer structure is based on the WRF sigma-pressure coordinates and the exact layer structure used can be found in Table 5-1.

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 a grid cell size of ~ 4 km (U.S. EPA, 2014). Our selection of modeling domains and grid resolution is consistent with this 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 50 mb) are anywhere from 14 to 35 vertical layers. For the present SIP, 18 vertical layers will be used in the CMAQ model. 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, 0.8709, 0.8431, 0.8107, 0.7733, 0.6254, 0.293, 0.0788, and 0.0. As previously noted, this also ensures that the majority of the layers are in the planetary boundary layer.

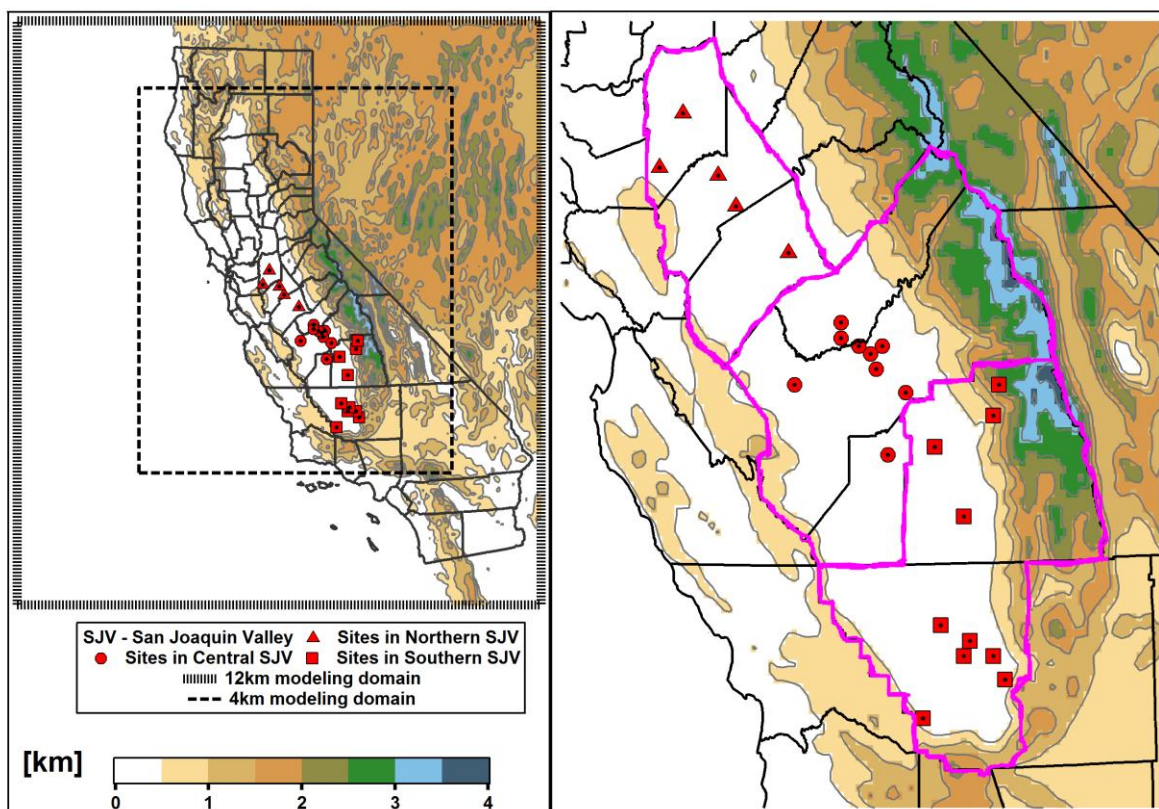


Figure 5-2. The CMAQ modeling domains used in this SIP modeling. The outer box of the left panel is the California statewide 12 km modeling domain, while the inner box shows the 4km modeling domain covering Central California. The shaded and gray line contours denote the gradients in topography (km). The insert on the right shows the zoomed-in view of the spatial extent (magenta lines) and the location of sites in the Northern (red triangle markers), Central (red circle makers) and Southern (red square markers) sub regions in the Valley that have been used in evaluating model performance for ozone. (Figure adapted from Kulkarni et al., 2014)

5.2.2 CMAQ Model Options

Table 5-3 shows the CMAQv5.0.2 configuration that will be used to model ozone in the SJV. The same configuration will be used for all simulations for the base case, reference, and future years. CMAQv5.0.2 was compiled using the Intel FORTRAN compiler version 12.

Table 5-3. CMAQ v5.0.2 configuration and settings.

Process	Scheme
Horizontal advection	Yamo (Yamartino scheme for mass-conserving advection)
Vertical advection	WRF-based scheme for mass-conserving advection
Horizontal diffusion	Multi-scale
Vertical diffusion	ACM2 (Asymmetric Convective Model version 2)
Gas-phase chemical mechanism	SAPRC-07 gas-phase mechanism with version "C" toluene updates
Chemical solver	EBI (Euler Backward Iterative solver)
Aerosol module	Aero6 (the sixth-generation CMAQ aerosol mechanism with extensions for sea salt emissions and thermodynamics; includes a new formulation for secondary organic aerosol yields)
Cloud module	ACM_AE6 (ACM cloud processor that uses the ACM methodology to compute convective mixing with heterogeneous chemistry for AERO6)
Photolysis rate	phot_inline (calculate photolysis rates in-line using simulated aerosols and ozone)

5.2.3 Photochemical Mechanism

The SAPRC07 mechanism will be utilized as the photochemical mechanism for the CMAQ simulations. SAPRC07, 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 (NO_x) (Carter, 2010a, 2010b). It represents a complete update to the SAPRC99 mechanism, which has been used for previous ozone SIP plans in the SJV. The well-known SAPRC family of mechanisms have been used widely in California and the U.S. (e.g., Baker, et al., 2015; Cai et al., 2011; Chen et al., 2014a; Dennis et al., 2008; Ensberg, et al., 2013; Hakami, et al., 2004a, 2004b; Hu et al., 2012, 2014a, 2014b; Jackson, et al., 2006; Jin et al., 2008, 2010b; Kelly, et al., 2010b; Lane et al., 2008; Liang and Kaduwela, 2005; Livingstone et al., 2009; Lin et al., 2005; Napelenok, 2006; Pun et al., 2009; Tonse et al., 2008; Ying et al., 2008a, 2008b; Zhang et al., 2010; Zhang and Ying, 2011).

The SAPRC07 mechanism has been fully reviewed by four experts in the field through a ARB funded contract. These reviews can be found at <http://www.arb.ca.gov/research/reactivity/rsac.htm>. Dr. Derwent's (2010) review compared ozone impacts of 121 organic compounds calculated using SAPRC07 and the Master Chemical Mechanism (MCM) v 3.1 and concluded that the ozone impacts using the two mechanisms were consistent for most compounds. Dr. Azzi (2010) used SAPRC07 to simulate ozone formation from isoprene, toluene, m-xylene, and evaporated fuel in environmental chambers performed in Australia and found that SAPRC07 performed reasonably well for these data. Dr. Harley discussed implementing the SAPRC07 mechanism into 3-D air quality models and brought up the importance of the rate constant of $\text{NO}_2 + \text{OH}$. This rate constant in the SAPRC07 mechanism in CMAQv5.0.2 has been updated based on new research (Mollner et al., 2010). Dr. Stockwell (2009) compared individual reactions and rate constants in SAPRC07 to two other mechanisms (CB05 and RADM2) and concluded that SAPRC07 represented a state-of-the-science treatment of atmospheric chemistry.

5.2.4 CMAQ Initial and Boundary Conditions (IC/BC) and Spin-Up period

Air quality model initial conditions define the mixing ratio (or concentration) of chemical and aerosol species within the modeling domain at the beginning of the model simulation. Boundary conditions define the chemical species mixing ratio (or concentration) within the air entering or leaving the modeling domain. This section discusses the initial and boundary conditions used by the ARB in air quality modeling that will support developing the 8-hour ozone SIP.

U.S. EPA guidance recommends using a model "spin-up" period by beginning a simulation 3-10 days prior to the period of interest (U.S. EPA, 2014). This "spin-up" period allows the initial conditions to be "washed out" of the system, so that the actual initial conditions have little to no impact on the modeling over the time period of interest, as well as giving sufficient time for the modeled species to come to chemical equilibrium. When simulating an entire ozone season, it is more computationally efficient to simulate each month in parallel rather than the entire season sequentially. For each month, the CMAQ simulations will include a seven day spin-up period (i.e., the last seven days of the previous month) for the outer 12 km domain to ensure that the initial conditions are "washed out" of the system. Initial conditions at the beginning of the seven day spin-up period will be based on the default initial conditions that are included with the CMAQ release. The 4 km inner domain simulations will utilize a three

day spin-up period, where the initial conditions will be based on output from the corresponding day of the 12 km domain simulation.

In recent years, the use of global chemical transport model (CTM) outputs as boundary conditions (BCs) in regional CTM applications has become increasingly common (Chen et al., 2008; Hogrefe et al., 2011; Lin et al., 2010; Lam and Fu, 2009; Lee et al., 2011), and has been shown to improve model performance in many cases (Appel et al., 2007; Borge et al., 2010; Tang et al., 2007, 2009; Tong and Mauzerall, 2006;). 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 mixing ratios. In the modeling for this SIP, the Model for Ozone And Related chemical Tracers (MOZART; Emmons et al., 2010a) will be used to define the boundary conditions for the outer 12 km CMAQ domain, while boundary conditions for the 4 km domain will be derived from the 12 km output. MOZART 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 (NCAR), the Max-Planck-Institute for Meteorology (in Germany), and the Geophysical Fluid Dynamics Laboratory (GFDL) of the National Oceanic and Atmospheric Administration (NOAA), and is widely used in the scientific community. In addition to inorganic gases and VOCs, BCs were extracted for aerosol species including elemental carbon, organic matter, sulfate, soil and nitrate. MOZART has been extensively peer-reviewed and applied in a range of studies that utilize its output in defining BCs for regional modeling studies within California and other regions of the U.S. (e.g., Avise et al., 2008; Chen et al., 2008, 2009a, 2009b; Fast et al., 2014; Jathar et al., 2015).

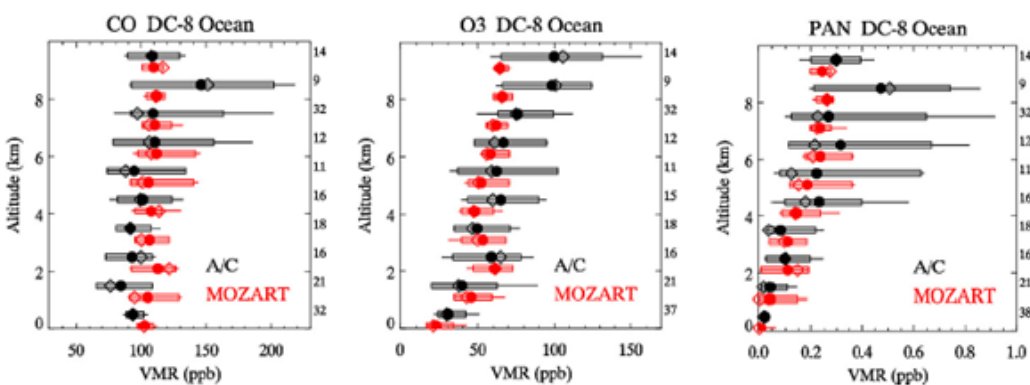


Figure 5-3. Comparison of MOZART (red) simulated CO (left), ozone (center), and PAN (right) to observations (black) along the DC-8 flight track. Shown are mean (filled symbol), median (open symbols), 10th and 90th percentiles (bars) and extremes (lines). The number of data points per 1-km wide altitude 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 5-3).

The specific MOZART simulations to be utilized in this SIP are the MOZART4-GEOS5 simulations by Louisa Emmons (NCAR) for the year 2012, which are available for download at <http://www.acom.ucar.edu/wrf-chem/mozart.shtml>. These simulations are similar to those of Emmons et al. (2010a), but with updated meteorological fields. Boundary condition data will be extracted from the MOZART-4 output and processed to CMAQ model ready format using the “mozart2camx” code developed by the Rambol-Environ Corporation (available at <http://www.camx.com/download/support-software.aspx>). The final BCs represent day-specific mixing ratios, which vary in both space (horizontal and vertical) and time (every six hours).

Per U.S. EPA guidance, the same MOZART derived BCs for the 12 km outer domain will be used for all simulations (e.g., Base Case, Reference, Future, and any sensitivity simulation).

5.3 Quality Assurance of Model Inputs

In developing the IC/BCs and Four Dimensional Data Assimilation (FDDA) datasets for WRF, quality control is performed on all associated meteorological data. Generally, all surface and upper air meteorological 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 may not be used in the modeling analyses.

In addition, the model-ready emissions files used in CMAQ will be evaluated and compared against the planning inventory totals. Although deviations between the model-ready and planning inventories are expected due to temporal adjustments (e.g., month-of-year and day-of-week) and adjustments based on meteorology (e.g., evaporative emissions from motor vehicles and biogenic sources), any excessive deviation will be investigated to ensure the accuracy of the temporal and meteorology based adjustments. If determined to be scientifically implausible, then the adjustments

which led to the deviation will be investigated and updated based on the best available science.

Similar to the quality control of the modeling emissions inventory, the chemical boundary conditions derived from the global CTM model will be evaluated to ensure that no errors were introduced during the processing of the data (e.g., during vertical interpolation of the global model data to the regional model vertical structure or mapping of the chemical species). Any possible errors will be evaluated and addressed if they are determined to be actual errors and not an artifact of the spatial and temporal dynamics inherent in the boundary conditions themselves.

6. METEOROLOGICAL MODEL PERFORMANCE

The complex interactions between the ocean-land interface, orographic induced flows from the mountain-valley topography, and the extreme temperature gradients between the ocean, delta region, valley floor, and mountain ranges surrounding the valley, make the SJV one of the most challenging areas in the country to simulate using prognostic meteorological models. Although there is a long history of prognostic meteorological model applications in the SJV (e.g., 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., 2010a, 2010b; Hu et al., 2010), there is no single model configuration that works equally well for all years and/or seasons, which makes evaluation of the simulated meteorological fields critical for ensuring that the fields reasonably reproduce the observed meteorology for any given time period.

6.1 Ambient Data Base and Quality of Data

Observed meteorological data used to evaluate the WRF model simulations will be obtained from the Air Quality and Meteorological Information System (AQMIS) database, which is a web-based source for real-time and official air quality and meteorological data (www.arb.ca.gov/airqualitytoday/). This database contains surface meteorological observations from 1969-2016, with the data through 2013 having been fully quality assured and deemed official. In addition ARB also has quality-assured upper-air meteorological data obtained using balloons, aircraft, and profilers.

6.2 Statistical Evaluation

Statistical analyses will be performed to evaluate how well the WRF model captured the overall structure of the observed atmosphere within the SJV during the five-month simulation period, using wind speed, wind direction, temperature, and humidity. The performance of the WRF model against observations will be evaluated using the METSTAT analysis tool (Emery et al, 2001) and supplemented using statistical software tools developed at ARB. The model output and observations for all five months in 2012 will be read, and data points at each observational site for wind speed, wind direction, temperature, and moisture data will be extracted. The following values will be calculated: Mean Obs, Mean Model, Mean Bias (MB), Mean (Gross) Error (ME/MGE), Normalized Mean Bias (NMB), Root Mean Squared error (RMSE), and the Index Of Agreement (IOA) when applicable.

The mathematical expressions for these quantities are:

$$MB = \frac{1}{N} \sum_1^N (\text{Model} - \text{Obs}) \quad (6-1)$$

$$ME = \frac{1}{N} \sum_1^N |\text{Model} - \text{Obs}| \quad (6-2)$$

$$NMB = \frac{\sum_1^N (\text{Model} - \text{Obs})}{\sum_1^N \text{Obs}} \times 100\%, \quad (6-3)$$

$$RSME = \sqrt{\frac{\sum_1^N (\text{Model} - \text{Obs})^2}{N}} \quad (6-4)$$

$$IOA = 1 - \frac{\sum_1^N (\text{Model} - \text{Obs})^2}{\sum_1^N [(\text{Model} - \text{Obs}) + (\text{Model} + \text{Obs})]^2}, \quad (6-5)$$

where, “*Model*” is the simulated values, “*Obs*” is the observed value, and *N* is the number of observations. These values will be tabulated and plotted for all monitoring sites within the SJV and summarized for three subregions: Northern SJV, Central SJV, and Southern SJV. Statistics may be compared to other prognostic model applications in the SJV to place the current model performance within the context of previous studies. In addition to the statistics above, model performance may also be evaluated through metrics such as frequency distributions, time-series analysis, and wind-rose plots. Based on previous experience with meteorological simulations in California, it is expected that the analysis will show wind speed to be overestimated at some stations with a smaller difference at others. The diurnal variations of temperature and wind direction at most stations are likely to be captured reasonably well. However, the model will likely underestimate the larger magnitudes of temperature during the day and smaller magnitudes at night.

6.3 Phenomenological Evaluation

In addition to the statistical evaluation described above, a phenomenological based evaluation can provide additional insights as to the accuracy of the meteorological model. A phenomenological evaluation may include analysis such as determining the relationship between observed air quality and key meteorological parameters (e.g., conceptual model) and then evaluating whether the simulated meteorology and air quality is able to reproduce those relationships. Another possible approach would be to generate geopotential height charts at 500 and 850 mb using the simulated results and compare those to the standard geopotential height charts. This would 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 National Centers for Environmental Prediction (NCEP) Reanalysis dataset. These can then be visually compared to the simulated meteorological fields to determine whether those large-scale meteorological conditions were accurately simulated and whether the same relationships observed in the NCEP reanalysis are present in the simulated data.

7. PHOTOCHEMICAL MODEL PERFORMANCE

7.1 Ambient Data

Observed air quality data used to evaluate the CMAQ model simulations will be obtained from the Air Quality and Meteorological Information System (AQMIS) database, which is a web-based source for real-time and official air quality and meteorological data (www.arb.ca.gov/airqualitytoday/). This database contains surface air quality observations from 1980-2016, with the data through 2014 having been fully quality assured and deemed official.

7.2 Statistical Evaluation

As recommended by U.S. EPA, a number of statistical metrics will be used to evaluate the model performance for ozone. These metrics include mean bias (MB), mean error (ME), mean fractional bias (MFB), mean fractional error (MFE), normalized mean bias (NMB), normalized mean error (NME), root mean square error (RMSE), and correlation coefficient (R^2). The formulae for estimating these metrics are given below.

$$MB = \frac{1}{N} \sum_1^N (\text{Model} - \text{Obs}) \quad (7-1)$$

$$ME = \frac{1}{N} \sum_1^N |\text{Model} - \text{Obs}| \quad (7-2)$$

$$MFB = \frac{2}{N} \sum_1^N \left(\frac{\text{Model} - \text{Obs}}{\text{Model} + \text{Obs}} \right) \times 100\%, \quad (7-3)$$

$$MFE = \frac{2}{N} \sum_1^N \left(\frac{|\text{Model} - \text{Obs}|}{\text{Model} + \text{Obs}} \right) \times 100\%, \quad (7-4)$$

$$NMB = \frac{\sum_1^N (\text{Model} - \text{Obs})}{\sum_1^N \text{Obs}} \times 100\%, \quad (7-5)$$

$$\text{NME} = \frac{\sum_1^N |\text{Model} - \text{Obs}|}{\sum_1^N \text{Obs}} \times 100\%, \quad (7-6)$$

$$\text{RSME} = \sqrt{\frac{\sum_1^N (\text{Model} - \text{Obs})^2}{N}} \quad (7-7)$$

$$R^2 = \left(\frac{\sum_1^N ((\text{Model} - \overline{\text{Model}}) \times (\text{Obs} - \overline{\text{Obs}}))}{\sqrt{\sum_1^N (\text{Model} - \overline{\text{Model}})^2 \sum_1^N (\text{Obs} - \overline{\text{Obs}})^2}} \right)^2 \quad (7-8)$$

where, “Model” is the simulated mixing ratio, “ $\overline{\text{Model}}$ ” is the simulated mean mixing ratio, “Obs” is the observed value, “ $\overline{\text{Obs}}$ ” is the mean observed value, and “N” is the number of observations.

In addition, for evaluating summertime O₃, we will also use mean normalized bias (MNB) and mean normalized gross error (MNGE). Definitions for these quantities are given below.

$$\text{MNB} = \frac{1}{N} \sum_1^N \left(\frac{\text{Model} - \text{Obs}}{\text{Obs}} \right) \times 100\%, \quad (7-9)$$

$$\text{MNGE} = \frac{1}{N} \sum_1^N \left(\frac{|\text{Model} - \text{Obs}|}{\text{Obs}} \right) \times 100\%. \quad (7-10)$$

In addition to the above statistics, various forms of graphics will also be created to visually examine and compare the model predictions to observations. These will include time-series plots comparing the predictions and observations, scatter plots for comparing the magnitude of the simulated and observed mixing ratios, box plots to summarize the time series data across different regions and averaging times, as well as frequency distributions. These plots will be created for paired observations and

predictions over time scales dictated by the averaging frequencies of observations (i.e., hourly, daily, monthly, seasonally) for the species of interest. Together, they will provide a comprehensive view of model performance during different time periods, in different sub-regions, and over different mixing ratio levels.

7.3 Comparison to Previous Modeling Studies

Previous U.S. EPA modeling guidance (U.S. EPA, 1991) utilized “bright line” criteria for the performance statistics that distinguished between adequate and inadequate model performance. In the latest modeling guidance from U.S. EPA (U.S. EPA, 2014) it is now recommended that model performance be evaluated in the context of similar modeling studies to ensure that the model performance approximates the quality of other studies. The work of Simon et al. (2012) summarized photochemical model performance for studies published in the peer-reviewed literature between 2006 and 2012. and this work will form the basis for evaluating the modeling utilized in this attainment demonstration.

7.4 Diagnostic Evaluation

Diagnostic evaluations are useful for investigating whether the physical and chemical processes that control ozone formation are correctly represented in the modeling. These evaluations can take many forms, such as utilizing model probing tools like process analysis, which tracks and apportions ozone mixing ratios in the model to various chemical and physical processes, or source apportionment tools that utilize model tracers to attribute ozone formation to various emissions source sectors and/or geographic regions. Sensitivity studies (either “brute-force” or the numerical Direct Decoupled Method) can also provide useful information as to the response exhibited in the modeling to changes in various input parameters, such as changes to the emissions inventory or boundary conditions. Due to the nature of this type of analysis, diagnostic evaluations can be very resource intensive and the U.S. EPA modeling guidance acknowledges that air agencies may have limited resources and time to perform such analysis under the constraints of a typical SIP modeling application. To the extent possible, some level of diagnostic evaluation will be included in the model attainment demonstration for this SIP.

8. ATTAINMENT DEMONSTRATION

The U.S. EPA modeling guidance (U.S. EPA, 2014) outlines the approach for utilizing models to predict future attainment of the 0.075 ppm 8-hour ozone standard. Consistent with the previous modeling guidance (U.S. EPA, 2007) utilized in the 2007 SIP for the 0.08 ppm 8-hour ozone standard and the 2013 SIP for the 0.12 ppm 1-hour ozone standard, the current guidance recommends utilizing modeling in a relative sense. A detailed description of how models are applied in the attainment demonstration, as prescribed by U.S. EPA modeling guidance, is provided below.

8.1 Base Year Design Values

The starting point for the attainment demonstration is with the observational based design value (DV), which is used to determine compliance with the standard at any given monitor. The DV for a specific monitor and year represents the three-year average of the annual 4th highest 8-hour ozone mixing ratio observed at the monitor. For example, a DV for 2012 would represent the average of the 4th highest 8-hour ozone mixing ratio from 2010, 2011, and 2012. The U.S. EPA recommends using an average of three DVs to better account for the year-to-year variability inherent in meteorology. Since 2012 has been chosen as the base year for projecting DVs to the future, site-specific DVs will be calculated for the three three-year periods ending in 2012, 2013, and 2014 and then these three DVs will be averaged. This average DV is called a weighted DV (in the context of this SIP, the weighted DV will also be referred to as the reference year DV or DV_R). Table 8-1 illustrates how the weighted DV is calculated.

Table 8-1. Illustrates the data from each year that are utilized in the Design Value calculation for a specific year (DV Year), and the yearly weighting of data for the weighted Design Value calculation (or DVR).

DV Year	Years Averaged for the Design Value (4 th highest observed 8-hr O ₃)				
2012	2010	2011	2012		
2013		2011	2012	2013	
2014			2012	2013	2014
Yearly Weightings for the Weighted Design Value Calculation					
2012-2014 Average	$DV_R = \frac{8hrO3_{2010} + (2)8hrO3_{2011} + (3)8hrO3_{2012} + (2)8hrO3_{2013} + 8hrO3_{2014}}{9}$				

8.2 Base, Reference, and Future Year Simulations

Projecting the weighted DVs to the future requires three photochemical model simulations described below:

1. Base Year Simulation

The base year simulation for 2012 is used to assess model performance (i.e., to ensure that the model is reasonably able to reproduce the observed ozone mixing ratios). Since this simulation will be used to assess model performance, it is essential to include as much day-specific detail as possible in the emissions inventory, including, but not limited to hourly adjustments to the motor vehicle and biogenic inventories based on observed local meteorological conditions, known wildfire and agricultural burning events, and exceptional events such as the Chevron refinery fire.

2. Reference Year Simulation

The reference year simulation is identical to the base year simulation, except that certain emissions events which are either random and/or cannot be projected to the future are removed from the emissions inventory. These include wildfires and events such as the Chevron refinery fire.

3. Future Year Simulation

The future year simulation is identical to the reference year simulation, except that projected future year (2031) anthropogenic emission levels are used rather than the 2012 emission levels. All other model inputs (e.g., meteorology, chemical boundary conditions, biogenic emissions, and calendar for day-of-week specifications in the inventory) are the same as those used in the reference year simulation.

The base year simulation is solely used for evaluating model performance, while the reference and future year simulations are used to project the weighted DV to the future as described in subsequent sections of this document.

8.3 Relative Response Factors

As part of the model attainment demonstration, the fractional change in air pollutant mixing ratios between the model future year and model reference year are calculated for each monitor location. These ratios, called “relative response factors” or RRF, are calculated based on the ratio of modeled future year maximum daily average 8-hour (MDA8) ozone to modeled baseline year MDA8 (Equation 8-1).

$$\text{RRF} = \frac{\text{average MDA8 ozone}_{\text{future}}}{\text{average MDA8 ozone}_{\text{reference}}} \quad (8-1)$$

The MDA8 values used in calculating the RRF are based on the maximum simulated ozone within a 3x3 array of cells surrounding the monitor (Figure 8-1). The future and base year ozone values used in RRF calculations are paired in space (i.e., using the future year MDA8 ozone value at the same grid cell where the MDA8 value for the base year is located within the 3x3 array of cells). The days used to calculate the average MDA8 for the reference and future years are inherently consistent, since the same meteorology is used to drive both simulations.

Not all modeled days are used to calculate the average MDA8 ozone from the reference and future year simulations. The form of the 8-hour ozone NAAQS is such that it is geared toward the days with the highest mixing ratios of any ozone season (i.e., the 4th highest MDA8 ozone). Therefore, the modeled days used in the RRF calculation should also reflect days with the highest ozone levels. As a result, the current U.S. EPA guidance suggests using the top 10 modeled days when calculating the RRF. Since the relative sensitivity to emissions changes (in both the model and real world) can vary from day-to-day due to meteorology and emissions (e.g., temperature dependent emissions or day-of-week variability) using the top 10 days ensures that the calculated RRF is robust and stable (i.e., not overly sensitive to any single day used in the calculation).

When choosing the top 10 days, the U.S. EPA recommends beginning with all days in which the simulated reference MDA8 is ≥ 60 ppb and then calculating RRFs based on the top 10 high ozone days. If there are fewer than 10 days with MDA8 ozone ≥ 60 ppb then all days ≥ 60 ppb are used in the RRF calculation, as long as there are at least 5 days used in the calculation. If there are fewer than 5 days ≥ 60 ppb, an RRF cannot be calculated for that monitor. To ensure that only modeled days which are consistent with the observed ozone levels are used in the RRF calculation, the modeled days are further restricted to days in which the reference MDA8 ozone is within $\pm 20\%$ of the observed value at the monitor location.

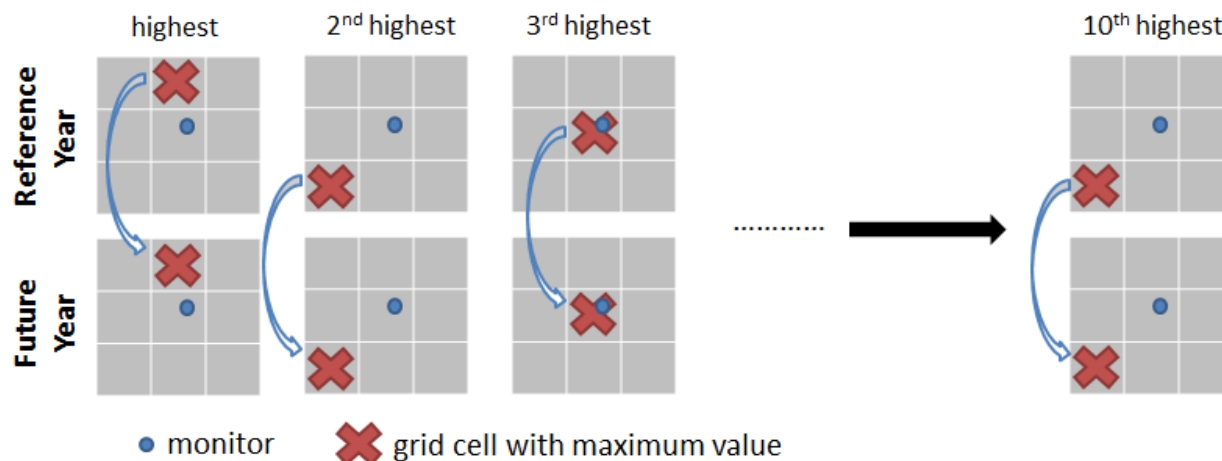


Figure 8-1. Example showing how the location of the MDA8 ozone for the top ten days in the reference and future years are chosen.

8.4 Future Year Design Value Calculation

A future year DV for each monitor is calculated by multiplying the corresponding reference year DV by the site-specific RRF from Equation 8-1 (Equation 8-2).

$$DV_F = DV_R \times RRF \quad (8-2)$$

where,

DV_F = future year design value,

DV_R = reference year design value, and

RRF = the site specific RRF from Equation 8-1

The resulting future year DVs are then compared to the 8-hour ozone NAAQS (75 ppb) to demonstrate whether attainment will be reached under the future emissions scenario utilized in the future year modeling. A monitor is considered to be in attainment of the 75 ppb ozone standard if the estimated future design value does not exceed the level of the standard.

8.5 Unmonitored Area Analysis

The unmonitored area analysis is used to ensure that there are no regions outside of the existing monitoring network that would exceed the NAAQS if a monitor was present (U.S. EPA, 2014). U.S. EPA recommends combining spatially interpolated design value fields with modeled ozone gradients and grid-specific RRFs in order to generate gridded future year gradient adjusted design values. This analysis can be done using the Model

Attainment Test Software (MATS) (Abt, 2014); however this software is not open source and comes as a precompiled software package. To maintain transparency and flexibility in the analysis, in-house R codes (<https://www.r-project.org/>) developed at ARB will be utilized in this analysis.

The steps followed in the unmonitored area analysis are as follows:

Step 1: For each grid cell, calculate the average of the top-10 modeled maximum daily average 8-hour ozone mixing ratios from the reference year simulation.

Step 2: Interpolate the monitor-specific weighted base-year DVs to an unmonitored grid cell using normalized inverse distance squared weightings for all monitors within a grid cell's Voronoi Region (calculated with the R tripack library; <https://cran.r-project.org/web/packages/tripack/README>), and adjusted based on the ozone gradient between the grid cell and the corresponding monitor from Step 1. Interpolation is done only within the geographic region constrained by the monitoring network, since extrapolating to outside of the monitoring network is inherently uncertain.

Step 3: For each grid cell, calculate an RRF based on the reference- and future-year modeling following the same approach outlined in Section 8.3, except that the +/- 20% limitation on the simulated and observed maximum daily average 8-hour ozone is not applicable because observed data do not exist for grid cells in unmonitored areas.

Step 4: Multiply the gradient-adjusted interpolated DVs from Step 2 by the gridded RRFs from Step 3 to calculate future-year gridded DVs.

Step 5: Examine the future-year gridded DVs to determine if there are peak values higher than those at the monitors, which could cause violations of the 8-hour ozone NAAQS.

The R codes used in this analysis will be made available upon request.

8.6 Banded Relative Response Factors

The “Band-RRF” approach expands upon the standard “Single-RRF” approach to account for differences in model response to emissions controls at varying ozone levels. The most recent U.S. EPA modeling guidance (U. S. EPA, 2014) accounts for some of these differences by focusing on the top ten modeled days, but even the top ten days may contain a significant range of ozone mixing ratios. The Band-RRF approach accounts for these differences more explicitly by grouping the simulated ozone into bands of lower, medium, and higher ozone mixing ratios. Specifically, daily peak 8-hour ozone mixing ratios for all days meeting model performance criteria (+/- 20% with the observations) can be stratified into 5 ppb increments from 60 ppb upwards (bin size and mixing ratio range may vary under different applications). A separate RRF is calculated for each ozone band following a similar approach as the standard Single-RRF. A linear regression is then fit to the data resulting in an equation relating RRF to ozone band. Similar to the Single-RRF, this equation is unique to each monitor/location.

The top ten days for each monitor, based on observed 8-hour ozone, for each year that is utilized in the design value calculation (see Table 8-1) is then projected to the future using the appropriate RRF for the corresponding ozone band. The top ten future days for each year are then re-sorted, the fourth highest 8-hour ozone is selected, and the future year design value is calculated in a manner consistent with the base/reference year design value calculation. More detailed information on the Band-RRF approach can be found in Kulkarni et al. (2014) and the SJV 2013 1-Hour Ozone SIP.

9. PROCEDURAL REQUIREMENTS

9.1 How Modeling and other Analyses will be Archived, Documented, and Disseminated

The air quality modeling system covers the central portion of California with 4x4 km² grids. In total there are over half a million grid cells in each simulation (192 x 192 cells in the lateral direction and 18 vertical layers). 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 require ~200 DVDs to hold one TB). Please note that this estimate is for simulated surface-level pollutant output only. If three-dimensional pollutant data are needed, it would add a few more TB to this total. 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
Air Quality Planning and Science 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.

9.2 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 year 8-hour ozone Design Values
- Access to input data and simulation results

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