# PHOTOCHEMICAL MODELING PROTOCOL

# Photochemical Modeling for the 8-Hour Ozone and Annual/24-hour PM$_{2.5}$ State Implementation Plans

## Prepared by
California Air Resources Board

## 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

BCs – Boundary Conditions

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

CCOS - Central California Ozone Study

CMAQ Model – Community Multi-scale Air Quality Model

CIT – California Institute of Technology

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

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

FEM – Federal Equivalence Monitors

FRM – Federal Reference Monitors

$HNO_3$ – Nitric Acid

ICs – Initial Conditions

IMPROVE – Interagency Monitoring of Protected Visual Environments

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

NARR - North American Regional Reanalysis

NCAR – National Center for Atmospheric Research

NCEP – National Centers for Environmental Prediction

$NH_3$ – Ammonia

NOAA - National Oceanic and Atmospheric Administration

$NO_x$ – Oxides of nitrogen

OC – Organic Carbon

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

$PM_{10}$ – 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

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

SAPRC – Statewide Air Pollution Research Center

SARMAP – SJVAQS/AUSPEX Regional Modeling Adaptation Project

SCAQMD – South Coast Air Quality Management District

SIP – State Implementation Plan

SJV – San Joaquin Valley

SJVAB – San Joaquin Valley Air Basin (SJVAB)

SJVUAPCD – San Joaquin Valley Unified 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

SMAQMD – Sacramento Metropolitan Air Quality Management District

SMAT – Application of the Speciated Modeled Attainment Test

SOA – Secondary Organic Aerosol

$SO_x$ – Oxides of Sulfur

STN – Speciated Trend Network

UCD – University of California at Davis

U.S. EPA – United States Environmental Protection Agency

VOC – Volatile Organic Compounds

WRF Model – Weather and Research Forecast Model

# 1. INTRODUCTION

The purpose of this modeling protocol is to detail and formalize the procedures for conducting the photochemical modeling that forms the basis of the attainment demonstration for the 8-hour ozone and annual/24-hour $PM_{2.5}$ State Implementation Plans (SIPs) for California.  The protocol is intended to communicate up front how the model attainment test will be performed.  In addition, this protocol discusses analyses that are intended to help corroborate the findings of the model attainment test.

## 1.1    Modeling roles for the current SIP

The Clean Air Act (Act) establishes the planning requirements for all 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.

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

## 1.2    Stakeholder participation

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, the Air Districts 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 Districts' Governing Boards and subsequently by the ARB Board. These documents will include descriptions of the technical aspects of the SIP. Stakeholders have the choice to provide written and in-person comments at any of the Plan workshops and public Board hearings. The agencies take the comments into consideration when finalizing the Plan.

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

During the development of the modeling protocol for the 2012 SJV 24-hour $PM_{2.5}$ SIP (SJVUAPCD, 2012), ARB and the San Joaquin Valley Air Pollution Control District (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:

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

The current approach to regional air quality modeling has not changed significantly since the 2012 SJV 24-hour $PM_{2.5}$ SIP (SJVUAPCD, 2012), 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 this 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.

## 1.4  Schedule for completion of the Plan

Final area designations kick-off the three year SIP development process. For the first two years, efforts center on updates and improvements to the Plan's technical and scientific underpinnings. These include the development of emission inventories, selection of modeling periods, model selection, model input preparation, model performance evaluation and supplemental analyses. During the last year, modeling, further supplemental analyses and control strategy development proceed in an iterative manner and the public participation process gets under way. After thorough review the District Board and subsequently the ARB Board consider the Plan. The Plan is then submitted to U.S. EPA. Table 1-1 in the Appendix corresponding to the appropriate region/standard (e.g., SJV 0.075 ppm 8-hour ozone) summarizes the overall anticipated schedule for Plan completion.

# 2.  DESCRIPTION OF THE CONCEPTUAL MODEL FOR THE NONATTAINMENT AREA

See Section 2 in the Appendix corresponding to the appropriate region/standard (e.g., SJV 0.075 ppm 8-hour ozone).

# 3.  SELECTION OF MODELING PERIODS

## 3.1  Reference Year Selection and Justification

From an air quality and emissions perspective, ARB and the Districts have selected 2012 as the base year for design value calculation and for the modeled attainment test.

For the SJV, the PM$_{2.5}$ model attainment test will utilize 2013 instead of 2012.  These baseline values will serve as the anchor point for estimating future year projected design values.

The selection of 2012/13 is based on the following four considerations:
- Most complete and up to date emissions inventory, which reduces the uncertainty associated with future emissions projections.
- Analysis of meteorological adjusted air quality trends to determine recent years with meteorology most conducive to ozone and PM$_{2.5}$ formation and buildup.
- Availability of research-grade wintertime field measurements in the Valley, which captured two significant pollution episodes during the DISCOVER-AQ field study (January-February 2013).
- The SJV PM$_{2.5}$ design values for year 2013 were some of the highest in recent years, making 2013 a conservative choice for attainment demonstration modeling.

Details and discussion on these analyses can be found in the Weight of Evidence Appendix.


## 3.2  Future Year Selection and Justification

The future year modeled is determined by the year for which attainment must be demonstrated.  Table 3-1 lists the year in which attainment must be demonstrated for the various ozone and PM$_{2.5}$ standards and non-attainment regions in California.

Table 3-1. Future attainment year by non-attainment region and NAAQS. 0.08 ppm and 0.075 ppm refer to the 1997 and 2008 8-hour ozone standards, respectively. 15 ug/m$^3$ and 12 ug/m$^3$ refer to the 1997 and 2012 annual PM$_{2.5}$ standards, respectively. 35 ug/m$^3$ refers to the 2006 24-hour PM$_{2.5}$ standard, and 1-hr ozone refers to the revoked 1979 0.12 ppm 1-hour ozone standard.

| Area | Year | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| | 2031 | 2026 | 2025 | 2024 | 2023 | 2021 | 2020 | 2019 | 2017 |
| South Coast | 0.075 ppm | -- | -- | -- | 0.08 ppm | 12 µg/m$^3$ | -- | -- | -- |
| Mojave/Coachella | -- | 0.075 ppm | -- | -- | -- | -- | -- | -- | 0.08 ppm |
| Imperial County | -- | -- | -- | -- | -- | 12 µg/m$^3$ | -- | -- | 0.075 ppm |
| Ventura County | -- | -- | -- | -- | -- | -- | 0.075 ppm | -- | -- |
| San Diego | -- | -- | -- | -- | -- | -- | -- | -- | 0.075 ppm |
| San Joaquin Valley | 0.075 ppm | -- | [1]12 µg/m$^3$ | 35 µg/m$^3$ | -- | [2]12 µg/m$^3$ | 15 µg/m$^3$ | 35 µg/m$^3$ | 1-hr ozone |
| Sacramento Metropolitan | -- | 0.075 ppm | -- | -- | -- | -- | -- | -- | -- |
| Portola-Plumas County | -- | -- | -- | -- | -- | 12 µg/m$^3$ | -- | -- | -- |
| East Kern | -- | -- | -- | -- | -- | -- | -- | -- | 0.075 ppm |
| W. Nevada County | -- | -- | -- | -- | -- | -- | -- | -- | 0.075 ppm |

[1] Serious classification attainment date
[2] Moderate classification attainment date

## 3.3 Justification for Seasonal/Annual Modeling Rather than Episodic Modeling

In the past, computational constraints restricted the time period modeled for a SIP attainment demonstration to a few episodes (e.g., 2007 SJV 8-hr ozone SIP (SJVUAPCD, 2007), 2007 SC 8-hr ozone SIP (SCAQMD, 2012) and 2009 Sacramento 8-hr ozone SIP (SMAQMD, 2012)). However, as computers have become faster and

large amounts of data storage have become readily accessible, there is no longer a need to restrict modeling periods to only a few episodes.  In more recent years, SIP modeling in California has covered the entire ozone or peak $PM_{2.5}$ seasons (2012 SC 8-hour ozone and 24-hour $PM_{2.5}$ SIP (SCAQMD, 2012), 2012 SJV 24-hour $PM_{2.5}$ SIP (SJVUAPCD, 2012) and 2013 SJV 1-hr ozone SIP (SJVUAPCD,2013) ), or an entire year in the case of annual $PM_{2.5}$ ( 2008 SJV annual $PM_{2.5}$ SIP (SJVUAPCD, 2008)) The same is true for other regulatory modeling platforms outside of California (Boylan and Russell, 2006; Morris et al., 2006; Rodriguez et al., 2009; Simon et al., 2012; Tesche et al., 2006; U.S. EPA, 2011a, b).

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; Vizuete et al., 2011). This enables a more complete assessment of ozone response to emission controls under a wide range of meteorological conditions.  The same is true for modeling conducted for peak 24-hour $PM_{2.5}$.  Consistent with the shift to seasonal or annual modeling in most regulatory modeling applications, modeling for the 8-hour ozone standard will cover the entire ozone season (May – September), modeling for the annual 24-hour $PM_{2.5}$ standard will be conducted for the entire year, and modeling for the 24-hour $PM_{2.5}$ standard will, at a minimum, cover the months in which peak 24-hour $PM_{2.5}$ occurs (e.g., October – March in the SJV) and will be conducted annually whenever possible.

# 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 modeling platform, the Weather and Research Forecasting (WRF) model (Skaramock et al, 2005) will be used 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 32 km horizontal resolution.  Boundary conditions to WRF are updated at 6-hour intervals for the 36 km 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.
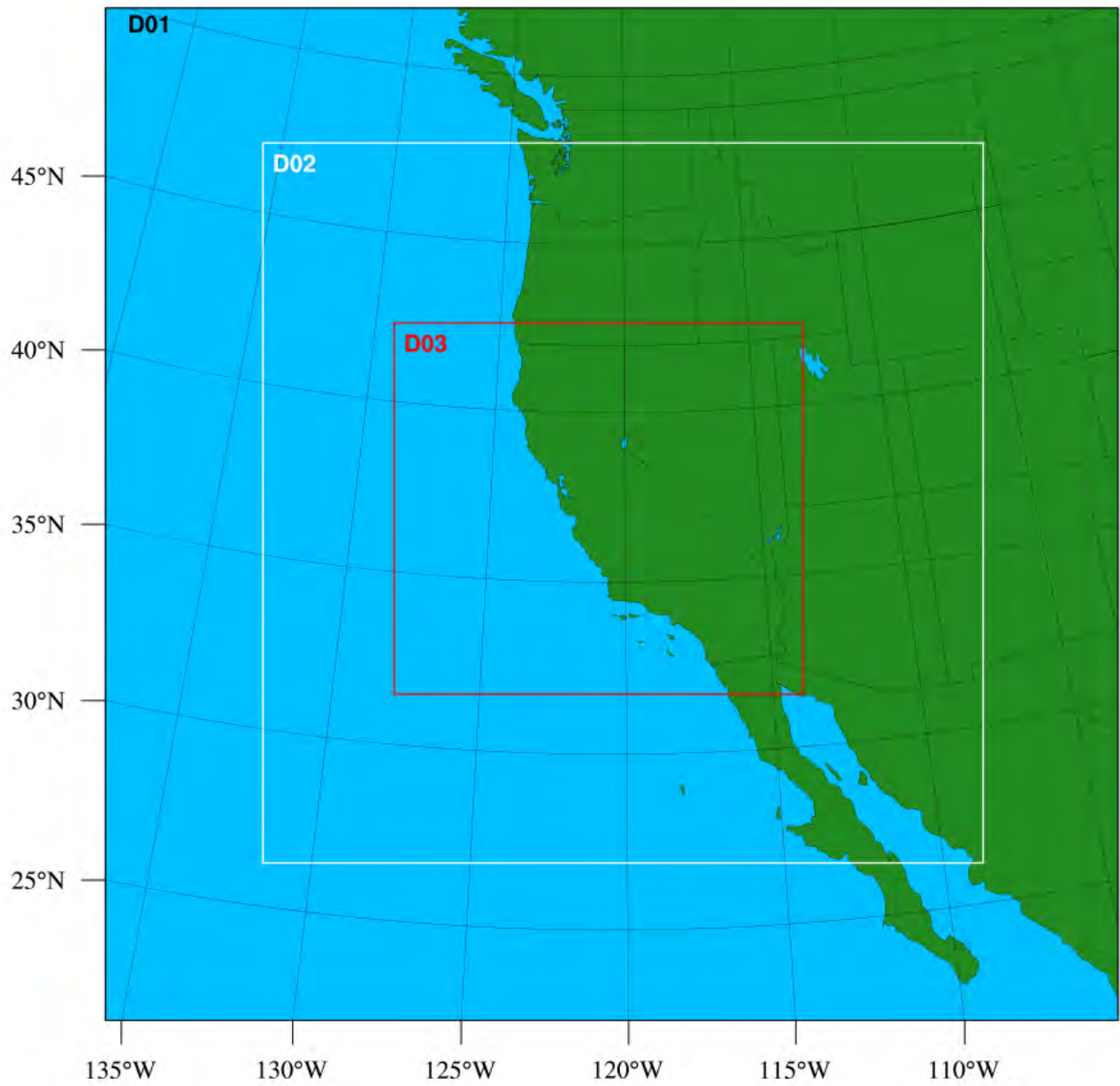


Figure 5-1. The three nested grids for the WRF model (D01 36km; D02 12km; and D03 4km).

Table 5-1. WRF vertical layer structure.

| Layer Number | Height (m) | Layer Thickness (m) | Layer Number | Height (m) | Layer Thickness (m) |
|---|---|---|---|---|---|
| | | | | | |
| 29 | 14890 | 1134 | | | |
| 28 | 13756 | 1081 | | | |
| | | | | | |
| 26 | 11643 | 996 | | | |
| 25 | 10647 | 970 | | | |
| 24 | 9677 | 959 | | | |
| 23 | 8719 | 961 | | | |
| | | | | | |
| 21 | 6779 | 993 | | | |
| 20 | 5786 | 967 | | | |
| 19 | 4819 | 815 | | | |
| 18 | 4004 | 685 | | | |
| | | | | | |
| 16 | 2744 | 482 | | | |
| 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

The U.S. EPA modeling 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.  In ARB's SIP modeling platform, the Community Multiscale Air Quality (CMAQ) Modeling System has been selected as the air quality model for use in attainment demonstrations of NAAQS for ozone and $PM_{2.5}$.

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 (SJVUAPCD, 2008), the 2012 SJV 24-hour $PM_{2.5}$ SIP (SJVUAPCD, 2012) and the 2013  SJV 1-hr ozone SIP (SJVUAPCD, 2013).  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; Smyth et al., 2006; Sokhi 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.

The version 5.0.2 of the CMAQ model released in May 2014, (http://www.airqualitymodeling.org/cmaqwiki/index.php?title=CMAQ_version_5.0.2_%28April_2014_release%29_Technical_Documentation), will be used in this SIP modeling platform. Compared to the previous version, CMAQv4.7.1, which was used for the 2012 SJV 24-hour $PM_{2.5}$ SIP (SJVUAPCD, 2012) and the 2013 SJV 1-hour ozone SIP (SJVUAPCD, 2013), 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_CMAQv5.0_-.C2.A0February_2012).

## 5.2.1 Photochemical Modeling Domain

Figure 5-2 shows the photochemical modeling domains used by ARB in this modeling platform. The larger domain (dashed black colored box), 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 4 km Northern (green box) and Southern (red box) modeling domains are nested within the outer 12 km domain and utilized 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.  A third 4 km resolution modeling domain (blue box) is nested within the Northern California domain and covers the SJV air basin.  This smaller SJV domain may be utilized for $PM_{2.5}$ modeling in the SJV if computational constraints (particularly for annual modeling) require the use of a smaller modeling domain.  In prior work, modeling results from the smaller SJV domain were compared to results from the larger Northern California domain and no appreciable differences were noted, provided that both simulations utilized chemical boundary conditions derived from the same statewide 12 km simulation.

For the coarse portions of nested regional grids, the U.S. EPA guidance (U.S. EPA, 2014) 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 recommendation.  The U.S. EPA guidance (U.S. EPA, 2014) 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 50-100 mb) are anywhere from 14 to 35 vertical layers.  In the ARB's current SIP modeling platform, 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.
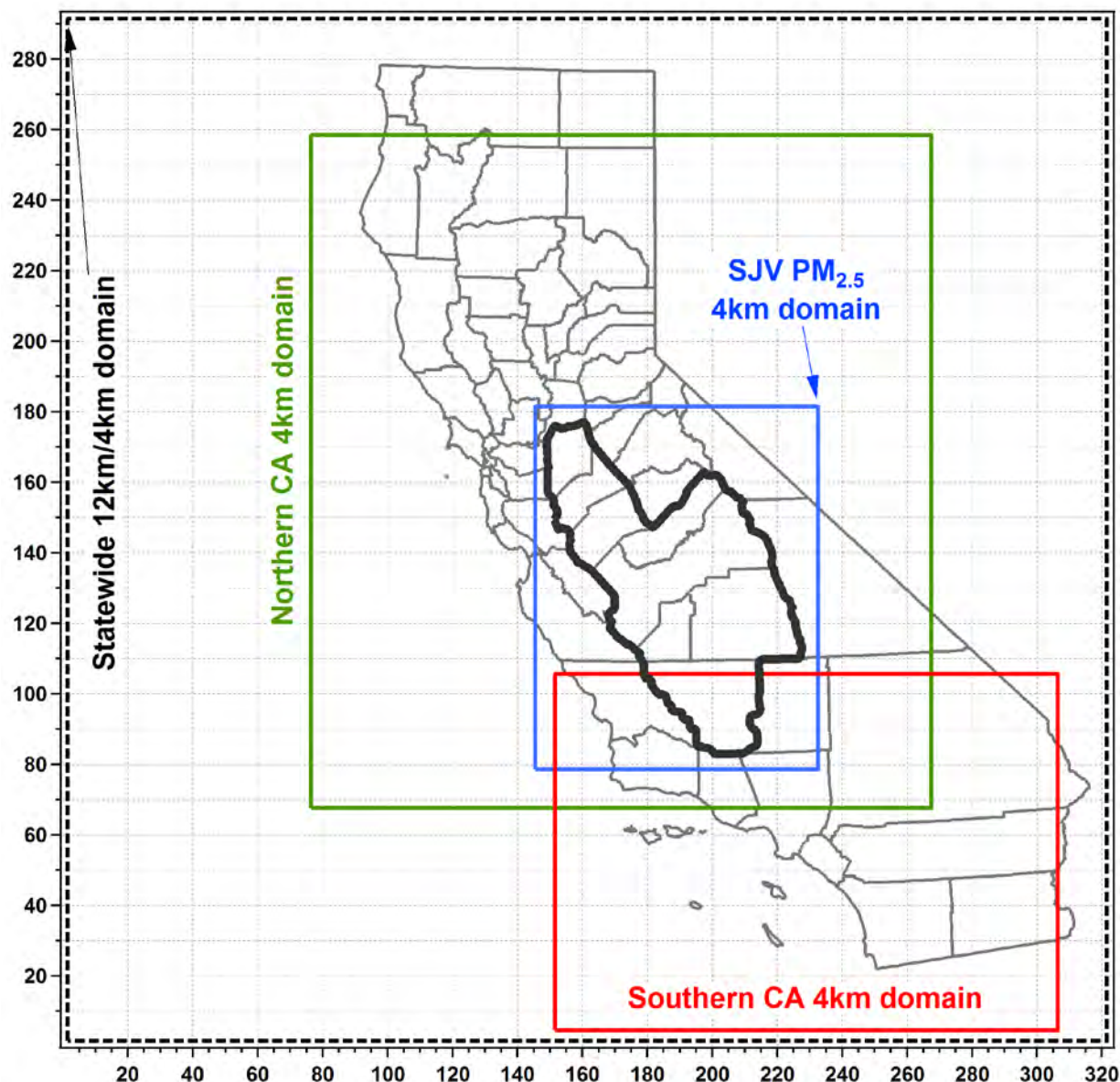
Figure 5-2. CMAQ modeling domains used in this SIP modeling platform. The outer domain (dashed black line) represents the extent of the California statewide domain (shown here with a 4 km horizontal resolution, but utilized in this modeling platform with a 12 km horizontal resolution). Nested higher resolution 4 km modeling domains are highlighted in green and red for Northern/Central California and Southern California, respectively. The smaller SJV PM$_{2.5}$ 4 km domain (colored in blue) is nested within the Northern California 4 km domain.

## 5.2.2 CMAQ Model Options

Table 5-3 shows the CMAQv5.0.2 configuration utilized in this modeling platform. The same configuration will be used in all simulations for both ozone and $PM_{2.5}$, and for all modeled years. The Intel FORTRAN compiler version 12 will be used to compile all source codes.

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 | SAPRC07 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 chemical mechanism will be utilized for all 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., 2014; 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 an 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 $NO_2$ + 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 Aerosol Module

The aerosol mechanism with extensions version 6 with aqueous-phase chemistry (AE6-AQ) will be utilized for all SIP modeling.  When coupled with the SAPRC07 chemical mechanism, AE6-AQ simulates the formation and evaporation of aerosol and the evolution of the aerosol size distribution (Foley et al., 2010).  AE6-AQ includes a comprehensive, yet computationally efficient, inorganic thermodynamic model ISORROPIA to simulate the physical state and chemical composition of inorganic atmospheric aerosols (Fountoukis and Nenes, 2007).  AE6-AQ also features the addition of new $PM_{2.5}$ species, an improved secondary organic aerosol (SOA) formation module, as well as new treatment of atmospheric processing of primary organic aerosol (Appel et al., 2013; Carlton et al., 2010; Simon and Bhave, 2011).  These updates to AE6-AQ in CMAQv5.0.2 continue to represent state-of-the-art treatment of aerosol processes in the atmosphere (Brown et al., 2011).

## 5.2.5 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 utilized in the ARB modeling system.

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 conducting annual or seasonal modeling, it is computationally more efficient to simulate each month in parallel rather than the entire year or 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; Lam and Fu, 2009; Lee et al., 2011; Lin et al., 2010), 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 ARB's SIP modeling system, the Model for Ozone And Related chemical Tracers (MOZART; Emmons et al., 2010) 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., 2010). 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).
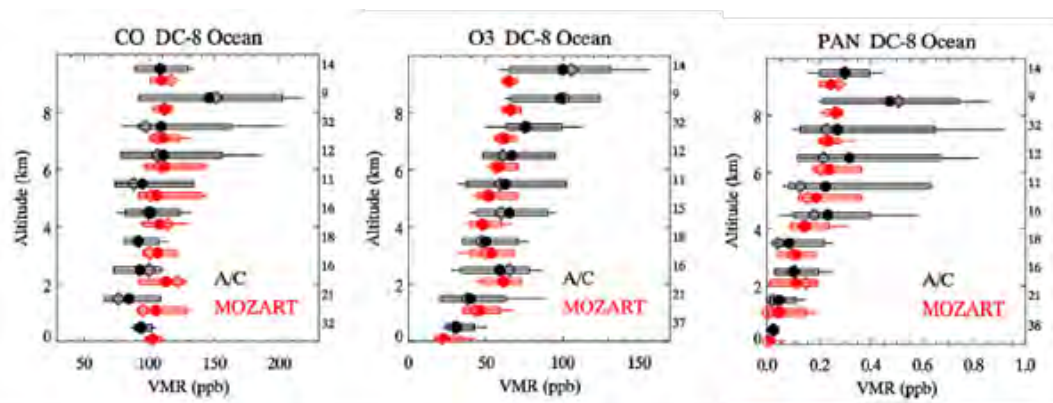


Figure 5-3. Comparison of MOZART (red) simulated CO (left), ozone (center), and PAN (right) to observations (black) along the DC-8 flight track.  Shown are mean (filled symbol), median (open symbols), 10th and 90th percentiles (bars) and extremes (lines). The number of data points per 1-km wide altitude 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 modeling platform are the MOZART4-GEOS5 simulations by Louisa Emmons (NCAR) for the years 2012 and 2013, 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. (2010), 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 California (e.g., Bao et al., 2008; Hu at al., 2010; Jackson et al., 2006; Jin et al., 2010a, 2010b; Livingstone et al., 2009; Michelson et al., 2010; Seaman, Stauffer, and Lario-Gibbs, 1995; Stauffer et al., 2000; Tanrikulu et al., 2000), 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 during the 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 will be processed, 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.  Additional statistical analysis may also be performed.

The mathematical expressions for these quantities are:

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

$$ME = \frac{1}{N}\sum_{1}^{N}\left|\text{Model - Obs}\right| \qquad (6\text{-}2)$$

$$NMB = \frac{\sum_{1}^{N}(\text{Model} - \text{Obs})}{\sum_{1}^{N}\text{Obs}} \times 100\%, \qquad (6\text{-}3)$$

$$RSME = \sqrt{\frac{\sum_{1}^{N}(\text{Model} - \text{Obs})^{2}}{N}} \qquad (6\text{-}4)$$

$$IOA = 1 - \frac{\sum_{1}^{N}(Model - Obs)^{2}}{\sum_{1}^{N}\left[(Model - Obs) + (Model + Obs)\right]^{2}}, \qquad (6\text{-}5)$$

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 air basin of interest, and summarized by subregion when there are distinct differences in the meteorology within the basin.  Statistics may be compared to other prognostic model applications in California 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 modeling.  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

Air quality observations are routinely made at state and local monitoring stations.  Gas species and PM species are measured on various time scales (e.g., hourly, daily, weekly).  The U.S. EPA guidance recommends model performance evaluations for the following gaseous pollutants: ozone ($O_3$), nitric acid ($HNO_3$), nitric oxide (NO), nitrogen dioxide ($NO_2$), peroxyacetyl nitrate (PAN), volatile organic compounds (VOCs), ammonia ($NH_3$), $NO_y$ (sum of $NO_x$ and other oxidized compounds), sulfur dioxide ($SO_2$), carbon monoxide (CO), and hydrogen peroxide (H2O2).  The U.S. EPA recognizes that not all of these species are routinely measured (U.S. EPA, 2014) and therefore may not be available for evaluating every model application.  Recognizing that $PM_{2.5}$ is a mixture, U.S. EPA recommends model performance evaluation for the following individual $PM_{2.5}$ species: sulfate ($SO_4^{2-}$), nitrate ($NO_3^-$), ammonium ($NH_4^+$), elemental carbon (EC), organic carbon (OC) or organic mass (OM), crustal, and sea salt constituent (U.S. EPA, 2014).

Table 7-1 lists the species for which routine measurements are generally available in 2012 and 2013.  When quality assured data are available and appropriate for use, model performance for each species will be evaluated.  Observational data will be

obtained from the Air Quality and Meteorological Information System (AQMIS), 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.

Table 7-1. Monitored species used in evaluating model performance.

| Species | Sampling frequency |
| --- | --- |
| $O_3$ | 1 hour |
| NO | 1 hour |
| $NO_2$ | 1 hour |
| $NO_x$ | 1 hour |
| CO | 1 hour |
| $SO_2$ | 1 hour |
| Selected VOCs from the PAMS measurement | 3 hours (not every day) |
| $PM_{2.5}$ measured using FRM[1] | 24 hours (daily to one in six days) |
| $PM_{2.5}$ measured using FEM | Continuously |
| $PM_{2.5}$ Speciation sites | 24 hours (not every day) |
| Sulfate ion | 24 hours (not every day) |
| Nitrate ion | 24 hours (not every day) |
| Ammonium ion | 24 hours (not every day) |
| Organic carbon | 24 hours (not every day) |
| Elemental carbon | 24 hours (not every day) |
| Sea salt constituents | 24 hours (not every day) |

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

These species cover the majority of pollutants of interest for evaluating model performance as recommended by the U.S. EPA.  Other species such as $H_2O_2$, $HNO_3$, $NH_3$, and PAN are not routinely measured.  During the DISCOVER-AQ field campaign, which took place in January and February 2013 in the SJV, aircraft sampling provided daytime measurements for a number of species (including $HNO_3$, $NH_3$, PAN, alkyl nitrates, and selected VOC species) that are not routinely measured. Modeled concentrations will be compared to aircraft measurements for these species, except for the gaseous $HNO_3$ measurements, which were contaminated by particulate nitrate (Dr. Chris Cappa, personal communication).

## 7.2  Statistical Evaluation

As recommended by U.S. EPA, a number of statistical metrics will be used to evaluate model performance for ozone, speciated and total $PM_{2.5}$, as well as other precursor species.  These metrics may 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), correlation coefficient ($R^2$), mean normalized bias (MNB), and mean normalized gross error (MNGE).  The formulae for estimating these metrics are given below.

$$MB = \frac{1}{N}\sum_{1}^{N}(Model - Obs) \tag{7-1}$$

$$ME = \frac{1}{N}\sum_{1}^{N}|Model - Obs| \tag{7-2}$$

$$MFB = \frac{2}{N}\sum_{1}^{N}\left(\frac{Model - Obs}{Model + Obs}\right)\times 100\%, \tag{7-3}$$

$$MFE = \frac{2}{N}\sum_{1}^{N}\left(\frac{|Model - Obs|}{Model + Obs}\right)\times 100\%, \tag{7-4}$$

$$NMB = \frac{\sum_{1}^{N}(Model - Obs)}{\sum_{1}^{N}Obs} \times 100\%, \qquad (7\text{-}5)$$

$$NME = \frac{\sum_{1}^{N}|Model - Obs|}{\sum_{1}^{N}Obs} \times 100\%, \qquad (7\text{-}6)$$

$$RSME = \sqrt{\frac{\sum_{1}^{N}(Model - Obs)^2}{N}} \qquad (7\text{-}7)$$

$$R^2 = \left(\frac{\sum_{1}^{N}((Model - \overline{Model}) \times (Obs - \overline{Obs}))}{\sqrt{\sum_{1}^{N}(Model - \overline{Model})^2 \sum_{1}^{N}(Obs - \overline{Obs})^2}}\right)^2 \qquad (7\text{-}8)$$

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

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

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

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

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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. For $PM_{2.5}$ the so called "bugle plots" of MFE and MFB from Boylan and Russell (2006) will also be generated. The plots described above 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 detailed view of model performance during different time periods, in different sub-regions, and over different concentrations and 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 those 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 the attainment demonstration.

## 7.4 Diagnostic Evaluation

Diagnostic evaluations are useful for investigating whether the physical and chemical processes that control ozone and $PM_{2.5}$ 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.

In addition to the above analysis, the 2013 DISCOVER-AQ field campaign in the SJV offers a unique dataset for additional diagnostic analysis that is not available in other areas, in particular, the use of indicator ratios in determining the sensitivity of secondary $PM_{2.5}$ to its limiting precursors. As an example, the ratio between free ammonia (total ammonia – 2 x sulfate) and total nitrate (gaseous + particulate) was proposed by Ansari and Pandis (1998) as an indicator of whether ammonium nitrate formation is limited by $NO_x$ or ammonia emissions. The DISCOVER-AQ dataset will be utilized to the extent possible to investigate $PM_{2.5}$ precursor sensitivity in the SJV as well as analysis of upper measurements and detailed ground level AMS measurements (Young et al., 2016).

# 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 most recent 8-hour ozone (2007), annual $PM_{2.5}$ (2008), and 24-hour $PM_{2.5}$ (2012) SIPs, the current guidance recommends utilizing modeling in a relative sense. A detailed description of how models are applied in the attainment demonstration for both ozone and $PM_{2.5}$, 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, 98th percentile of the 24-hour $PM_{2.5}$ concentration, or annual average $PM_{2.5}$ concentration, depending on the standard, observed at the monitor. For example, the 8-hr $O_3$ DV for 2012 is the average of the observed 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 that year (DV Year), and the yearly weighting of data for the weighted Design Value calculation (or $DV_R$). "obs" refers to the observed metric (8-hr $O_3$, 24-hour $PM_{2.5}$, or annual average $PM_{2.5}$).

| DV Year | Years Averaged for the Design Value ($4^{th}$ highest observed 8-hr $O_3$, $98^{th}$ percentile 24-hour $PM_{2.5}$, or annual average $PM_{2.5}$) | | | | |
|---|---|---|---|---|---|
| 2012 | 2010 | 2011 | 2012 | | |
| 2013 | | 2011 | 2012 | 2013 | |
| 2014 | | | 2012 | 2013 | 2014 |
| **Yearly Weightings for the Weighted Design Value Calculation** | | | | | |
| 2012-2014 Average | $DV_R = \dfrac{obs_{2010} + (2)obs_{2011} + (3)obs_{2012} + (2)obs_{2013} + obs_{2014}}{9}$ | | | | |

## 8.2  Base, Reference, and Future Year Simulations

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

1. *Base Year Simulation*
   The base year simulation for 2012 or 2013 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 in 2012.

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 2012 Chevron refinery fire.

3. *Future Year Simulation*
   The future year simulation is identical to the reference year simulation, except that the projected future year anthropogenic emission levels are used rather than the reference year 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 ozone or $PM_{2.5}$ between the model future year and model reference year are calculated for each monitor location. These ratios, called "relative response factors" or RRFs, are calculated based on the ratio of modeled future year ozone or $PM_{2.5}$ to the corresponding modeled reference year ozone or $PM_{2.5}$ (Equation 8-1).

$$\text{RRF} = \frac{\text{average } (O_3 \text{ or } PM_{2.5})_{\text{future}}}{\text{average } (O_3 \text{ or } PM_{2.5})_{\text{reference}}} \tag{8-1}$$

### 8.3.1 8-hour Ozone RRF

For 8-hour ozone, the modeled maximum daily average 8-hour (MDA8) ozone is used in calculating the RRF.  These MDA8 ozone values 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 reference? 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 in 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 (U.S. EPA, 2014) 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 ± 20% of the observed value at the monitor location.
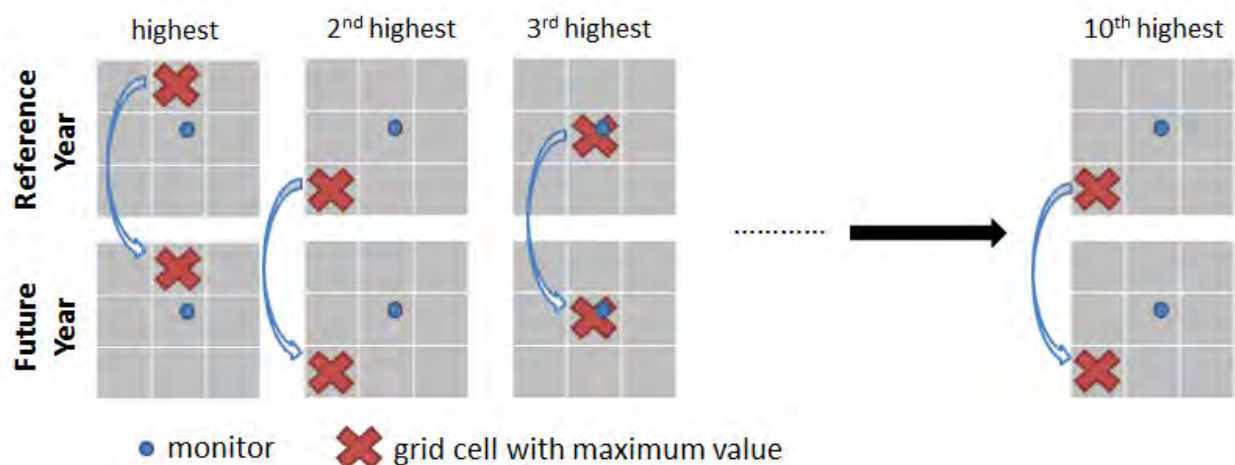


Figure 8-1. Example showing how the location of the MDA8 ozone for the top ten days in the reference and future years are chosen.

## 8.3.2 Annual and 24-hour PM$_{2.5}$ RRF

The U.S. EPA (2014) guidance requires RRFs for both the annual and 24-hour PM$_{2.5}$ attainment tests be calculated on a quarterly basis (January-March, April-June, July-September, and October-December) and for each PM$_{2.5}$ component (sulfate, nitrate, ammonium, organic carbon, elemental carbon, particle bound water, salt, and other primary inorganic components).

For annual PM$_{2.5}$, the quarterly RRFs are based on modeled quarterly mean concentrations for each component, where the concentrations are averaged over the 9 model grid cells within the 3x3 array of grid cells surrounding each monitor. For the 24-hour PM$_{2.5}$ attainment test, the quarterly RRFs are calculated based on the average for

each component over the top 10% of modeled days (or the top nine days per quarter) with the highest total 24-hour average $PM_{2.5}$ concentration. Peak $PM_{2.5}$ values are selected and averaged using the $PM_{2.5}$ concentration simulated at the single grid cell containing the monitoring site for calculating the 24-hour $PM_{2.5}$ RRF (as opposed to the 3x3 array average used in the annual $PM_{2.5}$ RRF calculation).

## 8.4 Future Year Design Value Calculation

### 8.4.1 8-hour Ozone

For 8-hour ozone, a future year DV at each monitor is calculated by multiplying the corresponding reference year DV by the site-specific RRF from Equation 8-1 (Equation 8-2).

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

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 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 8-hour ozone standard if the estimated future design value does not exceed the level of the standard.

### 8.4.2 Annual and 24-hour $PM_{2.5}$

#### 8.4.2.1 Sulfate, Adjusted Nitrate, Derived, Water, Inferred Carbonaceous Material Balance Approach (SANDWICH) and Potential Modifications

Federal Reference Method (FRM) $PM_{2.5}$ mass measurements provide the basis for the attainment/nonattainment designations. For this reason it is recommended that the FRM data be used to project future air quality and progress towards attainment. However, given the complex physicochemical nature of $PM_{2.5}$, it is necessary to consider individual $PM_{2.5}$ species as well. While the FRM measurements give the mass

of the bulk sample, a method for apportioning this bulk mass to individual $PM_{2.5}$ components is the first step towards determining the best emissions controls strategies to reach NAAQS levels in a timely manner.

The FRM measurement protocol finds its roots in the past epidemiological studies of health effects associated with $PM_{2.5}$ exposure. It is upon these studies that the NAAQS are based. The FRM protocol is sufficiently detailed so that results might be easily reproducible and involves the measurement of filter mass before and after sampling together with equilibrating at narrowly defined conditions. Filters are equilibrated for more than 24 hours at a standard relative humidity between 30 and 40% and temperature between 20 and 23 ºC. Due to the sampler construction and a lengthy filter equilibration period, FRM measurements are subjected to a number of known positive and negative artifacts. FRM measurements do not necessarily capture the $PM_{2.5}$ concentrations in the atmosphere and can differ substantially from what is measured by speciation monitors including the Speciation Trends Network (STN) monitors (see http://www.epa.gov/ttnamti1/specgen.html for more details). Nitrate and semi-volatile organic mass can be lost from the filter during the equilibration process, and particle bound water associated with hygroscopic species like sulfate provides a positive artifact. These differences present an area for careful consideration when one attempts to utilize speciated measurements to apportion the bulk FRM mass to individual species. Given that (1) attainment status is currently dependent upon FRM measurements and (2) concentrations of individual $PM_{2.5}$ species need to be considered in order to understand the nature of and efficient ways to ameliorate the $PM_{2.5}$ problem in a given region, a method has been developed to speciate bulk FRM $PM_{2.5}$ mass with known FRM limitations in mind. This method is referred to as the measured **S**ulfate, **A**djusted **N**itrate, **D**erived **W**ater, **I**nferred **C**arbonaceous material balance approach or "SANDWICH" (Frank, 2006). SANDWICH is based on speciated measurements from other (often co-located) samplers, such as those from STN, and the known sampling artifacts of the FRM. The approach strives to provide mass closure, reconciliation between speciated and bulk mass concentration measurements, and the basis for a connection between observations, modeled $PM_{2.5}$ concentrations, and the air quality standard (U.S. EPA, 2014).

The main steps in estimating the $PM_{2.5}$ composition are as follows:

### (1) Calculate the nitrate retained on the FRM filter using hourly relative humidity and temperature together with the STN nitrate measurements,

The FRM does not retain all of the semi-volatile $PM_{2.5}$ mass, and at warmer temperatures, loss of particulate nitrate from filters has been commonly observed (Chow et al., 2005). In order to estimate how much nitrate is retained on the FRM filter,

simple thermodynamic equilibrium relations may be used. Necessary inputs include 24-hour average nitrate measurements and hourly temperature and relative humidity data. Frank (2006) suggests the following methodology for estimating retained nitrate. For each hour $i$ of the day, calculate the dissociation constant, $K_i$ from ambient temperature and relative humidity (RH).

For RH < 61%:

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

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

For RH ≥ 61%, $K_i$ is replaced by:

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

where, $a_i$ is "fractional" relative humidity and

$$\ln(P_1) = -135.94 + 8763/T_i + 19.12 \times \ln(T_i),$$
$$\ln(P_2) = -122.65 + 9969/T_i + 16.22 \times \ln(T_i),$$
$$\ln(P_3) = -182.61 + 13875/T_i + 24.46 \times \ln(T_i).$$

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

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

where, $T_R$ is the daily average temperature for the sampled air volume in Kelvin, $K_i$ is the dissociation constant for $NH_4NO_3$ at ambient temperature for hour i, and $(\kappa - \gamma)$ relates to the temperature rise of the filter and vapor depletion from the inlet surface and is assumed to have a value equal to one (Hering and Cass, 1999).

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

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

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

**(4) Add 0.5 µg/m³ as blank mass, and**

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

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

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

After having calculated the species concentrations as outlined above, we will calculate the percentage contribution of each species to the measured FRM mass (minus the blank concentration of 0.5 µg/m³) for each quarter of the years represented by the speciated data. Note that blank mass is kept constant at 0.5 µg/m³ between the base and future years, and future year particle bound water needs to be calculated for the future year values of nitrate, ammonium, and sulfate.

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

Speciation data from available STN (speciation) sites will be used to speciate the FRM mass for all FRM sites.  For those sites not collocated with STN monitors, surrogate speciation sites will be determined based on proximity and evaluation of local emissions or based on similarity in speciation profiles if such data exists (e.g., such as the speciated data collected in the SJV during CRPAQS (Solomon and Magliano, 1998)).

### 8.4.2.3 Speciated Modeled Attainment Test (SMAT)

Following U.S. EPA modeling guidance (U.S. EPA, 2014), the model attainment test for the annual $PM_{2.5}$ standard will be performed with the following steps.

> Step 1: For each year used in the design value calculation, determine the observed quarterly mean $PM_{2.5}$ and quarterly mean composition for each monitor by multiplying the monitored quarterly mean concentration of FRM derived $PM_{2.5}$ by the fractional composition of $PM_{2.5}$ species for each quarter.

> Step 2: Calculate the component specific RRFs at each monitor for each quarter as described in section 8.3.2.

> Step 3: Apply the component specific RRFs to the quarterly mean concentrations from Step 1 to obtain projected quarterly species estimates.

> Step 4: Calculate future year annual average $PM_{2.5}$ estimates by summing the quarterly species estimates at each monitor and then compare to the annual $PM_{2.5}$ NAAQS. If the projected average annual arithmetic mean $PM_{2.5}$ concentration is ≤ the NAAQS, then the attainment test is passed.

For the 24-hour $PM_{2.5}$ standard, the attainment test is performed with the following steps (U.S. EPA, 2014):

> Step 1:  Determine the top eight days with the highest observed 24-hour $PM_{2.5}$ concentration (FRM sites) in each quarter and year used in the design value calculation (a total of 32 days per year), and calculate the 98th percentile value for each year.

Step 2: Calculate quarterly ambient species fractions on "high" $PM_{2.5}$ days for each of the major $PM_{2.5}$ component species (i.e., sulfate, nitrate, ammonium, elemental carbon, organic carbon, particle bound water, salt, and blank mass). The "high" days are represented by the top 10% of days in each quarter. Depending on the sampling frequency, the number of days captured in the top 10% would range from three to nine. The species fractions of $PM_{2.5}$ are calculated using the "SANDWICH" approach which was described previously. These quarter-specific fractions along with the FRM $PM_{2.5}$ concentrations are then used to calculate species concentrations for each of the 32 days per year determined in Step 1.

Step 3: Apply the component and quarter specific RRF, described in Section 8.3.2, to observed daily species concentrations from Step 2 to obtain future year concentrations of sulfate, nitrate, elemental carbon, organic carbon, salt, and other primary $PM_{2.5}$.

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

Step 5: Sum the concentration of each of the species components to calculate the total $PM_{2.5}$ concentration for each of the 32 days per year and at each site. Sort the 32 days for each site and year, and calculate the 98th percentile value corresponding to each year.

Step 6: Calculate the future design value at each site based on the 98th percentile concentrations calculated in Step 5 and following the standard protocol for calculating design values (see Table 8-1). Compare the future-year 24-hour design values to the NAAQS. If the projected design value is ≤ the NAAQS, then the attainment test is passed.

## 8.4.2.4 Sensitivity Analyses

Model sensitivity analysis may be conducted if the model attainment demonstration does not show attainment of the applicable standard with the baseline future inventory, or for determining precursor sensitivities and inter-pollutant equivalency ratios. For both ozone and $PM_{2.5}$, the sensitivity analysis will involve domain wide fractional reductions of the appropriate anthropogenic precursor emissions using the future year baseline emissions scenario as a starting point.  In the event that the model attainment demonstration does not show attainment for the applicable standard, it is important to know the precursor limitation to assess the level of emissions controls needed to attain the standard.

In order to identify what combinations of precursor emissions reductions is predicted to lead to attainment, a series of modeling sensitivity simulations with varying degrees of precursor reductions from anthropogenic sources are typically performed. These sensitivity simulations are identical to the baseline future year simulation discussed earlier except that domain-wide fractional reductions are applied to future year anthropogenic precursor emission levels and a new future year design value is calculated. The results of these sensitivity simulations are plotted on isopleth diagrams, which are also referred to as carrying capacity diagrams. The isopleths provide an estimate of the level of emissions needed to demonstrate attainment and thereby inform the development of a corresponding control strategy.

For ozone, this would likely entail reducing anthropogenic $NO_x$ and VOC emissions in 25% increments including cross sensitivities (e.g., 0.75 x $NO_x$ + 1.00 x VOC; 1.00 x $NO_x$ + 0.75 x VOC; 0.75 x $NO_x$ + 0.75 x VOC; 0.5 x $NO_x$ + 1.00 x VOC; ….).  Typically, a full set of sensitivities would include simulations for 25%, 50%, and 75% reduction in $NO_x$ and VOC, along with the cross sensitivities (for a total of 16 simulations including the future base simulation).  After design values are calculated for each new sensitivity simulation, an ozone isopleth (or carrying capacity diagram) as a function of $NO_x$ and VOC emissions is generated and used to estimate the additional $NO_x$ and VOC emission reductions needed to attain the standard. The approach for $PM_{2.5}$ is similar, except that additional precursor emissions must be considered.  Typically, the precursors considered for $PM_{2.5}$ would include anthropogenic $NO_x$, $SO_x$, VOCs, $NH_3$, as well as direct $PM_{2.5}$ emissions (Chen et al., 2014).  Cross sensitivities for generating $PM_{2.5}$ carrying capacity diagrams would be conducted with respect to $NO_x$, which would include the following precursor pairs: $NO_x$ vs. primary $PM_{2.5}$, $NO_x$ vs. VOC, $NO_x$ vs. $NH_3$, and $NO_x$ vs. $SO_x$.

In addition to the $PM_{2.5}$ carrying capacity simulations, precursor sensitivity modeling may be conducted for determining the significant precursors to $PM_{2.5}$ formation and for

developing inter-pollutant equivalency ratios.  These simulations would follow a similar approach to the carrying capacity simulations described above, but would involve only a single sensitivity simulation for each precursor, where emissions of that precursor are reduced between 30% and 70% from the future base year.  The "effectiveness" of reducing a given species can be quantified at each FRM monitor as the change in μg $PM_{2.5}$ (i.e., change in design value) per ton of precursor emissions (corresponding to the 15% change in emissions).  Equivalency ratios between $PM_{2.5}$ precursors (i.e., $NO_x$, $SO_x$, VOCs, and $NH_3$) and primary $PM_{2.5}$ will be determined by dividing primary $PM_{2.5}$ effectiveness by the precursors' effectiveness.


## 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 could exceed the NAAQS if a monitor was present at that location (U.S. EPA, 2014).  The U.S. EPA recommends combining spatially interpolated design value fields with modeled gradients for the pollutant of interest (e.g. Ozone and $PM_{2.5}$) and grid-specific RRFs in order to generate gridded future year gradient adjusted design values. The spatial Interpolation of the observed design values is done only within the geographic region constrained by the monitoring network, since extrapolating to outside of the monitoring network is inherently uncertain.   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 basic steps followed in the unmonitored area analysis for 8-hour ozone and annual/24-hour $PM_{2.5}$ are described below.

### 8.5.1 8-hour Ozone

In this section, the specific steps followed in 8-hr ozone unmonitored area analysis are described briefly:

Step 1: At each grid cell, the top-10 modeled maximum daily average 8-hour ozone mixing ratios from the reference year simulation will be averaged, and a gradient in this top-10 day average between each grid cell and grid cells which contain a monitor will be calculated.

Step 2: A single set of spatially interpolated 8-hr ozone DV fields will be generated based on the observed 5-year weighted base year 8-hr ozone DVs from the available monitors.  The interpolation is done 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 gradients between the grid cell and the corresponding monitor from Step 1.

Step 3: At each grid cell, the RRFs are calculated 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: The future year gridded 8-hr ozone DVs are calculated by multiplying the gradient-adjusted interpolated 8-hr ozone DVs from Step 2 with the gridded RRFs from Step 3

Step 5: The future-year gridded 8-hr ozone DVs (from Step 4) are examined to determine if there are any peak values higher than those at the monitors, which could potentially cause violations of the applicable 8-hr ozone NAAQS.

## 8.5.2 Annual PM$_{2.5}$

The unmonitored area analysis for the annual PM$_{2.5}$ standard will include the following steps:

Step 1: At each grid cell, the quarterly average PM$_{2.5}$ (total and by species) will be calculated from the reference year simulation, and a gradient in these quarterly averages between each grid cell and grid cells which contain a monitor will be calculated.

Step 2: Interpolated spatial fields, based on the observed PM$_{2.5}$ (FRM) and each component species of PM$_{2.5}$, will be generated for each quarter using normalized inverse distance squared weightings for all monitors within a grid cell's Voronoi Region. The ambient interpolated spatial fields are then adjusted based on the gradients in predicted quarterly mean concentrations from Step 1.

Step 3: The component specific RRFs are calculated at each grid cell for each quarter as described in section 8.3.2.

Step 4: The quarterly mean concentrations from Step 2 are then multiplied by the corresponding component specific RRF (from Step 3) to obtain the corresponding projected quarterly species estimates.

Step 5: The future year annual average $PM_{2.5}$ estimates are calculated by summing the quarterly species estimates at each grid cell and then compared to the annual $PM_{2.5}$ NAAQS to determine compliance.

### 8.5.3 24-hour $PM_{2.5}$

The unmonitored area analysis for the 24-hour $PM_{2.5}$ standard will include the following steps:

Step 1: At each grid cell, the quarterly average of the top 10% of the modeled days for 24-hour $PM_{2.5}$ (total and by species for the same top 10% of days) will be calculated from the reference year simulation, and a gradient in these quarterly averages between each grid cell and grid cells which contain a monitor will be calculated.

Step 2: The top 8 days with observed high $PM_{2.5}$ (FRM) are identified for each quarter and for each of the five years (a total of 32 days per year), used in the base year DV calculation. The speciated $PM_{2.5}$ (FRM) values are then interpolated for each of the "high" $PM_{2.5}$ days (identified above) using normalized inverse distance squared weightings for all monitors within a grid cell's Voronoi Region. These ambient interpolated spatial fields are then adjusted based on the appropriate gradients in predicted concentrations from Step 1.

Step 3: The component specific RRFs are calculated at each grid cell for each quarter as described in section 8.3.2.

Step 4: The observed daily species concentrations from Step 2 are multiplied by the component and quarter specific RRF (from Step 3) to estimate the future year concentration of each $PM_{2.5}$ species using the method outlined in section 8.4.2.3

Step 5: The concentration of each of the component $PM_{2.5}$ species is summed to calculate the total $PM_{2.5}$ concentration for each of the 32 days per year (8 days per quarter) and at each grid cell. For each year, the 98th percentile value is calculated by the sorting the 32 days for that particular year at each grid cell.

Step 6:  The future design value at each grid cell is calculated based on the 98$^{th}$ percentile concentrations calculated in Step 5 and following the standard protocol for calculating design values (see Table 8-1).  The future-year 24-hour design values are then compared to the 24-hour PM$_{2.5}$ NAAQS to determine compliance with that standard.

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

## 8.6  Banded Relative Response Factors for Ozone

The "Band-RRF" approach expands upon the standard "Single-RRF" approach for 8-hour ozone 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 2013 SJV 1-hour ozone SIP (SJVUAPCD, 2013).

# 9. PROCEDURAL REQUIREMENTS

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

The computational burden of modeling the entire state of California and its sub-regions requires a significant amount of computing power and large data storage requirements. For example, there are over half a million grid cells in total for each simulation based on the Northern CA domain (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 Design Values
- Access to input data and simulation results

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