Appendix E

Modeling Protocol

2013 Plan for the Revoked 1-Hour Ozone Standard
SJVUAPCD

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PHOTOCHEMICAL MODELING PROTOCOL

Photochemical Modeling for the 1-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

APCD – Air Pollution Control District

AQMD – Air Quality Management District

ARB – Air Resources Board

AUSPEX – Atmospheric Utility Signatures, Predictions and Experiments

BC – Boundary Conditions

BEIGIS – Geographic Information System based model for estimating BVOC emissions

BVOC – Biogenic Volatile Organic Compounds

CARB – California Air Resource Board

CBIV – Carbon Bond IV Chemical Mechanism

CCAQS – Central California Air Quality Studies

CCOS – Central California Ozone Study

CEFS – California Emission Forecasting System

CEIDARS – California Emission Inventory Development and Reporting System

CMAQ – Community Multiscale Air Quality model

CRPAQS – California Regional PM10/PM2.5 Air Quality Study

CO – Carbon Monoxide

DTIM – Direct Travel Impact Model

EIC – Emission Inventory Code

EMFAC – ARB's tool for estimating emissions from on-road vehicles

FDDA – Four Dimensional Data Assimilation

FORTRAN – The IBM Mathematical **For**mula **Tran**slating System

FR – Federal Register

GIS – Geographic Information System

IC – Initial Conditions

MEGAN – Model of Emissions of Gases and Aerosols from Nature

MM5 – Mesoscale Meteorological Model Version 5

MOZART – Model for Ozone and Related chemical Tracers

NAAQS – National Ambient Air Quality Standards

NAICS – North American Industry Classification System

NAMS – National Air Monitoring Station

NCAR – National Center for Atmospheric Research

NCEP – National Centers for Environmental Prediction

NO_x – Oxides of nitrogen

PAMS – Photochemical Assessment Monitoring Station

PM – Particulate Matter

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

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

ROG – Reactive Organic Gas

RSAC – Reactivity Scientific Advisory Committee

SAPRC – State-wide Air Pollution Research Center chemical mechanism

SARMAP – SJVAQS/AUSPEX Regional Modeling Adaptation Project

SFBA – San Francisco Bay Area

SJV – San Joaquin Valley

SJVAQS – San Joaquin Valley Air Quality Study

SIP – State Implementation Plan

SIP-GICG – The SIP Gridded Inventory Coordination Group

SLAM – State and Local Air Monitoring Stations

SCC – Source Classification Code

SIC – Standard Industrial Classification

SMOKE – Sparse Matrix Object Kernel Emission

SO_x – Oxides of Sulfur

SPM – Special Purpose Monitoring

TOG – Total Organic Gas

VMT – Vehicle Miles Traveled

VOC – Volatile Organic Compounds

U.S. EPA – United States Environmental Protection Agency

WRF – Weather and Research Forecasting Model

1 INTRODUCTION

1.1 Purpose

The previous 1-hour ozone State Implementation Plan (SIP) for the San Joaquin Valley (SJV) extreme ozone nonattainment area was submitted to the U.S. EPA effective May 17, 2004 (69 FR 20550) and was fully approved on March 8, 2010 (75 FR 10420). However, the U.S. Court of Appeals for the Ninth Circuit in Sierra Club *et. al* v. EPA, 671 F.3d 955 (9th Cir. 2012) remanded the 2010 approval. As a result, on November 9, 2012, U.S. EPA withdrew its March 8, 2010 approval of the San Joaquin Valley's 2004 1-Hour Ozone SIP (77 FR 58078). A new 1-hour SIP for the San Joaquin Valley extreme ozone nonattainment area is now due. The air quality modeling protocol that is presented in this document will form the basis for developing a new 1-hour ozone SIP for the SJV. This document describes the input data, technical decisions, and procedures that will be used for computer-based simulations of 1-hour ozone concentrations. It also describes how model results will be evaluated with field measurements and how future year air quality will be simulated.

1.2 Approach

The modeling approach draws heavily on the products of large-scale, scientific studies in the region, collaboration among technical staff of State and local regulatory agencies, as well as from participation in technical and policy groups within the region. It is also consistent with the modeling approach used for the 2012 24-hour $PM_{2.5}$ SIP that was submitted to the U.S. EPA in early 2013.

1.3 History of Field Studies in the Region

The San Joaquin Valley (SJV) airshed is perhaps the second most studied airshed in the world, in terms of the number of publications in peer-reviewed international scientific/technical journals and other major reports. The Los Angeles airshed is the first. Major field studies that have taken place in the SJV and surrounding areas are listed in Table 2-1. A comprehensive listing of publications (reports and peer-reviewed

journal articles) up to 2005, compiled by Professor John Watson of the Desert Research Institute, can be found at http://www.arb.ca.gov/airways/crpaqs/publications.htm.

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

While CCOS is still very relevant to the current 1-hour O_3 SIP, there are two subsequent studies that are noteworthy for several different reasons. Either of these studies would not form the technical basis for a future SIP itself, but they contributed significantly to our understanding of various atmospheric processes.

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

- How good is our current understanding of the HO_x-NO_x-O_3-aerosol photochemical system over the Los Angeles Basin as represented in air quality models?
- How should upwind boundary conditions for simulating air quality in California be specified?
- How do ship emissions and long-range transport affect the sulfur budget in southern California?
- What are the state's emissions of VOCs and greenhouse gases from urban and industrial activities, agricultural operations, and wildfires?

The analyses of ARCTAS-CARB data are still in progress, but some of the findings could be applicable to the current 1-hour O_3 SIP (Kaduwela and Cai, 2009; Huang et al., 2010; Singh et al., 2010; Pfister et al., 2011a,b; Huang et al., 2011; D'Allura et al., 2011; Singh et al., 2012; Ren et al., 2012; Huang et al., 2013). Note, however, that the ARCTAS-CARB field work was conducted during June-July, 2008 but the high 1-hour O_3 concentrations in SJV occur during late summer months.

The ARCTAS-CARB campaign was considered to be the pilot phase for a more comprehensive multi-platform study known as CalNex 2010 (Research at the Nexus of Air Quality and Climate Change conducted in 2010)(www.esrl.noaa.gov/csd/calnex/). This campaign was coordinated by NOAA and CARB together with researchers from several universities and national laboratories. It involved several instrumented aircraft, an instrumented ship, two surface supersites (one in Bakersfield and another in Pasadena), and networks of meteorological and ozonesonde measurements. It was designed to answer a much broader set of questions than ARCTAS-CARB did, however the data analysis phase is still in progress and only preliminary air quality modeling has been conducted to date (Cai and Kaduwela, 2011; Kelly et al., 2011; Angevine et al., 2012).

Table 1.1: Major Field Studies in Central California and surrounding areas.

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

Year	Study	Significance
1999-February 2001	Quality Study (CRPAQS) and Central California Ozone Study (CCOS)	both O_3 and $PM_{2.5}$
December 1999 to present:	Fresno Supersite	First multi-year experiment with advanced monitoring technology
July 2003	NASA high-resolution lidar flights	First high-resolution airborne lidar application in SJV in the summer
February 2007	U.S. EPA Advanced Monitoring Initiative	First high-resolution airborne lidar application in SJV in the winter
June 2008	ARCTAS - CARB	First measurement of high-time resolution (1-10s) measurements of organics and free radicals in SJV.
May-July 2010	CalNex 2010 (Research at the Nexus of Air Quality and Climate Change)	Expansion of ARCTAS-CARB type research-grade measurements to multi-platform and expanded geographical area including the ocean.
January-February 2013	DISCOVER-AQ (Deriving Information on Surface Conditions from COlumn and VERtically Resolved Observations Relevant to Air Quality)	The overarching objective of the DISCOVER-AQ investigation is to improve the interpretation of satellite observations to diagnose near-surface conditions relating to air quality.

1.4 Background

The shaded relief maps provided at the end of this section illustrate the topography of California as well as the Air Basin and County political boundaries (Figure 1.1) and Air District and County boundaries (Figure 1.2).

Generally, the weather conditions that lead to high ozone levels in the San Joaquin Valley include large-scale high-pressure systems that develop over the Western United States, low wind speeds, and high temperatures. These conditions occur frequently in the San Joaquin Valley between May and September and may persist for several days.

The complex airflow within the region contributes to various types of ozone episodes in the San Joaquin Valley, the Sacramento Valley, the Mountain Counties, and the San Francisco Bay Area. Ozone and its precursors are distributed throughout the mixed layer by turbulent diffusion. When meteorological conditions are favorable, daytime sea breezes are funneled through the Carquinez Strait and nearby mountain passes, bringing ozone and precursors into the northern part of the San Joaquin Valley. Some inflow is also observed through the Pacheco Pass on the west side of the Valley.

Depending upon the nature of the airflow in the region, ozone episodes in the San Joaquin Valley or Sacramento region can be generated predominantly from locally derived pollutants or by pollutants transported from upwind regions. In the San Francisco Bay Area (SFBA), ozone concentrations are elevated when airflow from the Bay Area to the Central Valley is limited. Elevated ozone concentrations are observed in the Mountain Counties mostly due to transported pollutants. The conditions that promote the formation of a nocturnal jet within the Valley may limit ventilation of the Valley. During the day, pollutants may be transported from the San Joaquin Valley to the Mojave Desert via the Tehachapi Pass. Outflow from the San Joaquin Valley to the coast in the vicinity of San Luis Obispo area has also been observed.

Except for the warmest days, an inversion is almost always present within the Central Valley throughout the year. This inversion tends to trap pollutants either emitted within the Valley or transported into the Valley from surrounding regions. In this regime, mesoscale flow patterns such as sea breeze intrusion, local eddies, bifurcation and convergence, and mountain/valley flows are especially important in determining the distribution of pollutants throughout the region. These mesoscale characteristics are described in more detail below, and provide a reference for features to consider during qualitatively assessing meteorological model performance, which is discussed further in Chapter 7:

Sea Breeze and Marine Air Intrusion: Differential heating between the land and ocean causes a pressure gradient between the cooler, denser air over the ocean and the warmer air over the land. The resulting pressure gradient draws marine air into the Valley during the day. Typically, with calm coastal winds during mornings, rush hour

pollutants can accumulate in the coastal source region. As the sea breeze develops by mid-day, ozone and its precursors can enter the Valley, encountering warmer temperatures and higher insolation.

Nocturnal jet and eddies: A low-level nocturnal wind maximum can develop during evening hours. As surface temperatures cool overnight, a strong stable layer within the Central Valley can result. As this stable layer forms, the wind aloft may be decoupled from the surface and accelerate. The result is an overnight wind flow that may carry pollutants from one end of the Valley to the other. While this nocturnal jet may be present in other seasons, it has been observed during the ozone season (Smith et al. 1981; Blumenthal, 1985; Thuillier et al. 1994). It is believed to be a pollutant transport mechanism during the summer months. The rangers of high mountains in the southern Valley force the air to turn north along the Sierra foothills at the southeastern edge of the Valley. Smith et al. (1981) mapped the northerly flow, sometimes called the Fresno eddy, with pibals and described an unusual case where it extended as far north as Modesto. During the Southern San Joaquin Ozone Study, Blumenthal et al. (1985) measured the Fresno eddy extending above 900 meters above ground level about 50% of the time. Neff et al. (1991) measured the eddy using radar wind profilers during the SJVAQS/AUSPEX study.

Bifurcation and Convergence Zones: Marine air entering the Sacramento River Delta region from the west may diverge. It may flow into the San Joaquin Valley to the south and Sacramento Valley to the north. The position of this bifurcation zone may shift and can determine the relative proportion of Bay Area pollutants transported to each downwind basin. The dynamics of this bifurcation zone are currently not well understood. However, this zone may also prevent transport between air basins by functioning as a block to air moving north to south within the Delta. For example, the effect of convergence zones on air quality is provided by Blumenthal et al. (1985), where it is hypothesized that the increase in mixing heights (~200 m higher than in the northern SJV) at the southern end of the San Joaquin Valley was due to damming of the northerly flow against the Tehachapi Mountains at the southern end. Without this

damming effect, the mixing levels over Bakersfield, Arvin, and Edison would be lower, with correspondingly higher ozone concentrations.

Up-slope and Down-slope Flows: The increased daytime heating in mountain canyons and valleys adjacent to the Central Valley causes significant upslope flows during the afternoons in the San Joaquin and Sacramento Valleys. This can act as a removal mechanism, and can lift mixing heights on the edges of the valleys, relative to the mixing heights at valley center. During the nighttime, mountain valleys and canyons may cool relative to the Valley floor, resulting in a reversal of the flow. Myrup et al. (1989) studied transport of aerosols from the San Joaquin Valley into Sequoia National Park. They found a net up-slope flow of most pollutant species. The return flow can bring pollutants back down. Smith et al. (1981) used tracer data to estimate pollutant budgets due to slope flow fluxes (and other ventilation mechanisms). Smith et al. suggested that polluted air at higher elevations is diluted, thus down-slope flows may result in lower pollution levels within the San Joaquin Valley.

Up-Valley and Down-Valley Flows: Up-valley and down-valley flows are similar to up-slope and down-slope flows, but take place along the valley on a larger scale. During the summer, the Sacramento River Delta tends to have cooler air temperatures during the day and warmer temperatures at night than at the extreme ends of the Central Valley due to higher humidity within the Delta. During the daylight hours, up-valley flow draws air south into the San Joaquin Valley and north into the Sacramento Valley. At night, down-valley drainage winds tend to ventilate both valleys. Hayes et al. (1984) described both regimes for the Central Valley.

Figure 1.1: California Air Basins and Counties.

Figure 1.2: California Air Districts and Counties.

2 SELECTION OF THE MODELING PERIODS

From an air quality perspective, ARB and the District have selected 2007 baseline design values for the modeled attainment test. These baseline concentrations values will serve as the anchor point for estimating future year projected concentrations. The modeling period is from May 2007 to September 2007. Table 2.1 shows the 2007 ozone design values for the San Joaquin Valley.

Table 2.1: The 2007 Ozone Design Values for the San Joaquin Valley

Site	2007 1-Hour Ozone Design Values (ppb)
Arvin-Bear Mountain Blvd	131
Bakersfield- 5558 California Avenue	117
Bakersfield- Golden State Highway	108
Edison	135
Maricopa-Stanislaus Street	100
Oildale-3311 Manor Street	112
Shafter-Walker Street	105
Clovis-N Villa Avenue	125
Hanford-S Irwin Street	110
Sequoia and Kings Canyon Natl Park	119
Sequoia Natl Park- Lower Kaweah	113
Visalia-N Church Street	112
Fresno-1st Street	130
Fresno-Drummond Street	110
Fresno-Sierra Skypark #2	124
Parlier	121
Madera-Pump Yard	95
Merced-S Coffee Avenue	102
Modesto-14th Street	109
Turlock-S Minaret Street	104

2.1 Available Observational Data

Model performance will be based on comparing model predictions with observational data collected from routine field measurements. The data networks for the routine collected data are described below.

2.2 Routinely Collected Data

Routine meteorological and air quality data are collected through different network systems, including (1) the State and Local Air Monitoring Stations (SLAMS) network, (2) the National Air Monitoring Station (NAMS) network, (3) the Photochemical Assessment Monitoring Station (PAMS) network and (4) Special Purpose Monitoring (SPM) that is performed at some sites. More detailed information on routinely available data can be obtained from the California Air Resources Board web site at: http://www.arb.ca.gov/html/ds.htm

The existing routine ozone and nitrogen oxides monitoring sites are shown in Figure 2.1.

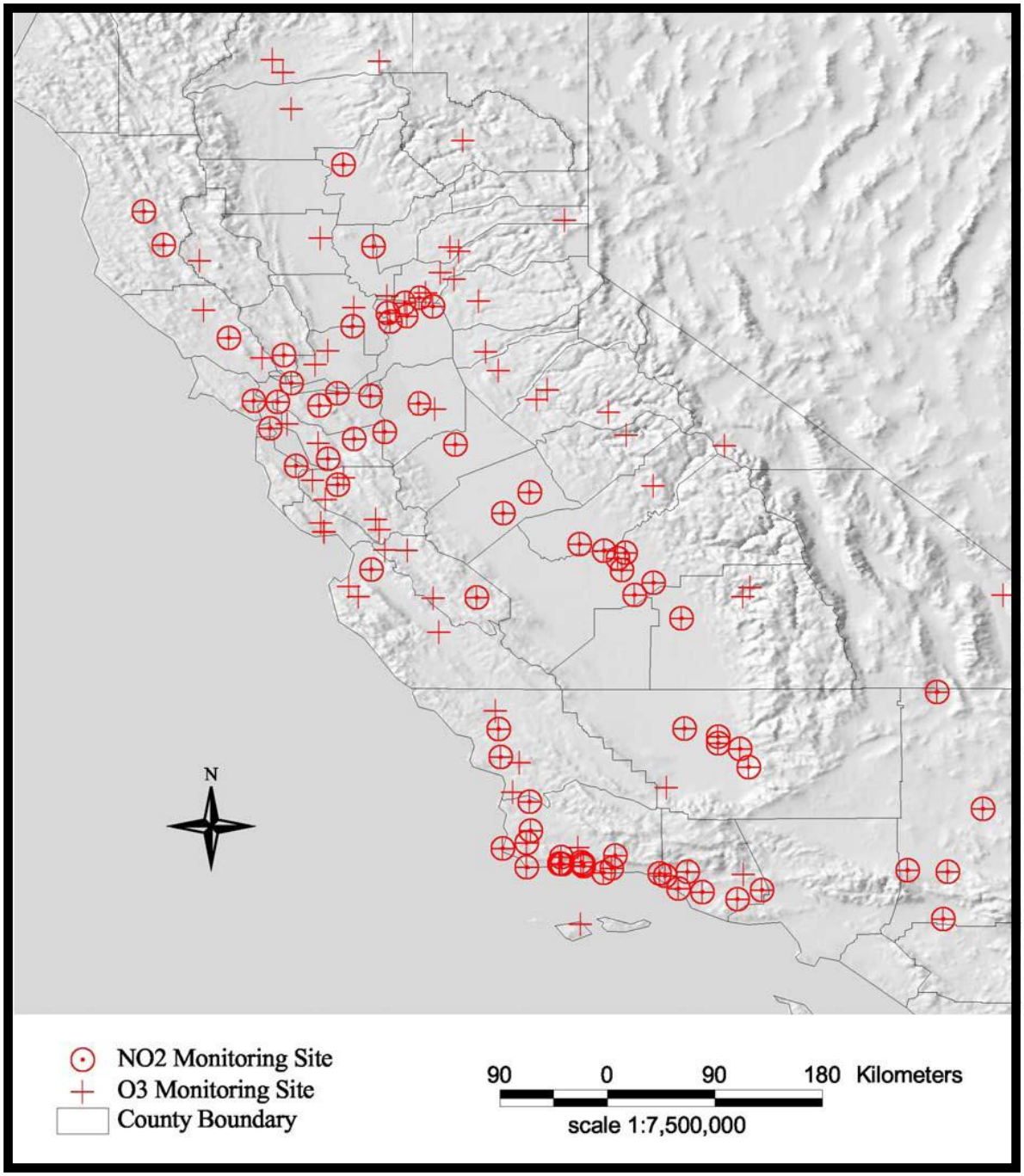


Figure 2.1: Existing routine ozone and nitrogen oxides monitoring sites

3 MODEL SELECTION

This chapter describes the selection of the meteorological and air quality models used for this effort.

3.1 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, etc. 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, the models under consideration for meteorological modeling are:

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

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

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

Since then NCAR has devoted its resources to the development of the WRF model, which was designed to be the replacement for MM5. The WRF model is being continually updated, and WRF fields produced by ARB have shown comparable results with MM5. Therefore, the WRF numerical model was chosen to generate meteorological fields for this SIP. For a more detailed description of prognostic meteorological models and their known limitations in the complex terrain of California, see Section 7.1.

3.2 Photochemical Model

U.S. EPA guidance requires several factors to be considered as criteria for choosing a qualifying air quality model to support the attainment demonstration. These criteria include: (1) documentation and proven track record of candidate models in similar applications; (2) advanced science and technical features available in the model and/or modeling system; (3) experience of staff and available contractors; (4) required time and resources versus available time and resources; and (5) in the case of regional applications, consistency with regional models applied in adjacent regions (U.S. EPA, 2007).

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 understanding of the atmospheric chemistry and physics. It is a three-dimensional Eulerian modeling system that simulates ozone, particulate matter, toxic air pollutants, visibility, and acidic pollutant species throughout the troposphere (UNC, 2010). The CMAQ model has undergone peer review every few years and was found to be state of the science (Aiyyer et al.,

2007). The CMAQ model is regularly updated to incorporate new mechanisms, algorithms, and data as they become available in the scientific literature (e.g., Foley, et al., 2010). In addition, the CMAQ model is well documented in terms of its underlying scientific algorithms as well as guidance on operational uses (e.g., Binkowski and Roselle, 2003; Byun and Ching, 1999; Byun and Schere, 2006; Carlton et al., 2010; Foley et al., 2010; Kelly, et al., 2010a; UNC, 2010).

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

CMAQv4.7.1 (Foley et al., 2010) will be used. While U.S. EPA released CMAQ version 5.0 in October 2011 and v5.0.1 in July 2012, the stable production version at ARB is v4.7.1. ARB is currently testing the v5.0.1 with the research-grade data obtained during two recent field studies: The California portion of the Arctic Research of the Composition of the Troposphere from Aircraft and Satellites (ARCTAS) and California Research at the Nexus of Air Quality and Climate Change (CalNex). ARB intends to use v5.01.1 with SAPRC07 chemistry for the next 8-hour ozone SIP.

4 MODELING DOMAIN AND GRID STRUCTURE

4.1 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 4.1). The purpose of the coarse, 36 km grid (D01) is to provide synoptic-scale conditions to all three grids; while the purpose of the 12 km grid (D02) is to provide input data to the 4 km grid (D03). The D01 grid is centered at 37 N x 120.5 W while the two inner grids, D02 and D03, are placed within the coarser grid such that they are not too close to the lateral boundaries. The D01 grid consists of 70 x 70 grid cells. The D02 grid consists of 132 x 132 grid cells and the D03 grid consists of 327 x 297 grid cells having an origin at -696 km x -576 km (Lambert Conformal projection). All three grids were run simultaneously, and the D03 grid is intended to resolve the fine details of atmospheric motion. Both D02 and D03 grids are used to feed the air quality modeling simulations. The vertical layer structure has 30 layers, as shown in Table 4.1.

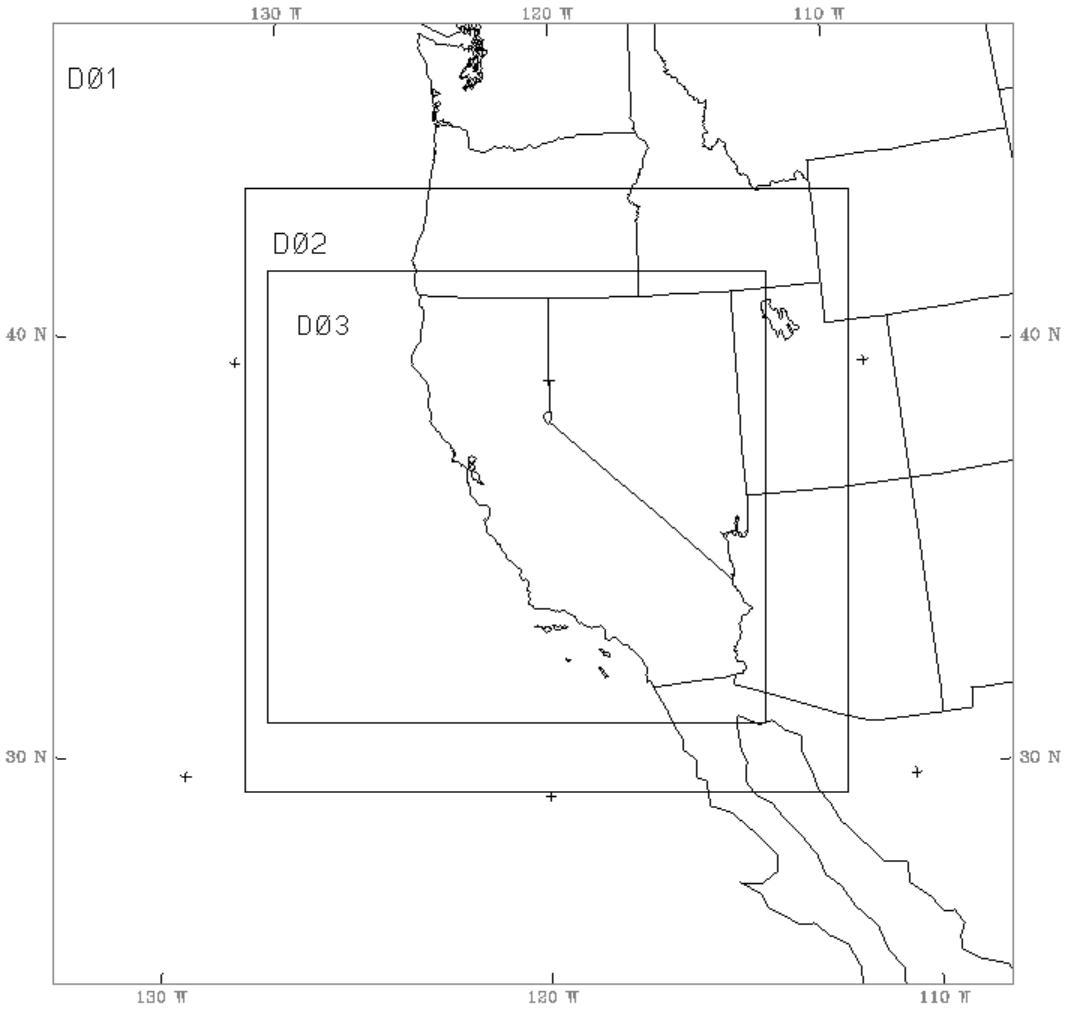


Figure 4.1: The three nested grids for the WRF model (D01 36km; D02 12km; and D03 4km).

Table 4.1: WRF 30 Vertical Layer Configuration for the modeling period.

Layer No.	Height (m)	Layer Thickness (m)
30	15674	998
29	14676	982
28	13694	976

27	12718	970
26	11748	972
25	10776	973
24	9803	979
23	8824	983
22	7841	994
21	6847	1002
20	5845	972
19	4873	818
18	4055	687
17	3368	577
16	2791	484
15	2307	407
14	1900	339
13	1561	285
12	1276	238
11	1038	199
10	839	166
9	673	139
8	534	115
7	419	97
6	322	81
5	241	67
4	174	56
3	118	47
2	71	39
1	32	32
0	0	0

4.2 Photochemical Modeling Domain

Figure 4.2 shows the modeling domains used by ARB. The two modeling domains that are proposed for this work are shown in blue (12 km coarse domain) and magenta (4 km nested domain). The coarse domain (blue) includes 107x97 lateral 12 km grid cells for each vertical layer. This domain extends from the Pacific Ocean in the west to the Eastern Nevada in the east and runs from the U.S.-Mexico border in the south to the California-Oregon border in the north. The nested domain (magenta) covers Central California with 192x192 lateral 4 km grid cells. The domain is based on 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, respectively.

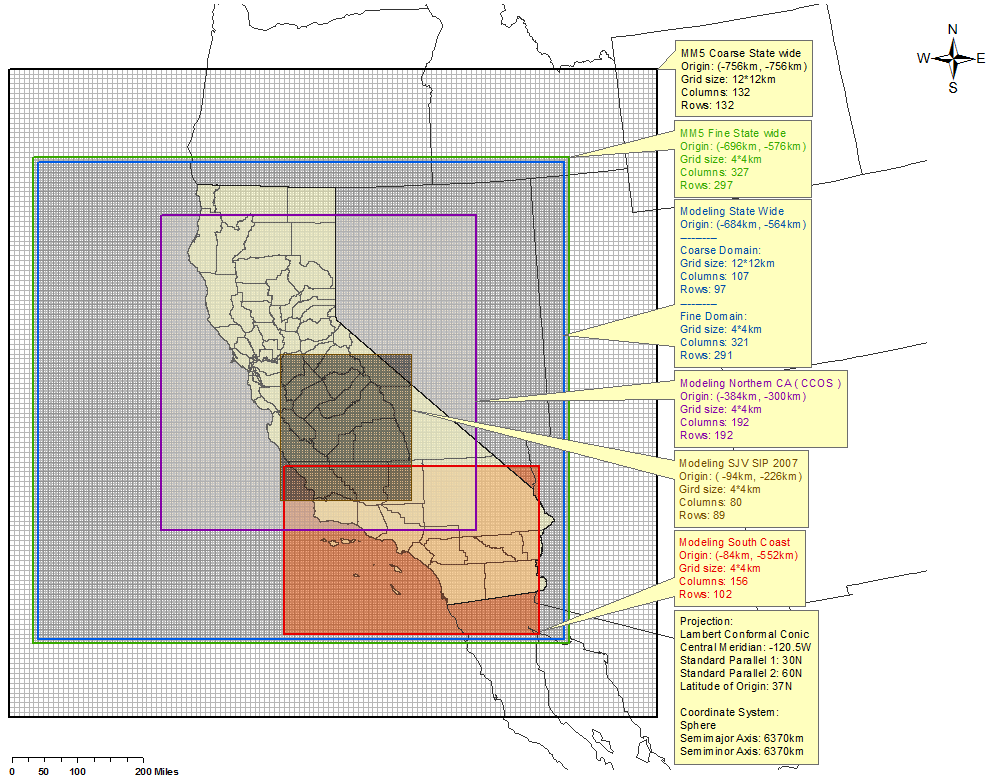


Figure 4.2: Modeling domains used by ARB

Table 4.2: Vertical Layer Heights (m) of Photochemical Modeling.

Layer No.	30 -Layer WRF configuration Height (m)
15	15674
14	12718
13	7841
12	3368
11	1900
10	839
9	673
8	534
7	419
6	322
5	241
4	174
3	118
2	71
1	32

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

although typical applications of "one- atmosphere" models (with the model top at 100 mb) employ 12 to 21 vertical layers. For the present SIP, 15 vertical layers will be used in the CMAQ model, extending from the surface to 100 mb. The vertical structure is based on the sigma-pressure coordinate, with the layers separated at 1.0, 0.9958, 0.9907, 0.9846, 0.9774, 0.9688, 0.9585, 0.9463, 0.9319, 0.9148, 0.8946, 0.7733, 0.6254, 0.293, 0.0788, and 0.0. This ensures that the majority of the layers are in the planetary boundary layer. The vertical layer structure in meters is shown in Table 4.2.

5 MODEL INITIALIZATION AND BOUNDARY CONDITIONS

Regional meteorological and air quality models must be initialized so that the chemical and physical conditions at the start of a model simulation approximate ambient conditions. This chapter is divided into two sub-sections that cover the initialization of the meteorological model (WRF) and the air quality model (CMAQ) separately. Each section briefly covers the data upon which model initialization is based.

5.1 Initialization of the Meteorological Model

WRF is a complex numerical model that requires setting a large number of input parameters and model options. Some of these requirements include: the specification of initial and boundary conditions (IC/BCs); gathering and processing representative data to be used for initial/boundary conditions as well as Four Dimensional Data Assimilation (FDDA); and the selection of a variety of algorithms to calculate meteorological parameters, such as winds, temperature, humidity, pressure, soil temperature, the depth of the planetary boundary layer, cloud microphysics, and radiative transfer.

There is no prior guidance on the specific data or options to be used in WRF. Rather, these decisions are determined based on optimizing model performance. Thus, during the preparation of preliminary meteorological fields for the modeling period, vast amounts of data were processed and many combinations of model options were tested. Based on the best model performance for these preliminary tests, the most successful

WRF model options and input datasets were determined. These are described in the following sections.

5.1.1 WRF Model Options

As indicated above, many sensitivity studies were conducted to choose a set of model options that result in scientifically reasonable meteorological fields that are representative of the specific conditions experienced during the modeling period. The physics options are shown in Table 5.1.

Table 5.1: WRF Physics Options.

Physics Option	D01	D02	D03
Microphysics	WSM 6-class graupel scheme	WSM 6-class graupel scheme	WSM 6-class graupel scheme
Surface Layer	MM5 Monin-Obukhov scheme	MM5 Monin-Obukhov scheme	MM5 Monin-Obukhov scheme
Land Surface Model	Unified Noah land-surface model	Unified Noah land-surface model	Unified Noah land-surface model
Planetary Boundary Layer Scheme	YSU scheme	YSU scheme	YSU scheme
Cumulus	Kain-Fritsch (new Eta) scheme	Kain-Fritsch (new Eta) scheme	None
Longwave Radiation Scheme	RRTM	RRTM	RRTM
Shortwave Radiation Scheme	Dudhia scheme	Dudhia scheme	Dudhia scheme
Number of Soil Layers	thermal diffusion scheme for temp only	thermal diffusion scheme for temp only	thermal diffusion scheme for temp only

5.1.2 WRF Initial and Boundary Conditions (IC/BC)

The initial and boundary conditions (IC/BCs) for WRF were prepared based on NCEP Eta 212 grid (40km) model output that is archived at NCAR. These data are archived

from global simulations and have a 40 km horizontal resolution. Initial conditions to WRF were updated at 6-hour intervals for the 36 and 12 km grids. In addition, surface and upper air synoptic observations obtained from NCEP are also used to further refine the IC/BCs.

5.1.3 WRF Four Dimensional Data Assimilation

The WRF model was nudged toward observed meteorological conditions by using the analysis nudging option of the Four Dimensional Data Assimilation (FDDA) for the 36km grid only.

5.1.4 Meteorological Data Quality Assurance

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

5.2 Initialization of the Air Quality Model

5.2.1 CMAQ Model Options

Table 5.2 shows the CMAQ v4.7.1 configuration that will be used to model ozone in the SJV. The same configuration will be used for all simulations for the base, reference, and future years. CMAQv4.7.1 will be compiled using the Portland Group FORTRAN Compiler version 10.9.

Table 5.2: CMAQ v4.7.1 Schemes used for Current Simulations.

Processes	**Scheme**
Horizontal advection	PPM (piecewise parabolic method)
Vertical advection	PPM (piecewise parabolic method)
Horizontal diffusion	Multi-scale
Vertical diffusion	Eddy
Gas-phase chemical mechanism	SAPRC99
Chemical solver	EBI
Aerosol module	Aero5
Cloud module	ACM_AE5
Photolysis rate	Table Generated by the JPROC

5.2.2 Photochemical Mechanism

Historically, over the last several decades, air quality modeling for ozone SIPs throughout California have predominately been conducted using the Carbon Bond IV (CBIV) chemical mechanism. The CBIV mechanism uses 36 chemical species and 89 chemical reactions (may vary somewhat among different air quality models) to describe the relationship between ozone and ozone precursors in the atmosphere. Over the last decade, more complex chemical mechanisms, such as the 1999 State-wide Air Pollution Research Center chemical mechanism (SAPRC99; Carter, 2000), have been developed. SAPRC99, developed by Dr. William Carter at the University of California, Riverside, is a detailed mechanism describing the gas-phase reactions of volatile

organic compounds (VOCs) and oxides of nitrogen (NOx). It is a well-known chemical mechanism and has been used widely in California and the U.S. (e.g., Hakami, et al., 2004a, 2004b; Liang and Kaduwela, 2005; Lin et al., 2005; Jackson, et al., 2006; Napelenok, 2006; Dennis et al., 2008; Jin et al., 2008, 2010; Lane et al., 2008; Tonse et al., 2008; Ying et al., 2008; Livingstone et al., 2009; Pun et al., 2009; Kelly, et al., 2010b; Zhang et al., 2010; Zhang and Ying, 2011).

CARB established the Reactivity Scientific Advisory Committee (RSAC) in April 1996. RSAC is a group of independent scientists who make non-binding recommendations on the science related to the reactivity of VOCs. RSAC consists of the following members: Drs. John Seinfeld (Chair, California Institute of Technology), Roger Atkinson (University of California at Riverside), Jack Calvert (National Center for Atmospheric Research), Harvey Jeffries (University of North Carolina at Chapel Hill), Jana Milford (University of Colorado at Boulder), and Armistead Russell (Georgia Institute of Technology). In 1998, RSAC recommended that the SAPRC99 mechanism undergo a scientific review. Following RSAC's recommendation, CARB contracted Dr. William R. Stockwell in 1999 to conduct a review of the SAPRC99 mechanism, its documentation, and the Maximum Incremental Reactivity scale derived from SAPRC99. Stockwell (1999) compared the chemical kinetic data used in the SAPRC99 mechanism with values from standard kinetic databases (e.g., Atkinson et al., 1994, 1997; DeMore et al., 1997) and the most recent literature available at the time. The kinetic parameters checked included the reactions, rate constants, product yields, and lumping methods. Stockwell's (1999) comments led to the revision of the mechanism and identification of outstanding issues to be resolved with further experimental studies. Stockwell (1999) concluded that SAPRC99 reflected the best available science at its completion date, and RSAC approved both the SAPRC99 peer review and the mechanism in October 1999. They also recommended that the SAPRC family of mechanisms be used for regulatory photochemical modeling activities in California.

Since SAPRC-99 has been thoroughly peer-reviewed, ARB's Reactivity Scientific Advisory Committee recommended unanimously in October of 1999 that ARB use SAPRC-99 instead of CBIV for SIP modeling.

In central and northern California, SAPRC has been the mechanism of choice for over a decade. Consistent with this and with the expectation of better representation of atmospheric chemical behavior for ozone modeling, the SAPRC99 chemical mechanism was selected for all 1-hour ozone air quality modeling in California.

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

Air quality model initial conditions define the concentration distributions of chemical species within the modeling domain at the beginning of the model simulation. Boundary conditions define the chemical species concentration distributions for air entering or leaving the modeling domain. To some extent the initial and boundary conditions need to reflect the modeling domain dimensions, and the characteristics of the model being used. This section discusses the initial and boundary conditions used by the CARB in air quality modeling that will support developing the 1-hour ozone SIP.

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

The boundary conditions for the coarse domain were extracted from the global atmospheric chemical transport Model for Ozone and Related chemical Tracers (MOZART). The MOZART model 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, the Max-Planck-Institute for Meteorology (in Germany), and the Geophysical Fluid Dynamics Laboratory of the National Oceanic and Atmospheric Administration, and is widely used in the scientific community. In addition to inorganic gases and VOCs, boundary conditions

were extracted for aerosol species including elemental carbon, organic matter, sulfate, soil and nitrate. The boundary conditions for the coarse domain for the reference year will be used for future years as well, consistent with U.S. EPA guidance.

The boundary conditions for the nested domain were extracted from the output for the coarse domain simulation using the BCON program in the CMAQ modeling system.

Overall, using a 4 km nested domain within the 12 km coarse domain will reduce the computational burden without compromising the accuracy of the modeling results when compared to a simulation using a 4 km grid for the entire outer domain.

6 EMISSION INPUTS

One of the necessary inputs to air quality modeling is an emission inventory with temporally and spatially resolved emissions estimates. Emissions are broadly categorized into major stationary or point sources, area sources (which include off-road mobile sources), on-road mobile sources, and biogenic sources.

6.1 Emission Inventory Development

To support the body of work conducted by stakeholders, modeling inventories have been developed by ARB staff on an on-going basis for the modeling period. The following sections describe how emissions estimates required by the selected air quality models (commonly and interchangeably referred to as 'modeling inventories' or 'gridded inventories') are estimated and how they will be used to develop base case and future year emissions estimates for modeling used to prepare the SIP. As modifications to basic inventory inputs are approved by the responsible regulatory agencies, including ARB, they will be incorporated into final SIP modeling. Once final SIP modeling is complete, the specific versions of the emission inputs used will be documented and summarized. The Air Resources Board convened the following inventory coordination group:

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

In addition to the coordination group described above, a great deal of work preceded this modeling effort through the Central California Air Quality Studies (CCAQS). CCAQS consists of two studies: 1) the Central California Ozone Study (CCOS); and 2) the California Regional $PM_{10}/PM_{2.5}$ Air Quality Study (CRPAQS). More details on CCAQS can be found at the following link: http://www.arb.ca.gov/airways/ccaqs.htm

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

6.1.1 Background

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

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

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

ARB maintains an electronic database of emissions and other useful information. Annual average emissions are stored for each county, air basin, and district. The database is called the California Emission Inventory Development and Reporting System (CEIDARS). Emissions are stored in CEIDARS for criteria and toxic pollutants. The criteria pollutants are total organic gases (TOG), carbon monoxide (CO), oxides of nitrogen (NOx), oxides of sulfur (SOx), and total particulate matter (PM). Reactive organic gases (ROG) and particulate matter 10 microns in diameter and smaller (PM_{10}) are calculated from TOG and PM, respectively. Following are more details on how emissions are estimated for point and area sources, on-road motor vehicles, and biogenic sources. Additional information on emission inventories can be found at http://www.arb.ca.gov/ei/ei.htm

6.1.2 Terminology

There can be confusion regarding the terms “point sources” and “area sources”. Traditionally, these terms have had two different meanings to the developers of emissions inventories and the developers of modeling inventories. Table 6.1 summarizes the difference in the terms. Both sets of terms are used in this document. In modeling terminology, “point sources” refers to elevated emission sources that exit from a stack and have a potential plume rise. “Area sources” refers collectively to area-wide sources, stationary-aggregated sources, and other mobile sources (including aircraft, trains, ships, and all off-road vehicles and equipment). That is, “area sources” are low-level sources from a modeling perspective. In the development of the

inventories, all point sources were treated as possible elevated sources. Processing of the inventory for the photochemical model will determine which vertical layer the emissions from a process will be placed into. So, for the modeling inventories, the use of the term "point sources" is the same whether using the modeling or emission inventory definition.

Table 6.1: Inventory Terms

Modeling Term	Emission Inventory Term	Examples
Point	Stationary – Point Facilities	Stacks at Individual Facilities
Area	Off-Road Mobile	Farm Equipment, Construction Equipment, Aircraft, and Trains
Area	Area-wide	Consumer Products, Architectural Coatings, and Pesticides
Area	Stationary - Aggregated	Industrial Fuel Use
On-Road Motor Vehicles	On-Road Mobile	Automobiles
Biogenic	Biogenic	Trees

6.2 Point and Area Source Emissions

6.2.1 Development of Base-Year Emission Inventory

The stationary source component of the emission inventory is comprised of more than 20,000 individual facilities, called "point sources", and about 160 categories of

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

The area-wide source component includes several hundred source categories and is made up of sources of pollution mainly linked to the activity of people. Examples of these categories are emissions from consumer products, architectural coatings, pesticide applications, and wind-blown dust from agricultural lands. The emissions for these categories are located mostly within major population centers. Some of the emissions in these categories come from agricultural centers and construction sites.

The off-road mobile source inventory is based on the population, activity, and emissions estimates of the varied types of off-road equipment. The major categories of engines and vehicles include agricultural, construction, lawn and garden, and off-road recreation, and include equipment from hedge trimmers to cranes. ARB's OFFROAD model estimates the relative contribution of gasoline, diesel, compressed natural gas, and liquefied petroleum gas powered vehicles to the overall emissions inventory of the state. In previous versions of the inventory, emissions from the OFFROAD model were aggregated into about 100 broad categories. Since April 2006, the inventory reports emissions in about 1800 detailed categories that match what is produced by the OFFROAD model. Carrying this level of detail allows for more accurate application of control measures as well as more specific assignments of speciation and spatial distribution. For more information, see http://www.arb.ca.gov/msei/offroad/offroad.htm.

Local air districts estimate emissions from point sources. The districts provide point source information to ARB to update the annual average CEIDARS database. Estimating emissions from area sources is a cooperative effort between ARB and air

district staffs. Updating the emission inventory is a continual process, as new information becomes available.

6.2.2 Quality Assurance of Base Year Emissions

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

In particular, facility location, stack data, and temporal data were closely checked. This information is critical whenever photochemical modeling is conducted, such as during SIP preparation or special studies such as CCAQS. However these data are not always of sufficient quality in the inventory database since this information is not needed in the actual calculation of emissions and resources are limited. ARB ran several types of QA reports on the inventory to assist the districts in locating errors or incomplete information. This QA process began with the 1999 CEIDARS database, and continued with the 2002 CEIDARS database that was used for previous $PM_{2.5}$ and ozone inventory preparation. The QA process has continued with the 2005 and subsequent CEIDARS databases. The 2005 CEIDARS database is the basis for the modeling inventories developed for the 24-hour $PM_{2.5}$ SIPs in northern California. Staff of the South Coast AQMD is using the 2008 CEIDARS database for their modeling effort covering southern California (approximately the Tehachapi Mountains southward).

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

Location data – The report checks for missing or wrong Universal Transverse Mercator) UTM coordinates. The report lists missing UTM coordinates for both facilities and stacks. UTM coordinates are also checked to ensure that they are in the range for

a given county. Another report is also run that shows the UTM coordinates for a facility grouped by the city in which the facility is located. This allows staff to look for outliers that may indicate facilities whose locations are in the county, but not in the correct location. Additionally, ARB staff reviewed location coordinates for accuracy and completeness. Comparisons were made using address or zip code mapping.

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

Code Assignments – Source Classification Codes (SCC) and Standard Industrial Classification Codes (SIC) were reviewed for accuracy. The SCC is used to determine the speciation profile assigned (speciation is discussed in Section 6.10). The SIC and SCC combined determine emission control rules that may apply for forecasting emissions (see Section 6.3) along with the categorization of emissions for reporting purposes.

6.3 Future Year (Forecasted) Emissions

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

ARB's model to forecast or backcast emissions is known as the California Emission Forecasting System (CEFS). The CEFS model is designed to generate year-specific emissions estimates for each county/air basin/district combination taking into account two factors: 1) the effects of growth and 2) the effects of adopted emission control rules. It does this by linking these growth and control factors directly to CEIDARS emission categories for a particular base year (2002 for this project). A key component of the model is the Rule Tracking Subsystem (RTS). The RTS was developed to link year-

specific implementation of emission control rules to the emission process level. The emission process level is identified in one of two ways. For facilities, the Source Classification Code (SCC) and Standard Industrial Classification (SIC) are used. For all other sources, the Emission Inventory Code (EIC) is used. In total, the emission process level comprises more than 30,000 possible emission categories statewide.

Reports of year-specific emissions are available to district staff on-line. District staffs should contact their emission inventory liaisons for URL and password information. The reports can be generated for a variety of years, pollutants, source types, seasons, and geographical areas.

6.3.1 Growth Factors

Growth factors are derived from county-specific economic activity profiles, population forecasts, and other socio/demographic activity. These data are obtained from a number of sources, such as: districts and local regional transportation planning agencies (RTPAs) when they are available; economic activity studies contracted by the ARB; and demographic data such as population survey data from the California Department of Finance (DOF) and Vehicle Miles Traveled (VMT) data from the California Department of Transportation (Caltrans).

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

6.3.2 Control Factors

Control factors are derived from adopted State and Federal regulations and local district rules that impose emission reductions or a technological change on a particular emission process. These data are provided by the agencies responsible for overseeing

the regulatory action for the particular emission categories affected. For example, the ARB staff develops the control factors for sectors regulated by the ARB, such as consumer products and clean fuels. The districts develop control factors for locally enforceable stationary source regulations that affect emissions from such equipment as internal combustion engines or power plant boilers. The Department of Pesticide Regulation (DPR) supplies control data for pesticides. In general, control factors account for three variables:

Control Efficiency which estimates the technological efficiency of the abatement strategy

Rule Effectiveness which estimates the "real-world" application of the strategy taking into account factors such as operational variations and upsets

Rule Penetration which estimates the degree a control strategy will penetrate a certain regulated sector taking into account such things as equipment exemptions.

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

6.4 Day-Specific Emissions

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

6.4.1 Wildfires and Prescribed Burns

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

For 2007 model performance, day-specific 2007 wildfire emission estimates are used. However, for RRF determination, average-day emissions from wildfires and prescribed fires are used and, to avoid overly influencing the RRF calculation, fire emissions were held constant between the base and future years. Since the fire emissions used in the RRF determination are based on a 10-year average, fire emissions were distributed equally throughout the first ten model layers (i.e. fire-specific plume rise calculations are not made).

6.4.2 Agricultural Burn Data for San Joaquin Valley

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

To determine the location of the burn, district staff created spatial allocation factors for each 4 kilometer grid cell used in modeling. These factors were developed for "burn

zones" in the San Joaquin Valley based on the agricultural land coverage. Daily emissions in each "agricultural burn zone" were then distributed across the zone/grid cell combinations using the spatial allocation factors. Emissions were summarized by grid cell and day.

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

6.4.3 Ocean-Going Vessels

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

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

6.5 Temporally and Spatially Resolved Emissions

Emission inventories that are temporally and spatially resolved are needed for modeling purposes, for both the base year and future years. Annual average emissions for point and area sources were used as input to version 2.6 of SMOKE (Sparse Matrix Object

Kernel Emission). The SMOKE processor was developed by the MCNC-North Carolina Supercomputing Center, Environmental Sciences Division, with U.S. EPA cooperation and support. Temporal information is input into SMOKE. Adjustments are made for variations in months, day of week and hour of day. Emissions are estimated for each county, air basin, and district combination for each day of the year. The SMOKE processor also distributes emissions to each grid cell. The spatial allocation of emissions is discussed in Section 6.9.

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

6.6 Surface Temperature and Relative Humidity Fields

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

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

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

Compute the relative weights of each surface observation station to each grid cell (the weight is inversely proportional to the distance between the surface observation station and grid cell center).

Adjust all surface temperatures to sea level. In this step, a lapse rate of -0.0049 ^{o}C/m is used (this lapse rate is based on private communication with Gary Moore of Earth Tech, Inc., Concord, MA). This lapse rate (=2.7 F/1000 feet) is based on observational data.

Use the weights to compute a spatially-averaged sea-level temperature in each grid cell.

Correct all sea-level temperatures back to 10 m height above ground level (i.e. the standard height of surface temperature measurement) using the lapse rate of -0.0049 ^{o}C/m again.

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

Calculate actual vapor pressure from observed relative humidity and temperature at all meteorological stations. The McRae (1980) method is used to calculate the saturated vapor pressure from temperature;

Compute the relative weights of each surface observation station to each grid in question, exactly as done by CALMET to compute the temperature field;

Use the weights from step 2 to compute a spatially-averaged estimate of actual vapor pressure in each grid cell;

For each grid cell, calculate relative humidity from values for actual vapor pressure and temperature for the same grid cell.

6.7 On-Road Mobile Source Emissions

As described in the prior sections, air quality models require gridded, hourly emission inputs. However, California's official on-road motor vehicle emission inventory model, EMFAC, is designed to produce *county-level, average-day* estimates. As a result, emission estimates from EMFAC must be disaggregated spatially and temporally from county-level, average-day estimates into gridded, hourly estimates. The general methodology that ARB has used to disaggregate EMFAC emission estimates in the past is described below and will be used again. Basically, it involves using the Direct Travel Impact Model (DTIM) (Systems Applications, Inc. 2001) to produce gridded, hourly emission estimates, and then uses these estimates as a gridded hourly spatial surrogate to distribute EMFAC emissions. The methodology has been peer reviewed by UCI under a Central California Ozone Study (CCOS) contract.

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

6.7.1 General Methodology

Day-Specific Temperature and Relative Humidity. Mobile source emissions are sensitive to ambient temperature and humidity. Both EMFAC and DTIM account for meteorological effects using day-specific inputs (the gridded, hourly meteorological data

used are described under the prior section titled “Surface Temperature and Relative Humidity Fields”). For EMFAC-LD, hourly gridded temperature and humidity fields are averaged by county using a gridded VMT weighted average (i.e. weighted proportional to the VMT per grid cell in a county). DTIM accepts gridded, hourly data directly.

EMFAC-LD provides vehicle-class-specific emissions estimates for exhaust emissions, evaporative emissions, tire wear emissions and brake wear emissions. EMFAC-LD also produces estimates of fuel consumption, vehicle miles traveled (VMT), and the number of vehicles in use. Day-specific temperature and relative humidity adjustments are not made to heavy-duty diesel vehicles; EMFAC-HD provides winter and summer emission estimates.

More information on EMFAC is available at the following link.
http://www.arb.ca.gov/msei/modeling.htm

Temporal Adjustment (Day-of-Week adjustments to EMFAC daily totals): Day-of-Week (DOW) adjustments are made to the total daily emissions estimated by EMFAC for Friday, Saturday, Sunday, and Monday. The logic behind this is that EMFAC produces emission estimates for an average weekday. It is assumed that EMFAC’s average weekday emissions generally represent Tuesday, Wednesday, and Thursday. Day of week adjustment factors were developed using Automatic Vehicle Classifier (AVC) count data from the California Department of Transportation (Caltrans). These data were collected at 139 sites in the state during the summer of 2004 (specifically, data for the months of June, July and August were used, excluding data from July 2-5 to remove unusual traffic patterns around the July 4th holiday). Three factors were developed: (1) passenger cars (LD), (2) light and medium duty trucks (LM), and (3) heavy-heavy duty trucks (HHDT). An example of the prior assignment of these factors to EMFAC2007 classifications is summarized below in Table 6.2.

Table 6.2: EMFAC2007 Classifications

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

* Vehicle classes are being updated for use with EMFAC2011

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

Temporal Adjustment (Hour-of-Day re-distribution of hourly travel network volumes): The travel networks provided by local government agencies and used for DTIM represent an average weekday hourly distribution. It is assumed that these average weekday hourly distributions lack the day-of-week temporal variations known to occur on specific days of the week. To rectify this, hour-of-day profiles for every day of the week, Monday through Sunday, were developed for each Caltrans District using Caltrans data. These profiles are used to re-allocate the hourly travel network distributions for all vehicle classes used in DTIM.

Spatial Adjustment: The spatial allocation of countywide EMFAC emissions is accomplished using gridded, hourly emission estimates from DTIM normalized by county. DTIM uses emission rates from EMFAC along with activity data, digitized roadway segments (links) and traffic analysis zone centroids to calculate gridded, hourly emissions for travel and trip ends. DTIM considers fewer vehicle categories than EMFAC outputs, so a mapping between EMFAC and DTIM vehicle categories is necessary (this is being updated to work with EMFAC2011). DTIM emission categories are presented in the Table 6.3. The categories are represented by the listed source classification codes (SCC) and depend on vehicle type, technology, and whether the vehicle is catalyst, non-catalyst, or diesel. Light- and medium-duty vehicles are separated from heavy-duty vehicles to allow for separate reporting and control strategy applications. The light- and medium-duty vehicles include LDA, LDT1, LDT2, MDV, LHDT1, LHDT2, UBUS, MH and MCY. The heavy-duty vehicles include MHDT, HHDT, OBUS and SBUS.

Table 6.3: DTIM Emission Categories

SCC for light-duty and medium-duty gasoline vehicles	SCC for heavy-duty gasoline vehicles	SCC for light-duty and medium-duty diesel vehicles	SCC for heavy-duty diesel vehicles	Description
202	302			Catalyst Start Exhaust
203	303			Catalyst Running Exhaust
204	304			Non-catalyst Start Exhaust
205	305			Non-catalyst Running Exhaust
206	306			Hot Soak
207	307			Diurnal Evaporatives
		808	408, 508	Diesel Exhaust
209	309			Running Evaporatives
210	310			Resting Evaporatives
211	311			Multi-Day Resting
212	312			Multi-Day Diurnal
213	313	813	413, 513, 613, 713	PM Tire Wear
214	314	814	414, 514, 614, 714	PM Brake Wear
215	315			Catalyst Buses
216	316			Non-catalyst Buses
		817	617, 717	Diesel Bus
218	318			Catalyst Idle
219	319			Non-catalyst Idle
		820	420, 520, 620, 720	Diesel Idle
221	321			PM Road Dust

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

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

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

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

Step 4 (DTIM emission factor inputs for HD). Merge the HD emission rate by process (ERP) data and the EMFAC-LD ERP data (EMFAC-LD produces these data files directly as an option) and generate a look-up table of on-road mobile source emission factors by speed, temperature, and relative humidity for each county. The HD ERP data came from the HD model. The HD model also provides hourly county emissions for annual, summer and winter. However, only summer and winter are used.

Step 5 (DTIM inputs – redistribute countywide roadway network hourly volumes using Caltrans District data)

5a. Calculate Daily Total Volumes. Sum the hourly volumes by vehicle type and county on the roadway network into daily totals.

5b. Day-of-Week (DOW) adjustment. Modify daily total daily volume from step 5a using Caltrans District DOW adjustment factors to reflect day-of-week differences. For Tuesday through Thursday, no DOW adjustment is made (i.e. the DOW adjustment factor is 1.0) since the data already reflect an average mid-week (Tues-Thurs) allocation. For Friday, Saturday, Sunday, and Monday different DOW factors are applied to county-wide network data based on the Caltrans District associated with each county.

5c. Hour-of-Day adjustments. Hour-of-day profiles for every day of the week, Monday through Sunday, were developed for each Caltrans District using

Caltrans data. Each District is 'assigned' to one or more counties. For each county, the profiles are used to re-allocate the hourly travel network distributions for all vehicle classes used in DTIM.

Step 6 (Run DTIM and spatially/temporally distribute EMFAC emissions)

6a. For each county, run DTIM with revised roadway network activity from Step 5 for light and medium duty gasoline vehicles, heavy duty gasoline vehicles, light and medium duty diesel vehicles and heavy duty diesel vehicles (one run for each group; four runs per county).

6b. Sum DTIM emissions by county and SCC.

6c. Distribute EMFAC emissions. EMFAC daily, countywide emissions (adjusted for weekend days, if needed), are disaggregated by category into grid-cells for each hour of the day using the DTIM output as a spatial and temporal surrogate. The disaggregation follows the equation:

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

where:

E = grid cell emissions

EF = EMFAC emissions

DTIM = DTIM emissions

P = pollutant

ij = grid cell

hr = hourly emissions

cat = Emission Category

daily = daily emissions

cnty = county

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

6.8 Biogenic Emissions

Development of effective ozone control strategies in California requires accurate emission inventories, including biogenic volatile organic compounds (BVOCs) such as isoprene and monoterpenes. Due to the heterogeneity of vegetation land cover, species composition, and leaf mass distribution in California, quantifying BVOC emissions in this domain requires an emission inventory model with region-specific input databases and a high degree of spatial and temporal resolution. In response to this need, the California Air Resources Board (CARB) has developed a Geographic Information System (GIS)-based model for estimating BVOC emissions, called BEIGIS (Scott and Benjamin, 2003), which uses California-specific input databases with a minimum spatial resolution of 1 km^2 and an hourly temporal resolution. To take advantage of recent scientific advances in biogenic emissions modeling, CARB has recently transitioned from the BEIGIS model to the Model of Emissions of Gases and Aerosols from Nature (MEGAN) version 2.04 (Guenther et al., 2006). MEGAN is a state-of-the-science biogenic emissions model, which represents an evolution of the Biogenic Emissions Inventory System (BEIS), and is being integrated into the Community Multi-scale Air Quality (CMAQ) modeling system by U.S. EPA scientists.

MEGAN estimates biogenic emissions as a function of normalized emission rates (i.e., emission rates at standard conditions), which are adjusted to reflect variations in temperature, light, leaf area index (LAI), and leaf age (estimated from changes in LAI). MEGAN requires input datasets of Emission Factors (EF; at standard conditions: temperature = 303 ˚K, LAI = 5, photosynthetically active radiation ~ 1500 μmol $m^{-2}s^{-1}$), Plant Functional Type (PFT), and hourly surface temperature and insolation. The default MEGAN input databases for EFs, PFTs, and LAI are not used in the application of MEGAN in California. Instead, California-specific emission factor and PFT databases were translated from those used in BEIGIS to improve emission estimates and to maintain consistency with previous California biogenic emission inventories. LAI data is derived from the MODIS 8-day LAI satellite product. Hourly surface temperatures are from observations gridded with the CALMET meteorological model and insolation (light reaching the surface) data is provided by the MM5 meteorological model. Emissions of

isoprene, monoterpenes, and methylbutenol are estimated from California-specific gridded emission factor data, while emissions of sesquiterpenes, methanol, and other volatile organic compounds are estimated from California-specific PFT data and PFT derived emission rates. For urban areas, land use/vegetation land cover databases were developed from regional planning agency data and botanical surveys (Horie et al. 1990; Nowak 1991; Sidawi and Horie 1992; Benjamin et al. 1996, 1997; McPherson et al. 1998). Natural areas are represented using the GAP vegetation database (also satellite-derived and air photo interpreted) developed by the U.S.G.S. Gap Analysis Program (Davis et al. 1995). Agricultural areas are represented using crop land cover databases developed by the California Department of Water Resources (*http://www.waterplan.water.ca.gov*).

Biogenic emissions are not estimated for future years because future inputs to BEIGIS, such as changes in climate and land use/land cover, are highly uncertain. Photochemical modeling for future years uses the biogenic emissions developed for the base year.

Table 6.4: SJV domain-wide biogenic emissions for 2007 in tons/day.

	Isoprene	Methylbutenol	Terpenes	Other ROG	Total ROG
Jan	4	14	13	24	55
Feb	6	18	24	58	106
Mar	117	78	70	142	407
Apr	163	111	92	161	526
May	436	251	159	276	1121
Jun	734	400	261	427	1821
Jul	941	495	341	522	2300
Aug	771	394	303	440	1908
Sep	336	182	160	220	899
Oct	43	63	60	88	255
Nov	11	29	28	45	113
Dec	2	8	9	19	39

The biogenic emissions for the modeling domain are shown in Table 6.4 in tons/day. Note that all biogenic emissions are higher during the warm and sunny summer months and lower in cold and gloomy winter months.

6.9 Spatial Allocation

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

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

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

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

Emissions are also distributed vertically into their proper layer in the air quality model. The vertical layer is determined from the calculation of buoyancy for those emissions that are released from an elevated height with a significant upward velocity and/or buoyancy. Most vertical allocation is from significant point sources with stacks. In most modeling exercises, low-level point sources are screened out at this point and placed with the area sources. However, in this modeling exercise, all point sources from the

inventory were kept as possible elevated sources. The air quality model will then place the point sources in the appropriate layer of the model. Additionally in this modeling exercise, day-specific wildfire emissions were also distributed vertically.

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

6.9.1 Grid Definition

The ARB emissions inventory domain, shown in Figure 6.1, is defined to match the WRF model domain, which is used to generate the meteorological parameter fields used for air quality modeling. WRF uses a Lambert projection and assumes a spherical Earth. The emission grid is defined in a similar way to match as closely as possible.

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

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

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

MAP PROJECTION
Lambert Conformal Conic
Datum: NONE (Clarke 1866 spheroid)
1st Standard Parallel: 30.0° N
2nd Standard Parallel: 60.0° N

Central Meridian: -120.5° W

Latitude of Projection Origin: 37.0° N

COORDINATE SYSTEM

Units: Meters

Semi-major Axis: 6370 km

Semi-minor Axis: 6370 km

DEFINITION OF GRID

321 x 291 cells (4 km x 4 km)

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

Geographic Origin @ -120.5° Latitude and 37.0° Longitude

DEFINITION OF SUBGRID (CCOS)

192 x 192 cells (4 km x 4 km)

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

Geographic Origin @ -120.5° Latitude and 37.0° Longitude

6.9.2 Spatial Surrogates

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

In support of CRPAQS and CCOS, Sonoma Technology, Inc. (Funk et al. 2001) developed gridded spatial allocation factors for a 2000 base-year and three future years (2005, 2010, and 2020) for the entire state of California. STI's work was based on the statewide 4-kilometer (km) grid cell domain defined by the ARB. The definition and extent of the 4-km grid were used to create a 2-km nested grid for which spatial allocation factors were developed. In 2007, STI was contracted by CCOS again to

update the spatial allocation factors. STI updated the underlying spatial data and updated the spatial surrogate cross-reference file to account for new emission source categories (Reid et al., 2006). STI then updated spatial allocation factors for ARB's statewide modeling domain for a base year of 2000 and future years of 2010, 2015, and 2020. This task was completed in March 2008.

In preparation for modeling for the Ozone SIPs, ARB staff reviewed the STI spatial surrogates associated with the highest emissions to see which surrogates were candidates for update. ARB staff searched for more recent or improved sources of data, since the underlying data used by STI were pre-recession, then updated 15 of the surrogates using more recent data. A total of 61 unique surrogates are available for use. A summary of the spatial surrogates for which spatial allocation factors were developed is listed in the Table 6.4.

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

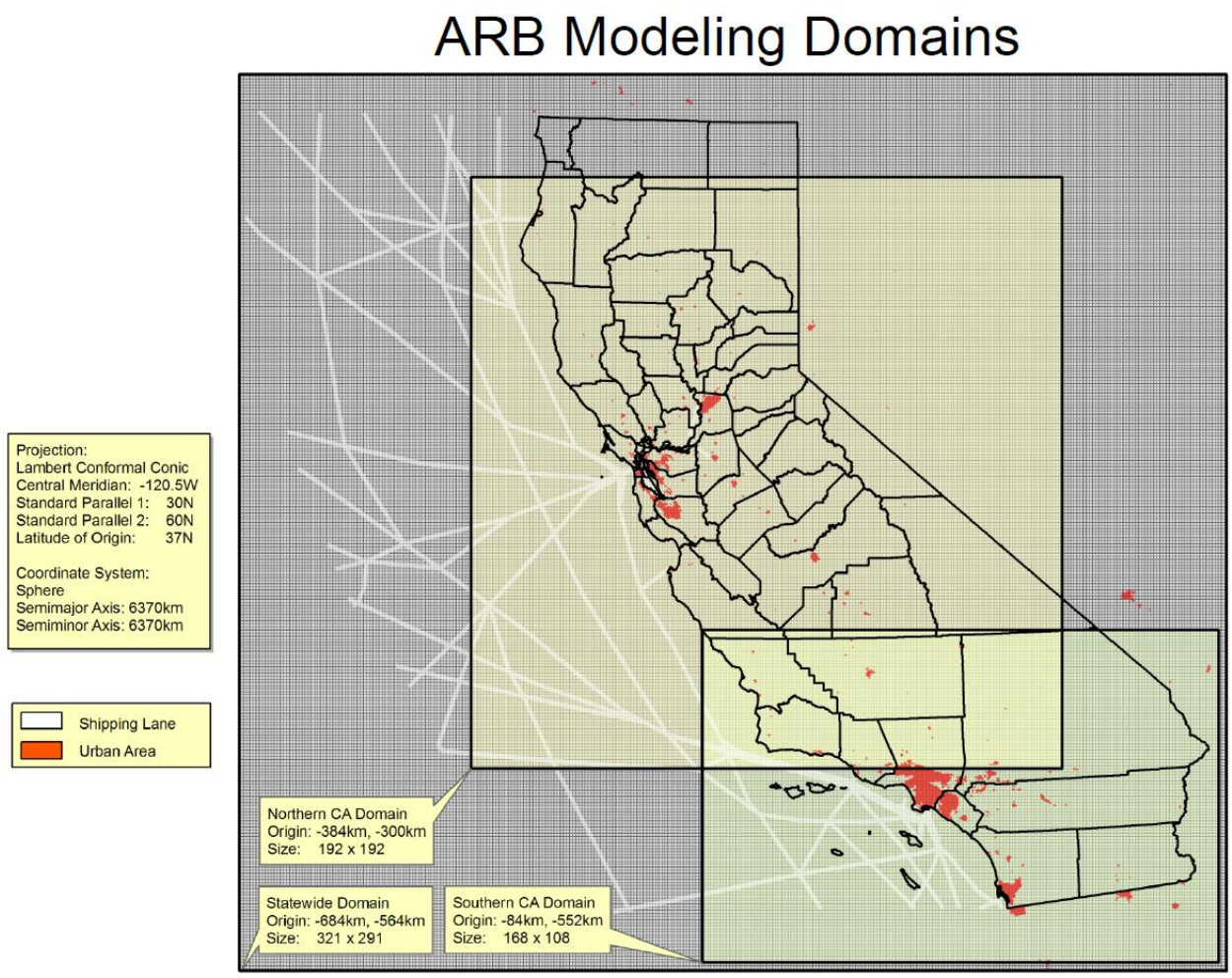


Figure 6.1: ARB Modeling Domain with urban areas and shipping lanes shown.

Table 6.5: Summary of spatial surrogates

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

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

6.10 Speciation

The ARB's emission inventory and photochemical air quality models both quantify organic compounds as Total Organic Gases (TOG). Photochemical models simulate the physical and chemical processes in the lower atmosphere, and include all emissions of the important compounds involved in photochemistry. Organic gases are one of the most important classes of chemicals involved in photochemistry. Organic gases emitted

to the atmosphere are referred to as total organic gases (TOG). ARB's chemical speciation profiles (CARB 2006) are applied to characterize the chemical composition of the TOG emitted from each source type.

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

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

6.10.1 Speciation Profiles

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

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

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

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

The Organic Speciation Profiles (ORGPROF) file contains the weight fraction data (expressed as percent for ease of display) of each chemical in each profile. Each chemical fraction is multiplied by the Total Organic Gas (TOG) emissions for a source category to get the amount of each specific constituent chemical. In addition to the chemical name for each chemical constituent, the file also shows the chemical code (a 5-digit internal identifier) and the Chemical Abstracts Service (CAS) number, which is a unique identifying code (up to 9 digits) assigned to chemicals by the CAS Registry Service.

Also available for download from ARB's web site is a cross-reference file that indicates which Organic Gas profile is assigned to each source category in the inventory. The inventory source categories are represented by an 8-digit Source Classification Code (SCC) for point sources, or a 14-digit Emission Inventory Code (EIC) for area and

mobile sources. This file also contains the fraction of reactive organic gas (FROG) values for organic profiles. Some of the Organic Gas Speciation Profiles related to motor vehicles and fuel evaporative sources vary by the inventory year of interest, due to changes in fuel composition and vehicle fleet composition over time.

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

6.10.2 Chemical Mechanisms

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

For State Implementation Plan (SIP) attainment demonstrations and evaluations, the U.S. EPA has approved the California Air Resources Board's photochemical air quality models. The air quality models used by the ARB for SIP attainment demonstrations use the SAPRC photochemical mechanism. This mechanism is based on extensive scientific research and is documented in the scientific literature (Carter 2000). Table 6.5 shows modeled ROG species (or species categories) for the SAPRC-99 chemical mechanism. Table 6.6 shows modeled species for NOx.

Table 6.6: ARB's SAPRC-99 Emitted Organic Model Species

Model Species	Description
HCHO	Formaldehyde
CCHO	Acetaldehyde
RCHO	Lumped C3+ Aldehydes
ACET	Acetone
MEK	Ketones and other non-aldehyde oxygenated products
PROD	
RNO3	Lumped Organic Nitrates
PAN	Peroxy Acetyl Nitrate
PAN2	PPN and other higher alkyl PAN analogues
BALD	Aromatic aldehydes (e.g., benzaldehyde)
PBZN	PAN analogues formed from Aromatic Aldehydes
PHEN	Phenol
CRES	Cresols
NPHE	Nitrophenols
GLY	Glyoxal
MGLY	Methyl Glyoxal
MVK	Methyl Vinyl Ketone
MEOH	Methanol
HC2H	Formic Acid
CH4	Methane
ETHE	Ethene
ISOP	Isoprene
TERP	Terpenes
MTBE	Methyl Tertiary Butyl Ether
ETOH	Ethanol
NROG	Non-reactive
LOST	Lost carbon

Model Species	Description
ALK1	Alkanes and other non-aromatic compounds that react only with OH, and have kOH <
ALK2	Alkanes and other non-aromatic compounds that react only with OH, and have kOH
ALK3	Alkanes and other non-aromatic compounds that react only with OH, and have kOH
ALK4	Alkanes and other non-aromatic compounds that react only with OH, and have kOH
ALK5	Alkanes and other non-aromatic compounds that react only with OH, and have kOH
ARO1	Aromatics with kOH < $2x10^4$ ppm-1 min-1.
ARO2	Aromatics with kOH > $2x10^4$ ppm-1 min-1.
OLE1	Alkenes (other than ethene) with kOH < $7x10^4$ ppm-1 min-1.
OLE2	Alkenes with kOH > $7x10^4$ ppm-1 min-1.

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

Table 6.7: Model Species for NOx

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

6.11 Quality Assurance

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

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

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

6.11.1 Examples of Standard Tabular Summaries

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

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

CO	NOX	SOX	TOG	PM	NH3	ROG	PM10	PM25
17,939.63	4,308.18	285.01	7,334.56	4,109.78	762.98	3,620.07	2,472.03	810.70

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

EIC1	DESCRIPTION	CO	NOX	SOX	TOG	PM	NH3	ROG	PM10	PM25
0	FUEL COMBUSTION	384.18	406.63	48.20	148.62	45.55	5.49	34.17	40.08	37.24
1	WASTE DISPOSAL	2.18	3.02	0.67	1,245.77	1.62	42.56	14.86	0.83	0.73
2	CLEANING AND SURFACE COATINGS	0.15	0.40	0.04	381.17	0.39	2.13	279.20	0.38	0.36
3	PETROLEUM PROD AND MARKETING	10.08	13.97	58.60	536.56	4.90	1.85	219.60	3.05	2.26
4	INDUSTRIAL PROCESSES	53.52	96.16	31.57	95.55	174.20	9.22	79.44	100.22	51.50
5	SOLVENT EVAPORATION	0.00	0.00	0.00	475.95	0.03	37.45	419.42	0.03	0.03
6	MISCELLANEOUS PROCESSES	2,545.81	156.27	9.64	1,811.66	3,726.68	538.27	300.23	2,173.18	586.03
7	ON-ROAD MOTOR VEHICLES	12,726.85	2,315.33	11.27	1,343.71	74.73	75.25	1,233.16	74.09	57.91
8	OTHER MOBILE SOURCES	2,216.86	1,316.41	125.03	484.40	81.69	0.00	431.80	80.18	74.65
9	NATURAL SOURCES	0.00	0.00	0.00	811.17	0.00	50.76	608.19	0.00	0.00

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

EIC3	DESCRIPTION	CO	NOX	SOX	TOG	PM	NH3	ROG	PM_{10}	PM_{25}
010	ELECTRIC UTILITIES	56.74	51.52	4.76	30.97	6.82	2.35	4.97	6.35	5.89
020	COGENERATION	49.01	30.87	1.87	17.27	4.43	0.18	4.04	4.03	3.72
030	OIL AND GAS PRODUCTION	22.66	45.18	7.44	26.59	2.09	0.10	4.15	2.08	2.08
040	PETROLEUM REFINING	10.22	46.03	12.75	3.52	4.26	0.61	1.79	4.06	3.98
050	MANUFACTURING AND INDUSTRIAL	52.77	86.07	14.52	20.28	5.92	1.63	3.96	5.71	5.45
052	FOOD AND AGRICULTURAL	111.24	22.60	2.69	7.72	3.02	0.10	6.06	2.94	2.89
060	SERVICE AND COMMERCIAL	71.00	104.86	3.66	35.62	8.31	0.40	6.90	8.24	8.19
099	OTHER (FUEL COMBUSTION)	10.55	19.50	0.50	6.65	10.70	0.11	2.31	6.68	5.05
110	SEWAGE TREATMENT	0.25	0.39	0.28	1.29	0.03	0.25	0.70	0.02	0.02
120	LANDFILLS	0.85	0.67	0.21	1,182.55	0.89	9.78	7.92	0.40	0.35
130	INCINERATORS	1.01	1.77	0.14	0.94	0.23	0.09	0.16	0.11	0.10
140	SOIL REMEDIATION	0.06	0.09	0.03	0.49	0.11	0.00	0.34	0.04	0.03
199	OTHER (WASTE DISPOSAL)	0.01	0.10	0.00	60.49	0.36	32.42	5.74	0.25	0.25
210	LAUNDERING	0.00	0.00	0.00	8.60	0.00	0.00	0.84	0.00	0.00
220	DEGREASING	0.00	0.00	0.00	178.79	0.00	0.00	99.87	0.00	0.00
230	COATINGS AND RELATED PROCESS	0.11	0.16	0.04	122.45	0.32	0.03	114.08	0.30	0.29
240	PRINTING	0.01	0.05	0.00	25.31	0.05	0.04	25.31	0.05	0.04
250	ADHESIVES AND SEALANTS	0.00	0.00	0.00	35.84	0.01	0.00	31.80	0.01	0.01
299	OTHER (CLEANING AND SURFACE	0.03	0.19	0.00	10.17	0.02	2.06	7.30	0.02	0.02
310	OIL AND GAS PRODUCTION	1.91	3.32	0.53	104.11	0.10	0.00	53.90	0.08	0.08
320	PETROLEUM REFINING	6.03	9.85	58.06	49.04	3.99	1.85	38.43	2.54	2.08
330	PETROLEUM MARKETING	2.14	0.80	0.00	382.93	0.81	0.00	126.85	0.43	0.10
399	OTHER (PETROLEUM PROD AND	0.00	0.00	0.00	0.47	0.00	0.00	0.42	0.00	0.00
410	CHEMICAL	0.44	1.82	2.69	34.07	5.99	0.25	27.38	5.09	4.71

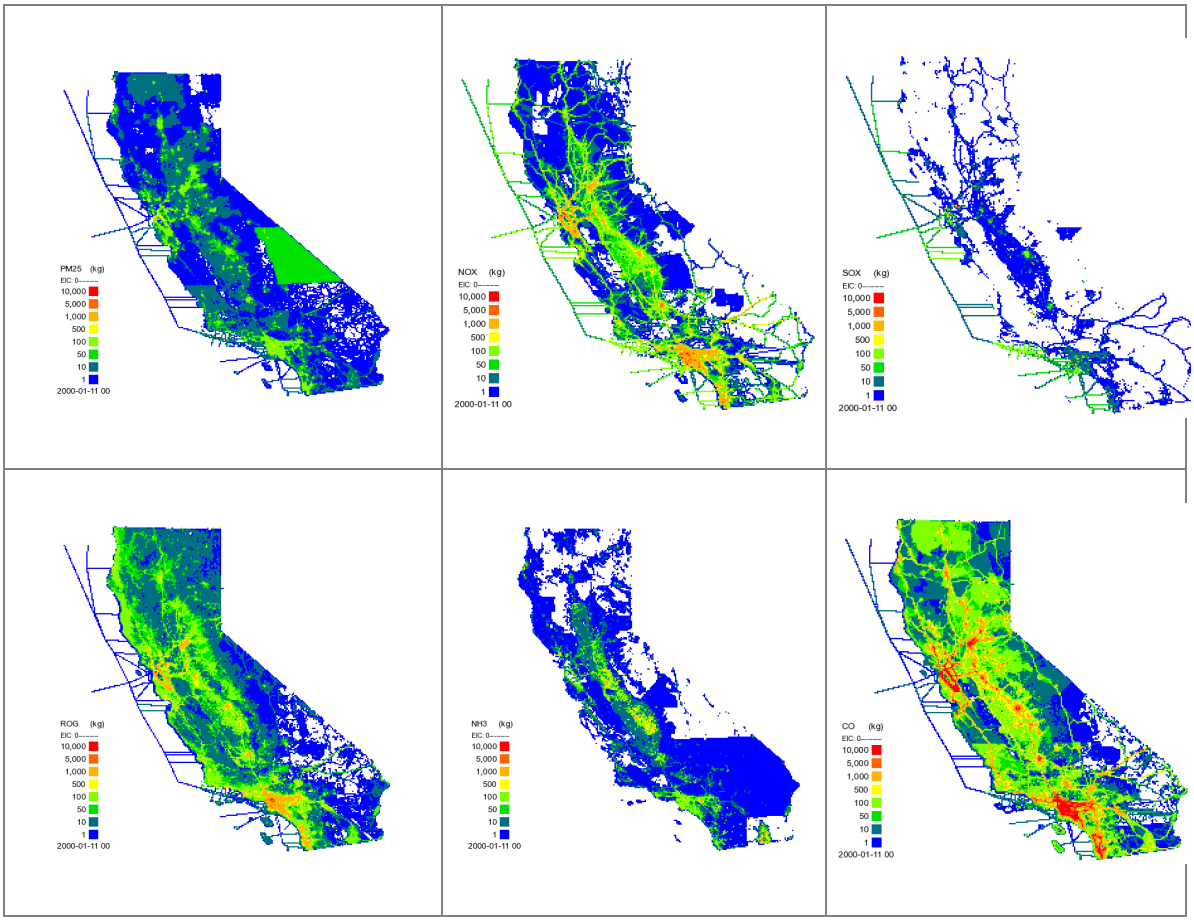
EIC3	DESCRIPTION	CO	NOX	SOX	TOG	PM	NH3	ROG	PM_{10}	PM_{25}
420	FOOD AND AGRICULTURE (Note:	2.71	9.60	2.52	23.33	29.67	0.07	21.15	12.05	2.79
499	OTHER (INDUSTRIAL PROCESSES)	10.37	9.31	0.85	22.72	18.20	8.82	18.42	11.70	7.86
510	CONSUMER PRODUCTS	0.00	0.00	0.00	305.34	0.00	0.00	259.30	0.00	0.00
520	ARCHITECTURAL COATINGS AND	0.00	0.00	0.00	111.39	0.00	0.00	108.74	0.00	0.00
530	PESTICIDES/FERTILIZERS	0.00	0.00	0.00	39.41	0.00	37.45	32.38	0.00	0.00
540	ASPHALT PAVING / ROOFING	0.00	0.00	0.00	19.82	0.03	0.00	19.01	0.03	0.03
610	RESIDENTIAL FUEL COMBUSTION	1,741.05	129.11	8.59	274.46	270.85	12.36	120.38	253.79	244.63
620	FARMING OPERATIONS	0.00	0.00	0.00	1,419.61	147.04	467.32	113.57	72.64	17.07
630	CONSTRUCTION AND DEMOLITION	0.00	0.00	0.00	0.00	415.08	0.00	0.00	203.10	20.30
640	PAVED ROAD DUST	0.00	0.00	0.00	0.00	810.83	0.00	0.00	370.71	55.62
645	UNPAVED ROAD DUST	0.00	0.00	0.00	0.00	235.99	0.00	0.00	140.25	14.02
650	FUGITIVE WINDBLOWN DUST	0.00	0.00	0.00	0.00	1,718.35	0.00	0.00	1,016.94	135.06
660	FIRES	10.14	0.24	0.00	1.01	1.17	0.00	0.71	1.15	1.08
670	WASTE BURNING AND DISPOSAL	793.31	26.85	1.05	107.70	92.67	4.64	59.38	90.31	83.67
690	COOKING	0.16	0.00	0.00	8.77	33.40	0.00	6.13	23.38	14.03
699	OTHER (MISCELLANEOUS	1.15	0.07	0.00	0.10	1.31	53.95	0.07	0.92	0.55
700	On-Road Motor Vehicles	12,726.85	2,315.33	11.27	1,343.71	74.73	0.00	1,233.16	74.09	57.91
710	LIGHT DUTY PASSENGER (LDA)	0.00	0.00	0.00	0.00	0.00	41.86	0.00	0.00	0.00
722	LIGHT DUTY TRUCKS - 1 (LDT1)	0.00	0.00	0.00	0.00	0.00	9.32	0.00	0.00	0.00
723	LIGHT DUTY TRUCKS - 2 (LDT2)	0.00	0.00	0.00	0.00	0.00	15.73	0.00	0.00	0.00
724	MEDIUM DUTY TRUCKS (MDV)	0.00	0.00	0.00	0.00	0.00	5.82	0.00	0.00	0.00
732	LIGHT HEAVY DUTY GAS TRUCKS - 1	0.00	0.00	0.00	0.00	0.00	1.20	0.00	0.00	0.00
733	LIGHT HEAVY DUTY GAS TRUCKS - 2	0.00	0.00	0.00	0.00	0.00	0.38	0.00	0.00	0.00
734	MEDIUM HEAVY DUTY GAS TRUCKS	0.00	0.00	0.00	0.00	0.00	0.26	0.00	0.00	0.00
736	HEAVY HEAVY DUTY GAS TRUCKS	0.00	0.00	0.00	0.00	0.00	0.14	0.00	0.00	0.00
742	LT HEAVY DUTY DIESEL TRUCKS - 1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

EIC3	DESCRIPTION	CO	NOX	SOX	TOG	PM	NH3	ROG	PM_{10}	PM_{25}
743	LT HEAVY DUTY DIESEL TRUCKS - 2	0.00	0.00	0.00	0.00	0.00	0.01	0.00	0.00	0.00
744	MED HEAVY DUTY DIESEL TRUCKS	0.00	0.00	0.00	0.00	0.00	0.03	0.00	0.00	0.00
746	HEAVY HEAVY DUTY DIESEL	0.00	0.00	0.00	0.00	0.00	0.09	0.00	0.00	0.00
750	MOTORCYCLES (MCY)	0.00	0.00	0.00	0.00	0.00	0.05	0.00	0.00	0.00
760	HEAVY DUTY DIESEL URBAN BUSES	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
762	HEAVY DUTY GAS URBAN BUSES	0.00	0.00	0.00	0.00	0.00	0.02	0.00	0.00	0.00
770	SCHOOL BUSES (SB)	0.00	0.00	0.00	0.00	0.00	0.01	0.00	0.00	0.00
776	OTHER DIESEL BUSES	0.00	0.00	0.00	0.00	0.00	0.04	0.00	0.00	0.00
780	MOTOR HOMES (MH)	0.00	0.00	0.00	0.00	0.00	0.26	0.00	0.00	0.00
810	AIRCRAFT	249.71	54.02	2.81	40.28	9.03	0.00	35.91	8.81	8.72
820	TRAINS	28.90	194.16	8.05	13.29	4.40	0.00	11.12	4.40	4.05
830	SHIPS AND COMMERCIAL BOATS	38.84	276.79	109.70	17.62	20.28	0.00	14.77	19.62	18.94
840	RECREATIONAL BOATS	126.38	3.82	0.01	36.92	1.39	0.00	34.86	1.25	0.95
850	OFF-ROAD RECREATIONAL	135.10	1.08	0.25	41.00	0.80	0.00	38.28	0.72	0.54
860	OFF-ROAD EQUIPMENT	1,536.69	680.34	3.49	259.95	39.32	0.00	225.28	38.92	35.52
870	FARM EQUIPMENT	101.24	106.20	0.72	24.87	6.47	0.00	21.29	6.46	5.93
890	FUEL STORAGE AND HANDLING	0.00	0.00	0.00	50.46	0.00	0.00	50.28	0.00	0.00
910	BIOGENIC SOURCES	0.00	0.00	0.00	709.42	0.00	14.54	578.69	0.00	0.00
920	GEOGENIC SOURCES	0.00	0.00	0.00	101.75	0.00	36.22	29.50	0.00	0.00

6.11.2 Spatial Plots

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

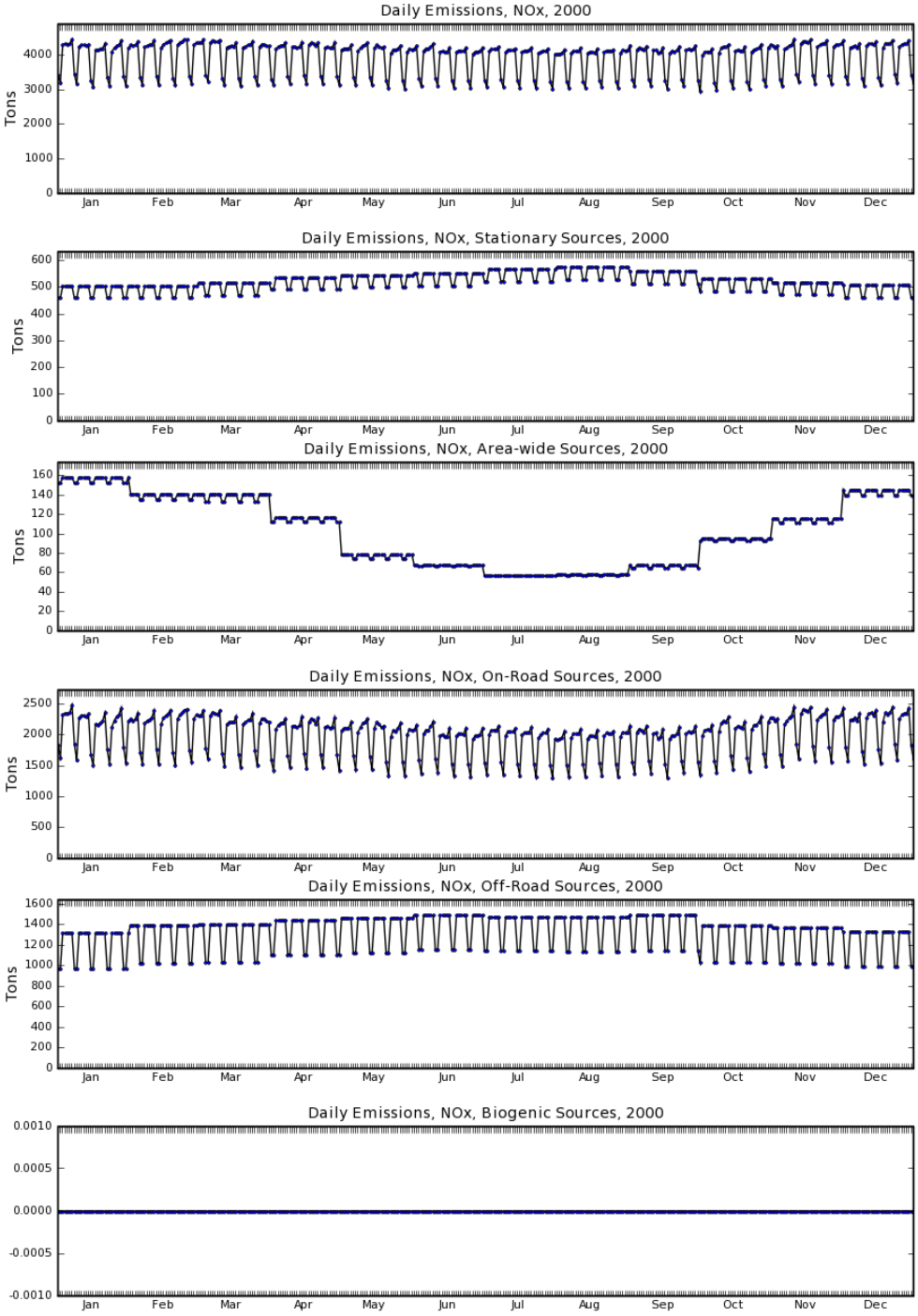
Plots by Pollutant and Time Period for Baseline and Adjusted Emissions



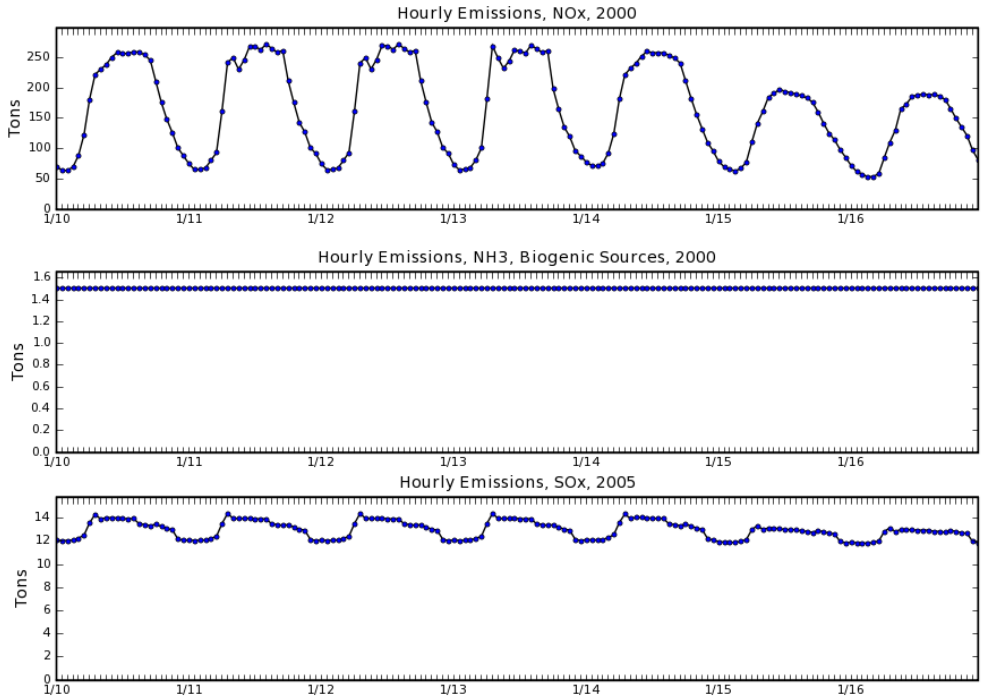
6.11.3 Time Series Plots

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

Weekly Time-Series Plots of Emissions by Year



Hourly Time-Series Plots of Emissions by Week



7 MODEL PERFORMANCE EVALUATION

The following subsections summarize the model performance evaluation procedures that will be used for the meteorological and photochemical models (based on: Emery & Tai, 2001; Tesche et al., 2002; U.S. EPA, 1991 & 2005).

7.1 Meteorological Model Performance Evaluation

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

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

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

When a dense network of representative meteorological measurements are not available, one can use a set of non-linear partial differential equations, known as governing equations, which describe the time evolution of the atmospheric system through space and time. The governing equations are comprised of the equations of conservation of mass, motion, heat, and water (Pielke, 1984). Meteorological models that integrate the set of governing equations through space-time are known as prognostic models. There is a long history of prognostic meteorological model applications in the SJV (Seaman, Stauffer, and Lario-Gibbs, 1995; Stauffer et al., 2000; Tanrikulu et al., 2000; Jackson et al., 2006; Bao et al., 2008; Livingstone et al., 2009; Michelson et al., 2010; Jin et al., 2010; Hu at al., 2010).

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

The second undesirable consequence is due to the complex terrain of California itself as shown in Figure 7.1. The centered finite difference scheme used in prognostic models works well when the terrain features are smooth and continuous. However, the SJV is bounded by three steep and rugged mountain ranges. The elevation can change by tens to hundreds of meters in one 4 km grid cell. The Coastal Range on the west is near the ocean-land interface which is also difficult to simulate. This makes the terrain in California complex compared to other parts of the country where the application of prognostic models have been more successful. To overcome this difficulty, the grid sizes were reduced from 4 km to 1.33 km as a test. The minor improvements in the fine-scale meteorological fields did not justify the nine fold increase in the computational time. Another option is to investigate the effect of using different model options,

especially those related to sub-grid-scale processes. This is being done now in collaboration with Professor Robert Fovell of the University of California at Los Angeles with funding from the San Joaquin Valley Study Agency.

7.1.2 Ambient Data Base and Quality of Data

The Air Quality and Meteorological Information System (AQMIS) is a web-based source for real-time and official air quality and meteorological data (www.arb.ca.gov/airqualitytoday/). This database contains 1969-2011 meteorological data (partial months for 2011). The data until the end of 2008 are quality assured and deemed official. In addition ARB also has quality-assured upper-air meteorological data obtained using balloons, aircraft, and profilers.

7.1.3 Model Performance Evaluation Procedures and Metrics

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

Figure 7.1: Terrain height changes along with counties and major rivers and lakes in California (http://geology.com/state-map/california.shtml).

7.1.3.1 Statistical Evaluation

Statistical analyses will be performed to evaluate how well the WRF model captured the overall structure of the observed atmosphere during the five-month simulation period, using wind speed, wind direction, and temperature. Since observed moisture data are very scarce, relative humidity or mixing ratio will not be used in these comparisons. It is

quite common to see, especially in such a long numerical simulation period, that observed statistical characteristics of atmospheric flow may be captured well by the model during a certain time period and/or within some sub-domain while the agreement between the model and observations may not be reasonably good at other times and/or locations. As a result, the very first sign that we look for in the model results is whether the model can capture the overall characteristics of the atmosphere in a statistical sense during the entire simulated period and within the entire domain. Then, the same statistical calculations will be repeated within each subregion to find out in which subregions model predictions are good or acceptable and are not acceptable in others, so that the reason for weak model performance issues in a subregion can be investigated.

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

The mathematical expressions for these quantities are:

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

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

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

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

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

where, "*Model*" is the simulated concentrations, "*Obs*" is the observed value, and *N* is the number of observations. The model performance expectations are shown in Table7.1.

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

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

Table 7.1: Model Performance Expectations.

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

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

7.1.3.2 Phenomenological Evaluation

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

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

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

7.2 Air Quality Model Performance Evaluation

The U.S. EPA (1991) and ARB (1990) outline a number of procedures for analysis of base year, air quality model performance. These include spatial and time-series plots, statistical analyses, comparing simulated and observed pollutant concentrations, as well as sensitivity analysis of selected input fields. The purpose of the performance analysis is to provide some confidence that the air quality simulations – which are the basis of future-year ozone concentration estimates – are performing properly and for the right reasons.

The application of air quality modeling results to demonstrate attainment of the federal 1-hour ozone standard emphasized the simulated unpaired peak ozone concentration. Three statistical measures were recommended to evaluate model performance: unpaired peak ratio (UPR), paired mean normalized bias (NB), and paired gross error

(GE). These statistical measures were calculated for the modeling domain as a whole, and the NB and GE were calculated from all hourly concentrations in excess of 60 ppb (to avoid biasing the statistical measures with low concentrations). To meet performance guidelines, recommendations were that the UPR should be within ±20%, NB should be within ±15%, and the GE less than 35%. However, California's geography is very complex and modeling domains have evolved to cover large geographic areas. Thus it is recommended that the domains be divided into subregions, and that the performance measures be calculated independently for each subregion. The configuration of these subregions is somewhat arbitrary; however, they should be configured to isolate "common" regions of higher ozone. Figure 7.2 illustrates the proposed subregions for the statewide domain.

Along with the statistical measures discussed above, the graphical and statistical tests recommended by the U.S. EPA (1991 and 2005) and shown in Tables 7.1 and 7.2 will be used to assess overall model performance. Several sensitivity tests recommended by the U.S. EPA (1991) will also be used for qualitative evaluation. While the results of these sensitivity analyses are inherently subjective, they are designed to provide confidence that the air quality model is not only performing well, but is also properly responding to changes in inputs.

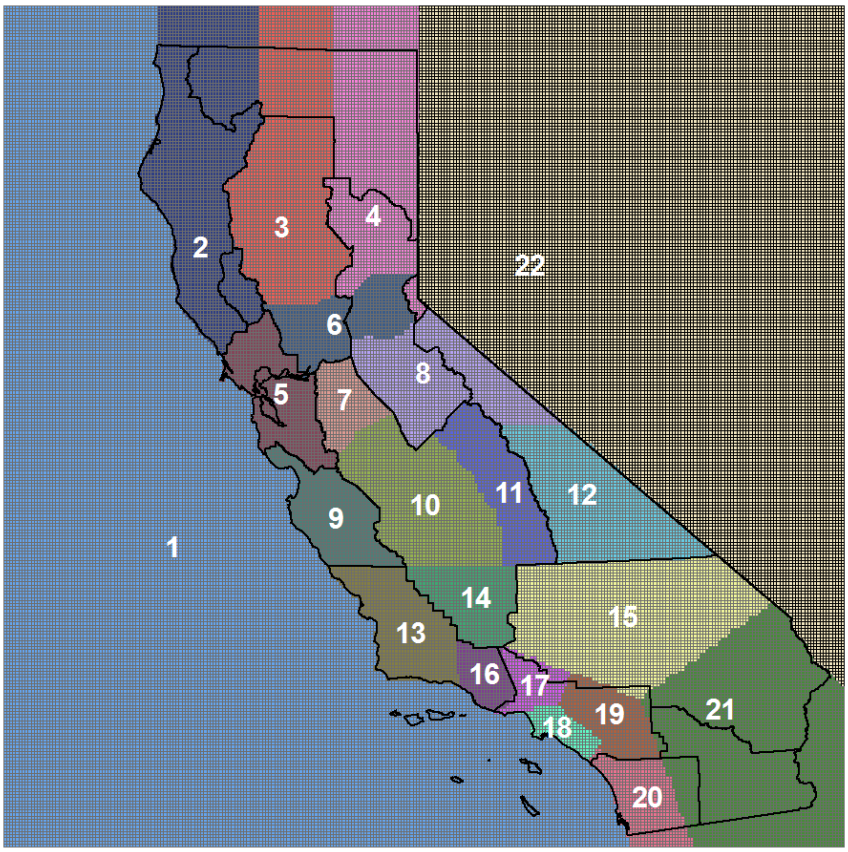


Figure 7.2: Sub-regions of air quality model performance evaluation (7: Northern San Joaquin Valley region, 10: Central San Joaquin Valley region, 11: San Joaquin Valley APCD About 3000 feet region, 14 Southern San Joaquin Valley region).

Table 7.2: Statistics for evaluating base year air quality model performance for all sub-regions.

- Mean normalized bias for all 1-hour ozone concentrations (60 ppb), unpaired in time and space for all sites
- Mean normalized gross error for all 1-hour ozone concentrations (≥60 ppb), unpaired in time and space for all sites
- Peak 1-hour ozone concentration ratio, unpaired in time and space

Table 7.3: Graphical tools for evaluating base year air quality model performance.

• Time-series plots comparing 1-hour measured and simulated concentrations of ozone, NO, NO2, and CO for each site. • Hourly spatial plots of 1-hour measured and simulated concentrations of ozone, NO, NO2, and CO for the CCOS modeling domain. • Scatter plot of 1-hour ozone concentrations for each day, and for each subregion of the modeling domain.

8 ATTAINMENT DEMONSTRATION

The U.S. EPA has not issued new guidance that prescribes how attainment for the 1-hour ozone National Ambient Air Quality Standard (NAAQS) should be demonstrated. Therefore, following previous EPA guidance for the 8-hour O_3 NAAQS (U.S. EPA, 2007), we propose to use the modeling results in a relative sense (i.e., using relative response factors or RRFs) to demonstrate attainment of the 1-hour O_3 NAAQS. The RRFs are calculated as the ratio of future-year and reference year ozone concentrations for each site. The RRF is then multiplied by a site-specific design value to estimate the future-year design value.

8.1 Criteria for Use of Modeled Days in RRF Calculations

Adequate model performance is a requirement for use of modeled results. The lack of acceptable performance greatly increases uncertainty in the use of the modeling results, and casts doubt on conclusions based on the modeling. Therefore only those days which satisfy the previously described model performance criteria will be utilized in RRF calculations.

In addition to the issue of model performance, analyses conducted by the U.S. EPA (2005) suggest that air quality models respond more to emission reductions at higher predicted ozone values. Correspondingly, the model predicts less benefit at lower concentrations. This is consistent with preliminary modeling in support of the 1-hour ozone standard conducted by the ARB and the districts. These results imply that RRF calculations should be restricted to days with predicted high ozone concentrations. It is thus reasonable to establish a minimum threshold for predicted peak 1-hour ozone concentrations in the reference year.

Based on the above discussion, we propose the following methodology for determining sites and modeled days to be used in the RRF calculations:

1) The modeled daily 1-hour peak ozone concentration of the site for the base year (model performance year) of the modeling must be within ±20% of the observed value at the site.

2) The modeled daily 1-hour peak ozone concentration of the site in the reference year must be 85 ppb or greater.

3) The sub-regional 1-hour statistical measures of NB and GE must fall within the thresholds of ±15% and 35%, respectively.

8.2 Relative Reduction Factors

As discussed above, the RRF is a monitor-specific value that is calculated based on daily peak 1-hour ozone concentrations simulated in a future year, divided by daily peak concentrations simulated in a reference year. To be consistent with the principle that the modeled attainment test and design values should be robust and stable over a number of different types of meteorology, the RRF should be based on multiple simulated days. The following methodology will be used to calculate site-specific RRFs:

Site-specific RRFs will be calculated as the ratio of the average daily peak 1-hour modeled ozone concentration in the future year, divided by the average daily peak 1-hour modeled ozone concentration in the reference year. Only those days satisfying the model performance and threshold criteria described below shall be included in the RRF calculation.

$$RRF_{AVG} = \frac{(FY_{1\text{–}hr})_{AVG}}{(RY_{1\text{–}hr})_{AVG}}$$

where RRF_{AVG} = *the average relative reduction factor for a monitor*

$(FY_{1\text{-}hr})_{AVG}$ = *the average future year 1-hour daily maximum concentration predicted near the same monitor, averaged over those days which satisfy model performance and threshold criteria*

$(RY_{1\text{-}hr})_{AVG}$ = *the modeled reference year 1-hour daily maximum concentration predicted near the same monitor, averaged over those days which satisfy model performance and threshold criteria*

As stated in the 8-hour ozone modeling guidance (U.S. EPA, 2007), the U.S. EPA recognizes that higher ozone values are more responsive to emissions controls. To emphasize this observation, we have extended the concept of average RRFs to form band RRFs. Here, we segment the simulated ozone concentrations into several bands that span the range of values. An average RRF is then calculated for each band. These band RRFs are then used to project reference-year design values into the future.

Detailed information on this procedure will be included in the modeling documentation for this SIP. In brief:

- For the days that meet model performance, develop RRFs for bands of concentrations. For example, one can develop RRFs for base-year concentration ranges (bands) of 130-120 ppb, 119-110 ppb, 109-100 ppb, 99-90 ppb, etc. These band-RRFs represent the model's response to similar concentrations averaged over different meteorological and emissions conditions.

- Select the top N (e.g., 10) 1-hr concentrations during the three years ending in the base year. Using a relatively large (compared to four) number of base-year concentrations will ensure that we fully allow for possible reshuffling in the future year.

- Project each such concentration to the future year using the RRF for the band that concentration falls into. Since the simulated and observed concentrations are not perfectly correlated, use a correlation diagram of simulated to observed values to determine what RRF band a given observation would fall into.

- Re-sort the future-year concentrations and select the fourth highest value. This will be the future 1-hr design value that should be compared with the NAAQS.

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

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

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

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 1-hour ozone Design Values
- Access to input data and simulated results

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