PHOTOCHEMICAL MODELING PROTOCOL

FOR DEVELOPING STRATEGIES

TO ATTAIN THE FEDERAL 8-HOUR OZONE AIR

QUALITY STANDARD IN CENTRAL CALIFORNIA

California Air Resources Board
Planning and Technical Support Division
Sacramento, California 95814

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1 INTRODUCTION

1.1 Purpose

This modeling protocol is intended to both guide and describe the technical aspects of air quality modeling that is to be conducted in support of developing an 8-hour ozone State Implementation Plan (SIP) for central California. It will describe the data, technical decisions, and the procedures associated with producing computer-based simulations of ozone concentrations. It will also describe how model results will be evaluated with field measurements and how future year air quality will be simulated. The approach taken follows U.S. EPA modeling guidance for 8-hour ozone SIPs (2005).

1.2 Approach

The intent of this protocol is to utilize the best available science, technical tools, and data to develop the modeling system. Once the modeling system has demonstrated adequate performance, it will be used as a technical resource to assist decision makers in selecting the most effective future-year emission control measures to include in the SIP. Some examples of the types of questions that will likely be considered are:

- In terms of ozone formation, what are the regional and sub-regional effects of hydrocarbon emissions and emissions of oxides of nitrogen?

- With regard to reducing 8-hour ozone concentrations, what are the carrying capacities for the on-attainment areas in the region?

- What are the likely years that the non-attainment areas in the region will achieve attainment?

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. In particular, the following three groups provided substantial input:

- The 2000 Central California Ozone Study (CCOS) – More information on CCOS, including the organizational structure, CCOS products, and the Technical Committee (CCOS-TC) can be found via the following two links:

http://www.arb.ca.gov/airways/crpaqs/organization.htm

http://www.arb.ca.gov/airways/ccos/ccos.htm

- The Bay Area Modeling Advisory Committee (BA-MAC) – This technical group was established by the Bay Area Air Quality Management District (BAAQMD) to guide modeling in support of the 2004 Bay Area SIP revision. More information and results from this group can be found at:

  http://www.baaqmd.gov/pln/plans/ozone/2003_modeling/index.htm

- The SIP Gridded Inventory Coordination Group (SIP-GICG) – This group of regulatory agency staff (and, in some cases, their consultants) was established by ARB to coordinate the development and review of the emissions inventory inputs to SIP air quality modeling in central California.

The regular participants for each of these three groups are listed in the following two tables. Table 1.1a lists non-government participants and Table 1.1b lists government agency participants. The suite of candidate episodes, models, model inputs to consider, and, ultimately, the selected episodes, modeling tools, and inputs for use in SIP modeling were discussed within and among these technical groups, including via projects or contracts that were sponsored by them individually or collectively.

Table 1.1a – Consultants and Public/Private Stakeholder Representatives

Group	Employer	Representative	BA-MAC	CCOS-TC	SIP-GICG
Acadamia/Consulting	Alpine Geophysics	James Wilkinson	X		X
	Dowling and Associates	Carrie Anderson			X
	Envair	Steve Reynolds		X	
	ENVIRON	Chris Emery	X		X
	Golden Gate University	Ken Kloc	X		
	UC Berkeley	Rob Harley	X		
Environmental	West County Toxics Coalition	Henry Clark	X		
	Sierra Club	John Holtzclaw	X		
	Clean Air Partnership	Jude Lamare	X		
Industry	Chevron-Texaco	Steve Ziman	X	X	
	PG&E	Sam Altshuler	X		
	Shell	Christopher Rabideau	X	X	

Table 1.1b. Government Agency Stakeholder Representatives

Group	Employer*	Representative	BA-MAC	CCOS-TC	SIP-GICG
Federal Government	US-EPA (Region 9)	Carol Bohnenkamp	X	X	
	NOAA	James Wilczak	X	X	
Local Government	ABAG	Eugene Leong	X		
	BAAQMD	Amir Fanai	X		X
	BAAQMD	Gary Kendall	X		
	BAAQMD	Jean Roggenkamp	X		
	BAAQMD	Peter Hess	X		
	BAAQMD	Phil Martien	X	X	X
	BAAQMD	Saffet Tanrikulu	X	X	
	BAAQMD	Toch Mangat			X
	Fresno COG	Mike Bitner			X
	Monterey Bay APCD	Bob Nunes	X		
	MTC	Harold Brazil	X		X
	Sacramento Area COG	Gordon Garry			X
	San Joaquin Valley APCD	David Nunes	X	X	
	San Joaquin Valley APCD	Evan Shipp	X	X	X
	San Joaquin Valley APCD	James Sweet	X	X	
	San Joaquin Valley APCD	Gary Arcemont			X
	San Joaquin Valley APCD	Leland Villalvazo			X
	San Joaquin Valley APCD	Steven Shaw			X
	Sacramento Metro AQMD	Brigette Tollstrup	X		
	Sacramento Metro AQMD	Bruce Katayama	X	X	X
	Sacramento Metro AQMD	Charles Anderson	X		X
	Sacramento Metro AQMD	Hao Quinn			X
	Sacramento Metro AQMD	Larry Greene	X		
	TRANSDEF	David Schonbrunn	X		
	Yolo-Solano AQMD	Rene Toledo			X
State Government	CalTrans	Leonard Seitz			X
	ARB	Ajith Kaduwela	X	X	
	ARB	Anne Lin			X
	ARB	Bruce Tuter	X		
	ARB	Daniel Chau		X	
	ARB	Cheryl Taylor	X	X	X
	ARB	Eugene Yang		X	X
	ARB	Jeff Lindberg			X
	ARB	Jinyou Liang	X		
	ARB	John DaMassa	X	X	
	ARB	Martin Johnson			X
	ARB	Kemal Gurer		X	
	ARB	Mimi Sogutlugil			X
	ARB	Paul Allen			X
	ARB	Vernon Hughes	X	X	X

*NOAA – National Oceanic and Atmospheric Administration; ABAG – Assoc. of Bay Area Governments; BAAQMD – Bay Area Air Quality Management District; COG – Council of Government; APCD – Air Pollution Control District; MTC – Metropolitan Transportation Commission; AQMD – Air Quality Management District; CalTrans – California Department of Transportation.

1.3 Background

The shaded relief maps provided at the end of this section illustrate the topography in 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 features of airflow within the region contribute 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 to 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 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 due mostly 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 on 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:

<u>Sea Breeze and Marine Air Intrusion:</u> 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. Depending on the temperature structure of the Valley, the jet may not be able to exit through the Tehachapi Pass (~1400 m); in which case the air is forced 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 EPISODE SELECTION

As indicated in the first chapter, a large body of work already exists that has been produced by stakeholder groups towards the goal of determining representative, candidate episode periods for use in 8-hour ozone SIP modeling for the region. From this collective body of work, the following four episodes were identified as having the greatest potential for SIP modeling in the region:

- July 7-13, 1999 (captured with routine State and Local measurements)
- July 29-August 2, 2000 (CCOS-studied episode)
- September 17-21, 2000 (CCOS-studied episode)
- August 8-15, 2002 (captured with routine State and Local measurements)

Due to time constraints and based on model performance issues expressed by stakeholder efforts for the two later episodes, the first two episodes (July 7-13, 1999, and July 29-August 2, 2000) were determined to be the most adequate for the initial round of 8-hour ozone SIP attainment planning. Brief summaries of the two episodes selected for SIP modeling are contained in the following sections.

With regard to the two episodes being dropped from consideration, CCOS sponsored a project that was focused on developing the third (September, 2000) episode while the Sacramento Metropolitan Air Quality Management District (SMAQMD) sponsored a project to develop the fourth (August, 2002) episode. As indicated above, achieving adequate model performance for both of these periods was problematic. It should be noted, however, that a subsequent effort is now underway (via a pending 2007 CCOS Request for Proposals) to improve model performance for the September, 2000 episode. More information on efforts to initially develop or to improve these two dropped episodes can be found via the following links:

September 2000 (CCOS):

http://www.arb.ca.gov/airways/ccos/docs/03-01CCOS_Alpine_Final_Report_PDF.zip

http://www.arb.ca.gov/airways/ccos/RFPs/Sept_Modeling/RFP_septmodeling_FINAL.pdf

August 2002 (SMAQMD):

http://www.airquality.org/cleanairplan/modeling.shtml

2.1 July 7-13, 1999 (Routine Episode)

On July 8, 1999, high pressure began to build throughout the southern United States. Through July 10, the high pressure at 500mb increased and a relative high formed over the 4-Corners area. After July 10, the 500mb high began to regress westward and weaken after July 12. Winds aloft during this period were generally weak and variable.

During this episode period, the high-pressure ridges that formed were generally shallow. The maximum 500mb pressure-heights were in excess of 594 dm and are consistent with the high pressures and strong subsidence generally associated with the occurrence of high ozone concentrations within central California.

Ozone concentrations exceeded 125 ppb on July 8-13, 1999. On July 8, a concentration of 155 ppb was recorded at Parlier; however, this peak was isolated in time and space and was considered difficult to model. On July 10, high ozone concentrations were recorded throughout the Sacramento area, with a peak of 147 ppb. On July 11, high ozone concentrations were recorded from the San Francisco Bay Area into Sacramento, and continued into July 13 with a high ozone concentration of 156 ppb recorded at Concord. Concentrations declined thereafter and on July 13, the only concentration exceeding 125 ppb was the 132 ppb recorded at Merced.

The 8-hour ozone concentrations exceeding 85 ppb in this period were recorded on July 8, and occurred through July 13 (Table 2.1). In the San Joaquin Valley, ozone concentrations in excess of 85 ppb were recorded for at least 10 sites on each day of the episode period until July 13. The maximum 8-hour ozone concentration was recorded at the Fresno – First Street site on July 11. In the Sacramento Area, the peak 8-hour concentration was recorded at Folsom, also on July 11. In the San Francisco Bay Area, the maximum daily ozone concentrations did not exceed 85 ppb until July 10. However, the daily maximums and number of sites recording concentrations greater than 85 ppb increased on July 11 and 12. The maximum 8-hour ozone concentration in the San Francisco Bay Area during this episode period was 123 ppb recorded at Concord on July 12.

Table 2.1 The number of monitoring sites with measured 8-hour ozone concentrations exceeding 85 ppb and daily maximum measured concentrations**.**

	Total Sites	July 8		July 9		July 10		July 11	
		Sites	Max	Sites	Max	Sites	Max	Sites	Max
Bay Area	19	0	72	0	73	2	95	11	116
Sacramento Valley	17	4	96	8	116	13	129	14	124
San Joaquin Valley	20	13	110	13	102	15	108	19	123

	Total Sites	July 12		July 13	
		Sites	Max	Sites	Max
Bay Area	19	7	123	0	74
Sacramento Valley	17	13	107	4	91
San Joaquin Valley	20	11	116	8	117

2.2 July 29-August 2, 2000 (CCOS Episode)

During the 2000 CCOS field campaign, the duration of high pressure ridging, which fosters ozone production, was somewhat shorter than those recorded in previous summers. When compared to the 30-year climatology for June to September for Fresno and San Francisco, (Table 2.5-1, CCOS Field Study Plan, Fujita et al. 1999), the inland temperatures were statistically colder during CCOS, while the coastal temperatures were not. For example the study period daily temperature maximum at Fresno, 91.4±0.7 °F, was more than three standard deviations below the climatological value of 94.8 °F. The study period daily temperature maximum at San Francisco, 71.5±0.7 °F, was below the climatological value of 72.0 °F. This can be explained by the occurrence of fewer high pressure ridges and/or ridging of shorter duration passing over the western United States, where the inland sites are not as influenced by the mitigating effects of the Pacific Ocean (after Lehrman et. al., 2003). Statistical analyses indicate that this episode is in the upper range of poor air pollution dispersion meteorology that results in exceedances of the NAAQS in the San Joaquin Valley. Lehrman (2003) reported that all days during the July-August 2000 ozone episode fall into meteorological categories within one standard deviation of the mean for days greater than the NAAQS.

Inspection of 500-mb and surface daily weather maps shows that low-pressure troughs, cut-off lows, and zonal flow occurred during the first seven weeks of the study period, except for one brief incursion of an Eastern Pacific High, which brought some ridging over the West Coast. That occurred on June 14-15, which became the Practice Intensive Operating Period (IOP) on June 14 and 16. After this slow start to the study

period, ridging during IOP#1, July 23-24, brought a Four Corners High. Unfortunately, this 500-mb high positioning can also foster monsoonal flow. Too much positive vorticity (lifting) kept ozone concentrations low over much of the study area, in particular the southern San Joaquin Valley. This high persisted the next week and moved over the Great Basin during IOP#2, July 30-Aug 2. By August 6, the high had weakened and moved eastward leaving troughs or zonal flow over California for almost another week. IOP#3 was conducted on August 14 when the high had broadened to include southern California. But IOP#3 lasted only one day, as the high retreated from a trough moving down from the Gulf of Alaska. As the high retreated further east to Texas, Oklahoma, and Arkansas, a trough remained over the pacific Coast as far south as Northern California, but cut-off lows and zonal flow over southern California kept ozone concentrations relatively low. Because of the lack of suitable episodes during the originally scheduled end of the field study on September 3, the CCOS was extended to late September.

On September 11, zonal flow over the Pacific Northwest and a weak cut-off low off the California coast were adjacent to a new high expanding up from the south over Northern Mexico. Due to the slow start in the study period, IOP#4 was called for September 14. Unfortunately, a relatively strong cut-off low developed offshore of the US-Canadian border and kept the high to the east. As the cut-off low moved east over Idaho, a relatively strong high built in behind it over the eastern Pacific. IOP#5 was initiated on September 17, a ramp-up day, and continued through the 21st when the high had regressed back westward leaving strong northerly flow through a trough axis from Hudson Bay to San Francisco Bay. As the trough gave way to zonal flow over the next week, flights were conducted to monitor boundary conditions during zonal flow conditions during September 30 through October 2.

By July 25, the ridge had weakened slightly and dropped southeastward into eastern New Mexico, and a trough developed along the West Coast from Point Conception to British Columbia. This resulted in the lowering of 500 mb heights and 850 mb temperatures somewhat during July 25 and 26. However, on the 27th, the high-pressure ridge once again regressed towards the west and strengthened somewhat to become centered once again in the Four Corners area. With this regression of the ridge, the 850 mb temperature and 500 mb heights at Oakland (OAK) once again rose during that period and continued to rise through July 30, and the period of the next IOP. During the IOP of July 30 through August 2, the ridge remained strong and continued to slowly regress towards the west until it was centered near Reno, Nevada by July 31. The OAK 850 mb temperature during the IOP reached as high as 27°C and the 500 mb height topped at 5,970 m.

During the July-August 2000 CCOS episode, the highest ozone level was a recorded 151 ppb at Edison on August 2 in the southern portion of Central Valley. Peak ozone values on July 30 occurred in the San Joaquin Valley, where values near 130 ppb were recorded at Parlier and Edison; the Bay Area and Sacramento region experienced no federal 1-hour exceedances that day. On July 30, only the San Joaquin Valley exceeded the 1-hour NAAQS for ozone. Concentrations at Parlier and Edison were 129

and 128 ppb, respectively. The highest reading on July 31 occurred at Livermore in the Bay Area. The measured peak value was 126 ppb. This was the only exceedance of the federal standard on that day in the CCOS domain. The only federal 1-hour exceedances on August 1 occurred in the Sacramento region, which experienced its highest ozone readings of the episode. On that day a peak value of 133 ppb ozone was observed at the Sloughouse site. Similarly, the only exceedances on August 2 occurred in the San Joaquin Valley, which had peak readings of 131 ppb in the northern part of the valley (Turlock and Modesto) and the maximum concentration for the episode at Edison of 151 ppb.

Maximum daily 8-hour ozone concentrations exceeded 85 ppb beginning on July 30 (see Table 2.2). Most of these were located in the San Joaquin Valley with a maximum of 106 ppb at Parlier. On July 31, ozone concentrations exceeded 85 ppb in the San Francisco Bay Area, the Sacramento Area, and the San Joaquin Valley. The frequency of high 8-hour ozone concentrations within the Sacramento Area and the San Joaquin Valley increased on August 1 and 2, with the maximum of 113 ppb recorded at Edison on August 2.

During this episode period, there were a number of large wildfires in the southern part of the study domain. Model-based analyses suggested that these fires impacted ozone concentrations measured in Kern County.

Table 2.2 The number of monitoring sites with measured 8-hour ozone concentrations exceeding 85 ppb and daily maximum measured concentrations.

	Total Sites	July 30		July 31		August 1		August 2	
		Sites	Max	Sites	Max	Sites	Max	Sites	Max
Bay Area	11	0	66	2	90	1	91	2	94
Sacramento Valley	16	4	93	2	89	11	109	9	107
San Joaquin Valley	25	14	106	11	104	18	110	19	113

2.3 Available Observational Data

Model performance for the computer simulations of the two episodes characterized above will be based on comparing model predictions with observational data collected from both routine field measurement efforts as well as from the Central California Ozone Study. The data networks for both of these sources are described below.

2.3.1 Routinely Collected Data (1999)

Routine meteorological and air quality data are collected regularly 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/aqd/namslams/namslams.htm

2.3.2 Data Collected During CCOS (2000)

The Central California Ozone Study database is comprised of data collected during the summer of 2000 at a variety of special study stations, routine field stations, and supplemental sources. The CCOS monitoring network is illustrated in Figures 2.1 and 2.2. More specific information regarding the CCOS field study design and CCOS data collection efforts, including information on the supplemental data sources, can be found in the documents located under the following link:

http://www.arb.ca.gov/airways/CCOS/CCOS.htm

In addition, CCOS observational data collected during the summer, 2000, field study can be accessed via interactive web queries at:

http://www.arb.ca.gov/airways/Datamaintenance/default.asp

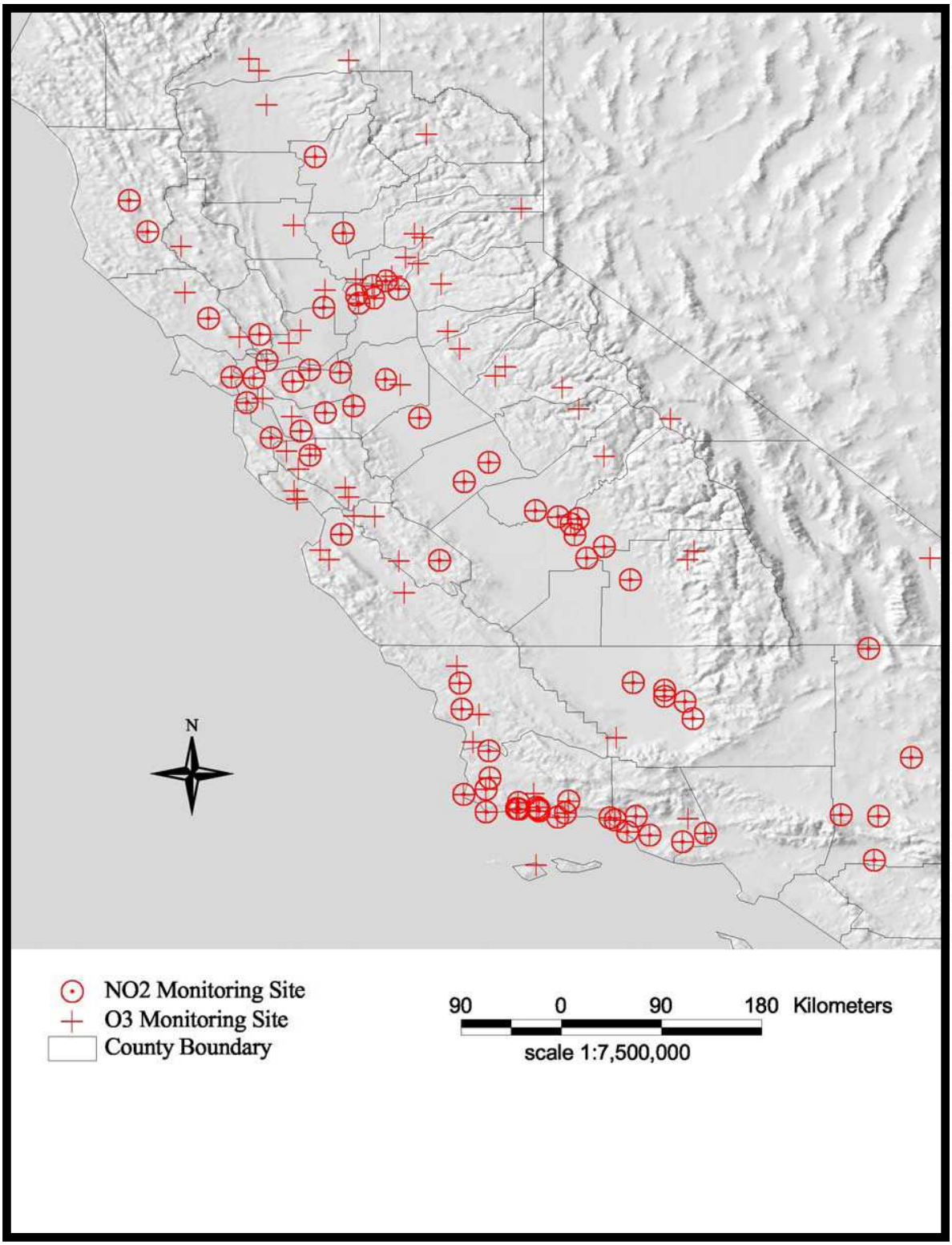


Figure 2.1 Existing routine ozone and nitrogen oxides monitoring sites.

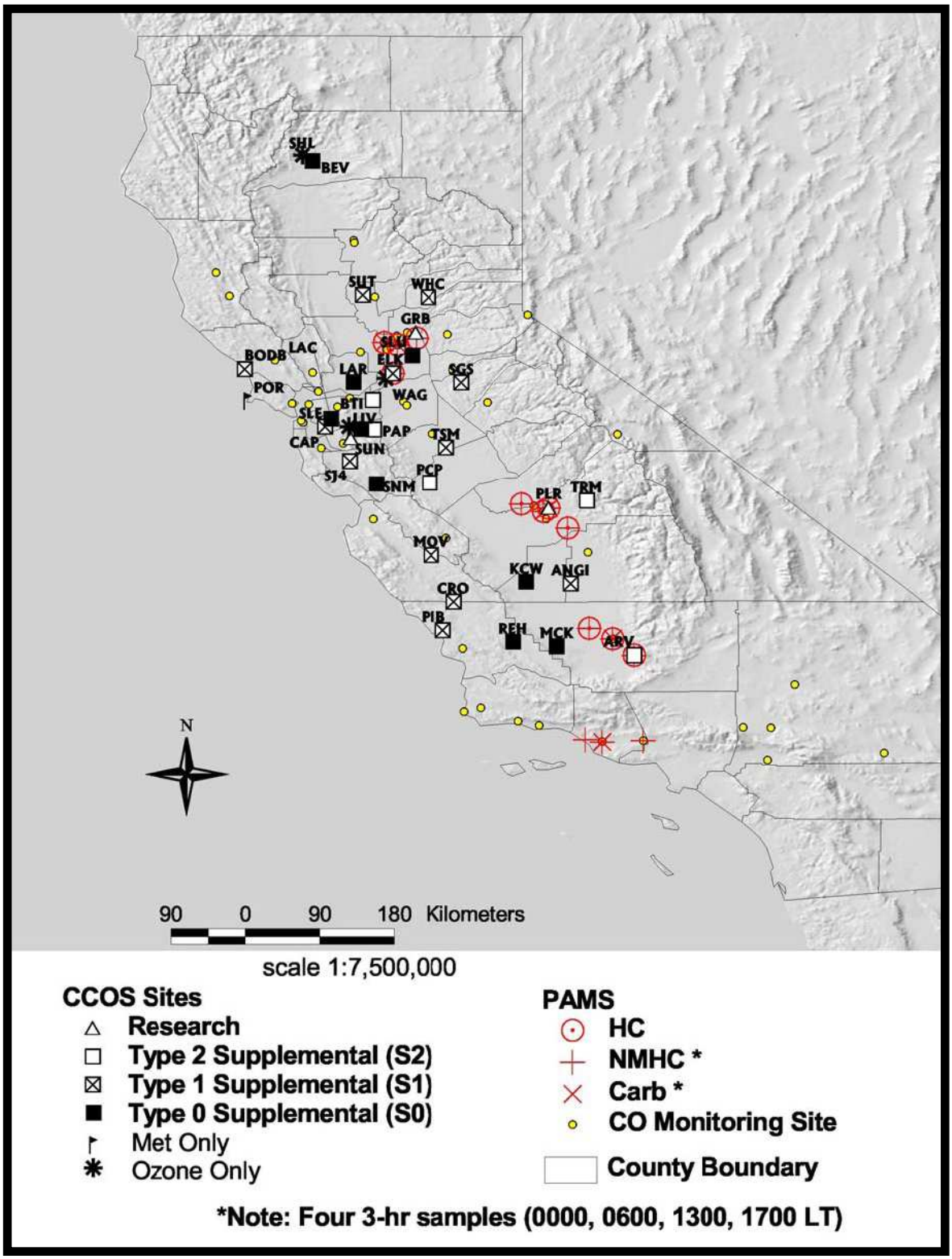


Figure 2.2 CCOS supplemental air quality and meteorological monitoring sites, and Photochemical Assessment Monitoring Stations.

3 MODEL SELECTION

This chapter describes the selection of the meteorological and air quality models to be used.

3.1 Meteorological Model

Meteorological model selection is based on a need to accurately simulate the synoptic and mesoscale meteorological features exhibited during the selected episodic periods. The main difficulties in accomplishing this are California's extremely complex terrain and its diverse climate. It is desirable that atmospheric modeling adequately represent essential meteorological 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 objective models to prepare meteorological fields for photochemical modeling. There are various numerical models that are used by the scientific community to study the meteorological characteristics of an air pollution episode. The models under consideration for SIP modeling are:

- NCEP ETA model (Mesinger et al, 1988),
- Regional Atmospheric Modeling System (RAMS) (Pielke et al, 1992),
- Mesoscale Meteorological Model Version 5 (MM5) (Grell et al, 1994), and
- Weather and Research Forecasting Model (WRF) (Skaramock et al, 2005).

The NCEP ETA model is primarily used by the National Weather Service as a forecast model and has been used only in limited applications as a research tool. The RAMS model has been used extensively both as a research tool as well as a forecast model by various scientific communities.

The Bay Area Air Quality Management District (BAAQMD) has been using RAMS along with MM5 over the last decade. The application of RAMS conducted by BAAQMD showed consistent results or no better than MM5 simulations for selected episodes. The recent air quality results of the BAAQMD indicated some undesirable model performance characteristics of RAMS (Martien, BAAQMD, 2004, personal communication). Also, the intensive effort from BAQQMD on improving the RAMS model during the past years was curtailed due to limited technical resources.

MM5 is a mesoscale, limited area, non-hydrostatic numerical model developed by Penn State and the National Center for Atmospheric Research (NCAR). It uses a terrain-following, Lambert Conformal, sigma coordinate system. MM5 allows users to study the atmospheric motions at small scales by explicitly treating the effects of convective motions on atmospheric circulations. It has been improved on an ongoing basis over

the last two decades by contributions from a broad scientific community and has been maintained by NCAR along with necessary meteorological and geographical input data. Based on the complexity of terrain in northern and central California, the MM5 model represents an appropriate tool for resolving dynamics and thermodynamics using nesting capabilities. The ARB has also been using the MM5 model over the last two decades, since it has been widely used and tested for various meteorological regimes over the world and has been supported by the NCAR.

NCAR is currently developing the WRF model to eventually replace MM5. However, the model is still under development and has not been extensively tested or demonstrated for SIP use. In addition, the preliminary tests that have been conducted by NCAR to date have not reported any significant improvement over MM5.

Based on preliminary work by the stakeholder groups mentioned in Chapter 1 as well as the long history of utilizing MM5 for SIP modeling, the MM5 numerical model will be used to generate meteorological fields for SIP modeling.

3.2 Photochemical Model

ARB considered several photochemical air quality models to simulate the two episodes under consideration:

- SAQM (Chang et. al.,1997),
- CAMx (ENVIRON, 2004), and
- CMAQ (USEPA 1999).

The SAQM (SARMAP Air Quality Model) model was used for the 1994 ozone SIP modeling for the San Joaquin Valley (SJVUAPCD, 1994). This model was built upon the basis of the RADM (Regional Acid and Deposition Model) in 1993 for the SARMAP air quality study domain with non-optimal numerical calculation and coding. The program was not coded in a modular fashion to facilitate updates (like alternative modules), the documentation is incomplete, and the model has not been successfully applied to ozone modeling problems outside of the San Joaquin Valley since the SARMAP study. Embarking on updating and recoding this model for the present day would require an unwarranted level of resources to adopt the most recent transport numerical schemes and photochemical mechanisms (or any other major modification).

The CMAQ model is a widely recognized and highly regarded photochemical model supported by the US EPA. It has been widely used throughout most of the United States for ozone, PM, and visibility analysis; however, its successful application within California has been limited. It is a flexible model and allows the selection of alternative modules, such as a different chemical mechanism, advection scheme, or chemical solver. The CMAQ model has been shown to run slower than alternative models; however it has been linked to the MPI (Multiple Processor Integration) software library package to run in parallel through a distributed process mode, significantly reducing episodic run times.

The CAMx model is used throughout the United States. It is widely viewed as one of the better documented and supported air quality models. Periodic updates from the developers ensure that more recent technical developments are incorporated. The CAMx model has also been shown to be very flexible. Alternative chemical mechanisms (CB-IV and SAPRC99) and advection schemes can be selected and meteorological inputs may be developed from objective/diagnostic or prognostic meteorological models. It also has two built-in probing tools, DDM (Decoupled Direct Method) for formal sensitivity analysis and PA (Process Analysis) for model dynamic examination. A PM module for simultaneous simulations of ozone and aerosols has recently been updated.

Tonneson (2003a) prepared test case simulations for the July-August, 2000 episode using the CAMx, SAQM, and CMAQ models. Within the allotted time, the simulations using CAMx were the only ones completed. However, the study strongly suggested better model performance by CAMx over the other two (Tonneson, 2003b). At CARB (CARB, 2003), the CAMx air quality model was configured for the July-August, 2000 episode in approximately 1 day (excluding the development of the required meteorological fields). The preparation of the SAQM took approximately 2 weeks, and the CMAQ model took approximately 2 months (much of this time was spent investigating the installation of the CMAQ code and the code for the IOAPI and MPI libraries on an LINUX system and addressing file-size limitations). Given this relative ease of use, its acknowledge stature as a state-of-the-art photochemical air quality model, and its flexibility in accepting meteorological inputs, the CAMx model was selected as the primary air quality model for the CCOS ozone modeling. This decision was reinforced by the selection of CAMx for SIP modeling by the South Coast Air Quality Management District (SCAQMD, 2005) and the hope that one model can be used throughout the State of California.

While selecting CAMx as the primary model of choice for CCOS modeling, it was also acknowledged that CMAQ is an alternative model that is being widely used across the United States for ozone SIP modeling. Therefore, as resources allow, the CMAQ photochemical model may also be run for the episodes to compare the performance of the two models.

4 MODELING DOMAIN AND GRID STRUCTURE

As described in Chapter 1, stakeholders have already produced a significant body of work, including model simulations, for the two selected modeling episodes. Selection of the domain and grid structure described in this chapter and to be used for SIP modeling are based on this prior experience.

4.1 Meteorological Modeling Domain

The MM5 meteorological modeling domain is consistent for both episodes. It consists of three nested grids: 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 subsequent two inner grids, D02 and D03, are placed within the coarser grids such that they are not too close to the lateral boundaries. The innermost grid D03 consists of 189 x 189 grid cells having an origin at -384 km x -300 km (Lambert Conformal projection). Although a nested grid structure is configured, each modeling domain was run independently using the output of its coarser, parent grid as input. The D03 grid is intended to resolve the fine details of atmospheric motion and is used to feed the air quality model simulations.

4.1.1 July-August, 2000 Episode Application

The vertical structure of the modeling domain for this episode was developed under CCOS (Chapter 1) and consists of 50 vertical layers, for which the top layer extends to a height of approximately 15,000 magl (Table 4.1). 20 vertical layers were placed within the first 1000 magl of the whole depth of the modeling domain to resolve the small boundary layer atmospheric flow features such as large eddies and vertical advection of the fluxes of all meteorological quantities. Model integration was executed between July 29, 2000 at 12Z and August 3, 2000 at 12Z.

4.1.2 July, 1999 Episode Application

The vertical layer structure for the July 1999 episode was developed in collaboration with the Bay Area MAC (Chapter 1) and is configured in 30 layers, as shown in Table 4.2.

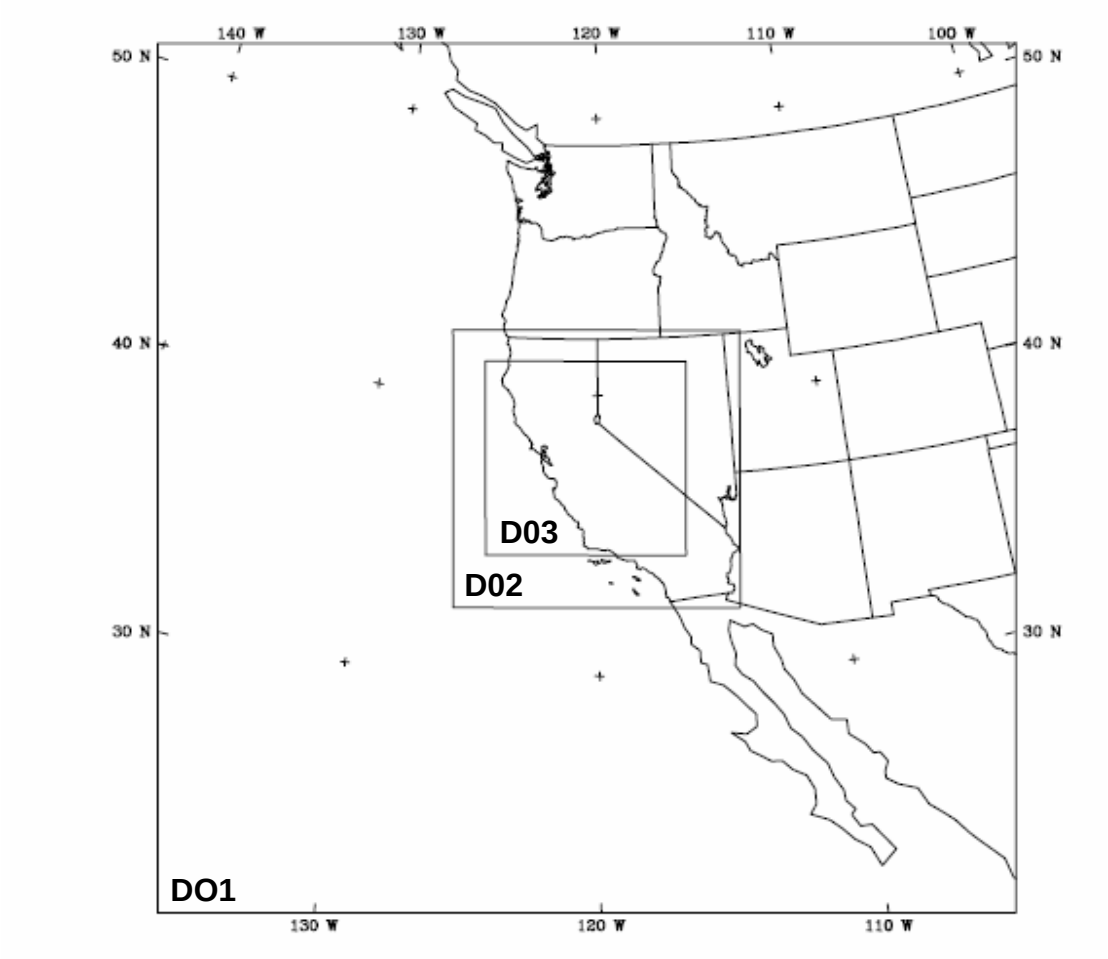


Figure 4.1: The structure of the three nested grids adopted for the numerical modeling for both SIP episodes using the MM5 model (D01 36km; D02 12km; and D03 4km).

Table 4.1 MM5 50 Vertical Layer Configuration for July-August 2000 Episode

Layer No.	Height (m)	Layer Thickness (m)
50	15674	1503
49	14171	1502
48	12669	1503
47	11166	1503
46	9663	1152
45	8511	993
44	7518	856
43	6662	738
42	5924	636
41	5288	547
40	4741	473
39	4268	408
38	3860	351
37	3509	303
36	3206	272
35	2934	246
34	2688	221
33	2467	199
32	2268	180
31	2088	162
30	1926	146
29	1780	131
28	1649	119
27	1530	106
26	1424	96
25	1328	87
24	1241	82
23	1159	81
22	1078	77
21	1001	74
20	927	71
19	856	69
18	787	65
17	722	63
16	659	61
15	598	59
14	539	56
13	483	54
12	429	50
11	379	48
10	331	44
9	287	41
8	246	39
7	207	36
6	171	34
5	137	31
4	106	29
3	77	27
2	50	26
1	24	24
0	0	0

Table 4.2 MM5 30 Vertical Layer Configuration for July 1999 Episode

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

The objectives of the SIP require that the photochemical modeling domain include all of the Central Valley of California and upwind areas. The constraints of the CAMx air quality model require that the domain be rectangular to accept meteorological input fields from MM5. The resulting ozone modeling domain is mapped in a Lambert Conformal, Conic Projection with parallels at 30°N and 60°N latitude, with a central meridian at 120.5°W longitude. The domain origin is defined at 37°N x 120.5°W. The photochemical modeling domain is defined horizontally as 185x185, 4x4-km grid cells, shown in Figure 4.2. The domain lower, left-hand corner is at -376 x -292 km from the defined origin. The MM5 output for the 4-km modeling domain consists of a grid of 189 x 189 grid cells having an origin at -384 km x -300 km, and has been processed to match the air quality model domain. The emissions inventory domain that has 190x190 grid cells is also processed in order to match the air quality model domain. The vertical structure of the air quality modeling domain, depending on the meteorological model configurations, will be adjusted accordingly to generate the required inputs for two episodes.

The 4-km resolution domain included areas of ocean and land, and terrain elevations (cell-averaged) from sea level to 3712 magl. The San Joaquin Valley is part of the larger Central Valley of California than runs roughly north/south and is surrounded by mountains, except in the vicinity of the SFBA.

There are two scenarios being evaluated for the determination of the height of the ozone modeling domain. In the first view, referred to herein as the 'MM5' view (although not used for all MM5-based air quality simulations) the vertical reach of the ozone modeling domain extends to the height of the top of the prognostic modeling domain at 100 millibars (~15 km). To reflect this view, the vertical structure of the ozone modeling domain was defined as 20 layers using the sigma coordinate system. In the sigma coordinate system, vertical layer heights were defined in terms of normalized pressure levels, therefore, the exact thickness of each layer varies somewhat as air temperature and density change across the domain. An additional justification for a vertical domain to 15,000 magl is that the presence of deep vertical layers aloft would dampen adverse effects from spurious vertical velocities that may occur in the wind fields from some meteorological models (ENVIRON, 2005a).

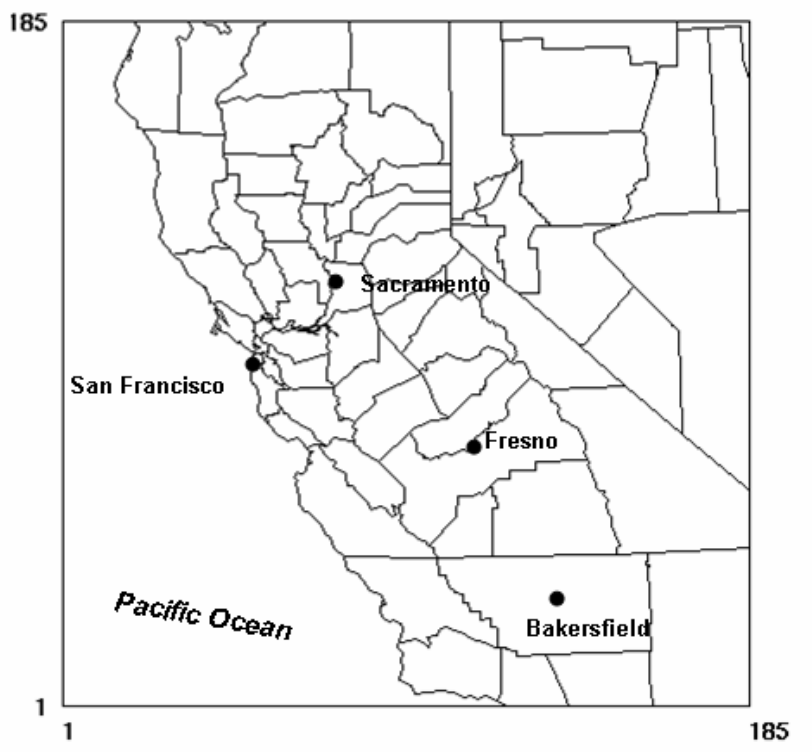


Figure 4.2 Photochemical Modeling Domain with185x185 Grid Cells at 4x4-km Horizontal Resolution

The number of vertical layers used in the ozone simulations will be tied closely to the meteorological model ultimately used. Configurations of 16-layer and 20-layer will be used for the July 1999 and July-August 2000 episodes, respectively, as shown in Table 4.3.

All photochemical model simulations will be run using a Pacific Daylight Time (PDT) time base.

Table 4.3 Vertical Layer Heights(m) of Photochemical Modeling for July-August 2000 and July 1999 Episodes.

Layer No.	July-August episode 50-Layer MM5 configuration Height(m)	July 1999 episode 30-Layer MM5 configuration Height(m)
20	15673	
19	12669	
18	9663	
17	7518	
16	5289	4873
15	3860	3368
14	2935	2306
13	2268	1560
12	1781	1275
11	1424	1037
10	1159	839
9	927	673
8	722	534
7	540	418
6	329	322
5	246	241
4	172	174
3	107	118
2	50	71
1	24	32

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 (MM5) and the air quality model (CAMx) separately. Each section briefly covers the data upon which model initialization is based.

5.1 Initialization of the Meteorological Model

MM5 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 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 apriori guidance on the specific data or options to be used in MM5. Rather, these decisions are determined based on optimizing model performance. Thus, during the preparation of preliminary meteorological fields for the July-August 2000 and July 1999 SIP episodes, 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 MM5 model options and input datasets were determined. These are described in the following sections.

5.1.1 MM5 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 during each of the two selected ozone episodes.

For the July-August 2000 episode, the Kain and Fritsch (1993) cumulus parameterization scheme was selected for coarse grids, while no cumulus parameterization was used for the 4 km grid. In addition, the ETA model for the parameterization of boundary layer flow (Janjic, 1994), Dudhia simple ice scheme for the treatment of cloud microphysics (Dudhia, 1989), the RRTM scheme for the calculation of radiation (Mlawer, 1997), and NOAH Land Surface Model for the calculation of surface energy balance (Chen and Dudhia, 2001) were used in all grids.

For the July 1999 episode, no cumulus parameterization scheme was used for any of the grids and a 5-layer slab model (Dudhia, 1996) was used for the calculation of surface energy balance for all grids. The cloud radiation scheme was used for the 4 km grid. All other model options were kept the same as those used for July-August 2000 episode.

5.1.2 MM5 Initial and Boundary Conditions (IC/BC)

The MM5 IC/BCs were prepared based on 3-D analyses of ETA model output that is archived at NCAR by the National Center for Environmental Prediction (NCEP). These data are archived for the continental United States and have a 40 km horizontal resolution. Initial conditions to MM5 were updated at 6-hour intervals for the 36 and 12 km grids. In addition, surface and upper air synoptic observations obtained by NCEP are also used to further refine the IC/BCs.

5.1.3 MM5 Four Dimensional Data Analysis (FDDA)

The MM5 model was forced to follow the meteorological conditions observed during the July-August 2000 and July 1999 episodes by using the analysis nudging option of the Four Dimensional Data Analysis (FDDA) for the 36 and 12 km grids only. Input conditions for the 4 km grid were obtained from the output of the 12 km grid, and observational nudging option of FDDA was used to enhance these input conditions for the two episodes. Only wind measurements were used for observational FDDA due to some inconsistent temperature measurements.

The extent of meteorological data available for developing FDDA input datasets is different for the July-August 2000 and July 1999 episodes. The July-August 2000 episode benefited from the extensive CCOS field campaign conducted during the summer of 2000. About 300 surface and 25 upper air meteorological stations were operated during CCOS field campaign (Section 2.3) and provided additional meteorological data in addition to the routine surface data that are available through the instruments operated by local air districts, ARB, and National Weather Service. Since a separate field campaign was not in place during the July 1999 episode, this episode had only six upper air meteorological stations plus the hourly surface data available from routine monitoring networks.

5.1.4 Meteorological Data Quality Assurance

In developing the IC/BCs and FDDA datasets, quality control is performed on all associated meteorological data (both inputs and outputs). 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 (e.g. after discussion with peers and stakeholders), the outlier data points are flagged as invalid and not used in the modeling analyses. Model-simulated meteorological

parameters such as 3-D winds, temperature, pressure, and humidity values are compared against surface and upper air observations to study the temporal and 3-D spatial structure of atmospheric motions as well as to evaluate the model performance. More details on the evaluation of model performance are provided in Chapter 7.

5.2 Air Quality Model Initial and Boundary Conditions

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, the episode, and the characteristics of the model being used.

This section discusses the initial and boundary conditions used by the Air Resources Board (ARB) in air quality modeling that will support developing the 8-hour ozone State Implementation Plan (SIP). The selected boundary conditions are summarized in Tables 5.2 and 5.3, while episode-specific initial conditions are provided in Table 5.4. These conditions were determined with stakeholder input at a March 10th, 2005, meeting of regulatory agency modeling staff.

5.2.1 *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 Air Pollution Research Center chemical mechanism (SAPRC99; Carter, 2000), have been developed; however, the use of SAPRC99 has historically been restricted by limited implementation in newer air quality models and the relatively large computational requirements.

Since SAPRC-99 is the most up-to-date chemical mechanism available (74 chemical species and 211 chemical reactions) and 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. Minutes of the October 8, 1999, Reactivity Scientific Advisory Committee (RRAC) can be found at:

http://www.arb.ca.gov/research/reactivity/rsac/oct99-min.html

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 8-hour ozone air quality modeling in California.

5.2.2 *Supporting Information*

This section discusses ambient concentrations available from measurements, related studies, as well as USEPA guidance on initial conditions, boundary conditions, and background concentrations of pollutants. Ideally, initial and boundary conditions used in modeling would be based upon measurements. Unfortunately, for a domain as large as that defined for CCOS, the boundaries are located in remote Pacific ocean areas (56km from northern coast line, 200km from S.F. coast line, and 360km from southern coast line) and there are few measurements that may be considered uncontaminated by anthropogenic sources.

The USEPA (1991) recommends default initial/boundary conditions based upon species for the Carbon Bond IV chemical mechanism. Table 5.1 shows USEPA's recommended initial concentrations for individual CBIV species, including 40 ppb ozone, 2 ppb NO_x, and approximately 22 ppbC ROG.

During the year 2000 CCOS field study, pollutant concentrations aloft were measured along several aircraft flight patterns and from ozonesondes at two locations (Granite Bay and Parlier). However, comparison of measurements taken along the coast of California versus historical data collected offshore suggest that the CCOS concentrations may not represent concentrations occurring over the Pacific Ocean. Thus, whether the CCOS samples are appropriate for the definition of top or lateral boundary concentrations is subject to interpretation.

Ozonesondes were launched four times per day from Parlier and Granite Bay during CCOS intensive measurement periods. However, these sites were located within the Sacramento and San Joaquin Valleys and are not necessarily well suited to represent ozone concentrations on the lateral domain boundaries, several hundreds of kilometers from the launch locations. During the July-August, 2000 episode, ozone concentrations at 5000 meters above ground level (magl) ranged between about 50 and 90 pbb. However, during other episode periods such as the September 18-20, 2000 episode, ozonesonde measurements showed ozone concentrations at 5000 magl of 40 ppb or less.

Unfortunately, the CCOS aircraft measurements were conducted at altitudes that rarely exceeded 1500 magl. Depending on the time of day and flight-path, ozone concentrations measured aloft from the aircraft ranged from 15 ppb to more than 100 ppb. Ozone concentrations during CCOS in the 70-80 ppb range were measured from aircraft as far as 160 km offshore (to the west); however, these flights were few and the evaluation of wind flow patterns during these flights casts doubt on the representativeness of these measurements for model boundary concentrations.

A study by Newchurch et. al. (2003) reported annual-average ozone concentrations aloft from ozonesondes at four sites in the U.S. Among them, the Trinidad Head site is located at the north coast of California as shown in Figure 5.2. Ozone measurements from two single day ozonesondes launched by the National Atmospheric and Oceanic Administration (NOAA) on July 21 and August 1, 2000, at Trinidad Head and two CCOS ozonesondes during a CCOS intensive measurement period (IOP #2) are plotted in Figure 5.3. NOAA's measurements at Trinidad Head show ozone concentrations at 15 km aloft of around 135 ppb. The CCOS measurements at Granite Bay and Parlier have higher ozone levels below 5000 magl than the ozonesonde at Trinidad Head. This is likely due to location – higher ozone levels in the Sacramento and San Joaquin Valleys are expected versus on the coastline. An analysis conducted by the Bay Area Air Quality Management District (BAAQMD) found a similar difference: that measured concentrations along the California coastline consistently have lower ozone levels in comparison with inland measurements.

Table 5.1 USEPA Default Background Concentrations for Carbon Bond-IV Species (1991).

Species	Species Names	Concentration (ppbC)
OLE	Olefins	0.60
PAR	Paraffins	14.94
TOL	Toluene	1.26
XYL	Xylene	0.78
FORM	Formaldehyde	2.10
ALD2	Higher Aldehydes	1.11
ETH	Ethene	1.02
CRES	Cresol, Higher Phenols	0.01
MGLY	Methyl Glyoxal	0.01
OPEN	Aromatic ring fragment Acid	0.01
PNA	Peroxynitric Acid	0.01
NXOY	Total Nitrogen Compunds	0.01
PAN	Peroxyacyl Nitrate	0.01
HONO	Nitrous Acid	0.01
H2O2	Hydrogen Peroxide	0.01
HNO3	Nitric Acid	0.01
MEOH	Methanol	0.10
ETOH	Ethanol	0.10
O3	Ozone	40.00 (ppb)
NO2	Nitrogen Dioxide	2.00 (ppb)
CO	Carbon Monoxide	350.00 (ppb)
ISOP	Isoprene	0.10 (ppb)

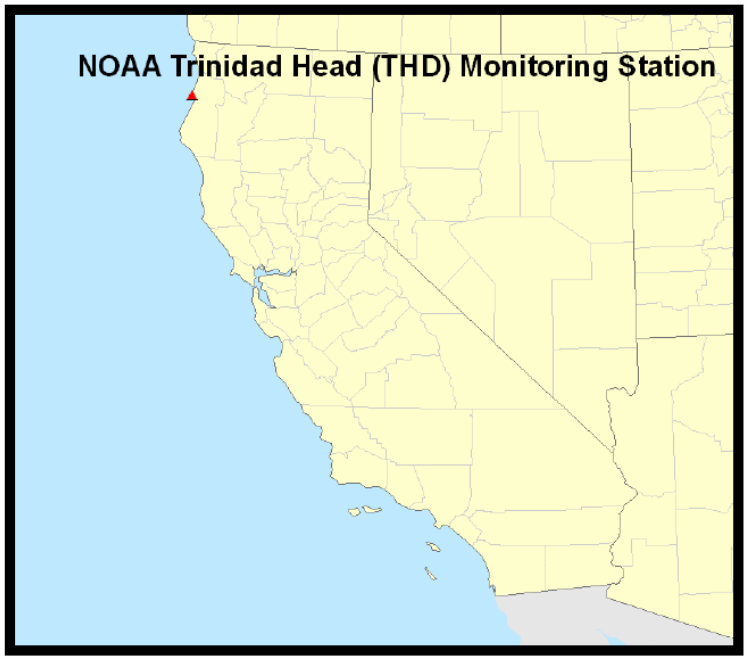


Figure 5.2. Trinidad Head ozonesonde site operated by NOAA.

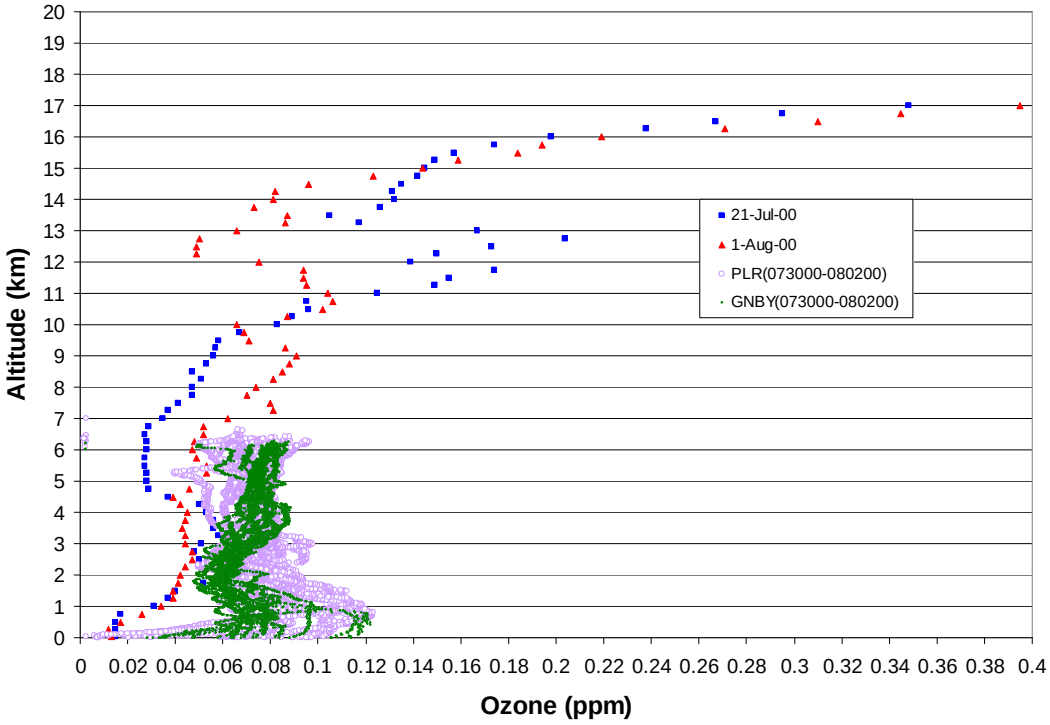


Figure 5.3. Ozone vertical profiles measured by ozonesonde at Trinidad Head (operated by the NOAA) as well as Granite Bay and Parlier (operated during CCOS).

The USEPA recommends a boundary condition for ozone of 40 ppb. However, analyses conducted by the BAAQMD (2005) suggested that lower concentrations are common at the surface near the Pacific coastline.

Reactive Organic Gases (ROGs) are the most difficult pollutant category to provide a measurement-based assessment of boundary concentrations, since there are only a limited number of measurements available. At the surface, all of the ROG samples collected during CCOS were made at sites located within the San Joaquin Valley, which are unlikely to represent boundary concentrations. A few dozen aircraft-based ROG samples were collected during the July-August, 2000, episode. However, the aircraft samples collected were of only short duration and an evaluation of the offshore flow patterns during these flights casts doubt on whether the measurements taken are representative of boundary concentrations.

For ROG boundary conditions, the U.S. EPA (1991) recommends default concentrations of 22 ppbC. However, ROG concentrations measured at the surface during CCOS were often higher than this. Aloft, concentrations of ROG measured during CCOS aircraft flights ranged from less than 10 to 100 ppbC. For most of the CCOS aircraft samples collected during the July-August, 2000 episode, ROG concentrations were between 20 and 40 ppbC. These data suggest that, while higher ROG concentrations occurred aloft, the concentrations aloft were not uniformly high. Analyses conducted by STI under a CCOS contract (2005) reported no significant correlation between high ROG concentrations aloft and high ozone concentrations observed throughout the episode. The data further suggested that the ROG concentration of 22 ppbC suggested by the USEPA was a reasonable estimate of clean air concentrations.

5.2.3 *Boundary Concentrations*

The recommended initial and boundary conditions are tabulated in Tables 5.2 and 5.3. More episode-specific details are provided in Attachment 1. The selected conditions were determined with BAAQMD, SJVAPCD, and SMAQMD stakeholder input at a March 10th, 2005, meeting of the SIP Modeling Working Group (Attachment 2).

Because of their relatively clean values, the boundary conditions for future years are kept the same as boundary conditions for the base years.

Table 5.2. Recommended air quality modeling domain boundary conditions.

	Region Top*	Over-Water Lateral	Over-Land Lateral
O_3 (ppb)	70	25-70	40-70
ROG (ppbC)	26	26	48
NO_2 (ppb)	1	1	1
CO (ppb)	200	200	200

* The July 1999 episode domain top is at approximately 5 km and the CCOS 2000 domain top is at approximately 15 km.

Table 5.3. Recommended SAPRC99 boundary conditions (ROG).

Over-Land			Over-Ocean	
Specie(s)	ppb*		Specie(s)	ppb*
HCHO	2.0		HCHO	2.0
RCHO	0.5		RCHO	0.5
ALK1	10.0		ALK1	6.0
ALK2	2.50		ALK2	1.0
OLE1	0.50		OLE1	0
OLE2	0.20		OLE2	0
ARO1	0.35		ARO1	0
ARO2	0.25		ARO2	0
ISOP	0.10		ISOP	0
ACET	1.0		ACET	1.0
PAN	0.005		PAN	0.005

* Based on USEPA (1991) and approximate 22 ppbC Carbon Bond IV ROG (chemical species not listed were set to concentrations of 0.00001).

Table 5.4. Summary of Episode-Specific Ozone & Precursor Boundary Conditions.

July 1999 (ppm)			
Layer	Elevation (m)	**Over water**	**Over land**
1	32	0.025000	0.040000
2	71	0.025000	0.040000
3	118	0.026000	0.042000
4	174	0.028000	0.043000
5	241	0.030000	0.045000
6	322	0.040000	0.050000
7	418	0.045000	0.052000
8	534	0.050000	0.055000
9	673	0.055000	0.058000
10	839	0.058000	0.060000
11	1,037	0.060000	0.062000
12	1,275	0.062000	0.064000
13	1,560	0.064000	0.065000
14	2,306	0.065000	0.066000
15	3,368	0.068000	0.068000
16	4,873	0.070000	0.070000

July-Aug. 2000 (ppm)			
Layer	Elevation (m)	**Over water**	**Over land**
1	24	0.025000	0.040000
2	50	0.025000	0.040000
3	107	0.026000	0.042000
4	172	0.027000	0.043000
5	246	0.028000	0.045000
6	379	0.030000	0.045000
7	540	0.030000	0.050000
8	722	0.040000	0.052000
9	927	0.045000	0.055000
10	1,159	0.050000	0.055000
11	1,424	0.055000	0.058000
12	1,781	0.058000	0.060000
13	2,268	0.060000	0.060000
14	2,935	0.062000	0.062000
15	3,860	0.063000	0.063000
16	5,289	0.064000	0.064000
17	7,518	0.065000	0.065000
18	9,663	0.066000	0.066000
19	12,669	0.068000	0.068000
20	15,673	0.070000	0.070000

Precursors (ppm)

	Over water	**Over land**
NO	0.000050	0.000050
NO2	0.001000	0.001000
CO	0.200000	0.200000
HCHO	0.002000	0.002000
RCHO	0.000500	0.000500
PAN	0.000005	0.000005
ALK1	0.006000	0.010000
ALK2	0.001000	0.002500
OLE1	0.000000	0.000500
OLE2	0.000000	0.000200
ARO1	0.000000	0.000350
ARO2	0.000000	0.000250
ISOP	0.000000	0.000100
ACET	0.001000	0.001000
ROG (ppbC)	26	48

5.2.4 *Initial Conditions and Spin-Up Period*

User-defined initial concentrations are often based on limited observational data and associated with a degree of uncertainty. To alleviate these uncertainties, the air quality model is started prior to the period of interest (i.e. a spin-up period) in an effort to allow the air quality model to generate appropriate initial conditions based on emissions and boundary conditions. Utilizing a spin-up period also reduces the affects of not specifying secondary reaction products or chemical radicals at start-up. That is, the spin-up period allows the model to use simulated meteorology and chemical transformation processes to generate more representative secondary and radical concentrations prior to beginning the simulation of air quality during the episode days of interest.

For both modeling episodes, a 2-day (48 hours) spin-up period will be utilized to minimize the impacts of the defined initial concentrations on the model predictions.

6 EMISSION INVENTORY DEVELOPMENT

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.

To support the body of work conducted by stakeholders, modeling inventories have been developed by ARB staff on an on-going basis for the July 1999 and July-August 2000 episodes. 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 State Implementation Plan (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.

To help coordinate the development of gridded inventories for CCOS modeling, an Emission Inventory Coordination Group (CCOS EICG) was established in February 1999. Participating in the group were many local air districts, regional transportation planning agencies (RTPAs), the California Department of Transportation (Caltrans), the California Energy Commission, the U.S. Environmental Protection Agency, and the ARB. Local air districts that participated included San Joaquin Valley APCD, Bay Area AQMD, Sacramento Metropolitan AQMD, Mendocino County APCD, Northern Sierra AQMD, Yolo/Solano AQMD, Placer County APCD, San Luis Obispo County APCD, and Monterey Bay Unified APCD. All local air districts in the CCOS region were invited to participate. The CCOS-EICG coordinated six studies through CCOS to improve the emission inventory:

- Small district assistance with point source updates (Contract 00-22CCOS, UC Davis). Section 6.2.1.3 describes this project in more detail.

- Small district assistance with area source updates (Contract 00-24CCOS, Sonoma Technology, Inc). Section 6.2.1.3 describes this project in more detail.

- Collect day-specific traffic count data and develop hourly distributions (Contract 00-04PM, UC Davis). Section 6.7.6 provides more detail.

- Develop the Integrated Transportation Network (ITN) and run the Direct Travel Impact Model (DTIM) (Contract 93-2PM, Alpine Geophysics). Section 6.7.9 describes this project in more detail.

- Validate databases for modeling biogenic emissions (Contract 00-16CCOS, UC Cooperative Extension). Section 6.8 provides more detail.

- Develop spatial surrogates for gridding area and off-road sources (Contract 00-24CCOS, Sonoma Technology, Inc.). Section 6.9 describes this project in more detail.

The CCOS EICG met on a regular basis to discuss CCOS emission inventory development issues into 2002.

As indicated in Chapter 1, as modeling inventories became available for the 1-hour ozone SIPs, the Air Resources Board established a SIP Gridded Inventory Coordination Group (SIP-GICG) in February 2003. The GICG consists primarily of government agencies and their contractors that are responsible for the variety of data used to develop gridded emission inventories for SIP purposes. Many of the same participants in the CCOS-EICG participate in the SIP-GICG. The purpose of the SIP-GICG is to conduct quality assurance of the emissions, and to distribute and coordinate the development of emission inputs for SIP modeling. In February 2005, the focus was changed to inventory development for the 8-hour ozone SIPs. Minutes from the SIP-GICG meetings are provided in Appendix A.

6.1 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

6.2 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 17,000 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.

6.2.1.1 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 6.2 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 CCOS inventories, all point sources were treated as possible elevated sources. Processing of the inventory for the photochemical model (e.g. CAMx) will determine which vertical layer the emissions from a process will be placed into. So, for the CCOS modeling inventories, the use of the term "point sources" is the same whether using the modeling or emission inventory definition.

Table 6.2 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, Trains
Area	Area-wide	Consumer Products, Architectural Coatings, Pesticides
Area	Stationary - Aggregated	Industrial Fuel Use
On-Road Motor Vehicles	On-Road Mobile	Automobiles
Biogenic	Biogenic	Trees

6.2.1.2 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 many local districts, including the Bay Area AQMD, Monterey Bay Unified APCD, Sacramento Metro AQMD and San Joaquin Valley APCD conducted extensive quality assurance to provide an accurate and complete inventory. Districts in the southern part of California had recently completed a similar exercise to improve their inventories as part of the Southern California Ozone Study (SCOS).

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 CCOS. 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 that was used initially for CCOS and 1-hour ozone SIP inventory preparation. This QA process has continued with the 2002 CEIDARS database, which is the basis for the modeling inventories being developed for the 8-hour ozone SIP.

- 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.

6.2.1.3 Improvements to Base Year Emissions for CCOS

In addition to the extensive QA checks described above, the CCOS Emission Inventory Coordination Group agreed to assist the small districts in the CCOS domain. Many small districts in the CCOS region have limited staff and resources to provide updated emission inventories to the ARB. After discussion with staff from districts in the Sacramento Valley and Mountain Counties Air Basins, two studies were decided upon. One study would focus on point sources and the second on area sources.

District staff said that they did have emission estimates for their point source facilities, but that they did not have the resources to provide the data to ARB. The first study sent engineering students from UC Davis (Kleeman, 2000) to visit several districts to gather the emissions and related data for 1999. The students then put the information into ARB's CEIDARS database. Two teams containing three students and one ARB staff person each visited Amador County APCD, Butte County AQMD, Colusa County APCD, El Dorado County APCD, Feather River AQMD, Glenn County APCD, Northern Sierra AQMD, Placer County APCD, Shasta County AQMD, Tehama County APCD, Tuolumne County APCD, and Yolo/Solano AQMD. The results of this project have been incorporated into the 1999, 2000, and 2002 CEIDARS inventories.

For area sources, district staff said that the best way to provide assistance would be to have a contractor develop emission estimates for the area source categories for which the districts were responsible. The CCOS study contracted with Sonoma Technology, Inc. (STI) (Coe, 2003) to prepare revised emissions estimates. STI would format the emissions and related data for input into the CEIDARS database. District staffs have

included these updates in the 2002 database. STI developed protocol memoranda that contained the following elements:

- Description of emission source
- Emission factors
- Activity data
- Emissions calculations, including a sample calculation
- Temporal allocation
- References and contacts

The protocols were pulled together from a variety of resources, including local air districts' past methods documents, U.S. Environmental Protection Agency documents, ARB documents, and original ideas based on the discovery of new information sources through library research, Internet research, and telephone contacts. Generally, STI attempted to incorporate data and information resources into the protocols that are readily available to the general public at no or low cost. And, while these methods and information resources are useful, it is recognized that it is more ideal to use highly customized or bottom-up emissions estimates when the costs of these efforts are warranted.

Emissions were estimated for the following counties: Amador, Butte, Calaveras, Colusa, E. Solano, El Dorado, Glenn, Mariposa, Mendocino, Nevada, Placer, Plumas, Sacramento, Shasta, Sierra, Sutter, Tehama, Tuolumne, Yolo, and Yuba. Area source methodologies were developed for the following broad categories:

- Asphalt paving/roofing
- Chemical and related products manufacturing
- Cleaning and surface coatings and related process solvents
- Fuel combustion:
    - Commercial natural gas
    - Commercial liquid fuels
    - Industrial natural gas
    - Industrial liquid fuels
    - Unspecified
    - Resource recovery
    - Petroleum production
- Cooking
- Wastes (e.g. livestock waste and landfills)
- Food and agriculture
- Mineral and metal processes
- Miscellaneous processes (e.g. miscellaneous industrial processes)
- Petroleum marketing

The protocol memoranda can be found on a password-protected project web site (URL: www.sonomatech.com/ccosii/; user name: "ccosii"; password: "emissions").

6.3 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
- 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 SIC. For area-wide and aggregated point sources, other growth parameters such as population, dwelling units, and fuel usage may be used.

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

As part of CCOS, the Emission Inventory Coordination Group (EICG), made up of ARB and district staff to guide inventory development for CCOS, requested that districts within the CCOS domain collect day-specific data from facilities and other sources within their jurisdiction. The EICG gathered hourly/daily emission information for:

1) large point sources (> 100 tons per year of NOx or ROG)
2) sources with large variability in emissions (e.g. power plants)
3) unusual events (e.g. source shut down, variances, breakdowns)
4) agricultural or prescribed burning
5) shipping emissions for the Bay Area
6) wildfires

6.4.1 Point Sources

Eleven air districts provided daily or hourly emission estimates for 67 facilities. The districts which provided data were Amador County APCD, Bay Area AQMD, Colusa County APCD, Monterey Bay Unified APCD, Placer County APCD, Sacramento Metro AQMD, San Joaquin Valley APCD, San Luis Obispo County APCD, Shasta County AQMD, Tehama County APCD, and Yolo/Solano AQMD. Day-specific emissions replaced emissions estimated from CEFS. Additionally, the Bay Area AQMD provided emission estimates from unusual events, such as equipment breakdowns. These emissions were added to the modeling inventories on the day when the unusual event occurred.

6.4.2 Area Sources

Three districts provided day-specific data for agricultural burning. In most districts, no agricultural burning occurred because no-burn days were declared during the episode.

6.4.3 Shipping in the Bay Area

Professor Bob Bornstein, San Jose State University, developed day-specific shipping adjustments for the Bay Area Air Quality Management District. Professor Bornstein provided factors that were applied to the annual average emission estimates for ships in the ocean and San Francisco Bay as well as for tugboats. Professor Bornstein developed factors for July 4 through July 14,1999, covering all the days needed for modeling (July 8 through 13, 1999). Professor Bornstein developed factors for July 29 through August 3, 2000. Since July 27 through August 2, 2000 is being modeled, August 3 was selected to approximate July 27 and 28, 2000.

Emissions from ships are estimated for two air basins: San Francisco Bay Area (SF) and the Outer Continental Shelf (OCS). Emissions from ships within 3 miles of the coast are considered in the SF air basin; emissions from ships beyond the 3-mile limit are in the OCS air basin. However, the current shipping surrogates used by the ARB to distribute emissions into grid cells differentiate by county, but not air basin. Emissions from ocean-going vessels in both the OCS and SF air basins are evenly distributed among the San Francisco Bay, the 3-mile coast, and the coast beyond the 3-mile limit. For ocean-going vessels, the factors developed by Professor Bornstein were applied only to grid cells that are within the 3-mile limit of the San Francisco coast. Grid cells beyond the 3-mile limit of the coast were not adjusted.

6.4.4 Wildfires

Emissions were estimated for known wildfires that occurred during the CCOS episodes. There were about 30 fires that occurred during episodes in the summer of 2000. All of the fires were less than 1,000 acres except for two. Two large wildfires occurred during the July-August 2000 episode. The Manter fire was a large-scale wildfire (over 73,000 acres) which occurred in Tulare County in the Sequoia National Forest and adjoining Bureau of Land Management areas on July 22 through August 9, 2000. The Plaskett2 fire was a large-scale wildfire (over 58,000 acres) which occurred in the Los Padres National Forest in Monterey County on July 23 through July 31, 2000. Due to these fires' duration, scale, and coincidence with the Central California Ozone Study, modeling staff requested that an estimate of fire emissions be developed in order to assess these fires' potential impacts on regional emissions and photochemistry.

To develop emission estimates, the ARB emission inventory staff turned to an on-going contract with UC Berkeley's Center for the Assessment and Monitoring of Forest and Environmental Resources (CAMFER) laboratory. In a prior ARB contract, CAMFER staff implemented the fire emissions module of the USDA Forest Service First Order Fire Effects Model (FOFEM, Reinhardt et al. 1997) within a Geographic Information System (GIS). FOFEM is a standard fire effects model used by federal and state land management agencies. The CAMFER model, called the Emissions Estimation System (EES), was initially devised to develop annual ARB fire emission inventories. In the

current contract, CAMFER was tasked to extend the EES to enable the model to estimate temporally-resolved emissions for individual fires, for an expanded suite of pollutants (CARB,2000).

The CAMFER EES runs within ArcView software and utilizes emission algorithms, emission factors, combustion efficiencies, fuel loadings, and other parameters from FOFEM. In the EES, GIS-based spatial data layers (polygon shapefiles), representing burned areas, are overlaid onto a GIS vegetation data layer in which vegetation community types are coupled with corresponding FOFEM biomass fuel profiles. For each fuel component (there are 10 fuel components representing foliage, litter, and stem diameter classes) in each vegetation type, the EES determines pre-burn fuel loadings (tons per acre), fuel mass consumed by the fire, combustion efficiency, and emissions released. Burning occurs in two distinct phases: flaming and smoldering. The temporal evolution of emissions from a burning area is therefore a function of the phase in which a fire is burning, and the time elapsed since ignition. The FOFEM and CAMFER EES models generate daily emissions from both phases. Emissions generated by the EES from flaming and smoldering phases are combined in the final outputs.

These emissions were then utilized to develop a plume profile, using the techniques outlined in a recent report of the Fire Emissions Joint Forum (FEJF) of the Western Regional Air Partnership (WRAP) (Air Sciences, 2004). Appendix B describes the vertical distribution of emissions in greater detail.

For all other fires in the summer of 2000, emissions were calculated based on the number of acres of three vegetation types: chaparral, grass, and timber. The U.S. Forest Service provided fuel loading and emission factors. The number of acres, vegetation type, fire duration, and location information were taken from California Department of Forestry (CDF) fire incident reports and newspaper articles. The vertical distributions of the plumes were calculated using the FEJF methodology referenced above.

There were also about 15 fires, totaling approximately 6,000 acres, which occurred during the July 1999 episode. Emissions from these fires have not been calculated.

6.5 *Temporally and Spatially Resolved Emissions*

In addition to forecasting emissions, CEFS can create temporally resolved inventories for modeling purposes, for the base year and future years. The annual average emissions are adjusted to account for monthly and weekly variations. CEFS generates an inventory for point and area sources (including off-road mobile sources) for a weekday and a weekend day in the year and months needed for an episode (e.g. July 1999 or August 2000). Emissions are estimated for each county, air basin, and district combination. In addition, information on how the daily emissions are distributed to each hour of the day is provided for later incorporation.

The emission inventories for CCOS were developed from the 2002 annual average CEIDARS inventory for TOG, NOx, SO_X, CO, PM, and ammonia. Since the episodes to be modeled (1999 and 2000) were earlier than the inventory base year (2002), emissions were backcasted from 2002 (see Section 6.3 for more information on forecasting emissions). Inventories for point and area sources were developed for a weekday and a weekend day for each of the 12 months for all years from 1990 to 2030. Note that all of these years may not have been processed into the formats needed for input to air quality models.

The backcasting of emissions for point and area sources usesg the best available data. Backcasting is handled differently for point and area sources. Point sources use historical data as stored in that year's CEIDARS inventory. In other words, the 1999 point source emissions come from the 1999 CEIDARS database and the 2000 point source emissions come from the 2000 CEIDARS database. Area source emissions are backcast from 2002 using growth and control factors. This procedure allows emissions to reflect changes that may have occurred due to updated emission calculation methodologies.

6.6 *Surface Temperature and Relative Humidity Fields*

The calculation of gridded emissions for some categories of the emissions inventory is dependent on gridded air temperature (T), relative humidity (RH), and solar radiation fields. Biogenic emissions are sensitive to air temperatures and solar radiation, and emissions from on-road mobile sources are sensitive to air temperature and relative humidity. Gridded temperature, humidity, and radiation fields are readily available from prognostic meteorological models such as MM5, used to prepare meteorological inputs for the air quality model. However, analysis of the MM5 outputs prepared for the July-August 2000 episode revealed poor agreement between simulated humidity and temperature fields and the available measurements.

As an alternative to the data fields generated using the prognostic meteorological model, air temperature and humidity fields for calculation of the emission inventory were prepared by objective analysis. In the objective analysis, hourly temperatures for each grid cell within the study domain were calculated using a distance-weighted average of the nearest three temperature measurements. Because few temperature measurements were available at higher terrain elevations, temperatures were adjusted using a vertical lapse rate (-0.0098 C/m to -0.0065 C/m) multiplied by elevation differences prior to averaging. Since this is an assumed constant, there may be uncertainty in temperatures at higher elevations.

Relative humidity measurements show a wide range of variability. Within the CCOS study domain, it was not unusual to find differences in relative humidity of 40% among sites within a 25-kilometer radius. To reduce large horizontal variations in the relative humidity fields developed for the emission inventory calculations, relative humidity fields

were calculated assuming a daily constant absolute humidity for each grid cell. The absolute humidity was calculated from the minimum daily temperature and assuming a maximum daily relative humidity of 80%.

The solar radiation fields needed for biogenic emission inventory calculations were taken from the MM5 simulation.

6.7 *On-Road Mobile Source Emissions*

EMFAC is the ARB approved on-road motor vehicle emission inventory model. The current version is EMFAC2007 v2.3 (November 2006) (CARB, 2006). ARB staff sought public input on this new version of EMFAC (see http://www.arb.ca.gov/msei/msei.htm for workshop notices and technical documentation). The improved inventories have undergone public review as part of the SIP outreach process.

Here are the main areas of change between the last version of EMFAC, EMFAC2002, and EMFAC2007:

Diesel Vehicles:

- Redistribution of heavy-duty diesel vehicle miles traveled (VMT)
- Adjustment to heavy-duty diesel emission factors
- Modifications to the speed correction factors for heavy-duty diesel vehicles
- The inclusion of high idle emission rates for heavy-duty diesel vehicles
- Diesel fuel correction factors

Gasoline Vehicles

- The impact of ethanol in gasoline on evaporative emissions
- Addition of areas into the Enhanced Smog Check program

The EMFAC model provides emission estimates for 13 classes of vehicles for exhaust, evaporation, and PM emissions from tire wear and brake wear. EMFAC also produces estimates of fuel consumption, vehicle miles traveled (VMT), and the number of vehicles in use. EMFAC does not output a gridded emission file. However, EMFAC will produce a file of emission rates that can be used with the Direct Travel Impact Model (DTIM) or other external on-road motor vehicle emission gridding program. These same emission rates are part of the information used by EMFAC to produce emission estimates for California counties or air basins.

DTIM4 (Systems Applications, Inc. 2001) is the latest version of DTIM, and is used to estimate gridded on-road motor vehicle emissions. In addition to the EMFAC emission rate file, DTIM4 uses digitized roadway segments (links) and traffic analysis zone activity centroids to allocate emissions for travel and trip ends. DTIM4 gridded emission files have fewer categories than EMFAC outputs. Each DTIM4 output category will be used to spatially allocate emissions for several EMFAC emission categories. There are

also several categories of emissions that EMFAC produces that are not estimated by DTIM4.

DTIM4 is used to estimate both the spatial and temporal distribution of all on-road motor vehicle emissions. It is important to recognize that EMFAC (and its associated activity), and not DTIM, is used to calculate county-specific emissions. DTIM output, using the Integrated Transportation Network (ITN) activity as inputs, was used to create hourly emission *ratios* for each grid cell in a county. These ratios were used to distribute county-specific, daily EMFAC emissions to each hour and grid cell. A horizontal grid resolution of 4 x 4 km is used.

Below we describe the procedures that were used with EMFAC2007 and DTIM4 to produce day-specific gridded on-road motor vehicle emission estimates. The procedures described here are carried out separately for each county in the CCOS modeling domain.

6.7.1 EMFAC Emissions Categories

EMFAC2007 produces emission estimates for the following 13 vehicle classes:

1. LDA Light Duty Autos
2. LDT1 Light Duty Trucks < 3,750 pounds GVW
3. LDT2 Light Duty Trucks > 3,750 - 5,750
4. MDV Medium Duty Vehicles > 5,750 – 8,500
5. LHD1 Light Heavy Duty Vehicles > 8,500 – 10,000
6. LHD2 Light Heavy Duty Vehicles > 10,000 – 14,000
7. MHD Medium Heavy Duty Vehicles > 14,000 – 33,000
8. HHD Heavy Heavy Duty Vehicles > 33,000
9. OB Other Buses
10. SBUS School Buses
11. UBUS Urban Buses
12. MH Motorhomes
13. MCY Motorcycles

Additionally, there are up to 3 technology groups within each vehicle type:

1. Catalyst
2. Non-catalyst
3. Diesel

For each of the combinations of vehicle type and technology there can be many emission categories:

1. Start Exhaust
2. Running Exhaust

3. Idle Exhaust
4. Hot Soak
5. Running Evaporatives
6. Resting Evaporatives
7. Partial Day Resting Evaporatives
8. Multi-Day Resting Evaporatives
9. Diurnal Evaporatives
10. Partial Day Diurnal Evaporatives
11. Multi-Day Diurnal Evaporatives
12. Break Wear PM
13. Tire Wear PM

A DTIM4 preprocessor calculates fleet average emission factors for each EMFAC technology type for each emission category. The vehicle type distribution used to calculate fleet emission factors is an input, so it can be varied as needed.

6.7.2 DTIM4 Emissions Categories

During DTIM4 operation, all emissions are collapsed into a total of 40 emission categories, represented by the SCCs below, which depend on vehicle type, the 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.

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

6.7.3 Creating the Emission Rate File

EMFAC will create an emission rate file for any desired combination of vehicle speeds, ambient temperatures, and relative humidities (RH). However, DTIM4 places restrictions on the total array size. The sets of values we use to build the array are:

Speed: 5, 10, 15, 20, 25, 30, 35, 40, 45, 50, 55, 60, 65

Temp: 30, 45, 60, 70, 75, 80, 85, 90, 100, 110

RH: 0, 30, 50, 70, 80, 90, 100

6.7.4 Day-Specific EMFAC Inventories

Emission estimates are produced by EMFAC for each day of each episode, by county. County average hourly temperatures, weighted by gridded VMT, are input to EMFAC to produce a 'BURDEN' inventory in a comma separated (.bcd) format. Both DTIM4 exhaust and evaporative emissions are scaled by category to the EMFAC emissions estimates for each county/air basin area. EMFAC bus and idle emission categories are not estimated by DTIM4. These categories are added to the gridded emission files.

6.7.5 CCOS Emissions Gridding

The method to estimate on-road mobile emissions at the grid cell level is described briefly in the following five steps:

Step 1. Gridded, hourly temperature (T) and relative humidity (RH) fields for each episode day are prepared for input to DTIM4. The T and RH fields are derived either from meteorological model predictions, observations, or some hybrid combination of model predictions and observations.

Step 2. EMFAC is run to prepare on-road mobile source emission factors by speed, temperatures, and relative humidity for each county.

Step 3. DTIM4 is run using data from the Integrated Transportation Network version 2 (ITNv2) and EMFAC to estimate gridded, hourly on-road mobile source emission estimates by day for DTIM4 categories.

Step 4. EMFAC is run again using episode-specific T and RH data to provide countywide on-road mobile source emission estimates by day for EMFAC categories. The episode-specific meteorological inputs for EMFAC are generated

via averaging (VMT-weighted) the gridded, hourly meteorology from Step1 by county and hour.

Step 5. Two sub-steps are taken:

Temporal adjustments

5a Sum the hourly volumes by vehicle type and county on the ITNv2 network.

5b For heavy-duty vehicles on core days (Tuesday through Thursday) redistribute the hourly emissions but make no daily VMT adjustment. Light duty vehicle emissions from EMFAC will not be adjusted at all for core days.

5c For Friday, Saturday, Sunday, and Monday, use Caltrans count data to develop a set of ratios of Caltrans daily VMT to core days. For example, develop ratios for Saturday to Tues-Thurs. Develop ratios for each Caltrans district for passenger cars, light and medium duty trucks, and heavy-duty trucks.

5d Apply Caltrans daily factors by county, and secondly, apply Caltrans' new hourly distributions by county to ITNv2 link activity.

5e Run DTIM with revised ITNv2 activity.

5f Run EMFAC with day-specific temperatures.

5g Adjust DTIM output emissions to EMFAC weekday by county.

5h For Friday, Saturday, Sunday, and Monday, apply daily ratios from step 5c to hourly DTIM emissions by county.

See Section 6.7.6 for more information.

Spatial/Temporal Distribution 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 DTIM4 output (Step 3) 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

6.7.6 Suggested Improvements for On-road Motor Vehicle Gridding

The five step process described above in section 6.7.5 is used to generate sets of day-specific, gridded on-road emissions. These emissions are our best estimates at the present time; however additional work in three areas would improve the estimates. One area of improvement, and likely the most important, is in the allocation of heavy-duty truck emissions. At present, the only transportation modeling done to explicitly model trucks is for Southern California counties covered by the Southern California Association of Governments (SCAG). For the remaining counties, heavy-duty trucks are assigned as a ratio of light-duty vehicles.

A second area of improvement is in developing emissions for weekend days. Both the spatial and temporal distribution of on-road motor vehicle emissions is different on weekend days than on weekdays. On-road motor vehicle emissions on weekend days should be considered an approximation since there are no transportation models to describe weekend traffic. In other words, people are still traveling to work; the emissions are just scaled down.

A third area of improvement is determining the hourly emissions from on-road motor vehicles. Local regional transportation agencies (RTPAs) and Caltrans supply traffic estimates for several time periods in a day. In the development of previous modeling inventories for CCOS, traffic within the time period was allocated to each hour using the hourly profiles that were developed by UC Davis. (Lam 2002). UC Davis developed two hourly profiles, one for weekdays and one for weekend days, which differed by county. However, there was no distinction by vehicle class. The same hourly profile

was used for heavy-duty vehicles as for light-duty vehicles within a county. This is of concern because trucks are known to have different diurnal distributions than cars and they have high NOx emissions.

Due to this concern, the Weekend Truck Subcommittee of the northern California SIP Gridded Inventory Coordination Group (GICG) was formed in 2004 to investigate a way to improve day-of-week adjustments, for vehicle types as needed, but particularly for heavy-duty trucks. Participants in the subcommittee are members of the GICG with particular knowledge and/or interest in improving the adjustment factors and include representatives from Caltrans, ARB, Bay Area AQMD, San Joaquin Valley APCD, and Alpine Geophysics (the developer of the ITN).

Caltrans staff acquired Automatic Vehicle Classifier (AVC) count data from about 139 sites in the state for calendar year 2004 (see Figure 6.1). Caltrans staff prepared hourly day of week factors for (1) passenger cars (LD), (2) light and medium duty trucks (LM), and (3) heavy-heavy duty trucks (HHDT). Caltrans count data are separated using the Federal Highway Administration (FHWA) vehicle classification scheme (see Table 6.3). Passenger cars are defined as FHWA classes 1 through 3. Light and medium heavy-duty trucks are defined as FHWA classes 7 and 8. Heavy-heavy duty trucks are defined as FHWA classes 9 through 14. Separate factors were prepared for each Caltrans District. One or more counties may fall into a single District. All counties within each Caltrans district will receive the same adjustment. Figure 6.2 shows a map of county and Caltrans district boundaries. Only counts during the summer of 2004 were used, specifically the months of June, July and August excluding data from July 2-5 to remove unusual traffic patterns around the July 4th holiday.

Temporal on-road activity adjustments by county were made for:

1. Heavy duty vehicles – all days
2. Light-duty vehicles – Friday, Saturday, Sunday, Monday

Daily total activity (daily VMT) adjustments were made for all vehicle types for Friday, Saturday, Sunday, and Monday. Tuesday, Wednesday, and Thursday are considered as one day. Adjustments applied to heavy-duty vehicles on Tuesdays, Wednesdays, and Thursdays were the same for each of the three days.

Since it is EMFAC emission estimates that are being adjusted to derive the final on-road inventory, the relation between EMFAC vehicle classes and Caltrans' adjustment factors is shown below.

EMFAC Class	Description	Caltrans' Factor
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	No data in ITNv2
10	School Bus	Unadjusted on weekdays, zero on weekend days
11	Urban Bus	LD
12	Motorhomes	LD
13	Motorcycles	LD

where LD based on count data for FhwA classes 1 through 3

LM based on count data for FhwA classes 7 and 8

HHDT based on count data for FhwA classes 9 through 14

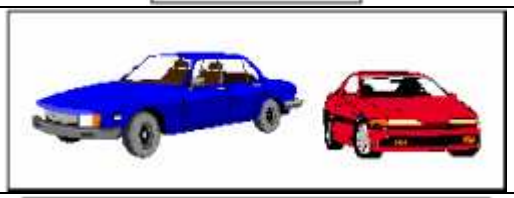
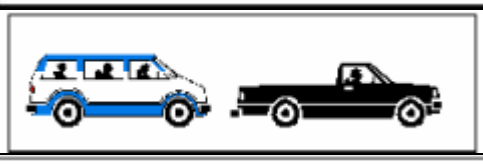
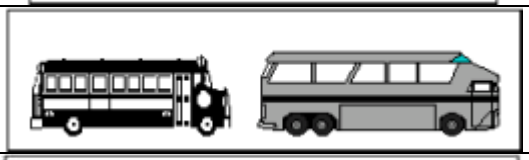
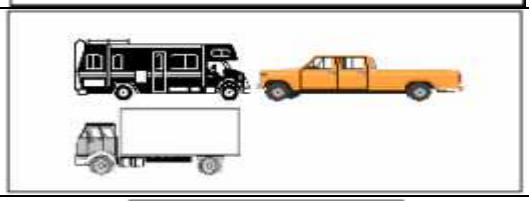
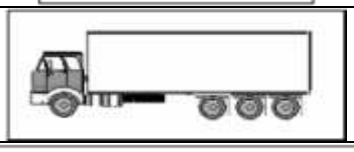
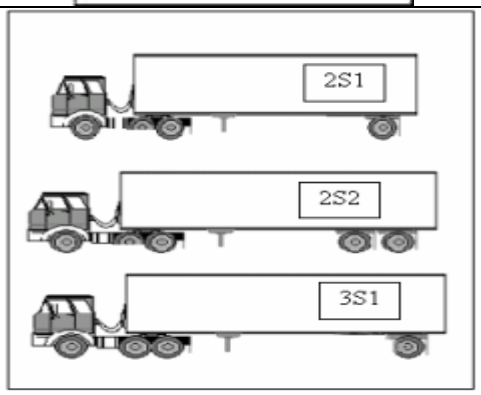
To summarize, for core days light- and medium-duty vehicle emissions will equal EMFAC emissions by county and hour. For core days, heavy-duty emissions will equal EMFAC but have Caltrans hourly distribution. For Friday through Monday, EMFAC weekday emissions will be scaled to reflect Caltrans day of week factors. Appendix C provides more detail on the methodology developed by the Weekend Truck Subcommittee.

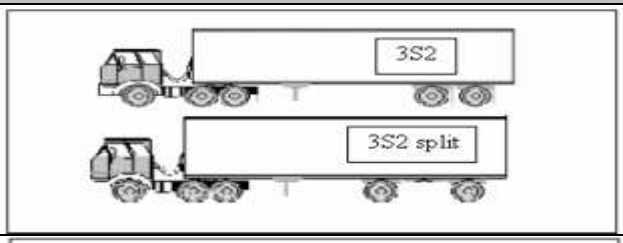
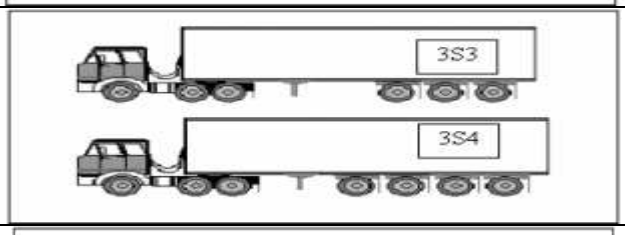
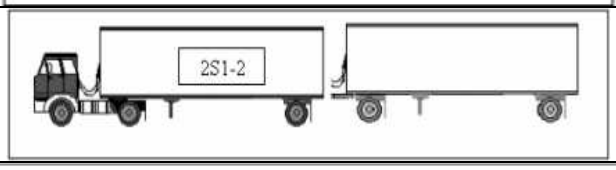
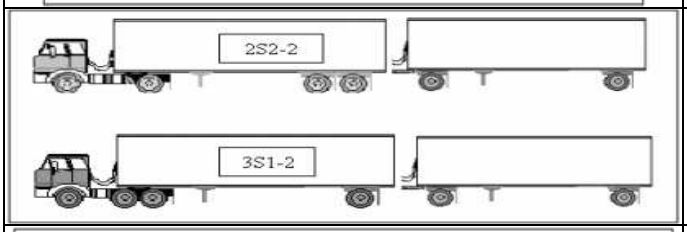
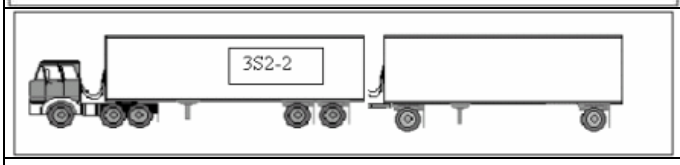
Although significant improvements have been made to improve the temporal distribution of on-road motor vehicles, some assumptions were made that may cause uncertainty in the adjustments. For example, one assumption is that the count data represent the temporal distribution of all road types, including local roads. The count data are gathered only on state highways. Another assumption is the link between EMFAC and FHWA classes. EMFAC classes are based on gross vehicle weight, whereas FHWA classes are based on type of vehicle and number of axles. It is not an easy process to determine which EMFAC class a specific type of vehicle falls into based on the number of axles, particularly for trucks. Additional work may provide improvements to estimating hourly emissions by vehicle type, especially on weekend days.

Figure 6.1 Caltrans Weigh-In-Motion Data Sites

Figure 6.2 Caltrans District and County Boundaries

Table 6.3 Federal Highway Administration (FHwA) Vehicle Classification

Graphic Depiction	FHWA Class	Description
	1	Motorcycles
	2	Passenger Cars (With 1- or 2-Axle Trailers)
	3	2 Axles, 4-Tire Single Units, Pickup or Van (With 1- or 2-Axle Trailers)
	4	Buses
	5	2D - 2 Axles, 6-Tire Single Units (Includes Handicappe-Equipped Bus and Mini School Bus)
	6	3 Axles, Single Unit
	7	4 or More Axles, Single Unit
	8	3 to 4 Axles, Single Trailer

Graphic Depiction	FHWA Class	Description
	9	5 Axles, Single Trailer
	10	6 or More Axles, Single Trailer
	11	5 or Less Axles, Multi-Trailers
	12	6 Axles, Multi-Trailers
	13	7 Axles, Multi-Trailers
No graphic available	14	5 Axles: 3 axle tractor pulling a 2 axle trailer (FHWA considers this type of truck a class 9;Caltrans counts these trucks separately for operational purposes.)

6.7.7 Fleet Emission Factors

An important input to DTIM4 is the vehicle type weighting for emission rate. The vehicle type VMT for each county/air basin output from EMFAC is used, which is then reformatted by the CONVIRS4 computer program and composited by vehicle type distribution from BURDEN in the IRS4 computer program. For the counties in CCOS that are covered by the ITN network, we process light/medium duty (LM) and heavy-duty vehicles (HDV) separately. The VMT for LM is the sum of EMFAC categories LDA, LDT1, LDT2, MDV, SBUS, UB, MCY and MH. The HDV VMT is the sum of LHD1, LHD2, MHD and HHD.

Besides the composite emission rate file, DTIM4 needs link and trip end activity files. All activity has been resolved to one-hour periods for each county using the method described in Sections 6.7.5 and 6.7.6 above. Specifically, temporal on-road activity (link and trip end) adjustments by county were made for:

- Heavy duty vehicles – all days
- Light-duty vehicles – Friday, Saturday, Sunday, Monday

Link and trip end activity adjustments were made for all vehicle types for Friday, Saturday, Sunday, and Monday. Tuesday, Wednesday, and Thursday are considered as one day. Adjustments applied to heavy-duty vehicles on Tuesdays, Wednesdays, and Thursdays were the same for each of the three days.

Additionally, EMFAC has different fleet mixes by county based on vehicle registrations. It is the fleet mixes in EMFAC that ultimately are the basis for the on-road mobile source emissions processing that has been done in support of CCOS. The fleet mixes in the DTIM4 runs are based on the fleet mixes in EMFAC. The DTIM4 runs are based on the composite emissions factors that are generated by EMFAC. During the preprocessing of the EMFAC output, which occurs prior to a complete DTIM4 run that is performed by the IRS/CONVIRS programs, there is generally an adjustment applied to the EMFAC emissions factors based on vehicle counts. In most cases, the regional transportation planning agencies (RTPAs) who supplied the transportation data provided the vehicle counts that were used to adjust the EMFAC emissions factors. In the remaining cases, the vehicle count data were taken directly from EMFAC.

6.7.8 Differences Between DTIM4 and EMFAC

6.7.8.1 Evaporative Emissions

DTIM4 and EMFAC use different methods to estimate evaporative emissions. However, as mentioned previously, we use the DTIM4 evaporative emissions as spatial and temporal "surrogates" to resolve EMFAC emission estimates. During processing, we drop the DTIM4 evaporative categories 211, 212, 311, and 312 (because those emissions are included in EMFAC's estimates for diurnal and resting emissions) and put all EMFAC resting emissions in DTIM4 category 210/310, and all diurnal emissions in DTIM4 category 207/307.

6.7.8.2 Exhaust Emissions

The exhaust emissions from EMFAC are also resolved spatially and temporally by DTIM4 emission estimates. Since transportation models do not estimate VMT for buses or excess idling categories, these are added to DTIM4 emissions. The exhaust CO, NOx, SOx, and PM emissions that DTIM4 allocates to category 1 are reassigned to catalyst starts, non-catalyst starts, catalyst stabilized, non-catalyst stabilized, and diesel exhaust categories according to the appropriate day-specific EMFAC inventory.

6.7.9 Integrated Transportation Network (ITN)

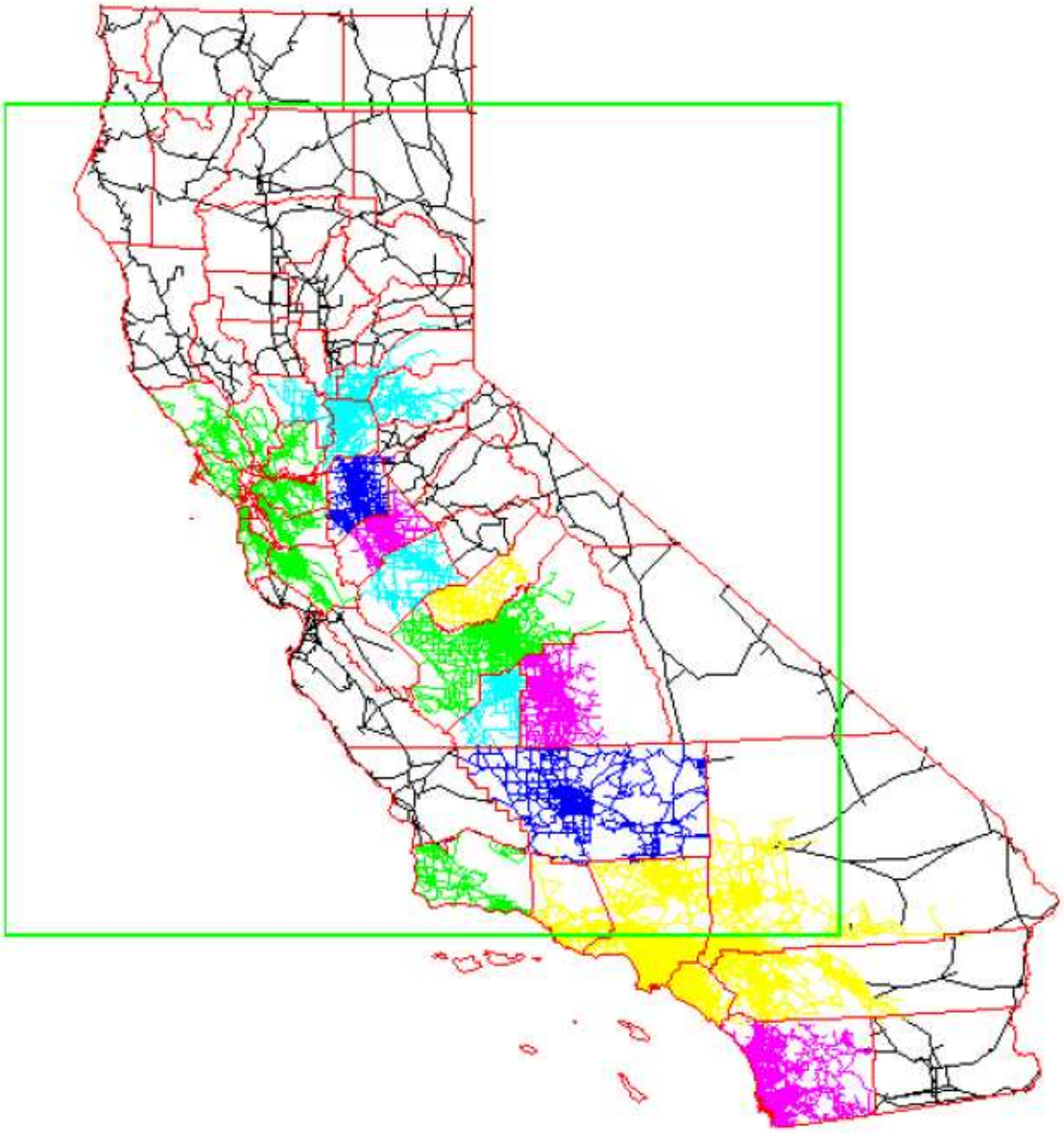
The Integrated Transportation Network (Wilkinson 2003) is a seamless on-road transportation network that covers all of California. The ITN was developed from many regional transportation planning agencies (RTPAs) as well as the California Department of Transportation (Caltrans) Statewide Model. The San Joaquin Valleywide Air Pollution Study Agency and Air Resources Board contracted with Alpine Geophysics to develop the ITN. After the ITN was developed, additional local transportation networks became available that were not included in the first version. Some RTPAs had also updated their networks since the original development. For these reasons, version two of the ITN (ITNv2.0) was developed (Wilkinson 2005). As mentioned earlier, the ITNv2.0 is used to spatially distribute the on-road mobile source emissions generated by EMFAC. Figure 6.3 shows the link-based ITNv2.0 for California.

Local networks were used for all or portions of the following counties: Alameda, Contra Costa, El Dorado, Fresno, Kern, Kings, Los Angeles, Madera, Marin, Merced, Napa, Orange, Placer, Riverside, Sacramento, San Bernardino, San Diego, San Francisco, San Joaquin, San Mateo, Santa Barbara, Santa Clara, Solano, Sonoma, Stanislaus, Sutter, Tulare, Ventura, and Yolo. Data that were provided for Imperial and San Luis Obispo could not be used because the parameters to conflate the networks to real world

coordinates were not available. The Caltrans statewide model was used to supplement the local data. More details on the ITNv2.0 can be found in Appendix D, the final report "Development of Version Two of the California Integrated Transportation Network (ITN)".

It is important to recognize that EMFAC (and the associated activity), and not DTIM4, will be used to calculate county-specific emissions. DTIM4 output, using the ITN activity as inputs, will simply be used to create hourly emission *ratios* for each grid-cell in a county. These ratios will be used to distribute county-specific, daily EMFAC emissions to each hour and grid-cell. This intended use negates the need to update countywide VMT on the ITN. That is, if up-to-date VMT in a specific county were 10% higher than is currently reflected in the ITN, all the VMT on ITN links for that county would be increased by 10%. Since both the county VMT and link VMT (in the same county) are factored by the same amount, the ratio of link-to-county VMT for every link in that county does not change. Similarly, DTIM4 grid-cell-to-county emissions *ratios* do not change. Thus, for the intended use and assuming no changes to ITN activity distribution, adjusting the ITN county totals to more accurate countywide VMT will not affect the outcome.

With regard to the spatial accuracy of the ITN, it is important to recognize that current modeling efforts in the region utilize square grid cells that are four kilometers on each side. Thus, the spatial accuracy of the statewide or local components of the ITN only requires enough resolution to distribute EMFAC emissions into the proper four by four kilometers grid cell. Given that the intended purpose of the ITN is for use in estimating on-road mobile source emissions for photochemical modeling efforts, this accuracy is sufficient.



Note: The county boundaries are in red. The Caltrans statewide network is in black. The various individual networks are in colors other than black or red. The 190 x 190 4 kilometer CCOS emissions modeling domain is shown as the green box.

Figure 6.3. Link-based Integrated Transportation Network (ITN) version 2.0

6.7.10 Motor Vehicle Activity

Motor vehicle activity data are an important part of EMFAC for estimating emissions. As part of an on-going effort to use the best data available, ARB periodically updates the vehicle miles traveled (VMT) and speed distributions by VMT used in the model. In November 2004, ARB sent letters to transportation planning agencies (TPAs) statewide requesting updated activity data for base years and forecasted years. A sample letter can be found in Appendix E. All major urban areas in the state responded. The data was reviewed and processed by ARB staff in coordination with the TPAs. ARB's Technical Memorandum on the activity data update is provided in Appendix F. The memorandum provides summaries of the data and refers to supporting documents that provide additional details as well as discussions of issues. ARB included additional updates as time permitted before finalizing EMFAC2007.

6.7.11 Forecasted Emissions for On-Road Motor Vehicles

Forecasted modeling inventories were developed for on-road motor vehicles as needed to complete the inventory inputs to episodes being modeled. For future year inventories, emissions and other needed data were taken from EMFAC for the desired future year. The method used to calculate the future year emissions was the same as the base year for each episode, including the same gridded, hourly temperature and relative humidity information.

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, which uses California-specific input databases with a minimum spatial resolution of 1 square kilometer (km^2) and an hourly temporal resolution.

The BEIGIS isoprene emission algorithm (Guenther et al. 1991, 1993) is of the form

$$I = I_S \times C_L \times C_T$$

where I is the isoprene emission rate (grams per gram dry leaf mass per hour) at temperature T and photosynthetically active radiation flux PAR. I_S is a base emission rate (grams per gram dry leaf mass per hour) at a standard temperature of 30 °C and

PAR flux of 1000 μmol $m^{-2}s^{-1}$. C_L and C_T are environmental adjustment functions for PAR and temperature, respectively. The monoterpene emission algorithm adjusts a base monoterpene emission rate by a temperature function (Guenther et al. 1993). Methylbutenol (MBO) emissions are modeled with an algorithm developed by Harley et al. (1998) similar to that for isoprene. Dry leaf mass/leaf area ratios, and base emission rates for isoprene, monoterpenes, and MBO are plant species-specific and assembled from the scientific literature. Modeled BVOC emissions for a given spatial domain therefore represent the contribution by various plant species (through their leaf mass and emission rates) to the total BVOC emissions.

The main inputs to BEIGIS are land use and vegetation land cover maps, gridded leaf area indices (LAI) derived from AVHRR satellite data (Nikolov 1999), leaf area/dry leaf mass factors, base emission rates, and gridded hourly ambient temperature and light intensity data (from a meteorological model). 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). Ground surveys have been funded by CCOS to validate the vegetation land cover and LAI input databases used in BEIGIS (Winer et al. 1998; Karlik and McKay 1999; Winer and Karlik 2001, Karlik 2002). Validation using flux measurements in the field is on going.

Using BEIGIS, the ARB developed hourly-resolved emissions of isoprene, monoterpenes, and methyl butanol (MBO), gridded at a 1-km resolution. Each 4-kilometer (km) grid cell, using the statewide 4-km grid cell domain defined by the ARB, was divided into 16 1-km grid squares. After the biogenic emissions were calculated, the emissions from the 1-km cells were aggregated for each 4-km grid cell. Two additions are then made to the biogenic emissions estimates for input to air quality models.

First, biogenic OVOCs (other VOCs) are added. Biogenic OVOCs comprise around twenty percent of some biogenic inventories and are known to affect air quality modeling predictions (e.g. Hanna et al., 2002). Guenther et al. (1994) estimates that the OVOCs comprise 8-73% of total BVOCs. OVOCs are estimated by ARB as an added fraction of 30%, scaled to the total isoprene, monoterpene, and MBO emissions.

The estimate of OVOC emissions used by ARB is the result of an August 2001 peer review of modeling procedures by Dr. William P. L. Carter (Carter 2001). During the discussion with ARB modeling staff, it was noted that estimates of OVOC were reported by some sources to be as great as the inventoried species (isoprene, m-butenol, and monoterpenes). Since OVOCs are very uncertain in both mass and species characterization, ARB had not been including them in the modeling programs. Dr. Carter suggested this omission was inappropriate. He recommended that OVOC

emissions be included with the best estimates we could make. During this discussion it was decided that doubling the known species would be like an upper limit which was felt to be too high. Collectively it was decided that an OVOC amount equal to 30% of the total known species would be a reasonable estimate.

ARB reviewed the literature to find a reasonable speciation to assign to OVOCs. Arthur Weiner sent a list of the compounds that were intended at that time to be included in BEIS-3. No amounts were fixed to species and ARB could not derive an OVOC profile. Allen Goldstein had published an article “In Situ Measurements of C2-C10 Volatile Organic Compounds Above a Sierra Nevada Ponderosa Pine Plantation” in the Journal of Geophysical Research (9-20-1999) which did allow us to create a profile to use until better information could be obtained. This profile is dominated by methanol and acetone and also contains ethene, propene, hexanal, and acetaldehyde. These compounds were all part of the species proposed for BEIS3.

ARB’s intention is to use this profile for all OVOC from all vegetation types until better information becomes available. In the future, use of information from BEIS-3 or other models may allow ARB to create BVOC inventories that contain enough compounds so that the additional step of adding a chosen amount of 'OVOCs' can be eliminated.

The second addition is to include biogenic NO emissions. Biogenic NO emissions were estimated using a soil NO algorithm found in BEIS-3.

For a more detailed description of the estimation of biogenic emissions, see Appendix G.

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.

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, 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 CCOS modeling domain is described below in Section 6.9.1.

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. Section 6.9.2 discusses in detail the spatial surrogates developed for CCOS.

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. Please refer to section 6.4.4 and Appendix C for more information.

The spatial treatment of area and point sources has been described above. The spatial allocation of on-road motor vehicles is based on activity on the Integrated Transportation Network version 2 (ITNv2.0) as described in Section 6.7.9. For biogenic emissions, the spatial allocation is built “from the ground up” since ARB’s biogenic model, BEIGIS, estimates emissions using a Geographic Information System (GIS) at a 1 square kilometer resolution. Section 6.8 describes how biogenic emissions are estimated.

6.9.1 Grid Definition

The CCOS emissions inventory domain was defined based on the MM5 model used to generate the meteorological parameter fields used for air quality modeling. However, the MM5 model uses only an approximation to the shape of the Earth. Therefore, there was a small offset error between the MM5-defined domain and the emissions domain defined using GIS software, which uses a more exact Earth shape.

The emissions inventory domain was defined using a Lambert Conical Projection with two parallels. The Parallels were at 30 and 60 N latitude, with a central meridian at 120.5 W longitude. The coordinate system origin was offset to 37 N latitude. The emissions inventory was gridded with a resolution of 4 km. However, because of differences between the MM5-defined domain and the GIS defined domain, the lower,

left-hand corner of the emissions inventory domain was not a integer multiple of 4-km (cell size) from the domain origin. The specifications of the emissions inventory domain grid were:

DEFINITION OF GRID
190 x 190 cells (4 km x 4 km)
Lambert Origin @ (-385131.6m , -302910.3m)
Geographic Origin @ -124.7423 deg. Latitude and 34.1210 deg. Longitude

MAP PROJECTION
LAMBERT
Units: Meters
Datum: NONE (Clarke 1866 spheroid)

PARAMETERS
1st Standard Parallel: 30 0 0.000
2nd Standard Parallel: 60 0 0.000
Central Meridian: -120 30 0.00
Latitude of Projection Origin: 37 0 0.000
X-Shift (meters): 0.0000
Y-Shift (meters): 0.0000

6.9.2 Spatial Surrogates

Spatial allocation factors are used to geographically distribute countywide area source emissions to individual grid cells. These spatial allocation factors were developed from spatial surrogate data. Spatial surrogates are economic, demographic, and land cover patterns that vary geographically.

In this context, “area source emissions” refers to all source categories that are not point sources, biogenics, or on-road motor vehicles (see Table 6.2 for description). 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 allocated by DTIM4 (see Section 6.7). Biogenic emissions are allocated by BEIGIS (see Section 6.8).

In support of CRPAQS and CCOS, Sonoma Technology, Inc. (Funk et al. 2001) was contracted to develop spatial allocation factors. Using a GIS-based approach, STI developed gridded spatial allocation factors for a 2000 base-year and three future years (2005, 2010, and 2020) for the entire state of California 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.

Each area source category is assigned a spatial surrogate. This assignment provides a cross-reference between the spatial allocation factors and the emission inventory categories. A total of 65 unique surrogates were developed as part of this project. A summary of the spatial surrogates, for which spatial allocation factors were developed, is listed in Table 6.4.

A listing of all surrogates and spatial allocation factors, and their corresponding spatial surrogate codes (SSC), are contained in Appendix H. Appendix H also includes the surrogate-to-emission inventory cross-reference list. Designating the surrogate-to-emission inventory assignments was an iterative process among STI staff, ARB staff, and local air district staff. Note that the spatial allocation factors and emissions category assignments vary by county depending on the data available for each county.

Three basic types of surrogate data were used to develop the spatial allocation factors:

- land use and land cover
- facility location
- demographic and socioeconomic data

Land use and land cover data are associated with specific land uses, such as agricultural tilling, feedlots, 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). Table 6.5 shows the sources of land use and land cover data as well as facility location information used to develop spatial allocation factors. Table 6.6 shows the sources of demographic and socioeconomic data used to develop spatial allocation factors. Table 6.7 provides a list of the counties covered by each data set. To develop spatial allocation factors of high quality and resolution, local socioeconomic and demographic data were used when available; for rural regions for which local data were not available, the Caltrans Statewide Transportation Model data were used.

Table 6.4 Summary of spatial surrogates developed as part of the CCOS gridded surrogate project

Surrogate Description
Agricultural cropland
Agricultural land
Feedlots
Feedlots, dairies, and poultry farms
Non-pasture agricultural land
All airports
Commercial airport locations
Total employment & road density
Total housing and locations of auto body/refinishing shops
Locations of hospitals, institutions, population, and commercial employment
Total housing, service, commercial, golf courses
Industrial employment and locations of auto body/refinishing shops
Road density & housing/employment (ft2/person)
Population, institutions, and commercial employment
Total housing and locations of restaurants/bakeries
Single dwelling units and non-urban land
Housing/employment (ft2/person)
Computed surrogate - residential
Computed surrogate - non-residential
Computed surrogate - residential & non-residential
Industrial employment + computed surrogate (residential & non-residential)
Population
Residential, service, commercial, golf courses
Industrial employment and population
Total housing and commercial employment
Total employment
Total housing
Total housing and total employment
Single dwelling units
Single and multiple dwelling units
Non-retail employment
Industrial employment
Service and commercial employment
Elevation > 5000 ft
Forest land
Locations of bulk plants

Table 6.5. Sources of land use/land cover and facility locations

Data Source	Parameter	Resolution	Vintage	Coverage
United States Electronic Yellow Pages (ProCD Select Phone)	Autobody shops, dry cleaners, restaurants, gas stations, and wineries	Address locations	1997	Statewide
Environmental Systems Research Institute	Airports, parks, golf courses, hospitals, institutions	Coordinate locations and polygon coverages	1997	Statewide
U.S. Census Bureau (ESRI ADOL version)	Water bodies	Polygon coverages	2000	Statewide
United States Geological Survey	Land use and land cover for 38 counties	Gridded data	1993	Statewide
ARB CEIDARS Database	Bulk plant locations	Coordinate locations	1999	Statewide
National Atlas	Mine locations	Coordinate locations	1998	Statewide
Bureau of Transportation Statistics	Ports and shipping lanes	Coordinate locations and line coverages	Publication date is 2000; source date varies	Statewide
State Water Resources Control Board	Publicly owned water treatment works locations	Coordinate locations	2001	Statewide
Integrated Waste Management Board	Landfill locations	Coordinate locations	Downloaded from the Internet, no dates	Statewide
StreetWorks	Military bases	Polygon coverages	1995	Statewide
Digital Chart of the World	Elevation data	Polygon coverages	1993	Statewide
California Department of Oil and Gas	Oil and gas well and field locations	Coordinate locations and polygon coverages	1998	Statewide
California Teale Data Center (from ARB)	Urban and rural roads and railroads	Line and polygon coverages	RR, updated 1991; RDS, updated 1993	Statewide
Department of Water Resources (from ARB)	Agricultural land cover	Polygon coverages	1995	San Joaquin Valley

Table 6.6. Sources of statewide and local TPA demographic and socioeconomic surrogate data

Data Source	Parameter (Years)	Resolution and Coverage
Caltrans Statewide Transportation Model (Caltrans STM)	Population, housing, employment (base and future)	TAZ[a] – data for rural counties only
Association of Bay Area Governments (ABAG) and 1990 U.S. Census	Population, housing, employment (base and future)	Census Tract – San Francisco Bay Area
Sacramento Area Council of Governments (SACOG)	Population, housing, employment (base and future)	TAZ[a] – Sacramento Urban Region
Tahoe Regional Planning Agency (TRPA)	Population, housing, employment (base and future)[b]	TAZ[a] – Lake Tahoe Region
Association of Monterey Bay Area Governments (AMBAG) and 1990 U.S. Census	Population (base and future)	Census Tract – Monterey Bay Area
South Coast Association of Governments (SCAG)	Population, housing, employment (base and future)	TAZ[a] – South Coast Region
Amador County Transportation Commission (ACTC)	Population, housing, employment (base and future)[b]	Growth Allocation Districts (unincorporated areas) and incorporated areas – Amador County
Council of Fresno County Governments (FresnoCOG)	Population, housing, employment (base and future)	TAZ[a] – Fresno County
San Diego Association of Governments (SANDAG)	Population, housing, employment (base and future)	TAZ[a] – San Diego County
San Joaquin Council of Governments (SJCOG)	Population, housing, employment (base and future)	TAZ[a] – San Joaquin County
Tulare County Association of Governments (TCAG)	Population, housing, employment (base and future)	Incorporated and unincorporated areas – Tulare County
Stanislaus Council of Governments (StanCOG)	Population, housing, employment (base and future)	Incorporated and unincorporated areas – Stanislaus County
Kern Council of Governments (KernCOG)	Population, housing, employment (base and future)	TAZ[a] – Kern County

Table 6.7. Counties covered by each of the demographic and socioeconomic data sets listed in Table 6.6

Data Source	County Coverage
Caltrans STM	Alpine, Butte, Calaveras, Colusa, Del Norte, Glenn, Humboldt, Imperial, Inyo, Kings, Lake, Lassen, Mariposa, Madera, Merced, Mendocino, Modoc, Mono, Nevada, Plumas, east Riverside, east San Bernardino, San Luis Obispo, Santa Barbara, Shasta, Sierra, Siskiyou, Tehama, Trinity, Tuolumne
ABAG	Alameda, Contra Costa Marin, Napa, San Francisco, San Mateo, Santa Clara, Solano, Sonoma
SACOG/TRPA	El Dorado, Placer, Sacramento, Sutter, Yolo, Yuba
AMBAG	Monterey, San Benito, Santa Cruz
SCAG	Los Angeles, Orange, west Riverside, west San Bernardino, Ventura
ACTC	Amador
FresnoCOG	Fresno
SANDAG	San Diego
SJCOG	San Joaquin
TCAG	Tulare
StanCOG	Stanislaus
KernCOG	Kern

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 processes leading to ozone formation and fate in the lower atmosphere, and include all emissions of the important compounds involved in ozone photochemistry. Organic gases are one of the most important classes of chemicals involved in the formation of surface ozone. 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 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 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.

To the extent possible 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 6.8 shows modeled ROG species (or species categories) for the SAPRC-99 chemical mechanism. Table 6.9 shows modeled species for NOx.

Table 6.8 ARB's SAPRC-99 Emitted Organic Model Species

Model Species Name	Description
HCHO	Formaldehyde
CCHO	Acetaldehyde
RCHO	Lumped C3+ Aldehydes
ACET	Acetone
MEK	Ketones and other non-aldehyde oxygenated products
PROD	
RNO3	Lumped Organic Nitrates
PAN	Peroxy Acetyl Nitrate
PAN2	PPN and other higher alkyl PAN analogues
BALD	Aromatic aldehydes (e.g., benzaldehyde)
PBZN	PAN analogues formed from Aromatic Aldehydes
PHEN	Phenol
CRES	Cresols
NPHE	Nitrophenols
GLY	Glyoxal
MGLY	Methyl Glyoxal
MVK	Methyl Vinyl Ketone
MEOH	Methanol
HC2H	Formic Acid
CH4	Methane
ETHE	Ethene
ISOP	Isoprene
TERP	Terpenes
MTBE	Methyl Tertiary Butyl Ether
ETOH	Ethanol
NROG	Non-reactive
LOST	Lost carbon
ALK1	Alkanes and other non-aromatic compounds that react only with OH, and have kOH < 5×10^2 ppm-1 min-1. (Primarily ethane)
ALK2	Alkanes and other non-aromatic compounds that react only with OH, and have kOH between 5×10^2 and 2.5×10^3 ppm-1 min-1. (Primarily propane and acetylene)
ALK3	Alkanes and other non-aromatic compounds that react only with OH, and have kOH between 2.5×10^3 and 5×10^3 ppm-1 min-1.
ALK4	Alkanes and other non-aromatic compounds that react only with OH, and have kOH between 5×10^3 and 1×10^4 ppm-1 min-1.
ALK5	Alkanes and other non-aromatic compounds that react only with OH, and have kOH greater than 1×10^4 ppm-1 min-1.
ARO1	Aromatics with kOH < 2×10^4 ppm-1 min-1.
ARO2	Aromatics with kOH > 2×10^4 ppm-1 min-1.
OLE1	Alkenes (other than ethene) with kOH < 7×10^4 ppm-1 min-1.
OLE2	Alkenes with kOH > 7×10^4 ppm-1 min-1.

Table 6.9 Model Species for NOx

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

Both U.S. EPA's and ARB's models require estimates of total organic gases, which include the "exempt VOCs", and, to the extent data are available, any low vapor pressure compounds that become airborne. Model results for ozone non-attainment areas have demonstrated that even compounds with low photochemical reactivity or low vapor pressure 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.

The implementation of the chemical mechanism is unique in each air quality model. In the case of the CAMx model, the chemical species ETOH (ethanol), MTBE (methyl tert-butyl ether) and MBUT (methyl butenol) are not treated explicitly. These species are considered important to ozone chemistry in California because ETOH and MTBE are motor-vehicle fuel components and MBUT is emitted by vegetation. Therefore, to include emissions of these species in the emissions inventory for CAMx, they were mapped as follows:

(moles of ETOH)*1.3 = moles converted to ALK3
(moles of MTBE)*1.2 = moles converted to ALK3
(moles of MBUT)*1.8 = moles converted to OLE1

7 MODEL PERFORMANCE EVALUATION

The following subsections summarize the recommended model performance evaluation procedures (Emery & Tai, 2001; Tesche et al., 2002; USEPA, 1991 & 2005) for meteorological and photochemical models.

7.1 Meteorological Model Performance

Meteorological model performance is assessed both quantitatively using statistical metrics as well as qualitatively against known conceptual meteorological flows and observed episodic meteorological features.

7.1.1 Quantitative Performance Evaluation

There are a number of statistical and graphical approaches for evaluating meteorological model outputs. However, none of them are independently conclusive. Most of these approaches involve comparisons between observed and simulated meteorological parameter values. These analyses pose a difficult challenge, since most of the available meteorological monitoring stations are located in urbanized areas. Thus, the majority of observations tend to represent those areas versus the full complexity of meteorology throughout the CCOS domain. Furthermore, since the use of objective analysis and observational nudging forces the meteorological modeling results towards the observations, model performance problems can increase in areas away from observation locations.

It also needs to be recognized that output from the various meteorological models must be preprocessed for input into the air quality model. This preprocessing may inadvertently perturb the meteorological fields. Therefore, meteorological model performance should be based on the air quality model input files, rather than the meteorological model outputs.

The SIP modeling domain is geographically very complex and the observational data on which meteorological model outputs were evaluated are not distributed uniformly. Therefore, it is unreasonable to evaluate model performance for the domain as a whole. For purposes of meteorological model performance analysis, the CCOS domain is divided into sub-regions, representing areas of similar meteorological features. The graphical and statistical model evaluations will be done for each of these sub-regions.

A number of standard statistical and graphical techniques are used for meteorological model performance analysis. The most widely used application is the METSTAT program (Tesche, 1994, Tesche et al, 2001). Two graphical representations of the METSTAT statistics were used in meteorological model performance analysis conducted here: a) “Root Mean Square Error (RMSE) of Wind Speed” vs. “Gross Error (E) of Wind Direction”, and b) “Bias Error (B)” vs. “Gross Error (E)” for temperature.

Equations used for these comparisons were taken from the user documentation of the METSTAT program and are given below:

Bias Error (B): calculated as the mean difference in prediction-observation pairings with valid data within a given analysis region and for a given time period (hourly or daily):

$$B = \frac{1}{IJ} \sum_{j=1}^{J} \sum_{i=1}^{I} \left(P_j^i - O_j^i \right)$$

Here, *P* and *O* indicate model predictions and observations, respectively. Similarly, I and J are the indices of grid points in x and y directions, respectively.

Gross Error (E): calculated as the mean *absolute* difference in prediction-observation pairings with valid data within a given analysis region and for a given time period (hourly or daily):

$$E = \frac{1}{IJ} \sum_{j=1}^{J} \sum_{i=1}^{I} \left| P_j^i - O_j^i \right|$$

Note that the bias and gross error for winds are calculated from the predicted-observed residuals in speed and direction (not from vector components *u* and *v*). The direction error for a given prediction-observation pairing is limited to the range from 0 to ±180°.

Root Mean Square Error (RMSE): calculated as the square root of the mean squared difference in prediction-observation pairings with valid data within a given analysis region and for a given time period (hourly or daily):

$$RMSE = \left[\frac{1}{IJ} \sum_{j=1}^{J} \sum_{i=1}^{I} \left(P_j^i - O_j^i \right)^2 \right]^{1/2}$$

The RMSE, as is the gross error, is a good overall measure of model performance. However, since large errors are weighted heavily (due to squaring), large errors in small subregions may produce a large RMSE even though the errors may be small and quite acceptable elsewhere.

Table 7-1 shows the criteria used to decide if the results of a given model fall within acceptable performance limits.

Table 7-1 Statistical comparisons between observed and simulated meteorological parameter values. Statistical comparisons are made by model performance sub-regions.

Parameter	Abbreviation	Benchmark
Wind Speed	RMSE: Bias: IOA:	$\leq$ 2 m/s $\leq \pm$0.5 m/s $\geq$ 0.6
Wind Direction	Gross Error: Bias:	$\leq$ 30 deg $\leq \pm$10 deg
Temperature	Gross Error: Bias: IOA:	$\leq$ 2 ºK $\leq \pm$0.5 ºK $\geq$ 0.8

In an ideal situation, meteorological field evaluation would be done independent of the air quality model results. However, in practice, meteorological field evaluation is limited by the relative paucity of observational data, especially aloft. Therefore, base year air quality model performance was also considered in the selection of meteorological fields used for air quality simulations.

Table 7-2 Graphical analysis of meteorological model fields. Time series plots are made for each station and spatial plots are made over the whole modeling domain.

Time-series plots of hourly mean air temperature
Time-series plots of hourly mean wind speeds.
Spatial plots of hourly wind vectors
Spatial plots of hourly air temperatures

7.1.2 Qualitative Performance Analyses

Given episode-specific information on the meteorological features that were observed with field measurements, additional subjective analyses of observed versus predicted mesoscale features can be conducted. Examples of such qualitative analyses that will be considered are described below.

1. Determine and compare modeled and observed horizontal flow patterns throughout the modeling domain. Features to consider include flow splitting, the structure of the sea breeze, urban circulations, local flows such as Fresno and Schultz eddy circulations, slope and drainage flows, up/down valley flows, and the existence of cloud formations (Described in Chapter 1).

2. Study the 3-D spatial characteristics of the flow field by using time-height cross sections of wind profiler observations and the simulated wind field at the wind profiler location.

3. Determine the spatial and temporal characteristics of the mixing layer height using available upper air observations, and compare it with the simulated behavior of mixing layer heights.

4. Perform sensitivity tests to see the effects of certain model parameters on the model results, such as observational nudging vs. analysis nudging, the choice of soil physics, and boundary layer parameterizations.

7.2 Air Quality Model Performance

Air quality model results are used to develop strategies for attaining the federal 8-hour ozone standard. The development of these strategies relies on the use of relative reduction factors (RRFs). A more detailed discussion of RRFs is provided in other documents. However, the use of RRFs requires an evaluation of relative air quality model response at specific monitoring sites in the base year(s), a reference year, and a future year.

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. Although it is desirable to include as many days as possible in the RRF calculations, our experience has demonstrated that not all modeled days meet the minimum performance standards, and are thus not suitable for use. Therefore only those days that satisfy the following model performance criteria will be utilized in RRF calculations.

The USEPA (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 7-1 illustrates the proposed subregions for the CCOS domain.

The USEPA (2005) recommends that model performance be evaluated for 8-hour concentrations as well. The recommended statistical measures to assess simulated versus observed maximum 8-hour ozone concentrations include paired (in space, but

not time) peak prediction accuracy (PPPA), paired mean normalized bias (NB), and paired gross error (GE). Although limited performance analysis has been completed for 8-hour ozone modeling in California, it seems prudent at this point to carry forward the 1-hour statistical goals and apply them for the 8-hour standard (UPR within ± 20%, NB within ± 15%, and the GE less than 35%). However, these limits may need to be revised as 8-hour SIP modeling progresses and rigorous model performance evaluations are completed.

While statistical measures for 1-hour model performance were typically calculated independently for each modeled day available, the USEPA also suggests that PPPA, NB, and GE be calculated for each site over all modeled days. However, because the number of episode days available may be very limited, the statistical uncertainties in these latter calculations would be large and they are not recommended or used herein.

In order to have confidence in future year estimates from air quality models, there must be confidence in the air quality modeling for the base year. That is, days not meeting model acceptance criteria provide high uncertainty, and should not be used for the modeled attainment test.

In addition to the issue of model performance, analyses conducted by the USEPA (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 8-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 8-hour ozone concentrations in the reference year. Days for which the predicted daily peak 8-hour ozone concentrations at a site are less than the threshold, would not be used for calculating RRFs at that site. Consistent with USEPA's recommendation, we propose to use a value of 85 ppb for the reference year threshold. However, USEPA guidelines allow the use of the maximum 8-hour concentrations within 15km of the site for this purpose.

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

Only those modeled days meeting the following criteria will be used to calculate site-specific RRFs:

1) The modeled daily 8-hour peak ozone concentration within 15 km of the site for the base year of the modeling (the model performance year) must be within ±20% of the observed value at the site.
2) The modeled daily 8-hour peak ozone concentration within 15 km of the site in the reference year must be 85 ppb or greater.
3) The subregional 1-hour and 8-hour statistical measures of NB and GE must fall within the thresholds of ± 15% and 35%, respectively.

Of these three criteria, only the third is considered in this document.

Along with the statistical measures discussed above, the graphical and statistical tests recommended by the USEPA (1991 and 2005) and shown in Tables 7-3 and 7-4 will be used to assess overall model performance. Several sensitivity tests recommended by the USEPA (1991) will also be used (Table 7-5) 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.

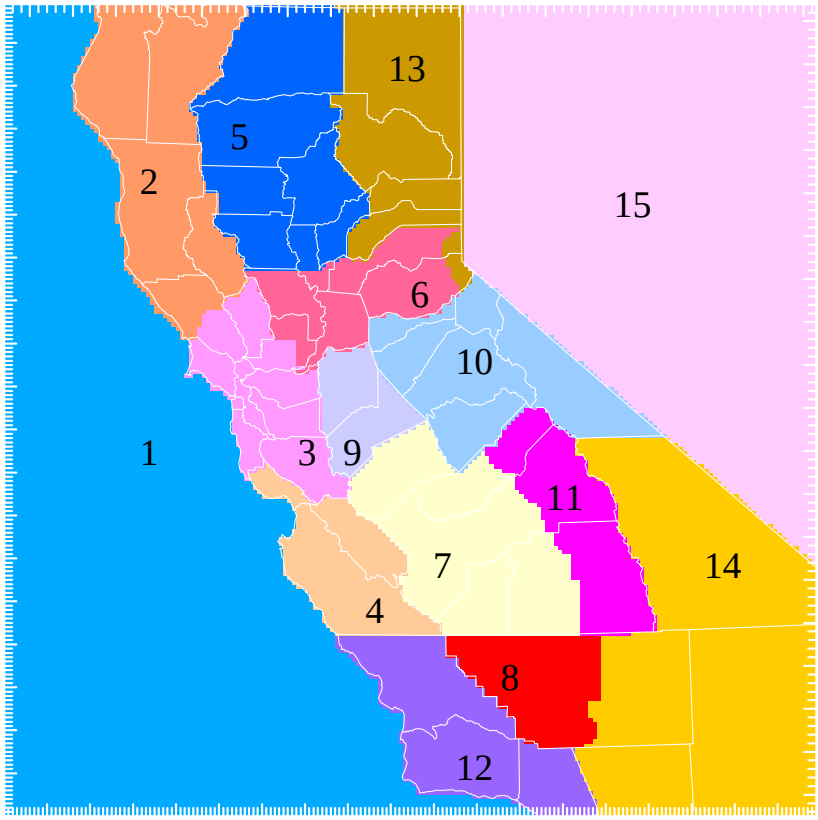


Figure 7-1 Sub-regions of air quality model performance evaluation (3: Bay Area region, 6: Sacramento Metro region, 7: Central San Joaquin Valley region , 8 Southern San Joaquin Valley region, 9: Northern San Joaquin Valley region).

Table 7-3. 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
- Mean normalized bias for all 8-hour ozone concentrations (≥60 ppb), unpaired in time for all sites
- Mean normalized gross error for all 8-hour ozone concentrations (≥60 ppb), unpaired in time for all sites
- Peak 8-hour ozone concentration ratio, unpaired in time and space

Table 7-4. 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.

Table 7-5. Sensitivity tests for evaluation of Base Year air quality simulations. The results of these analyses will be tabulated by subregion.

1	Minimize vertical diffusivity based on land cover
2	Zero anthropogenic emissions
3	Zero biogenic emissions
4	Set lateral ozone boundary conditions to 50 ppb
5	Set lateral ozone boundary conditions to 90 ppb
6	Set initial ozone conditions to 40 ppb everywhere
7	Set initial conditions to 0.1 ppb NO2 and 0.0 NO (run with all emissions)
8	Set initial conditions to 0.1 ppb NO2 and 0.0 NO (run with biogenic emissions only)
9	Double biogenic emissions
10	Remove wildfires
11	Zero mobile emissions
12	Set top ozone boundary conditions to 135ppb at 15km

8 FUTURE-YEAR AIR QUALITY MODELING

The current thinking for the use of air quality modeling results in attainment demonstrations is to utilize relative model response to predict future-year 8-hour ozone concentrations. The Relative Reduction Factor (RRF) is calculated as the ratio of future-year and reference year ozone concentrations at a site. The RRF is then multiplied by a site-specific design value to estimate the future-year design value. In principle, this concept is simple. In practice, it is confounded by the limited record of available observed ozone concentrations during the available episodes and the uncertainties inherent in air quality modeling.

The emphasis of this document is on site-specific RRFs and the estimation of future year design values at non-attainment monitoring sites; however, the USEPA (2005) also requires analysis to demonstrate that high ozone concentrations occurring away from monitors (e.g., unpaired in space) will also be controlled in future years to meet air quality standards. This latter analysis is not addressed in this document.

There are two primary components to the application of air quality modeling results for the estimation of future-year ozone concentrations. The first is model performance analysis. The USEPA (1991) outlines a number of procedures for analysis of base-year air quality model performance. These include spatial and time-series plots comparing simulated and observed pollutant concentrations, statistical analyses comparing simulated and observed pollutant concentrations, and sensitivity analysis of selected input fields. This document will only address the more basic statistical analysis tests. The purpose of the performance analyses is to provide some confidence that the air quality simulations on which the estimates of future-year ozone concentrations will be based, will have some semblance to reality. The second is the issue of representative ozone concentrations for base- and future-year concentrations at each site from which the RRFs will be calculated.

8.1 Estimation of Future Design Value (DV_F)

The application of photochemical ozone models has a long history in California, for uses ranging from the preparation of State Implementation Plans to research activities to regulatory development. The modeling community has applied these tools in the State for over 30 years, and much has been learned about their proper uses and limitations.

One of the fundamental understandings that has evolved is that photochemical models are best used to estimate the relative difference between scenarios, rather than for absolute concentration estimates. That is, their strength is in estimating the relative change in concentration levels from a reference condition (e.g., a current year) to an alternative scenario (e.g., a future year), rather than predicting the exact concentration level that will result from the alternative scenario.

The USEPA's guidance on the use of models for attainment demonstrations in support of 8-hour ozone planning (USEPA, 2005) is consistent with the fundamental strength of models described above. USEPA's recommended modeled attainment test is to utilize relative model response on a site-by-site basis, in the form of a relative reduction factor (RRF), to predict future-year 8-hour ozone design values. This methodology relies on the base year for the modeling for conducting model performance analyses, a reference year of 2002 for projecting forward site-specific design values, and a future year for the attainment test.

$$\mathbf{DV_F = (RRF)\ (DV_R)}$$

where DV_R = *a reference year (2002) concentration (design value) measured at a monitoring site*
DV_F = *the estimated future year design value at the same site*
RRF = *the relative reduction factor at the same site*

The RRF is calculated as the ratio of future year to reference year modeled ozone concentrations at a site:

$$\mathbf{RRF} = \frac{\mathbf{FY_{8-hr}}}{\mathbf{RY_{8-hr}}}$$

where RRF = *the relative reduction factor for a monitor*
$FY_{8\text{-}hr}$ = *the modeled future year 8-hour daily maximum concentration predicted near the same monitor*
$RY_{8\text{-}hr}$ = *the modeled reference year 8-hour daily maximum concentration predicted near the same monitor*

In principle, this concept is simple. Unfortunately, it can be confounded by a number of factors, including the limited number of modeled days available, the choice of year(s) to use for specification of the reference design value, the uncertainties inherent in air quality modeling, and the presence of a non-zero background level of ozone. As a result of this, EPA technical staff have indicated that there is flexibility in the application of RRFs, as long as the methodology is technically sound and is properly documented.

8.1.1 Estimating Reference Year (2002) Design Values

Specification of the reference design value is a key consideration in the modeled attainment test, since this is the value that is projected forward and used to test for attainment at each site. Since the reference design value is presumably reflective of conditions in the reference year, it should be representative of the emissions used for that year. However, many areas experience fluctuations in their year-to-year meteorology, as well as emissions levels. In recognition of this year-to-year variability, the reference design value should in some fashion also reflect this variability. A standard methodology for minimizing the influence of year-to-year variations is to calculate an average value over multiple years. Therefore, the following methodology is recommended for specification of the reference design value at each monitoring site:

> **The reference design value (DV_R) will be calculated as the average of the three design values for the three years commencing with the reference year of the modeling. The reference year for modeling in support of the 8-hour ozone SIPs is 2002. Therefore, the reference design value will be calculated at each monitoring site as the average of the design values for 2002, 2003, and 2004.**

California design values are calculated as the three-year average of the 4th highest 8-hour ozone peak values, and are assigned to the last year. Thus, a design value for 2002 would be based on data for 2000-2002. The recommendation above implies that the reference design value at each monitoring site will be calculated as the average of nine design values over five years: the three years which make up the 2002 design value (2000-2002), the 2003 design value (2001-2003), and the 2004 design value (2002-2004). This gives the greatest weight to 2002, since that year is included in the calculation of the design value for all three years.

The following table summarizes the recommended process for calculating the reference design value at each monitoring site.

Year	Years Averaged for Design Value				
2002	2000	2001	2002		
2003		2001	2002	2003	
2004			2002	2003	2004
	Yearly Weighting for Average Design Value for Modeled Attainment Test				
2002-2004 Average	$DV_R = \frac{Year_{2000} + (2)(Year_{2001}) + (3)(Year_{2002}) + (2)(Year_{2003}) + Year_{2004}}{9}$				

8.1.2 Relative Reduction Factors

As discussed above, the relative reduction factor (RRF) is a monitor-specific value that is calculated based on daily peak 8-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 8-hour modeled ozone concentration in the future year, divided by the average daily peak 8-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.

$$\mathbf{RRF_{AVG}} = \frac{(\mathbf{FY_{8-hr}})_{\mathbf{AVG}}}{(\mathbf{RY_{8-hr}})_{\mathbf{AVG}}}$$

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

$(FY_{8\text{-}hr})_{AVG}$ = *the average future year 8-hour daily maximum concentration predicted near the same monitor, averaged over those days which satisfy model performance and threshold criteria*

$(RY_{8\text{-}hr})_{AVG}$ = *the modeled reference year 8-hour daily maximum concentration predicted near the same monitor, averaged over those days which satisfy model performance and threshold criteria*

8.1.3 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. Although it is desirable to include as many days as possible in the RRF calculations, our experience has demonstrated that not all modeled days meet the minimum performance standards, and are thus not suitable for use. Therefore only those days which satisfy the following model performance criteria will be utilized in RRF calculations.

The USEPA (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.

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 sub-regions, and that the performance measures be calculated independently for each sub-region. The configuration of these sub-regions is somewhat arbitrary; however, they should be configured to isolate "common" regions of higher ozone.

The USEPA (2005) recommends that the emphasis for 8-hour model performance be based on concentrations occurring at, or in the vicinity of, individual monitoring sites. Specifically, modeled concentrations occurring within 15 km of a site are considered to be in the vicinity of the site. The recommended statistical measures to assess simulated versus observed maximum 8-hour ozone concentrations include paired (in space, but not time) peak prediction accuracy (PPPA), paired mean normalized bias (NB), and paired gross error (GE). Although limited performance analysis has been completed for 8-hour ozone modeling in California, it seems prudent at this point to carry forward the 1-hour statistical goals and apply them for the 8-hour standard (UPR within ± 20%, NB within ± 15%, and the GE less than 35%). However, these limits may need to be revised as 8-hour SIP modeling progresses and rigorous model performance evaluations are completed.

While statistical measures for 1-hour model performance were typically calculated independently for each modeled day available, the USEPA also recommends that PPPA, NB, and GE be calculated for each site over all modeled days. However, because the number of episode days available may be very limited, the statistical uncertainties in these latter calculations would be large and they are not recommended herein.

In order to have confidence in future year estimates from air quality models, there must be confidence in the air quality modeling for the base year. That is, days not meeting model acceptance criteria provide high uncertainty, and should not be used for the modeled attainment test.

In addition to the issue of model performance, analyses conducted by the USEPA (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 8-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 8-hour ozone concentrations in the reference year. Days for which the predicted daily peak 8-hour ozone concentration at a site is less than the threshold, would not be used for calculating RRFs at that site. Consistent with USEPA's recommendation, we propose to use a value of 85 ppb for the reference year threshold.

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 8-hour peak ozone concentration within 15 km of the site for the base year (model performance year) of the modeling must be within $\pm$ 20% of the observed value at the site.
2) The modeled daily 8-hour peak ozone concentration within 15 km of the site in the reference year must be 85 ppb or greater.
3) The sub-regional 1-hour and 8-hour statistical measures of NB and GE must fall within the thresholds of $\pm$ 15% and 35%, respectively.

8.1.4 Estimating Future-Year Design Values

As discussed above, the USEPA's 8-hour modeling guidance recommends utilizing relative model response on a site-by-site basis, in the form of an average relative reduction factor (RRF_{AVG}), to predict future-year 8-hour design values for attainment planning. The average RRF is then multiplied by a site-specific design value to estimate the future-year design value. One of the confounding factors in this approach is consideration of the effects that background levels have on the effectiveness of emission control programs.

There is a large body of information that suggests that ambient concentrations consist of some (perhaps nonlinear) background value and a contribution due to anthropogenic emissions. That is, if all man-made emissions could be zeroed out, ozone concentrations would not go to zero but rather some finite value. The literature suggests that 40 ppb is a reasonable global background ozone value, and it is quite likely that continental background is some other, somewhat higher, value. One possibility for estimating background ozone values in a given modeling domain would be to exercise the model without anthropogenic emissions, and to thus develop a gridded "background" ozone field. One concern with this approach is that at such low levels, the model's boundary conditions exert a large influence, and appropriate temporally- and spatially-resolved data to specify boundary conditions rarely exist. Thus boundary conditions can be subjective and uncertain. Whether the background value is established at some finite value (e.g., 40 ppb) or is model-derived, it represents that portion of a site's ozone problem that cannot be mitigated by anthropogenic emission controls.

According to EPA's 8-hour ozone modeling guidance, the modeled attainment test requires that a future year Design Value (DV_F) be calculated at each site and compared to the standard to determine if the site is predicted to be in attainment. To calculate the future year Design Value, the Design Value for the reference year (DV_R) is multiplied by RRF_{AVG}. Although EPA's guidance says nothing about background ozone, we propose to calculate the future year Design Value with consideration of background. The Table below illustrates calculation of the DV_F with and without background. Because the model's boundary conditions exert a large influence on modeled background ozone levels, 40 ppb will be used to represent background ozone concentrations.

Calculation of the Average Relative Reduction Factor and Future Year Design Values* with and without Consideration of Background Ozone

Without consideration of background	With consideration of background
$RRF_{AVG} = \frac{(FY)_{AVG}}{(RY)_{AVG}}$ $DV_F = (RRF_{AVG}) \times (DV_R)$	$RRF_{AVG} = \frac{(FY - BG)_{AVG}}{(RY - BG)_{AVG}}$ $DV_F = [(RRF_{AVG}) \times (DV_R - BG)] + BG$
Definitions DV_R = Design Value for the reference year RY = Reference year model prediction FY = Future year model prediction BG = Background ozone	

* Note: As per EPA guidance, future year design values are truncated rather than rounded.

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