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MODELING PROTOCOL FOR OZONE AND PARTICULATE MATTER MODELING IN SUPPORT OF THE SOUTH COAST AIR QUALITY MANAGEMENT DISTRICT 2007 AIR QUALITY MANAGEMENT PLAN UPDATE

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LIST OF ACRONYMS

Several acronyms are used in the modeling protocol document. For convenience, the acronyms used are listed below to aid the reader.

AAMA	–	American Automobile Manufacturer's Association
AGL	–	Above Ground Level
AQMD	–	Air Quality Management District
AQMP	–	Air Quality Management Plan
AQMPAG		Air Quality Management Plan Advisory Group
AUSPEX	–	Atmospheric Utility Signatures, Predictions, and Experiments
AVHRR	–	Advanced Very High Resolution Radiometer
BEIS	–	Biogenic Emission Inventory System
CAA	–	Clean Air Act Amendment of 1990
CAMx	–	Comprehensive Air-Quality Model with Extensions
CARB	–	California Air Resources Board
CBM	–	Carbon Bond Mechanism
CCAA	–	California Clean Air Act
CEFS	–	California Emission Forecasting System
CMAQ	–	Community Multi-scale Air Quality (model)
CO	–	Carbon Monoxide
COG	–	Council of Governments
DARS	–	Data Attribute Rating System
DWM	–	Diagnostic Wind Model
DTIM	–	Direct Travel Impact Model
EIWG	–	Emission Inventory Working Group
EKMA	–	Empirical Kinetics Modeling Approach
EMFAC	–	Emission Factor (model)
FCM	–	Flexible Chemical Mechanism
FDDA	–	Four-Dimensional Data Assimilation
GAP	–	Geographical Approach to Protection of Biological Diversity
GCM	–	Global Climate Model
ICAPCD	–	Imperial County Air Pollution Control District
IOP	–	Intensive Operation Period
LIDAR	–	Light Detection and Ranging
MDAQMD	–	Mojave Desert Air Quality Management District
MM5	–	Mesoscale Meteorological Model (5th generation)
MWG	–	Modeling Working Group
NAAQS	–	National Ambient Air Quality Standard
NDVI	–	Normalized Difference Vegetative Index

NOx – Nitrogen Oxides
NO2 – Nitrogen Dioxide
PDT – Pacific Daylight Time
PM – Particulate Matter
PM10 – Particulate Matter less than 10 microns equivalent aerodynamic diameter
PM2.5 – Particulate Matter less than 2.5 microns equivalent aerodynamic diameter
PMcourse – PM10 – PM2.5
PMfine – PM2.5
RADM – Regional Acid Deposition Model
RECLAIM – Regional Clean Air Incentives Market
ROG – Reactive Organic Gases
RRF – Relative Reduction Factor
SANDAG – San Diego Association of Governments
SAPRC – State Air Pollution Research Center
SAQM – SARMAP Air Quality Model
SARMAP – SJVAQS/AUSPEX Regional Model Adaptation Project
SBCAG – Santa Barbara County Association of Governments
SBCAPCD – Santa Barbara County Air Pollution Control District
SCAB – South Coast Air Basin
SCAG – Southern California Association of Governments
SCAQMD – South Coast Air Quality Management District
SCAQS – Southern California Air Quality Study
SCE – Southern California Edison
SCOS97 – Southern California Ozone Study (1997)
SDCAPCD – San Diego County Air Pollution Control District
SIP – State Implementation Plan
SJVAQS – San Joaquin Valley Air Quality Study
SOx – Sulfur Oxides
STMPRAG – Scientific, Technical, Modeling and Peer Review Advisory Group
TOG – Total Organic Gases
UAM – Urban Airshed Model
USEPA – United States Environmental Protection Agency
UTM – Universal Transverse Mercator
VCAPCD – Ventura County Air Pollution Control District
VMT – Vehicle Miles Traveled
VOC – Volatile Organic Compound
WSPA – Western States Petroleum Association

INTRODUCTION

The federal Clean Air Act (CAA) requires areas with unhealthy levels of ozone , carbon monoxide, nitrogen dioxide, sulfur dioxide, and inhalable particulate matter to develop plans, known as State Implementation Plans (SIPs), describing how they will attain national ambient air quality standards (NAAQS). The 2007 Air Quality Management Plan (AQMP or Plan) for the South Coast Air Basin (Basin) will meet the SIP update requirements for this area, demonstrating NAAQS attainment. The federal Clean Air Act (CAA) requires the use of photochemical grid models that are approved by the Unites States Environmental Protection Agency (USEPA) to perform the attainment demonstration. This document addresses the air quality modeling protocol for the 2007 AQMP, as developed through a joint cooperative effort between the staff of the South Coast Air Quality Management District (AQMD or District) and the California Air Resources Board (CARB), with technical oversight from the Scientific, Technical, Modeling and Peer Review Advisory Group (STMPRAG).

The objective of this modeling protocol is to define the methodology to be used for simulating the formation and transport of ozone and particulate matter in the Basin, including:

- the model(s) to be used;
- the modeling domain;
- the horizontal and vertical grid resolution;
- the annual PM period and ozone and PM episodes to be simulated;
- the model input data, including meteorology, emissions, initial conditions; and lateral and top boundary conditions;
- the process for model performance evaluation.

In addition, the protocol outlines the attainment demonstration process, including a review of the California Clean Air Act (CCAA) requirements. This protocol document is intended to be dynamic and will be updated in response to reviewer comments and to reflect the results of new information that will emerge during the AQMP modeling process.

In order to devote the maximum resources practicable to the development of the District's 2007 AQMP, the Executive Officers of CARB and AQMD have agreed to jointly develop the emissions and air quality modeling needed to determine the carrying capacity and attainment demonstration for the ozone and PM standards. The technical staffs of both agencies are working closely together to plan and carry out the necessary work for the

AQMP and are committed to intensive and timely coordination to ensure that it is based on the soundest science possible. Both agencies agree that their staffs will collaborate on this work such that the product will be mutually acceptable modeling analyses for use in the 2007 Plan.

Background

Regulatory Modeling Requirements and Guidance

The 1990 amendments to the federal CAA set new deadlines for attainment based on the severity of the pollution problem and launched a comprehensive planning process for attaining the NAAQS. The promulgation of the new national eight-hour ozone standard and the fine particulate matter (PM2.5) NAAQS in 1997 required additional statewide air quality planning efforts. In response to new federal regulations, SIPs must also address ways to improve visibility in national parks and wilderness areas. SIPs demonstrating attainment of the federal ozone standard must be adopted by the local air districts and CARB, and submitted to the USEPA by June 15, 2007.

USEPA's guidelines on air quality modeling previously recommended the use of the Urban Airshed Model (UAM) for attainment demonstrations involving entire urban areas. However, USEPA revised its recommendation (USEPA, 2001a) to no longer include a recommended air quality model for ozone. Instead, USEPA recommends that air quality models proposed for an ozone attainment demonstration be subjected to model performance evaluations to demonstrate that they are appropriate for attainment demonstration purposes.

USEPA issued the *Guideline for Regulatory Applications of the Urban Airshed Model* (USEPA, 1991) and *Guidance on the Use of Modeled Results to Demonstrate Attainment of 1-hour Ozone NAAQS* (USEPA, 1996) to assist states in preparing the attainment demonstration required by the CAA. In addition, the CARB *Technical Guidance Document: Photochemical Modeling* (CARB, 1992) provides photochemical modeling guidance for use by the districts to ensure the technical validity of the modeling results. Most recently, USEPA has finalized attainment demonstration guidance for the 8-hour ozone NAAQS (USEPA, 2005). The ozone modeling protocol in this document is based on these guideline documents. Guidance for the PM portion of the modeling protocol utilizes the *Draft Guidance for Demonstrating Attainment of Air Quality Goals for PM2.5 and Regional Haze* (USEPA, 2001b).

Under the federal Clean Air Act of 1990 (CAA), the South Coast Air Basin (Basin) was classified as an "extreme" nonattainment area for 1-hour ozone. Section 182(c)(2)(A) of the CAA set November 15, 1994 as the deadline for submission of a SIP to demonstrate attainment of the NAAQS for ambient 1-hour ozone of 0.125 parts per million (ppm) by December 2010. AQMD satisfied that CAA requirement with the submittal of the 1994 AQMP in September 1994. A subsequent revision was submitted to USEPA in February 1997. This was amended in 1999 to revise the Basin ozone portion of the 1997 AQMP due to its partial approval/disapproval by USEPA. The 2003 AQMP took advantage of information obtained from the 1997 Southern California Ozone Study (SCOS97) and emissions inventory enhancements. It updated the attainment demonstration for the ozone and PM10 particulate matter NAAQS, replaced the 1997 attainment demonstration for the CO NAAQS, and updated the maintenance plan for the NO2 NAAQS that the Basin has met since 1992. In 2005, AQMD submitted a CO attainment request and maintenance plan to CARB and USEPA; approval of this is pending.

In July 1997, the USEPA established new ozone NAAQS of 0.085 ppm based on an 8-hour average measurement. Due to legal challenges, the final form of the ozone NAAQS has been implemented in two phases. The Phase 1 ozone implementation rule, finalized on June 15, 2004, defined the classification scheme for 8-hour ozone nonattainment areas and revoked the 1-hour ozone NAAQS, while requiring states to maintain control programs which were included in their state implementation plans (SIP) for the 1-hour standard. Fifteen areas in California were designated that violate the federal 8-hour ozone standard. Each nonattainment area's classification and attainment deadline is based on the severity of its ozone problem. Southern California's nonattainment areas and attainment deadlines are: South Coast Air Basin (2021); Coachella Valley (2013); Ventura County (2010); Western Mojave Desert (2010); Antelope Valley (2010); San Diego (2009-2014); and Imperial County (2007).

The Phase 2 ozone rule, adopted November 9, 2005, described the actions that states must take to reduce ground level ozone and set the deadline for ozone SIP submittal of June 2007. The AQMD began air quality modeling analyses related to the 8-hour ozone standard during the 1997 AQMP, prior to the final NAAQS implementation. This analysis effort was continued for the 2003 AQMP. The 2007 AQMP modeling will expand the 8-hour ozone analysis and include an attainment demonstration for the current form of the NAAQS. The 2007 AQMP will include an analysis of 1-hour ozone to provide additional milestones for progress of ongoing control programs and for continuity with previous efforts.

AQMP Ozone Modeling History in the South Coast Air Basin

The first Air Quality Management Plan (AQMP) for the Basin was produced in 1979 as part of a revision to California's SIP. The 1979 AQMP indicated that it would not be possible to achieve the federal 1-hour ozone air quality standard of 0.12 ppm by 1982. Because the emission controls discussed in the 1979 AQMP would not be fully effective until after 1982, CARB and USEPA granted an extension to 1987 for achievement of the standard. As part of that extension, a revision to the AQMP was performed by the AQMD in 1982 which included a new series of modeling analyses to address concerns regarding the original 1979 modeling analysis.

For both the 1979 and 1982 AQMP revisions, the city-specific Empirical Kinetics Modeling Approach (EKMA) was applied. The 1979 AQMP used the city-specific EKMA procedures then in existence. The 1982 AQMP revision used a more sophisticated version of the EKMA procedures and also contained sensitivity analyses (Appendix VI-A of the 1982 AQMP revision). The UAM was used in conjunction with the EKMA analyses to evaluate the effect of applying all feasible control measures by 1987 (Appendix VI-E of the 1982 AQMP revision). On the basis of those modeling studies, it was determined that hydrocarbon reductions on the order of 75 percent or greater would be required to attain the federal standard by 1987, given a forecasted 23 percent reduction in oxides of nitrogen. Forecasted emission data indicated that only a 33 percent hydrocarbon reduction could be expected by 1987. Issues raised during the 1979 and 1982 AQMP revisions highlighted the need to use a three-dimensional, photochemical model such as the UAM to better understand the complex interactions between precursor emissions, meteorology, and the formation of ozone in the Basin.

For the 1989 AQMP revision, the UAM was applied to a single, multiday, ozone episode to demonstrate attainment of the National Ambient Air Quality Standard (NAAQS) for ozone. It was determined from the modeling analysis that hydrocarbon and oxides of nitrogen emission reductions of more than 80 percent would be needed in order to attain the 1-hour ozone NAAQS by the year 2007. The 1989 AQMP revision outlined three levels of controls (identified as Tiers I, II, and III) that separated the proposed control measures by known and proven technologies from those technologies anticipated to be available within the next 20 years.

For the 1991 AQMP, the AQMD used the UAM to further assess the effectiveness of the three tiers of control measures in reducing ambient ozone levels. To complement the single, multiday ozone episode used for the 1989 AQMP revision, two additional ozone episodes were modeled to investigate the effect of projected emission reductions on future ozone concentrations during a wider variety of meteorological conditions. Additional evaluations of model performance, including new graphical procedures and subregional performance statistics, were used to ensure adequate representation of the physical and chemical processes that influence ozone formation in the Basin.

A number of improvements were made to the modeling analysis for the 1994 AQMP. Growth factors for population and vehicle miles traveled (VMT) were revised to reflect the 1990 Census data and the economic climate of the early 1990s, and improved transportation modeling was considered. The modeling analysis benefited from a number of AQMD, CARB, and SCAG studies that improved the area source emission inventory (Appendix III-A). On-road, mobile emission estimates were improved with the use of the latest CARB emission factors program, EMFAC7F. Five ozone episodes were simulated to evaluate control strategy effectiveness. In addition to the June 5-7, 1985, episode used in the 1989 AQMP, and the two Southern California Air Quality Study (SCAQS) episodes (August 26-28, 1987, and June 23-25, 1987) added for the 1991 AQMP analysis, two additional episodes (July 13-15, 1987, a SCAQS episode, and September 7-9, 1987) were simulated for the 1994 AQMP. In this manner, control strategy decisions were based on a range of meteorological conditions, thereby reducing uncertainty in the control strategy's effectiveness. It was determined that hydrocarbon and oxides of nitrogen emission reductions on the order of 80 and 60 percent, respectively, would be needed in order to attain the NAAQS.

Based on the AQMD's experience with the five ozone episodes used in preparing the 1994 AQMP, it was decided to drop the June 1985 meteorological episode for the 1997 AQMP. The AQMD believed that the 1987 meteorological episodes were satisfactorily evaluated. Since the 1985 meteorological episode was based on routinely monitored data, it was believed that the 1987 SCAQS episodes provided improved performance. In October 1998, AQMD provided to the USEPA a "weight of evidence" analysis that indicated that even without the June 1985 episode, a viable ozone attainment demonstration could be made.

As a result of intense interest for aerometric databases to support *regional* ozone modeling, a large-scale field measurement program was carried out in southern California during the Summer of 1997 to collect sufficient aerometric data to allow data analysts and modelers to characterize and simulate ozone formation and fate in the region. Several agencies and others participated during the planning and operational phases of the field study, including CARB, USEPA, the local air districts, the US Navy, the US Marines, and the marine industry. The 1997 Southern California Ozone Study, or SCOS97, occurred over a four month period from June 15 through October 15, 1997 and captured several episodic ozone days.

The 2003 AQMP updated the attainment demonstration for the federal standards for ozone and PM10; replaced the 1997 attainment demonstration for the federal CO standard and provided a basis for a maintenance plan for CO for the future; and updated the maintenance plan for the federal NO2 standard that the Basin has met since 1992. New ozone episodes, including these from SCOS97, were included as complementary or replacement episodes in the 2003 AQMP. This revision to the AQMP also addressed several state and federal planning requirements and incorporated significant new scientific data, primarily in the form of updated emissions inventories, ambient measurements, new meteorological episodes and new air quality modeling tools. This revision pointed to the need for additional emission reductions (beyond those incorporated in the 1997/99 Plan) from all sources, specifically those under the jurisdiction of CARB and the USEPA which account for approximately 80 percent of the ozone precursor emissions in the Basin.

The 2007 AQMP modeling effort focuses primarily on recent ozone episodes in 2004 and 2005. These periods better reflect emissions conditions following the reformulation of gasoline in California. The August 1997 episode from SCOS97 will be retained for continuity with the previous AQMP analyses. The 2007 AQMP will be consistent with and will build upon the modeling approaches taken in the previous SIP efforts for the South Coast Air Basin, utilizing the latest tools and technical guidance.

AQMP PM Modeling History in the South Coast Air Basin

PM is a multicomponent pollutant including inorganic species such as sulfate, nitrate, ammonium, sodium, chloride, and organic compounds, elemental carbon, and a variety of trace metals. The PM10 modeling analysis shows that the annual average PM10 concentration is the controlling factor for attainment of the federal PM10 standards in the future. Although there were several PM10 modeling tools, there had been no single reliable annual PM10 model available to address the multicomponent nature of the PM10. Therefore, a multi-pronged modeling methodology was employed to assess regional PM10 and demonstrate future compliance with the federal PM standards.

For the 1989, l991, and 1994 AQMP, the Chemical Mass Balance (CMB) model for primary and secondary organic carbon and the Particle-In-Cell (PIC) model for sulfate and nitrate were used for annual PM10 analysis. And speciated linear rollback (SLR) was used for maximum 24-hour PM10 analysis.

For 1997 AQMP, a new annual PM10 modeling methodology, the UAM/LC model, was developed and applied. The Urban Airshed Model (UAM) (Ames, et al., 1985; and Morris, et al., 1990a, 1990b) was used as a host air quality model and the parameterized linear chemistry (LC) module was incorporated into the UAM. UAM was adapted to address the formation of particulate nitrate, sulfate, and ammonium and handling of primary particles by replacing the UAM standard chemical mechanism with the parameterized linear chemistry module. UAM/LC, unlike the PIC model, addresses the 3-dimensional aspects of transport and diffusion, varying mixing height, ammonia emissions change, and particulate nitrate concentrations. However, the UAM/LC model cannot handle secondary organic carbon because the current parameterized linear chemistry does not include organic chemistry. Secondary organic carbon is treated separately by the CMB model.

For the 2003 AQMP, UAM/LC model was further enhanced to include secondary organic carbon and PM2.5 partition. The resulting UAMAERO-LT model, for the first time, provided a more robust, stand-alone platform for primary and secondary annual PM2.5 and PM10 simulations.

2007 AQMP Modeling Analysis Goals

The 2007 AQMP modeling will focus primarily on the 8-hour ozone and the annual and 24-hour PM2.5 NAAQS attainment demonstration and reasonable further progress. The applicable NAAQS, along with the current attainment status of the South Coast Air Basin and recent design values, are presented in Table 1. Although the 1-hour federal standard was revoked in 2005, the analysis of 1-hour ozone will be retained as a benchmark of progress toward meeting the former 1-hour ozone NAAQS, as well as toward the State of California ozone standards. In addition to the PM2.5 NAAQS attainment demonstration, the particulate modeling analysis will include annual and 24-hour PM10 attainment demonstrations.

Further, the 2007 AQMP modeling will address maintenance plans for Carbon Monoxide (CO) and Nitrogen Dioxide (NO2).

The modeling effort may also include initial modeling strategy development toward demonstrating attainment of the inhalable coarse particle (PM10-2.5) NAAQS and a stricter PM2.5 NAAQS recently proposed by USEPA. The proposed standards are:

- PM10-2.5: 98^{th} percentile 24-hour PM10-2.5 in a year, averaged over 3 years not to exceed 70.4 $\mu g/m^3$; no annual standard;
- PM2.5: 98^{th} percentile 24-hour PM2.5 in a year, averaged over 3 years not to exceed 35.4 $\mu g/m^3$; no change to annual standard.

TABLE 1
National Ambient Air Quality Standards Compliance Status in the South Coast Air Basin

	8-Hour Ozone	**24-Hour PM2.5**	**Annual PM2.5**
Standard	3-year average of the 4th highest concentration not to exceed 0.084 ppm	3-year average of the 98th percentile of 24-hour concentrations not to exceed 65.4 $\mu g/m^3$	3-year average of 4 quarterly averages not to exceed 15.04 $\mu g/m^3$
Classification	Severe-17 [may petition for Extreme]	Non-Attainment	Non-Attainment
Attainment Date	2021 [2024, if Extreme]	2015	2015
Design Value	0.127 ppm (2002-2004)	67 $\mu g/m^3$ (2002-2004)	24.8 $\mu g/m^3$ (2002-2004)
	24-Hour PM10	**Annual PM10**	
Standard	3-year average of the 99th percentile of 24-hour concentrations not to exceed 154 $\mu g/m^3$	3-year average of 4 quarterly averages not to exceed 50.4 $\mu g/m^3$	
Classification	Serious Non-Attainment	Serious Non-Attainment	
Attainment Date	2006	2006	
Design Value	159 $\mu g/m^3$ (2002-2004)	57 $\mu g/m^3$ (2002-2004)	

Ozone Design Value Determination

Since the base year emissions are for 2004, air quality data from the three overlapping 3-year periods from 2000 through 2004 were used for calculation of the 8-hour ozone design values for each AQMD air monitoring station. These are shown in Table 2, along with the Relative Reduction Factors (RRF) needed. Per USEPA guidance, the design value averages are truncated (not rounded).

TABLE 2

Ozone Design Value (ppb) for Each Station, 2000-2004

(Average of the 4th highest 8-hour station concentration in each 3-year period)

Station	2000-2002 Design Value	2001-2003 Design Value	2002-2004 Design Value	Current Design Value (DVC)	RRF Required
AZUS	102.3	101.0	101.0	101.43	0.8284
BURK	91.7	91.3	91.3	91.43	0.9190
LGBH	61.7	60.7	60.7	61.03	
RESE	93.3	106.3	106.3	101.97	0.8235
POMA	89.7	96.7	96.7	94.37	0.8898
LYNN	51.0	53.3	53.3	52.53	
PICO	80.3	79.0	79.0	79.43	
CELA	79.3	78.3	78.3	78.63	
PASA	96.3	95.3	95.3	95.63	0.8787
SCLR	113.3	126.7	126.7	122.23	0.6874
WSLA	69.3	73.3	73.3	71.97	
HAWT	69.3	71.0	71.0	70.43	
GLEN	110.7	114.3	114.3	113.10	0.7427
ANAH	69.7	71.7	71.7	71.03	
LAHB	75.7	74.7	74.7	75.03	
CSTA	67.3	71.3	71.3	69.97	
MSVJ	80.0	82.7	82.7	81.80	
PLSP	105.3	108.3	108.3	107.30	0.7829
RIVR	108.0	112.7	112.7	111.13	0.7561
PERI	114.0	115.7	115.7	115.13	0.7298
INDI	92.3	96.7	96.7	95.23	0.8824
ELSI	104.3	109.0	109.0	107.43	0.7821
UCRI	113.3	117.3	117.3	115.97	0.7241
BNAP	110.3	118.7	118.7	115.90	0.7248
UPLA	114.0	113.0	113.0	113.33	0.7414
CRES	129.0	131.7	131.7	130.80	0.6422
FONT	112.3	123.0	123.0	119.43	0.7035
SNBO	114.7	118.7	118.7	117.37	0.7155
RDLD	120.0	128.3	128.3	125.53	0.6693
MLOM	103.0	106.0	106.0	105.00	0.8000
RHIS	130.3	136.7	136.7	134.57	0.6241

Overview of the Modeling Analysis

The analysis techniques currently recommended for attainment demonstrations using air quality models have changed significantly from those used in past demonstrations. In *Guidance on the Use of Models and Other Analyses in Attainment Demonstration for the 8-hour Ozone NAAQS* (USEPA, 2005), USEPA recommends that the air quality models be used in a relative sense in concert with observed air quality data rather than applying the air quality model in a deterministic sense. The Relative Reduction Factor (RRF) which takes the ratio of future to present predicted air quality is multiplied to an "ambient design value" to demonstrate attainment. The proposed ozone modeling analysis is comprised of the following tasks:

- Identify potential, new ozone meteorological episodes to be used. These episodes should represent the different meteorological conditions that are conducive to ozone formation in the Basin.
- Among the widely accepted state-of-the-science ozone models, CAMx was selected for the attainment demonstration. CMAQ may be employed in the sensitivity analysis and weight-of-evidence section as a supportive modeling tool.
- Develop model inputs. This task includes evaluation of the raw data and of the model input files developed from them. The input files will be evaluated using graphical and other techniques.
- Simulate each episode with the proposed ozone models. This task includes a separate performance evaluation for each episode and each model. Documentation of the simulation results and performance evaluations will be provided.
- Project ozone air quality with proposed control measures in effect for the years 2007, 2010, 2014, and 2020. This task includes the required attainment demonstration using RRF. Model projections for the year 2007 are necessary since that is the year that the CAA requires attainment for severe-17 areas, such as the Coachella Valley and Mojave Desert Ozone Nonattainment Areas. Ozone air quality projections to 2020 will be used to demonstrate that the control strategy maintains the ozone NAAQS and to establish emission budgets needed for conformity purposes.

The work to do the foregoing tasks will be divided between the AQMD and CARB staffs and they will fully share all analyses, model inputs and outputs, findings, and conclusions. Consensus on each component of the analysis shall be reached before proceeding with subsequent components. In the event of technical disagreement on any of the work elements, the

AQMD and CARB staffs shall attempt to reach consensus on a mutually acceptable approach. In the event that consensus cannot be reached, the disagreement will be elevated to the Executive Officers for resolution. Table 3 summarizes the model selection and application elements for the 2007 AQMP and the changes from the 2003 AQMP modeling.

TABLE 3
Summary of Proposed 2007 AQMP Model Selection and Application

2007 AQMP Element	2003 AQMP Element	Selection Process/Issues/Comments
Ozone Dispersion Platform: CAMx Chemistry: SAPRC99	*Ozone* Dispersion Platform: UAM Chemistry: SAPRC99	• Peer Group Recommendation to move to state-of-art mass-consistent model/chemistry • Integrates with numerical weather model output • CAMx used by several agencies for SIP development and supported by Environ • Option for one atmosphere modeling • Alternates CMAQ: Emissions preprocessing more extensive CALGRID: performance similar to CAMx with no one-atmosphere modeling
PM10/PM2.5 Annual and Episodic Dispersion Platform: CAMx <u>Chemistry:</u> • AERO-LT with CB-IV • Enhanced CFI scheme with CB-IV • Optional One Atmosphere Aerosol chemistry	*PM10/PM2.5* Dispersion Platform: UAM Chemistry: AERO-LT with CB-IV	• CAMx PM dispersion consistent with ozone discussion above. • Installed SCAQMD version of AERO-LT into latest CAMx code (V4.20). • Enhanced CAMx two section CFI aerosol scheme. It will be compared with AERO-LT.
Meteorology • MM5/4DDA • Hybrid MM5/CALMET • MM5 initialized using NCEP data	*Meteorology* • CALMET Objective Analysis • Hybrid *MM5/CALMET*	• EPA has expressed concerns about using the hybrid approach • MM5/4DDA is more mass consistent but doesn't capture localize wind impacts (transport to San Fernando Valley) • Testing several land use assumptions with prognostic model to optimize wind fields and vertical mixing/diffusivity fields. • Using Environ's and Aerospace met-model performance evaluation software. • Where possible take advantage of enhanced observation field data (e.g. 3D-Var)
Domain/ Coordinates SCOS97 Meteorology: Lambert Conformal Emissions and Model application: UTM Ozone: 16 layers PM10/2.5: 8 layers	*Domain* SCOS97 Meteorology: UTM Emissions and Model application: UTM Ozone & PM10 5-layers	• Maintained the SCOS97 domain however emissions inventories require coordinate system offsets to adjust from statewide modeling domain. Impacts are to biogenic and CEDARS output.

TABLE 3 (Continued)

2007 AQMP Element	2003 AQMP Element	Selection Process/Issues/Comments

Emissions Inventories
• 2002 Base year
• Enhanced aircraft/airport and shipping inventories
• POLA/POLB updates
• EMFAC2007
  o gross adjustments
  o "focused" inventories
  o Final public model
• Adjustments to fugitive PM10/PM2.5 categories
	Emissions Inventories
	• 1997 Ozone base year & 1995 PM10 base year
	• Updated aircraft/airport and shipping inventories
	• EMFAC2002V2.01 (major effort to develop surrogates for area sources)
		• 2002 Inventory will be used to back-cast 1997, 2000 and project inventories through 2030 for milestone years
		• Waiting on SCAGS' growth estimates based on 2004 RTP which is expected to differ only slightly from the 2007 RTP.
		• Episodic temperature and humidity fields submitted to CARB for biogenic emissions
		• CARB is adjusting temperature fields for planning inventory development
		• Gridded inventories awaiting focused on and off road model output and supplemental inventories
		• No weekend trip model output available from SCAG
		• CARB will develop a "weekend" overlay to mimic VMT based on Caltrans in-road counter data

Air Quality Model Performance <u>Ozone</u> • Assess model performance based on both 1-hour and 8-hour statistics • 60 ppb threshold (both indices) • Weight of Evidence Analysis • Mid-Course simulations PM10/PM2.5 (annual and episodic) • Base statistics at speciation sites • Weight of evidence analysis • Mid-Course simulations	*Air Quality Model Performance* Use EPA recommendations for 1-hour ozone and outline for PM10 and CO. <u>Ozone</u> • Mid-Course 2002 simulation • Comparative relative reduction for UAM/CAMx/CMAQ per Peer Advisory Group Recommendation <u>PM10</u> Analyzed "hot spot" grid cell emissions	• Will review thresholds and geographical zones used for ozone performance evaluation. • Conduct sensitivity simulations to test emissions mass, VOC/NOx ratios, emissions timing (daily and weekend vs. weekday), ammonia mass
Relative Reduction Factors RRF: sites specific applied to 3-year average of the design value (PM2.5 and ozone)	*Relative Reduction Factors* Tested for ozone and PM10 but not applied	

TABLE 3 (Continued)

2007 AQMP Element	2003 AQMP Element	Selection Process/Issues/Comments
Episode Selection Ozone • 1997 August 3-7 • 1997 Seasonal: August • 2004 June 3-7 • 2004 August 4-8 • 2005 May 17-24 • 2005 July 14-19 • 2005 August 25-29 PM10/2.5 • Annual 2005 (January – December) • 2005 October 19-25 • 2005 March 6-12	*Episode Selection* Ozone • 1997 August 4-7 PM10/2.5 • January – December 1995 • Episodic: Rollback CO • 1997 October 31-November 1	• Meteorological episodes include SCOS97 and post California Fuel reformulation (2003) • MATES-III meteorological data base development concurrent with AQMP data base development • Contract with Aerospace to provide additional observations data and MM5 initialization fields using (satellite ingest and 3DVAR
Initial/Boundary Conditions Ozone • EPA recommended boundary conditions • 40 ppb ozone top profiled to lower layers PM10/2.5 • Monthly varying emissions generated boundary conditions (simulate model with zero boundary conditions and let model generate boundary -- using 3-5 grid cells from model domain boundary as representative of boundary)	*Initial/Boundary Conditions* Ozone • Use EPA recommended boundary conditions • Per SCOS97 sampling tested 60 ppb ozone aloft PM10 Monthly varying boundary conditions based on coastal monitoring site data	• Will test varying top boundary concentration • Review alternate approaches for quantifying boundary conditions

2007 AQMP Schedule

The schedule of 2007 AQMP modeling efforts is driven by the regulatory deadlines for SIP submittal to USEPA, which is June 15, 2007 for 8-Hour Ozone. Table 4 outlines the tentative schedule of events leading up to the SIP submittal.

TABLE 4
Tentative 2007 AQMP Schedule

Task	Due Date
Episode Selection	January 2006
Air Quality and Meteorological Data Preparation	January 2006
Emission Inventory Preparation	April 2006
Performance Evaluation	May 2006
Control Strategy Development	May 2006
Attainment Demonstration	June 2006
Draft SIP Documents	September 2006
District Board Approval of Final SIP	November 2006
CARB Board Approval of Final SIP	February 2007
SIP Submittal to USEPA	June 15, 2007

[Add EIR Schedule,
Alternative Modeling,
Public Workshops]

AQMP Modeling Technical Oversight

The AQMD Governing Board has established several advisory groups to assist with technical oversight and scientific community and business involvement in air quality programs. The mission of the Air Quality Management Plan Advisory Group (AQMPAG), whose membership is appointed by the Board, is to review the overall aspects of a draft air quality management plan and to make recommendations concerning emission inventories, modeling, control measures, and socioeconomic impacts. Tasks of the AQMPAG, include:

- Provide review and comments on (1) studies relevant to advancing scientific and technical knowledge in support of AQMP preparation; (2) emissions inventory development and modeling approaches; (3) the development of new and revised control measures, including on-and off-road mobile sources; (4) socioeconomic data and evaluations.

- Foster coordinated approaches toward overall attainment strategies.
- Assist in resolving key technical issues.

In addition, the AQMD Governing Board has established a more focused technical oversight committee to review the technical aspects of the ongoing modeling analyses. Since the late 1980's the AQMD has had socioeconomic and modeling working groups, when the Governing Board passed a resolution to form the Modeling Working Group (MWG) during the adoption of the 1989 AQMP revision. The MWG, comprised of individuals with photochemical and aerosol modeling expertise, provided oversight and technical consensus on AQMP modeling issues. In 1997, the MWG was reconstituted as the Scientific, Technical, and Modeling Peer Review Advisory Group (STMPRAG). The STMPRAG role expands upon that of the MWG and includes experts in socioeconomic assessment and human health, providing review of AQMD modeling, monitoring and related scientific issues.

The STMPRAG assists AQMD in resolving technical issues related to air quality and socio-economic modeling by providing ongoing technical review and consensus of procedures and analyses. The objectives of the STMPRAG are as follows:

- Suggest methods to gather and process meteorological, aerometric and emission data with a specific focus on air quality modeling.
- Provide technical guidance to the air quality modeling efforts, with an emphasis on ozone and particulate matter. Some specific areas of technical guidance include: (1) Formulation of modeling approaches; (2) Selection and development of appropriate modeling techniques; and (3) Identification of model performance evaluation methods.
- Review and provide comments on the AQMP modeling procedures and analyses.
- Make recommendations on future modeling resource requirements (i.e., staffing and computational needs).
- Recommend methods for interpretation of modeling results.
- Provide a linkage between the air quality and socio-economic modeling communities, emphasizing the importance of future growth and economic factors on future air quality attainment demonstrations.

The STMPRAG consists of approximately 20 members appointed by the Governing Board, with representatives from USEPA, CARB, Southern California Association of Governments (SCAG), the California Small Business Alliance (CSBA), Southern California Edison (SCE), Western

States Petroleum Association (WSPA), and technical experts from universities and consultant firms.

Finally, as progress is made and products are available, interim results will be shared with the interested public at appropriate times and locations.

MODEL SELECTION

Meteorological Model

Background

Air quality models require three-dimensional, meteorological inputs. The key parameters are winds, mixing heights, temperature, and insolation. The windfields describe the transport and dispersion of pollutants. Mixing heights define the vertical extent of pollutant mixing near the surface. Temperature and insolation fields influence emission rates and the rates of chemical transformation. Because meteorological measurements can be made only at discrete locations, meteorological models are required to develop the 3-dimensional fields required by air quality models.

The meteorological models used to generate these three-dimensional fields are generally of three types: objective, diagnostic or prognostic. ***Objective models*** are the least sophisticated meteorological models. These models rely on interpolation of observations. Obtaining a reasonable field requires sufficient observations to accurately represent the atmosphere. This is especially true for windfields. In areas with complex terrain and bodies of water, such as the proposed modeling domain, the meteorology can be quite complex, and a successful objective analysis would require an extremely large number of observations.

Diagnostic models rely both on observations and constraints based on physical concepts such as the conservation of mass. A diagnostic wind model can simulate thermally induced circulations and the effects of surface friction. One example of this type of model is the Diagnostic Wind Model (DWM) which is distributed by the USEPA. For the DWM, the user first defines an initial-guess mean wind field that can be representative of synoptic scale patterns. The domain mean wind is then adjusted for the effects of terrain. Available observations are then used to develop meteorological fields using objective analysis. The initial guess and the objective analysis are then combined using a weighting function based on distance from observations. A criticism of diagnostic models is that the fields produced are not consistent from one hour to the next. Since the processes which create the wind, temperature, and mixing height fields are relatively independent, these models are also criticized for not being thermodynamically consistent between the meteorological parameter fields.

Prognostic models are the most sophisticated of the meteorological models. They are based on principles of atmospheric physics, i.e., conservation of mass, momentum, energy and moisture. As a result, they are computationally intensive. The use of four dimensional data assimilation (FDDA) or observational nudging – where observations are introduced to the model as an additional forcing term – is typically used in areas of complex meteorology to improve the accuracy of the outputs. Another approach is objective combination, in which observations are introduced after the model has estimated a value. Prognostic models are capable of explicitly incorporating many of the physical flow processes important in the domain. However, prognostic models have historically had problems estimating fine-scale flow features due to the limited resolution of datasets used for describing geographic features.

Previous AQMP Applications

In the past, CARB and AQMD have utilized prognostic, diagnostic, and objective models to generate meteorological inputs for modeling. The National Center for Atmospheric Research's prognostic, non-hydrostatic Mesoscale Model (MM5) was applied for modeling in support of attainment planning in the San Joaquin Valley. The SCAQMD also has experience with the SAIMM prognostic model. Diagnostic models (WIND2D, WIND3D, DWM) have been applied in the Sacramento area and in southern California to prepare meteorological input fields for the application of photochemical models in those areas. CARB and AQMD conducted a review of CALMET, which may be viewed as an improved version of the DWM and which is being distributed through the USEPA for air quality modeling applications. The CALMET model has an added feature that allows a hybrid meteorological field to be developed by merging the results from a prognostic model, such as the National Center for Atmospheric Research Mesoscale Model Version 5 (MM5), with an objective or diagnostic analysis characteristic of the CALMET model. This hybrid approach has the potential to take advantage of the prognostic capabilities of MM5 in areas of the domain where meteorological measurements are few, and utilizing measurements in an objective analysis where there are many.

2007 AQMP Meteorological Modeling Approach

The SCOS97 field study generated a dataset with a relatively high spatial density of meteorological observations. While this dataset suggests that an objective/diagnostic model could be adequate to develop the meteorological parameter fields required for air quality modeling of the August SCOS97 episode, there are large portions of the modeling domain—such as over the ocean or the inland desert—where there are few observations. The approach for the 2007 AQMP modeling will be to use the MM5 prognostic model with a 5 km grid resolution. The meteorological boundary conditions for MM5 are generated using the output from a Global Climate Model (GCM) with a relatively coarse grid of 45 km. The MM5 prognostic model uses more accurate and complete physics than the diagnostic models used previously. The MM5 has relatively good replication of meteorological features of the Basin, such as the coastal eddies, Santa Ana winds, recirculation, & strong inversions.

The recent air quality models are designed to use inputs from the prognostic models, such as MM5, and the use of such a model is strongly encouraged by USEPA. In the past, the use of MM5 meteorological fields in air quality models has brought limited success in the prediction of peak ozone concentrations that result from extreme meteorological conditions and complex distribution of precursor emissions. However, the prediction of ozone with MM5 meteorological fields on most days is comparable to the results using other models. Since the air quality model will be employed in more of a relative sense for the 2007 AQMP, with the use off relative reduction factors instead of peak concentration comparisons, the MM5 is an appropriate choice for the AQMP modeling. The premise is that the magnitude of RRF will reflect the ozone concentration resulting from the various meteorological episode classifications. With the use of the MM5 meteorological model, the AQMP modeling effort will move closer to the "one atmosphere" air quality modeling perspective (i.e., ozone and fine particles simulated with the same model). The successful application of this prognostic model is critical for the development of multipollutant control strategies.

Several MM5 initialization fields and data ingest options are also being explored for the 2007 AQMP modeling effort:

- MM5 model initialized with the National Centers for Environmental Prediction (NCEP) 12 km ETA/North American Model (NAM);
- MM5 model with Aerospace Corp 3DVAR forecast fields;
- Weather Research and Forecasting (WRF) community model using Aerospace Corporation 3DVAR;
- MM5 model with NCEP database of upper air and surface observations and the 1degree by 1 degree Global Tropospheric Analysis
- Above method of MM5 with NCEP database and Global Tropospheric Analysis and four-dimensional data assimilation (4DDA) of AQMD station meteorological data (this method is more mass consistent, but may be difficult to capture localized wind impacts (e.g., transport to San Fernando Valley);

- Hybrid CALMET with MM5 as background field

To supplement the MM5 meteorological modeling, the CALMET/MM5 hybrid meteorological model will be used to bolster the sensitivity analyses and weight-of-evidence discussions. The RRF can be adjusted or supported by the air quality modeling results using this alternative hybrid meteorological field. In this approach, the parameter fields will be overlaid using a weighting scheme that is based on the proximity to meteorological observations. The resultant fields benefit from the capabilities of the prognostic model in those areas of the modeling domain with few observations (such as offshore, in complex terrain, and in the desert areas), and benefit from the objective analysis component of the diagnostic model to force the fields to agree with observations. To develop the hybrid fields, the fields developed using CALMET and MM5 will need to be mapped into common horizontal and vertical coordinate domains. The CALMET model code is structured to facilitate this mapping.

Air Quality Model

Background

The air quality model employed for previous AQMP efforts, the Urban Airshed Model (UAM-IV (USEPA 1990), is widely acknowledged to have characteristics which limit its utility when applied to large modeling domains or to domains that are not geographically uniform. In addition, much of the science in the model is outdated, and both the USEPA and CARB are no longer recommending that model for most analyses. Several photochemical models have been developed to improve upon the UAM-IV. Among those models, CAMx and CMAQ were widely accepted models as the state of the science models that include the most up-to-date chemical mechanisms, physics and the efficient numerical algorithms. The following summarizes the current models.

- ***CALGRID***
  The CALGRID model (Yamartino et. al, 1989) was developed for CARB in the late 1980's. The model has been applied by various air pollution agencies around the world. It is modular to allow the user to substitute various types of wind fields and chemical mechanisms. CALGRID incorporates refined treatments of numerical advection, vertical transport and dispersion, and dry deposition. The model can be exercised with either the Carbon Bond IV (CB-IV) or SAPRC chemical mechanisms, and contains highly efficient chemical integration routines. The vertical structure of the atmosphere can be optionally defined

relative to a mixing height field, similar to the UAM, or can be based on fixed layer heights and a derived mixing height.

- ***Models-3***
  Models-3 (USEPA, 1998a) is a flexible software system designed for applications ranging from regulatory and policy analysis to understanding the complex interactions of atmospheric chemistry and physics. The Models-3 system is a framework that allows the user to go from developing model inputs to visualizing results all in one package. At the heart of the current version of Models-3 is the ***Community Multi-scale Air Quality (CMAQ) Model***. The capabilities of CMAQ include urban to regional scale air quality simulation of ozone, acid deposition, visibility and fine particles. CMAQ is a modular system capable of using output from the MM5 prognostic meteorological model, along with the CB-IV, RADM-2, or SAPRC-99 chemical mechanisms. The CMAQ model also includes a plume-in-grid module, vertical and horizontal growth due to turbulence and shear, a choice of advection schemes and a cloud- module to simulate precipitating and non-precipitating clouds. Since the Models-3 system is relatively new, some implementation and application problems are likely.

- ***SARMAP Air Quality Model (SAQM)***
  SAQM (Chang, et. al, 1997) is a three-dimensional non-hydrostatic model based upon the Regional Acid Deposition Model (RADM) (Chang et. al 1987, 1990). However, SAQM includes a number of improvements over RADM, including: a fixed vertical coordinate system that is compatible with MM5; a horizontal coordinate system defined in a Lambert-Conformal projection that accounts for curvature of the Earth; a mass conservation module for compatibility with non-hydrostatic meteorological inputs; the Bott advection scheme (Bott 1989a, 1989b) to reduce numerical diffusion and increase numerical accuracy; two-way nesting, and the capability to use either the CB-IV or SAPRC chemical mechanisms. A version of SAQM with plume-in-grid treatment is also available.

- ***Urban Airshed Model-Flexible Chemical Mechanism (UAM-FCM)***
  The UAM-FCM (Kumar et. al, 1995) is an alternate version of the UAM-IV that has been enhanced to allow the flexibility to incorporate any Carbon Bond- or SAPRC-type chemical mechanism. The FCM allows incorporation of reaction-specific photolysis rates. In addition, the UAM-FCM has a generalized methodology to solve the set of differential equations that is mechanism independent. However, the meteorological dispersion algorithms are the same as in UAM-IV.

- ***Urban Airshed Model-Variable (UAM-V)***
  The UAM-V (Systems Applications International, 1996) is an updated version of the Urban Airshed Model (UAM-IV) which incorporates many state-of-the-art enhancements in chemical mechanisms, meteorological models and the representation of emissions. Perhaps the most significant additions are: an updated CB-IV mechanism to include aqueous phase chemistry; plume-in-grid capabilities; an improved dry deposition algorithm; and an improved plume rise algorithm. Other enhancements over UAM-IV include allowing the user a fixed vertical structure as opposed to one that is relative to the diffusion break, the ability to use three dimensional inputs from prognostic models and two-way grid nesting. However, the present non-public domain status of UAM-V may preclude regulatory usage. The model developers have indicated that the model could be made available for any party to review if the party agrees that the use of the model would be solely for the review of the AQMP.

- ***Comprehensive Air-Quality Model with Extensions (CAMx)***
  CAMx (Environ, 1997) contains a number of advanced features, including grid nesting, sub-grid scale plume-in-grid simulation, alternative numerical advection solvers and the ability to use alternative chemical mechanisms. In addition it has the ability to tag emissions so that at the end of the simulation one can determine the sources of emissions impacting a particular receptor. Since CAMx is a relatively new model, thus there is a relatively short history of experience applying the model.

2007 AQMP Air Quality Modeling Approach

CAMx will be the primary air quality model for the attainment demonstration. This dispersion platform integrates well with numerical meteorological model output and it will be run using both the prognostic (MM5) and hybrid (CALMET/MM5) meteorological fields. The application of the MM5 and CAMx modeling system for both ozone and particulate matter simulation will bring AQMD closer to the “one atmosphere” modeling concept, where ozone and particulates are simulated in the same model. CMAQ model may also be run as a supporting model in the sensitivity analysis discussion.

The ozone air quality models will be run using the SAPRC (Carter 1999, 2001) chemical mechanism, based on chemical reactivity scales. At its meeting on October 8, 1999, CARB’s Reactivity Scientific Advisory

Committee (chaired by Dr. John Seinfeld, with participation by other members Dr. Roger Atkinson, Dr. Jack Calvert, Dr. Harvey Jeffries, Dr. Jana Milford, and Dr. Armistead Russell) discussed a peer review of the SAPRC-99 mechanism conducted by Dr. William Stockwell. Members of the committee agreed that the peer review was excellent, that SAPRC-99 was a state-of-the-art chemical mechanism, and they approved the peer review. The Committee then unanimously recommended that SAPRC-99, as the most up-to-date mechanism available, be used for SIP modeling.

The particulate matter air quality model will use CAMx with the AERO-LT/CB-IV chemical mechanism and the enhanced two-section CFI aerosol scheme with CV-IV. The AQMD version of the AERO-LT chemistry and the enhanced version of the CAMx CFI scheme have been installed in the latest CAMx code and comparative analyses will be presented. Advisory group recommendations have been to move toward a state-of-the-art, mass-consistent model and chemistry. This system will integrate well with numerical weather model output and with also use the MM5 model for meteorological fields.

MODELING DOMAIN

Meteorological Modeling Domain

Nested domains of 15 km and 5 km are defined within MM5 to simulate meteorological fields for the fine grid scale of the modeling domain. The modeling domain for MM5 is defined in a Lambert-Conformal projection with two parallels to account for curvature of the Earth within the modeling domain over such a large region. Figure 1 shows the nested MM5 domains. Figure 2 shows the finest scale (interior) MM5 domain, covering most of southern California. The vertical structure of MM5 is defined in a terrain-following, "sigma" coordinate system based upon a normalized pressure index. The 30 vertical layers defined for MM5 to approximately 15,000 m above ground level (AGL) can be transformed to fit the requirements of any air quality model. The MM5 meteorological fields are converted from Lambert-Conformal projection to UTM coordinates for input into the air quality models.

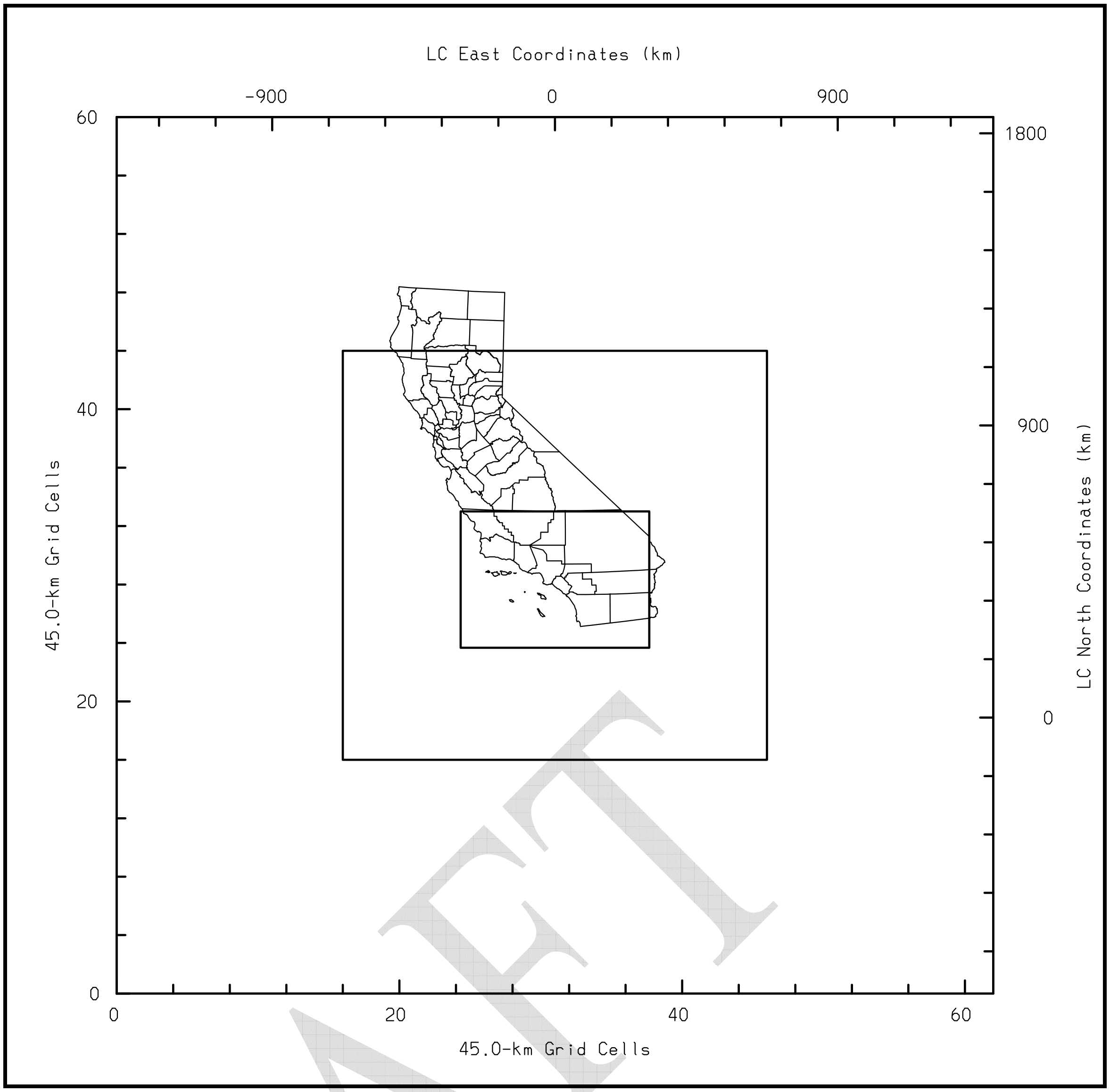

FIGURE 1
Nested MM5 Domains
The horizontal grid resolution of the outermost domain is 45 km, for the middle domain is 15 km, and for the fine scale domain is 5 km.

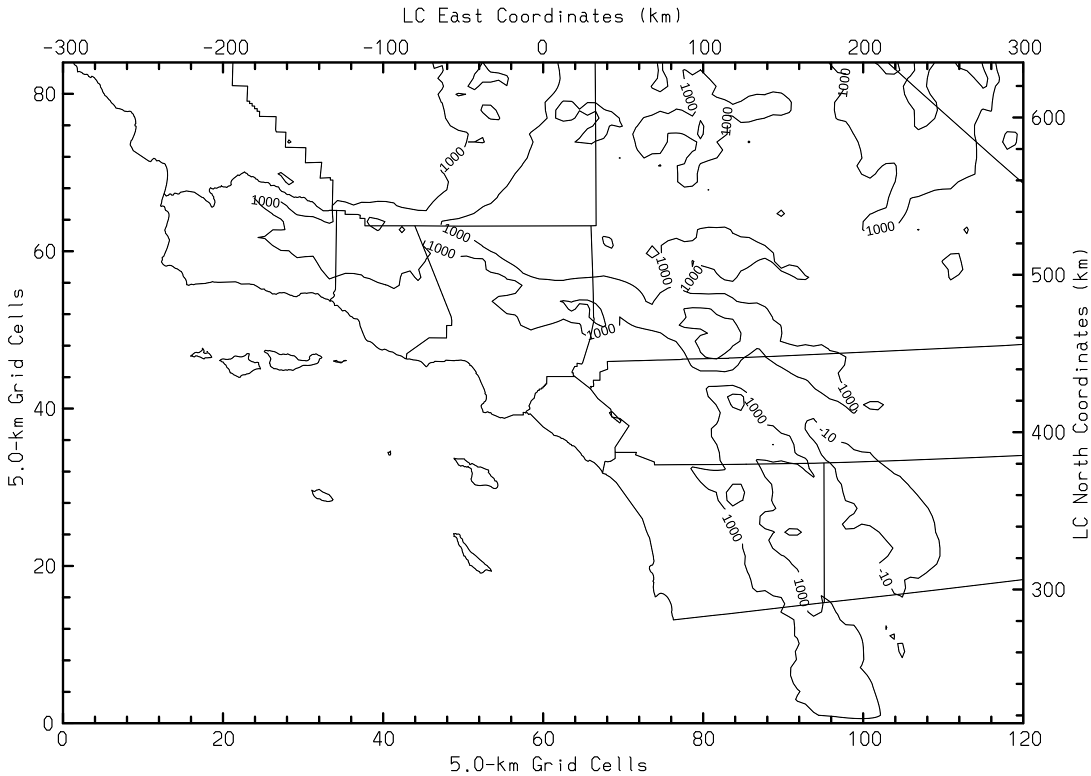

FIGURE 2
The Fine-Scale (5 km) MM5 Domain.

Ozone Modeling Domain

The proposed ozone regional modeling domain is that previously developed for the modeling of the SCOS97 field study episodes, encompassing a 600 km wide by 160 km area, as shown in Figure 3. Specifically, the UTM Zone 11 coordinates of the domain are 150-700 km UTM East and 3580-3950 km UTM North. This corresponds to 100 by 74 grid cells at 5 km grid spacing. The vertical modeling domain will extend to a height of approximately 5,000 m AGL for a more complete representation of atmospheric processes. This will contain observed high ozone concentrations aloft and allow three-dimensional wind flow patterns near elevated terrain features to be represented, providing accurate representation of pollutant transport and recirculation. This same domain will be used for all of the ozone episodes.

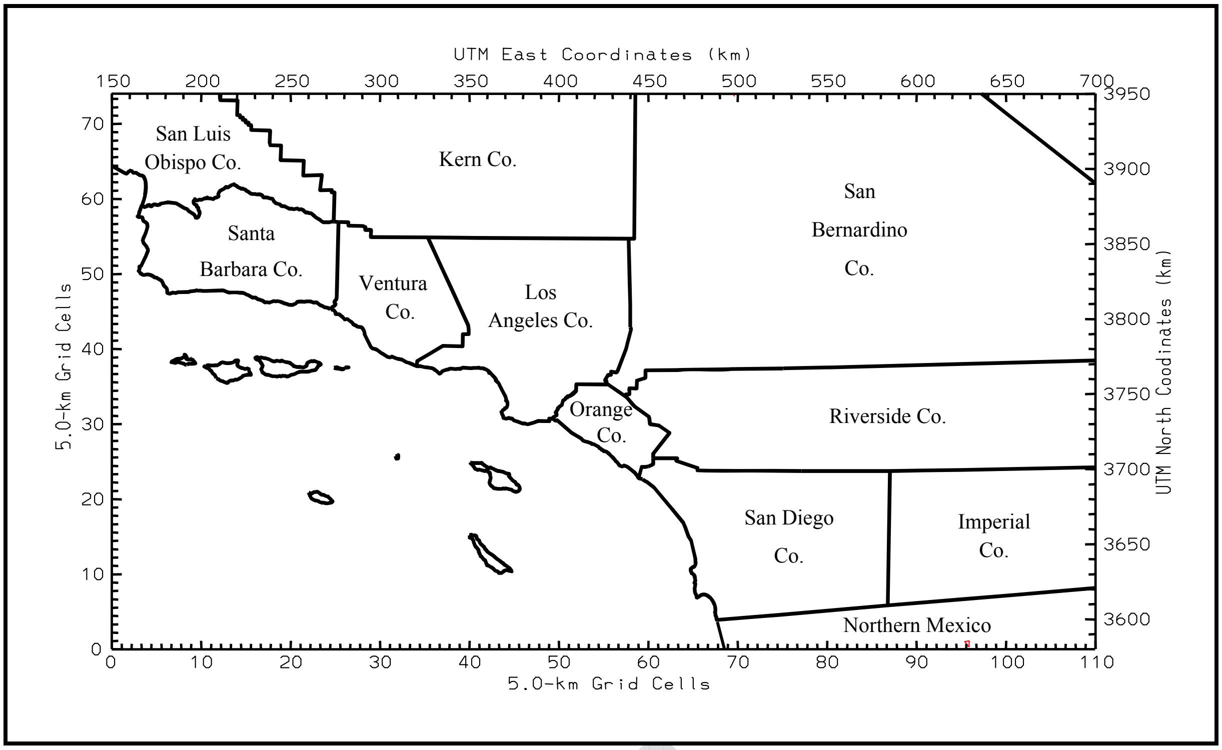

FIGURE 3
2007 AQMP Ozone Modeling Domain

The ozone modeling domain encompasses much of southern California, as follows: all of the South Coast Air Basin (including Orange County and the non-desert portions of Los Angeles, Riverside and San Bernardino Counties), the Coachella Valley and San Diego County; the California-Mexico border regions; most of Imperial County; most of the inland deserts; and almost all of the South Central Coast Air Basin (excepting a small piece of San Luis Obispo County). This large domain minimizes the influence of boundary conditions on simulation results and allows the effects of recirculation and interbasin transport to be better represented by the meteorological and photochemical model simulations. It also eliminates the need to define boundary concentrations between the air basins and it extends far enough offshore to contain wind flow patterns conducive to over-water recirculation.

PM Modeling Domain

The modeling domain for the particulate matter modeling will be smaller than the ozone domain, encompassing a 325 km wide by 200 km area, as shown in Figure 4. This corresponds to 65 by 40 grid cells at 5 km grid resolution. The reduced domain is due in part to the computational resource and time constraints of modeling the full 2005 year for annual PM. In addition, PM SIP modeling is not needed in the southernmost counties of California and adequate ammonia emissions inventories are not available from many areas surrounding the South Coast Air Basin.

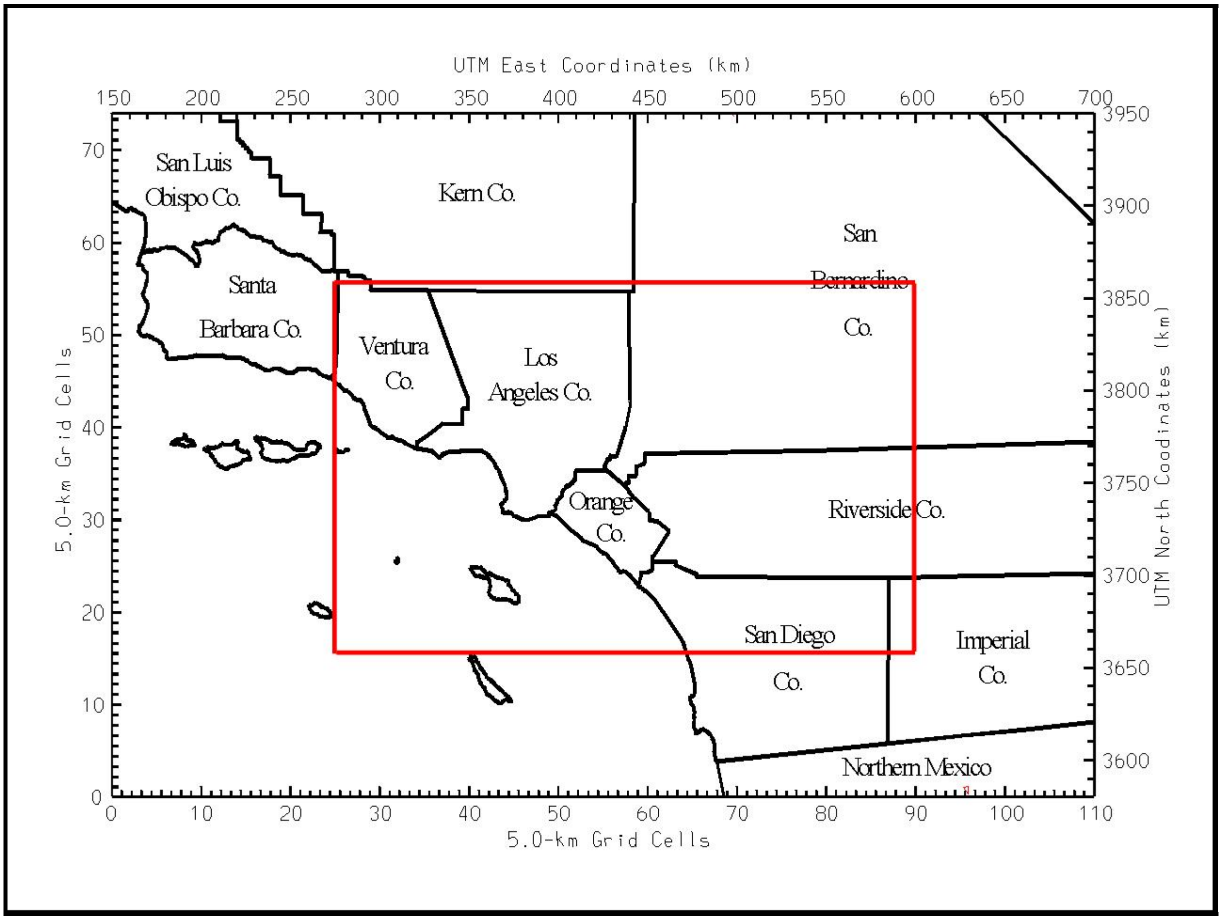

FIGURE 4
2007 AQMP PM Modeling Domain, inside the Ozone Modeling Domain

HORIZONTAL AND VERTICAL GRID RESOLUTION

Horizontal Grid Resolution

The horizontal grid resolution plays an important role in the modeling process. Large grid resolution tends to smooth emission gradients and meteorological inputs, which in turn leads to a smoothing of the resulting concentration fields. In general, the resolution should be sufficiently small to pick up emission gradients in urban areas and be consistent with the major terrain features which may affect the air flow. In the past, photochemical models have been applied in California with horizontal grid resolutions ranging from 2 x 2 km to 8 x 8 km. The specific grid resolution chosen was primarily dependent on the size of the modeling domain, computer resources available and the time and money available to carry out the simulations. In effect the final resolution was a compromise between the accuracy desired and the cost. However, the current generation of high-speed computers has minimized cost and resource constraints.

For the year 2007 AQMP ozone, particulate and meteorological modeling, a horizontal grid resolution of 5 km is proposed to be used for the air quality modeling. No grid nesting is anticipated. This resolution is consistent with the grid resolution used in earlier photochemical modeling studies for the South Coast Air Basin and for San Diego. In addition, this will reduce resources needed to create gridded emissions, which are based on 5 km grid cells. For the proposed ozone modeling domain, use of a 5 km resolution results in a modeling grid with 110 cells in the east-west direction and 74 cells in the north-south direction. The Universal Transverse Mercator (UTM) coordinate system is adopted as the primary coordinate system for the air quality modeling. There are variations in Lambert-Conformal map projection systems, such as the Normal Sphere (6471 km radius) used in MM5, the North American 1927 Clerk 1866 used in CARB's emissions development system, and the Arakawa-C or Arakawa-B variable configuration which assign meteorological parameters at grid points or the center of the grid. The selection of UTM simplifies translation from one grid system to another and the gridded emissions inventory is based on a UTM coordinate system.

Vertical Resolution

As with the selection of the horizontal grid resolution, the vertical resolution defined for air quality modeling domains has been limited by computational resources. In addition, available aloft meteorological and air quality databases were not sufficient to characterize conditions aloft. As a result, simulation results have been limited by a relatively small number of vertical layers within the atmospheric boundary layer, resulting in poor representation of the stratification of the atmosphere. The ability to better simulate the vertical structure of the atmosphere has improved significantly due to the increased availability of measurements aloft (including radar wind profilers and aircraft measurements), the emergence of higher-speed computers, and our increased experience with diagnostic and prognostic meteorological models.

Meteorological Modeling

For the terrain-following MM5 model, the proposed vertical layer consists of 34 layers to a height of over 15,000 meters AGL, as shown in Table 5. For input into the air quality model, the 34 layers are reduced to match the vertical resolution of the ozone or particulate matter air quality model.

TABLE 5
Vertical Structure for the MM5 Meteorological Model

Layer #	Sigma	P_0 (Pa)	Height (m)*	Depth (m)*
34	0.000	10000	15674	2004
33	0.050	14500	13670	1585
32	0.100	19000	12085	1321
31	0.150	23500	10764	1139
30	0.200	28000	9625	1004
29	0.250	32500	8621	900
28	0.300	37000	7720	817
27	0.400	41500	6903	750
26	0.300	46000	6163	693
25	0.450	50500	6461	645
24	0.500	55000	4816	604
23	0.550	59500	4212	568
22	0.600	64000	3644	536
21	0.650	68500	3108	508
20	0.700	73000	2600	388
19	0.740	76600	2212	282
18	0.770	79300	1930	274
17	0.800	82000	1657	178
16	0.820	83800	1478	175
15	0.840	85600	1303	172
14	0.860	87400	1130	169
13	0.880	89200	961	167
12	0.900	91000	794	82
11	0.910	91900	712	82
10	0.920	92800	631	81
9	0.930	93700	550	80
8	0.940	94600	469	80
7	0.950	95500	389	79
6	0.960	96400	310	78
5	0.970	97300	232	78
4	0.980	98200	154	39
3	0.985	98650	115	39
2	0.990	99100	77	38
1	0.995	99550	38	38
0	1.000	100000	0	0

** The vertical coordinate system for MM5 is based on a normalized pressure scale. The above layer heights were calculated from sea level using standard conditions. Layer heights are lower relative to ground level as terrain height increases.*

Air Quality Modeling

For sufficient vertical representation of the atmosphere, 16 vertical layers will be used for the CAMx ozone modeling, to a top height of nearly 5000 m AGL. Five of the layers will be below 500 m AGL (the nominal height of the summer afternoon mixing height within the Los Angeles coastal plain). The computational resources required for the annual particulate matter modeling necessitate a reduction in the number of layers used in the CAMx model for particulates. For this, eight vertical layers will used to a top height of approximately 5000 m AGL. The proposed vertical structure for the ozone and PM models are shown in Table 6, along side of the MM5 vertical structure.

TABLE 6

Vertical Structures for the CAMx Ozone and PM Simulations with Corresponding MM5 Meteorological Model Layers

MM5 Vertical Layer Heights (34)				Ozone Model Layers (16)		PM Model Layers (8)	
No.	Sigma	Height (m AGL)	Depth (m)	Height (m AGL)	Depth (m)	Height (m AGL)	Depth (m)
…	…	…	…				
24	0.500	4816	604	4816	1172	4816	2216
23	0.550	4212	568				
22	0.600	3644	536	3644	1044		
21	0.650	3108	508				
20	0.700	2600	388	2600	670	2600	670
19	0.740	2212	282				
18	0.770	1930	274	1930	274	1930	627
17	0.800	1657	178	1657	178		
16	0.820	1478	175	1478	175		
15	0.840	1303	172	1303	172	1303	508
14	0.860	1130	169	1130	169		
13	0.880	961	167	961	167		
12	0.900	794	82	794	164	794	325
11	0.910	712	82				
10	0.920	631	81	631	161		
9	0.930	550	80				
8	0.940	469	80	469	159	469	315
7	0.950	389	79				
6	0.960	310	78	310	156		
5	0.970	232	78				
4	0.980	154	39	154	78	154	116
3	0.985	115	39				
2	0.990	77	38	77	38		
1	0.995	38	38	38	38	38	38
0	1.000	0	0				

EPISODE SELECTION

Ozone Episodes

Five ozone episodes were simulated for the 2003 AQMP: June 24-25, 1987; August 27-28, 1987; August 3-7, 1997; September 26-29, 1997; and July 13-18, 1998. To maintain continuity with the last plan submittal, the model performance for the August 1997 episode will be reevaluated using updated emission data and modeling protocols. Five new recent episode periods from 2004 and 2005 will evaluated to better represent current conditions, including those associated with the reformulation of gasoline in the past several years. The six episodes are outlined in Table 7 and briefly described below.

TABLE 7
Summary of Ozone Episodes to be Simulated for the 2007 AQMP

Episode	Peak 1-Hr. Ozone	Peak 8-Hr. Ozone	Notes
August 3-7, 1997 (Sunday – Thursday)	**0.187 ppm** Tuesday, August 5 at Rubidoux	**0.117 ppm** Tue.& Wed., August 5 & 6	SCOS97 intensive measurement episode. Primary modeling episode from 2003 AQMP. Before California fuel reformulation.
June 3-7, 2004 (Thursday – Monday)	**0.163 ppm** Saturday, June 5 at Crestline	**0.145 ppm** Saturday, June 5 at Crestline	2004 Basin maximum 1-hour and 8-hour ozone concentrations.
August 4-8, 2004 (Wednesday – Sunday)	**0.156 ppm** Saturday, August 7 at Banning	**0.124 ppm** Saturday, August 7 at Crestline	
May 17 -24, 2005 (Tuesday – Tuesday)	**0.164 ppm** Sunday, May 22 at Santa Clarita	**0.145 ppm** Sunday, May 22 at Crestline	2005 Basin maximum 8-hour ozone concentration.
July 14-19, 2005 (Thursday – Tuesday)	**0.173 ppm** Saturday, July 16 at Santa Clarita	**0.143ppm** Friday, July 15 at Crestline	
August 25-29, 2005 (Thursday – Monday)	**0.182 ppm** Saturday, Aug. 27 at Crestline	**0.130 ppm** Saturday, Aug. 27 at Crestline	2005 Basin maximum 1-hour ozone concentration.

August 3-7, 1997 (Sunday – Thursday)

The episode period of August 3-7, 1997 was selected to provide continuity with the previous AQMP modeling effort. This episode was the primary modeling episode for the 2003 AQMP and it is representative of the most extreme meteorological conditions conducive to the highest ozone concentrations in the Basin. Unlike the more recent ozone episodes, the peak concentrations during this period did not occur on a weekend. Model input data supporting the August 1997 simulations were derived from intensive field monitoring that occurred during the 1997 Southern California Ozone Study (SCOS97). The SCOS97 study benefited from state-of-the art upper air wind and temperature monitoring and recently developed advances in particulate and oxides of nitrogen sampling technology.

The August 1997 episode included the peak ozone concentrations measured in the South Coast Air Basin during SCOS97 that were not associated with an exceptional event. A peak 1-hour ozone concentration of 0.187 ppm was measured at the AQMD Metropolitan Riverside County (Rubidoux) air monitoring station on Tuesday, August 5 and peak 8-hour concentrations of 0.117 ppm were measured on Tuesday, August 5 and Wednesday, August 6. High ozone concentrations were also observed in the Mojave Desert Air Basin (1-hour peak of 0.140 ppm) and in Ventura County (1-hour peak of 0.130 ppm, 8-hour peak of 0.115 ppm).

The August 1997 meteorological episode began on Sunday, August 3 under a ridge of high pressure aloft with 500 mb heights measured in excess of 5900 m each day. Weak onshore flow gave way to stagnant winds through the middle of the episode. Winds observed on August 5th, illustrate a classic "south route" transport regime that has been identified as characteristic of past severe Basin ozone meteorological episodes. Beginning late on August 6 and continuing into August 7, a well-defined coastal eddy developed that contributed to southerly flow and transport northward toward Ventura County. Peak inland afternoon temperatures crested over 100 degrees Fahrenheit on each day during the episode and downtown Los Angeles consistently reached the mid to upper 90's. The excessive regional surface temperatures and stagnant flow also contributed to a massive wildfire in the mountainous portions of eastern Ventura and southeastern Santa Barbara counties during the later part of the episode.

Ozone air quality reached the California Ozone Health Advisory level (0.150 ppm or higher) on two day during the episode at Redlands, San Bernardino, Rubidoux and Mira Loma. The peak observed value of 0.187

ppm occurred on the August 5 at Rubidoux. Eleven locations exceeded the federal 1-hour ozone standard. Areas such as Azusa, Pasadena, Glendora and Santa Clarita that routinely experience higher values of ozone during episodic conditions were spared the brunt of the impact due to excessive daytime heating that deepened the mixed layer. Overall, The peak concentrations in the Basin reached 0.140 ppm on the August 4 in the Central San Bernardino Mountains, 0.187 ppm at Rubidoux on August 5, 0.170 ppm and 0.150 ppm on August 6 and 7, respectively, in the Central San Bernardino Mountains. On August 6, ozone transport was observed through the Newhall pass to the Santa Clarita area and concentrations rose in Reseda and Ventura County as the coastal eddy developed.

June 3-7, 2004 (Thursday – Monday)

- Peak 1-hour Ozone: 0.163 ppm on Saturday, June 5 at Crestline (2004 Basin max 1-hour ozone)
- Peak 8-hour Ozone: 0.145 ppm on Saturday, June 5 at Crestline (2004 Basin max 8-hour ozone)

August 4-8, 2004 (Wednesday – Sunday)

- Peak 1-hour Ozone: 0.156 ppm on Saturday, August 7 at Banning
- Peak 8-hour Ozone: 0.124 ppm on Saturday, August 7 at Crestline

May 17-24, 2005 (Tuesday – Tuesday)

- Peak 1-hour Ozone: 0.164 ppm on Sunday, May 22 at Santa Clarita
- Peak 8-hour Ozone: 0.145 ppm on Sunday, May 22 at Crestline (2005 Basin max 8-hour ozone)

July 14-19, 2005 (Thursday – Tuesday)

- Peak 1-hour Ozone: 0.173 ppm on Saturday, July 16 at Santa Clarita
- Peak 8-hour Ozone: 0.143 ppm on Friday, July 15 at Crestline

The morning of July 13, 2005 had a low, strong temperature inversion layer in the Basin, which continued for several days, and hot weather except at the immediate coast. Skies were mostly clear, except for low clouds and fog offshore an at the coastline for most of the day. Ozone levels were starting to increase in the inland valley areas. The inland valley areas remained hot on July 14 while the coast remained much cooler with coastal low clouds and fog. On July 15, high pressures aloft, centered over the western U.S. deserts, helped to keep inland temperatures hot. Excessive heat warnings were in effect for many desert areas. The marine layer deepened a little with increased onshore flow, bringing night and morning low clouds and fog into the coastal valleys and transporting ozone and ozone precursors towards the Inland Empire with a 8-hour ozone peaking at Crestline (0.143 ppm). Skies in the Basin were mostly sunny with haze.

On July 16, the hot inland temperatures continued while coastal low cloud and fog in the morning clearing in the afternoon. .On July 17, the strong inversion layer continued along with the hot temperatures in the inland valley areas. Only the immediate coastal strip will escaped the hot weather due to low clouds and fog along the coastline and offshore. With strong high pressure aloft over the west coast, temperature will remain hot on July 18 and through the week with an excessive heat advisory and record temperature possible in some areas on Monday, July 18. A lower temperature inversion confined morning low clouds and fog to the coast, with hazy sunshine elsewhere. Little change occurred on July 19 as inland heating likely caused the inversion to break in the afternoon inland.

August 25-29, 2005 (Thursday – Monday)

- Peak 1-hour Ozone: 0.182 ppm on Saturday, August 27 at Crestline (2005 Basin max 1-hour ozone)
- Peak 8-hour Ozone: 0.130 ppm on Friday, August 27 at Crestline

Possible Seasonal Ozone Episode: Summer 1997

Ozone Episode Statistical Ranking

For the 2003 AQMP ozone attainment demonstration a statistical model was developed to characterize the ozone meteorological episodes selected for regional modeling evaluation. The statistical model related degree of ozone meteorological episode severity relative to the long term trend (1981-2002). Multi-variate regression was conducted using the Basin 1-hour average maximum ozone concentration and surface and upper air meteorological data for 1996 to generate an ozone prediction equation. This equation was applied to the air quality and meteorological data for the 22-year period to predict Basin daily maximum ozone and establish a daily ranking. The multiple linear regression analysis is discussed in Appendix V of the 2003 AQMP.

The statistical evaluation used in the 2003 AQMP used the daily maximum 1-hour ozone as the dependent variable to characterize the meteorological episodes. The meteorological conditions that give rise to higher 8-hour average concentrations are essentially a subset of those giving rise to peak 1-hour concentration. CART pattern recognition analysis (Cassmassi, 1998) demonstrated that the meteorological conditions that lead to high 1-hour average concentrations were the same as those for peak 8-hour concentrations. In addition, station specific correlations between maximum 1- and 8-hour average ozone concentrations generally explain more than 95 percent of the variance in the data. Given the consistency between the meteorological profiles contributing to both maximum 1- and 8-hour average concentrations, it was assumed that the algorithm used to rank episodes in the 2003 AQMP would be applicable for ranking the 8-hour episodes.

The 1997 episode ranking was taken directly from the 2003 AQMP. The statistical characterization was then extended to the 2004 and 2005 candidate episodes and their predicted daily maximum concentrations were compared to the 22-year distribution to determine relative rank. Table 6 summarizes the analysis.

Eleven of the 13 days ranked above the 95th percentile in episode severity with only August 6, 2004 failing to rank in the 90th percentile. The daily maximum 8-hour ozone averages were averaged by episode and compared to the 4th highest ozone value in the Basin (99th percentile) for each of the modeling years. The 1997 episode was a match for the annual design value while the 2004 and 2005 episodes bracketed the annual design values, each depicting episodes that were more or less severe than the design. The overall distribution listed in Table 8 may be enhanced at a later date if a seasonal modeling application is determined to be viable.

TABLE 8
Ozone Episode Characterization

Ranking Applied to Historical 22-Year Period (1981-2002)

Episode	Rank	Percentile	8-Hour Max Ozone (PPB)	Episode Average (PPB)	Annual 4th Highest Station (PPB)
8/5/97	198	98	124	127	127 San Bernardino
8/6/97	203	97	130		
6/5/04	83	99	148	138	116 Crestline
6/6/04	524	93	127		
8/6/04	1009	87	94	111	
8/7/04	331	96	127		
5/21/05	389	95	112	129	125 Crestline
5/22/05	50	99	145		
7/16/05	22	99	141	136	
7/17/05	15	99	141		
7/18/05	73	99	127		
8/27/05	160	98	130	126	
8/28/05	138	98	121		

PM Episodes

Annual particulate matter modeling will cover the entire year of 2005, taking advantage of additional speciated particulate measurements and meteorological data archived in association with the Multiple Air Toxics Exposure Study III (MATES-III) in the South Coast Air Basin. In addition, two PM2.5 episodes in 2005 will be modeled for 24-hour NAAQS compliance: October 19-25 and March 6-12, 2005. These two days were chosen since they were the highest PM2.5 episodes in 2005 that were not influenced by exceptional events. Both episode periods exhibited multiple-day buildups in the Beta Attenuation Monitor (BAM) continuous PM2.5 monitoring and affected multiple stations. Only July 5 had a higher PM2.5 concentration, but it was associated with fireworks on the night of July 4. Table 9 shows the days in 2005 with the highest Size Selective Inlet (SSI) sampler PM2.5 concentrations and the associated 24-hour BAM PM2.5 and SSI PM10 concentrations.

TABLE 9
Highest 24-Hour Averaged SSI PM2.5 Concentration in 2005
with BAM PM2.5 and SSI PM10 Concentrations

Date	Station	SSI PM2.5 ($\mu g/m^3$)	BAM PM2.5 ($\mu g/m^3$)	SSI PM10 ($\mu g/m^3$)
July 5, 2005	Azusa	132.7		
October 22, 2005	San Bernardino	106.3		
October 22, 2005	Rubidoux	98.7	120.6	123/124
October 22, 2005	Fontana	96.8		
October 23, 2005	Rubidoux	95.9	117.9	
October 22, 2005	Riverside	95.0		
October 22, 2005	Ontario	87.8		
October 21, 2005	Rubidoux	82.1	98.5	
July 5, 2005	Rubidoux	79.9	102.0	
March 10, 2005	Downtown LA	73.7	88.2	
March 11, 2005	Downtown LA	67.6	84.7	70

Annual PM: January 1 – December 31, 2005

- AQMP database development concurrent with MATES-III
- Peak Annual Average PM2.5: 23.3 $\mu g/m^3$ at Rubidoux
- Peak Annual Average PM10: 52.2 $\mu g/m^3$ at Rubidoux

Episodic PM10/2.5: October 19-25, 2005 & March 6-12, 2005

- Peak 24-Hour PM2.5 was 132.7 $\mu g/m^3$ at Azusa on July 5, 2005 (due to Independence Day fireworks)
- Second Peak 24-Hour Average PM2.5: 106.3 $\mu g/m^3$ at San Bernardino on October 22, 2005
- Rubidoux exceeded the 24-hour PM2.5 standard on the most days in 2005 (8 days)
- Peak 24-Hour Average PM10: 131 $\mu g/m^3$ at South Long Beach on May 4, 2005
- Second Peak 24-Hour Average PM10: 123 $\mu g/m^3$ at Rubidoux on October 22, 2005
- No 24-Hour NAAQS violations were measured in the Basin in 2005

INITIAL AND BOUNDARY CONDITIONS

Previous ozone modeling results in southern California proved sensitive to initial and boundary concentrations of air pollutants. This reflected the physical processes of recirculation of pollutants within southern California and the transport of pollutants from one air basin to another. However, because of the three-dimensional nature of transport and recirculation, it is difficult to take field study measurements that are adequate to determine boundary conditions. Ozonesonde measurements made during SCOS97 have shown high concentrations of ozone at heights above 3,000 m AGL. The modeling domain developed for the SCOS97 episodes, which will be used for the 2007 AQMP, has been expanded both horizontally and vertically from that of earlier studies in an attempt to minimize the influence of boundary conditions. With the boundaries extending horizontally well into the desert areas an over the ocean and vertically to 5000 m, the effects of recirculation and interbasin transport will be better represented by the meteorological and photochemical model simulations.

The sensitivity of the model simulations to initial and boundary conditions will be extensively examined with sensitivity analyses. Chemical species concentration measurements, where available from the SCOS97 field study archive and the PAMS measurements, will be used to check the initial and boundary conditions for reasonableness. For the large areas of the study domain in which there are few such measurements, initial and boundary conditions are often assigned “background” values based on the minimum concentrations measured from monitoring sites where measurements are available. The use of larger-domain air quality models to provide the initial, top and lateral boundary concentrations will also be explored. Speciated gridded pollutant and precursor profiles from the 36 km grid CMAQ model used for the WRAP visibility modeling is currently being evaluated to provide the initial and boundary conditions. The boundary profiles will vary with time and height level, as well as location, while the top boundary concentration will vary by time and grid location.

Initial Conditions

Initial conditions in the air quality models define the spatial distribution of chemical species concentrations throughout the 3-dimensional modeling domain at the time at which the air quality model simulation begins. There are two limitations inherent in defining initial conditions. The first is that chemical species concentrations are only measured at discrete locations and, for some species, for discrete time periods. In particular, observed VOC data is sparse although some PAMS monitoring stations data are available. Therefore, observed concentrations must be extrapolated to estimate concentrations throughout the modeling domain. The second limitation is that observed chemical species concentrations may not represent chemical equilibrium, especially since not all important chemical species are measured explicitly.

To minimize the importance of initial conditions on air quality model simulation results, the simulation is frequently started at some time interval before the period of interest. Historically, this “spin-up” time interval has ranged between 8 and 72 hours. For the 2007 AQMP episodes, the modeling period starts early in the morning (typically 0000 PDT) of the day before the first day of interest for spin-up. This allows a full diurnal cycle of sunlight for air quality model to reach chemical equilibrium. Since most of the modeling episodes encompass several days, the day with the worst air quality is typically well into the simulation.

Boundary Conditions

The top and lateral boundary conditions in the air quality models are the chemical species concentrations on the study domain boundaries and represent the concentrations for the air mass moving into the modeling domain. Unlike initial conditions which need to be defined only for the beginning of the simulation, boundary conditions must be defined for each hour of an air quality model simulation on the 2-dimensional, vertical planes on each of the horizontal boundaries of the domain and at the top of the modeling domain.

Ideally, the modeling domain boundaries are placed so remotely that simulation results are insensitive to boundary conditions. Even for the large SCOS97 modeling domain, the influence of boundary conditions on the simulation results may be problematic. Beyond the northern boundary, emissions from central California could have an impact on the domain. To the south, emissions from Mexico could have an impact. The western boundary is over the Pacific Ocean, where recirculation may be an issue.

Also, the determination of vertical profiles of chemical species is problematic. During SCOS97, ozone concentrations aloft were measured by launching balloon-borne ozonesondes. The measurements indicated that there are layers of high ozone ranging 60 to 80 ppb at near 3000 m. Prescribing a 60 ppb ozone concentration aloft in the model would contribute to high ozone concentrations at the surface due to advection or vertical diffusion. Ideally boundary conditions would be determined from measured chemical species concentrations, but these are rarely available for the most of the episode days or in all locations needed.

For the 2007 AQMP, AQMD proposes to use relatively clean initial and boundary conditions, based on the results of a larger domain model, the WRAP CMAQ visibility simulations. The SAPRC species for the initial and boundary conditions are shown in Table 10 for the ozone modeling. The use of relatively clean boundary conditions could significantly impact the predicted peak ozone concentration which results in poor model performance for ozone peak prediction. However, the use of clean boundary condition minimizes the uncertainty in future-year model predictions. The calculated RRF should only reflect the impact of anthropogenic emissions reductions. Also, as the future year air quality becomes close to background concentrations, the treatment of boundary conditions may be problematic, particularly in 8-hour ozone attainment demonstration. A part of the air quality model evaluation process, sensitivity analysis and weight of evidence analysis will be to assess the influence of boundary and initial concentrations on simulation results and RRF.

TABLE 10
SAPRC-99 Chemical Mechanism Species

Species	Species
ACET	ISPD
ALK1	MEK
ALK2	MEOH
ALK3	METH
ALK4	MGLY
ALK5	MPAN
ARO1	MVK
ARO2	NO
BACL	NO2
BALD	NOXY
CCHO	NPHE
CO	O3
CO2H	OLE1
CO3H	OLE2
COOH	PAN
CRES	PAN2
DCB1	PBZN
DCB2	PHEN
DCB3	PROD
ETHE	RC2H
GLY	RC3H
HC2H	RCHO
HC2H	RNO3
HCHO	ROOH
HNO3	SO2
HNO4	SULF
HO2H	TERP
HONO	XN
ISOP	

METEOROLOGICAL INPUTS

Meteorological Input Evaluation and Technical Review

The quality of the meteorological inputs can have a profound influence on the accuracy of the simulations concentrations of ozone, PM and other pollutants by the air quality models. It is therefore essential that the products of the meteorological models undergo a rigorous evaluation. By evaluating the flow characteristics of the wind fields, as well as the representativeness of the temperature, relative humidity and mixing height fields, the uncertainty in the air quality simulations can be minimized. AQMD and CARB staff will consider both qualitative and quantitative analyses in judging the meteorological fields and in reaching consensus on the appropriateness of those fields for use in the 2007 AQMP. Graphical and statistical analysis software is available to facilitate the meteorological input field evaluation.

The use of routine and special study monitoring data and model analysis archives provides a robust data set for comparing and analyzing the simulated meteorological fields. Some of the available data sets include:

- Routine surface meteorological network data, including:
    - South Coast AQMD (~32 stations),
    - Ventura County APCD,
    - San Diego County APCD,
    - Mojave Desert/Antelope Valley APCD,
    - NOAA/FAA Stations (METAR obs),
    - California Remote Access Weather Stations (RAWS),
    - California Irrigation Management Information System (CIMIS) Stations;
- Special study meteorological station data, such that from the Multiple Air Toxics Exposure Study III (MATES-III) project during part of 2004 and all of 2005;
- Marine buoy data from National Data Buoy Center (NDBC);
- Routine National Weather Service and military radiosonde observation (RAOB) data, including the stations at Miramar MCAS, Point Mugu NAS, San Nicolas Island NAS, Vandenberg AFB, Edwards AFB, China Lake NAS, Oakland, Mercury/Desert Rock, and Tucson;
- Southern California radar wind and temperature profiling network, including stations operated by:
    - South Coast AQMD (Los Angeles International Airport, Ontario International Airport and Moreno Valley),

  - Ventura County APCD (Simi Valley)
  - San Diego County APCD (Pt. Loma, Valley Center or Miramar)
  - NOAA project and SCOS97 profilers, when available (e.g., Goleta, San Clemente Island, Santa Catalina Island during SCOS97).
- National Center for Environmental Prediction (NCEP) gridded observational databases and model analysis fields, including:
  - NCEP ds353.4 ADP Global Upper Air Observations database,
  - NCEP ds464.0 ADP Global Surface Observations database,
  - NCEP ds083.2 Global Tropospheric Analyses, 1 degree x 1 degree gridded database,
  - NCEP ETA-12 km model forecast fields,
  - NCEP ETA-40 km Model Forecast Fields,
  - NCEP EDAS-40 km Gridded Data;
- Aerospace Corporation MM5/3-Dimensional Variational Analysis System (3DVAR) archives (incorporating surface, upper-air, ships, buoys, aircraft and satellite observations)

Qualitative Analyses

The qualitative analysis of modeled wind fields includes an evaluation of the gross circulation features in the modeling region to determine if the model is replicating those essential features (Mulberg, 1995, Lolk and Douglas, 1996). Such features include areas of convergence and divergence, eddy circulations, land/sea breezes, slope flows, and transport corridors. Since the modeling domain includes large overwater areas it is also necessary to evaluate offshore flows as well. Key features of the windfield are areas of convergence and divergence. These features result in vertical velocities which can transport pollutants upward (in the case of convergence) or bring pollutants from aloft down to the surface (with divergence). The evaluation will include a review of the convergence and divergence zones in the simulated windfield, and their impact on realistic vertical velocities, to determine agreement with measurements or conceptual models in terms of location, timing, and extent.

Synoptic forcing and mesoscale flow characteristics can sometimes result in eddy circulations. In the SCOS97 domain two key eddy features are prevalent: the Catalina Eddy (named since its center is often near Santa Catalina Island), and the Gaviota Eddy in the Santa Barbara Channel (Smith, et. al., 1984). Both eddy circulations are important transport mechanisms; they are capable of transporting precursors and aged ozone concentrations onshore and northward to Santa Clarita and sometimes Ventura and Santa Barbara Counties. Exceedances of the ozone standards are often observed with the presence of an eddy circulation and the deep of the marine layer that accompanies a mature coastal eddy can end an ozone episode. The timing of the onset, persistence, and spatial extent of eddy circulations, are a critical part of the windfield validation.

Land/sea breeze circulations are another important flow feature. The sea breeze is one method whereby pollutants generated in the Los Angeles Basin are transported eastward. That is, the strength of the sea breeze will determine how far precursors and ozone generated near the coast will be transported inland. Errors in the timing of the sea breeze can cause precursor emissions to be transported to the wrong locations instead of inland where peak concentrations are observed. It is essential that the onset of the sea and land breezes simulated by the model be compared to observations for reasonableness.

The onshore portion of the 2007 AQMP modeling domains includes areas of complex terrain. Slope flows are important as a recirculation mechanism that may influence ozone concentrations. Slope flows are probably the most challenging feature for prognostic meteorological models, due to the sparse observational data in complex terrain and these models have a tendency to overdo the speed of the slope flows. A proposed qualitative approach is to determine if wind speeds estimated by the model appear to be reasonable in areas of complex terrain.

As a qualitative and quantitative evaluation of the windfields, wind speeds are proposed to be statistically summarized and plotted by site and globally throughout the domain (Seaman et. al., 1995, Bigler-Engler et. al., 1996). Temporal plots for key sites will be examined to determine agreement with observations. Quantitative techniques will make use of statistical measures such as the mean gross error and mean bias to compare modeled and measured wind speeds (Mulberg, 1995).

Some of the methods being explored for the meteorological modeling incorporate observations, thus reasonably good agreement should be expected near those observation sites where data was used as input to the model. In order to diagnose the impact that incorporation of the observations has on the meteorological models, it may be useful to consider withholding some observations when executing the models to have an independent set of observations for comparison. The sites withheld should have some relation to the sites used to provide some assurance in the results from the comparison. This diagnostic evaluation is proposed to be conducted once acceptable meteorological fields have been prepared.

Temperature fields will also be examined. At the surface, qualitative analyses will include an examination of the diurnal and spatial variation of estimated and observed temperatures, as well as consistency of the gridded data within regions.. The interface at the coastline will be examined for the expected gradients between the ocean and the land. Mean bias and mean gross error statistics will also be calculated to provide quantitative measures of performance. In addition, the vertical temperature profiles generated by the models will be compared to those observed at rawinsonde sites and boundary layer wind and temperature profiler locations. The vertical temperature profile influences the stability characteristics of the modeling domain which significantly affects vertical mixing. The evaluation will include temporal and spatial evaluations of simulated vertical temperatures and mixing as compared to those estimated from observed soundings and profiler data. The timing of the onset and breakup of the inversion will also be evaluated, as this phenomenon has a profound effect on estimated ozone concentrations.

Quantitative Analyses

ENVIRON Corporation International (Emery, et al., 2001) proposed performance benchmarks and developed a statistical analysis software package, called METSTAT, to statistically and graphically analyze the meteorological fields. METSTAT is publicly available and widely used by the modeling community. It can read the MM5 output files and the observational data, and then calculate the following statistics: mean observation, mean prediction, bias error, gross error, root mean square error (RMSE), systematic root mean square error (RMSEs), unsystematic root mean square error (RMSEu), and index of agreement (IOA). It should be noted that the statistical evaluations are influenced by the number of stations and the duration of sampling period. The benchmark statistics will be applied to all observational stations available and to specific geographic groupings (e.g., coastal, mid-Basin, inland areas). Both daily and hourly statistics will be compiled for each modeled period.

Meeting the METSTAT benchmarks provides assurance that the model performance is comparable with performance achieved in the past. METSTAT can be used as a screening tool to identify the periods when the performance is poor that require further analysis. These statistics can also be used to identify stations where performance is consistently poor. Table 11 shows the proposed performance benchmarks for the meteorological inputs for the 2007 AQMP air quality modeling. In addition, temporal plots will provide direct comparison of modeled meteorological parameters at grid points corresponding to observational stations.

TABLE 11
Proposed Meteorological Input Performance Benchmarks

Parameter	**Benchmark**
Wind Speed Total RMSE	≤ 2.0 m/s
Wind Speed Bias	≤ ±0.5 m/s
Wind Speed IOA	≥ 0.6
Wind Direction Gross Error	≤ 30 degrees
Wind Direction Bias	≤ ±10 deg
Temperature Gross Error	≤ 2.0 K
Temperature Bias	≤ ±0.5 K
Temperature IOA	≥ 0.8
Humidity Gross Error	≤ 2 g/Kg
Humidity Bias	≤ ±1.0 g/Kg
Humidity IOA	≥ 0.6

[These benchmarks may be too stringent for MM5, especially Temperature. These may need to be reevaluated after seeing more results.]

EMISSION INVENTORY INPUTS

Ozone episodes occurring in 1997, 2004, and 2005 will be simulated for the 2007 AQMP. Gridded, hourly base year emissions inventories, including CO, NOx, SOx, and TOG emissions, for those years are needed for photochemical ozone modeling. The 2005 base year particulate matter emissions will also be needed to support inputs needed for aerosol modeling. The information needed to complete the emission inventory for the modeling region is obtained from the local air pollution control districts, transportation planning agencies and CARB. For the 2007 AQMP, the 2002 base year emissions will be used. The statewide emissions inventory will be gridded to the modeling domain. The 2002 emissions will be backcasted to the 1997 episode year and grown to the 2004 and 2005 episode years. Specific month and day-of-week emissions will be estimated from the annual average emissions, based on temperature corrections derived from ambient measurements. The emissions will also be grown to the attainment milestone and demonstration years of 2005, 2010, 2020 and, possibly 2015 and 2030.

Adjustments to the 2002 base year inventory for the 2007 AQMP will likely reflect the following changes from the 2003 AQMP inventory:

- Overall emissions inventory changes will likely include higher VOCs, lower NOx and lower CO emissions. New temperature and relative humidity profiles will be used for annual inventory adjustments.
- The stationary source inventory will reflect that the actual 2002 emissions were mostly lower than 2003 AQMP-projected emissions.
- The mobile source inventory will be projected with EMFAC Gross Adjustments (to be provided by Spring 2006). It will reflect increased VOC and NOx emissions from the 2003 AQMP inventory. Key areas of mobile source inventory adjustment include:
    - Truck Distribution/VMT/deterioration rate;
    - Ethanol & evaporatives and permeation issues;
    - Modified temperature distribution.
- For the particulate matter emissions categories, the new USEPA fugitive PM10/PM2.5 ratio will be evaluated and applied.
- Temperature and humidity corrections will be applied to the biogenic inventory.

Other potential emissions inventory changes will possibly result from improved inventories for ports, the Alameda Corridor, shipping, aircraft and airports. The 2007 AQMP on-road emissions will be based on technical-adjustments to the SCAG 2004 Regional Transportation Plan. No weekend trip model will be available from SCAG, so CARB will develop a "weekend" overlay to mimic VMT based on California Department of Transportation (Caltrans) in-road counter data. Air quality modeling analyses will stress emissions sensitivity runs, since the spatial distribution of emissions will be critical to model performance due to the use of Relative Reduction Factors (RRFs) instead of peak concentration performance metrics.

Emissions Characterization

Point Sources

Characterizing anthorpogenic point source emission is the responsibility of the local air districts. Emission inventories for point sources (including RECLAIM facilities) are compiled by local districts and reported to CARB. If annual emissions for a facility fall below 10 tons/year (this cutoff varies with district) the source is included in the area source inventory. Point sources are allocated to grid cells using the location that is stored as part of the point source emission database. Temporal codes which describe hours of operation are also included in the emission database. Factors are also stored to convert annual average emissions to a specific month and day of week. Point sources have been inventoried for 2002. SCAQMD's point source inventory for 2002 includes an update to locations (UTM coordinates) and stack parameters. Point source emissions will be estimated using the CARB California Emission Forecast System (Johnson, 1997) for the modeling episode base years and future years.

Area Sources

Area sources are comprised of emission source types that are difficult to inventory individually. Examples are architectural coatings, residential water heating, gasoline stations and off-road mobile sources not included in the CARB OFFROAD model. The area sources include point sources smaller than 10 tons per year and area surrogates are used for sources such as consumer products.

Districts and CARB share responsibility for estimating area source emissions according to a long-standing division of categories. CARB, 1997b describes methodologies used to estimate emissions from area sources. Factors are also included that allow estimates of specific month and day of week emissions from annual average emissions. Temporal codes which describe hours of operation are also included in the area source emission database. Area source categories have been inventoried for 2002. Emissions for the modeling episode base years and future years will be grown using CARB emission forecasting system.

On-Road Mobile Sources

On-road mobile source inventories are prepared using vehicle activity data from transportation planning agencies. The majority of travel is reflected in transportation plans developed by:

- Southern California Association of Governments (SCAG);
- San Diego Association of Governments (SANDAG);
- Santa Barbara County Association of Governments (SBCAG); and
- Kern Council of Governments (Kern COG).

Travel data for areas not covered by the transportation planning agencies are extracted from the California Statewide Planning Model maintained by the California Department of Transportation. Emission factors for on-road mobile sources will ultimately be estimated using the CARB EMFAC2007 emission factor model. However, the release of EMFAC2007 will likely be concurrent with the 2007 SIP submittal, so the modeling will proceed using the 2002 base year emissions inventory from the 2003 AQMP with gross EMFAC adjustments based on CARB technical documentation. DTIM4 will use both the emission factors and travel activity data to produce hourly gridded emission estimates for the SCOS97 region.

CARB is leading the effort to acquire all travel data needed for this modeling study. The network and travel activity data provided by transportation planning agencies is developed for peak and off-peak time periods, which will be processed into 24 hourly data sets. Day-specific traffic count data will be used to calibrate DTIM4 inputs for development of day-specific on-road mobile source emissions. CARB will use the network and travel activity data to produce gridded DTIM4 inventories for episode days.

Other Mobile Sources

Area source emissions from most categories of off-road mobile sources will be estimated using the CARB off-road mobile source emission model (OFFROAD). OFFROAD covers more than 12 off-road categories, including lawn and garden equipment, small utility and construction equipment, as well as farm equipment. Categories not estimated by OFFROAD will be covered under “area sources”. However, specific emissions for aircraft, marine vessels, and locomotives will be provided through separate special studies. OFFROAD will produce gridded emission inventories for each calendar year desired. The OFFROAD model will have the capability to estimate exhaust, starting, and evaporative emissions for differing spatial and temporal conditions.

Biogenic Emissions

The derivation of a gridded natural biogenic emission inventory requires data sets describing the spatial distributions of plant species, biomass, and emission factors that define rates of hydrocarbon emissions for each plant species. The Biogenic Emission Inventory System (BEIS 2.3) (USEPA, 1995) model, distributed by the USEPA for this purpose, is one source of these data sets for areas throughout the United States. However, the BEIS model has been shown to have limited use in California because of poor spatial resolution within the referenced data sets and a simplified scheme for assigning emission factors (e.g., Jackson, et al., 1996). The development of a gridded biogenic emission inventory for the SCOS97 domain will benefit from research conducted within California that describes the needed data sets in more detail than is defined within the BEIS model (Benjamin et. al., 1998).

CARB, in consultation with researchers at UCLA, developed a methodology to complete a gridded biogenics inventory for the SCOS97 modeling domain. The methodology involves the use of: (1) gridded plant species maps using the GAP data base (Davis et. al., 1995), an inventory of biomass diversity for the United States; (2) biomass distribution, determined using published correlations between biomass and Normalized Difference Vegetative Index (NDVI), an index of relative "greenness" from Advanced Very High Resolution Radiometer (AVHRR) satellite remote sensing data sets; (3) emission factors of isoprene, monoterpenes, methyl butenol, and other VOCs for various plant species known to exist within the modeling domain using taxonomic relationships between the plant species (Benjamin et. al., 1996). The gridded biogenic inventory, including the gridded plant species, biomass distribution and emission factor databases, are combined with ambient temperature and radiation data to produce gridded hourly emissions of isoprene, monoterpenes, methyl butenol, and other VOCs.

Organic Gas Speciation

Organic gas speciation profiles are applied to all categories of TOG emissions to obtain estimates for each organic gas species emitted in the modeling region. CARB maintains a database of current profiles that are routinely updated to reflect recent information. The most recent updates were for gasoline exhaust and evaporation, diesel exhaust and jet engine exhaust. The CARB publication *Identification of VOC Species Profiles* (CARB, 1991) documents the organic gas profiles.

Day-Specific Emissions

Emissions from many sources vary from day to day. Evaporative emissions from vehicles and vegetation increase with ambient temperature. Exhaust emissions are also a function of ambient temperature. Increased air conditioning demands on hot days also lead to increased emissions from electrical generation. Hourly surface temperatures for episode days are interpolated to each grid cell and are used in estimating emissions from vegetation and on-road mobile sources.

Criteria pollutant emissions from approximately 80 major point sources will also be estimated hourly for each specific episode day. Each district has acquired data from major point sources for the episode days and is developing day-specific point source inventories for those years. The districts also collect information on variances, temporary breakdowns and shutdowns. DTIM4 will be run to develop mobile source inventories for several episode days, including weekend days.

Where feasible, wildfire emissions will be estimated. Emissions from large ships in the shipping lanes are also estimated, using ship activity data (for commercial vessels) from shipping ports, ship-specific engine characteristics data, and the latest emission factors. Emissions from aircraft will be estimated using aircraft activity data, including hourly landing, takeoff, approach, climbout and cruise emission. This type of information will allow development of temporally and spatially resolved emission estimates.

Emissions Quality Assurance

CARB has provided specific guidelines to assist state and local agencies in implementing uniform and systematic approaches for collecting, compiling, and reporting emission inventory data. A comprehensive quality control and quality assurance plan was prepared to ensure good quality practices during development of the 2002 and future year emission inventories. These procedures include: quality control checks for collecting non-emission data, updating activity data, and using appropriate emission factors for calculating emissions; emission calculation methodology;

quality assurance evaluation using the Data Attribute Rating System (DARS); and quality review of the entire inventory. The DARS program, originally developed by the USEPA, will be used as an additional quality assurance tool to quantify the relative accuracy of the annual emission inventories. CARB has also provided the districts with a variety of quality assurance reports to aid in the review of inventory data important for modeling. These reports were intended to provide checks on the accuracy of the emission calculations, stack data, facility location data, temporal data, devices data, process data, etc.

Emission Projections

Future year emissions form the basis for an air quality emission reduction target. Future year emissions for area and point sources are projected by accounting for growth and control, generally using growth and control factors applied to the base year (2002) emissions. Control factors are derived based on adopted measures. Growth factors are derived from socioeconomic and demographic data provided by districts and local agencies, and CARB-sponsored research factors elsewhere. Area source and offroad emissions are gridded using the appropriate surrogates as used for 2002. Gridded future year surrogates for the entire modeling domain region and also being prepared for milestone and attainment demonstration years. Surrogates for other years can be interpolated as needed.

Future year traffic activity and network data are also prepared by local planning agencies. EMFAC will give estimates of future year emission factors. DTIM4 uses future year emission factors and network travel data to obtain gridded future year on-road mobile emissions. DTIM4 inputs for future years are being compiled and prepared. Ambient temperatures that occurred during 2002 are also used in calculating future year emissions for each episode day.

Biogenic emissions will not change for future years. Even though there may be a shift in farm or landscaping plans and species, the capability does not exist to incorporate any potential changes into the inventory. Seep emissions will also remain constant in future year inventories.

AIR QUALITY MODEL PERFORMANCE EVALUATION

It is a well established tenet of the modeling community that for an air quality modeling simulation to give reliable results, it must be capable of giving the right answers for the right reasons. That is, not only must the model be capable of reproducing observed air pollution measurements with a reasonable level of accuracy, but it must also pass a series of prescribed tests designed to ensure that the apparently accurate results are not produced by a combination of compensating errors. Several tests on the modeling simulations, both at the surface and aloft are proposed to be conducted as part of the model performance evaluation. Both precursor and secondary species will be evaluated, in addition to 1-hour and 8-hour ozone, PM10 and PM2.5 for each episode and model variation. Statistical and graphical analyses will compare simulated concentration to measured values, throughout the domain and by geographic region. Diagnostic simulations will be used to analyze the sensitivity of the model to the input parameters and assumptions. This performance evaluation should allow a determination that the model is working properly. The following evaluation tools are based on previous modeling practices, the CARB photochemical modeling guidance (CARB 1992), and the USEPA attainment demonstration guidance for ozone (USEPA, 2005) and particulate matter (USEPA, 2001b).

Statistical and Graphical Analyses

The model performance evaluation effort will include both graphical and statistical analyses. These will compare simulated pollutant concentrations with measured values from the routine air monitoring stations and special study sites, including the PAMS stations. The statistical evaluations for the particulate matter modeling will focus primarily on comparisons to the speciated particulate data from the MATES-III study. The graphical analyses will include time series plots showing temporal variations, contour plots showing spatial variations, scatter plots showing tendencies for over- or under- estimation, and residual plots showing the distribution of the differences between observed and predicted concentrations.

The statistical analyses will examine the accuracy of peak estimates (both paired and unpaired in time and space), mean normalized bias, mean absolute gross error, and mean absolute normalized gross error. The statistical performance criteria outlined in the CARB guidance document for Class B or better ozone performance will be used to guide the determination of acceptable model performance. These statistical criteria will be used as a criterion for acceptable model performance. However, other analyses (graphical, multi-species, aloft comparisons and the diagnostic simulations) will also be used to determine acceptable model performance, and ultimately a conclusion that the model is working properly must be made considering the evidence from all of the analyses. Table 12 shows some of the statistical performance goals for the ozone simulations.

TABLE 12

Performance Goals for 1-Hour Ozone

Statistic for 1-Hour Ozone	Criteria (%)	Comparison Basis
Normalized Gross Bias	≤ ±15	Paired in space and time
Normalized Gross Error	≤ 35	Paired in space (+2 grid cells) and time
Peak Prediction Accuracy	≤ ±20	Unpaired in space and time

Subregional Performance

The performance tests will be evaluated for the entire domain, by district or air basin, and for several geographic subregional zones to ensure that the domain-wide statistics do not mask subregional issues with the simulation. Since the modeling domains are very large, six geographic zones are proposed to be evaluated for model performance: San Fernando Valley, west (or coastal) Basin, mid-Basin, San Gabriel Valley, east Basin, and Coachella Valley. The same statistical acceptance criteria will be used for the subregions as for the entire domain.

Multi-Species Evaluations

To be useful for planning or other purposes, an air quality model must be able to replicate measured concentrations with reasonable accuracy. However, it is also important to compare estimated and measured concentrations of precursors and secondary species, to establish confidence that the chemistry is being simulated properly. The important ozone precursors are NO, NOx, HONO, and organic gas species; important secondary species are HNO3 and PAN. Organic gas concentrations will be lumped according to the scheme employed by each model’s chemical mechanism. Comparisons will be made for each of the estimated precursor species and lumped organic gas species, for each monitoring location. In addition, comparisons will also be made for NOx, and total ROG.

The multi-species comparisons may reveal modeling issues that were not obvious from the direct ozone comparison. Many of the precursor species have a secondary component as well. Concentrations of primary pollutants tend to have higher gradients than do secondary species. This makes it more difficult to assume that a measured concentration of a primary pollutant represents a grid cell average. For these reasons it is probably unreasonable to expect the same accuracy in replicating precursor concentrations as for ozone concentrations. Thus, use of a specific statistical error or bias criterion is not recommended. These comparisons should be viewed as more qualitative, to uncover potential problems in precursor and secondary performance.

Aloft Comparisons

Aloft air quality measurement data for the 2004 and 2005 episodes is minimal. The vertical profile of the chemical species will be evaluated qualitatively and a more quantitative analysis will be conducted whenever observational data are available. For the SCOS97 August 1997 episode, more extensive the upper air measurements are available. The concentrations of selected air pollutants were measured above the ground using aircraft, balloons and LIDAR. The primary component of these measurements is the oxidant concentrations measured with ozonesondes to a height of 5,000 m AGL. Ozonesondes were flown at seven sites, at 6-hour intervals, for selected episode days. Also, four aircraft were flown up to three times per day and an ozone LIDAR was operated continuously on selected episode days.

When air quality data aloft is available, the performance of air quality model simulations above the ground will be determined by quantitatively comparing simulated oxidant and ozone concentrations with measurements, at reasonable close times and locations. Measured concentration profiles will be averaged for the vertical layer increments corresponding to those of the air quality model. Due to the vertical resolution of the air quality models, the vertical resolution of the aloft comparisons is likely to be somewhat inconclusive and the evaluation will be of a more qualitative nature.

In addition to measuring ozone, three of the SCOS97 aircraft measured oxides of nitrogen and collected samples for later hydrocarbon analysis. Comparisons between these precursor data and concentrations simulated using the air quality models will also be made. However, there are relatively few samples and because an aircraft is not in one grid cell for an hour, comparisons may not be consistent with modeled concentrations. Comparisons to see if any large discrepancies exist between modeled and measured concentrations aloft will be made.

Acceptable Model Performance

While it is expected that acceptable model performance can be achieved for the ozone and particulate episodes, this is not always feasible given the regulatory deadlines for plan submittals. While the modeling results of some episodes may not meet all the performance goals, the episode can still be used for carrying capacity and attainment demonstration purposes assuming the relative reduction factors reflect the change in emission reduction. The RRF will be extensively evaluated with sensitivity analyses and such issues will be described in the weight-of-evidence discussions.

Sensitivity Analyses

Diagnostic Simulations

Several diagnostic or investigative simulations will be employed to further determine the fidelity of the model results. These sensitivity analyses will help evaluate potential concerns regarding such factors as emissions mass, VOC/NOx ratios, ammonia mass, and emissions timing, including daily and weekend vs. weekday emissions. The diagnostic simulations that are anticipated help evaluate model sensitivity and performance will include the following:

- ***Zero emissions –*** all anthropogenic and biogenic emissions will be set to zero to test the model's sensitivity to emissions and to ensure that the base case results are influenced appropriately by the emission inputs.
- ***Double anthropogenic emissions –*** all anthropogenic emissions will be doubled to test the model's sensitivity to increased man-made emissions. In addition, as separate tests of anthropogenic emissions affects, only mobile source emissions will be doubled and only stationary source emissions will be doubled.
- ***Emissions adjusted based on uncertainty analysis results –*** The anthropogenic emissions estimate include various inherent uncertainties because of the nature of human activity, such as the possibility that some VOC sources could not be accounted and uncertainty in the spatial distribution of the emission sources. The adjustment factors will be developed based on the ambient VOC species adjusted within the

bounds of the uncertainty. Various emissions estimate scenarios will be tested to diagnose model sensitivity and performance.

- ***Zero biogenic emissions –*** biogenic emissions will be set to zero to test the model's sensitivity to biogenic emissions.
- ***Zero surface deposition –*** deposition will be turned off for all species to examine the effects of dry deposition on ozone estimations.
- ***Reduced wind speeds –*** reducing the wind speeds by 50% is proposed to test the model's sensitivity to that parameter. However, it is possible that the resulting wind fields will not be dynamically consistent, so these results will need to be approached with caution.
- ***Zero and estimated or measured boundary and initial conditions –*** A range of boundary and initial conditions will be analyzed to test the sensitivity of the models to these inputs. The modeling results using the following initial and boundary conditions will be analyzed: (1) the boundary conditions at the top and sides of the modeling domain and the three-dimensional initial conditions will be set to zero; (2) the observed air quality data is interpolated for the initializations hours, using data from PAMS and other measurements as available to prepare estimated speciated initial and boundary profiles; (3) a range of boundary and initial conditions will be evaluated, based on the larger scale WRAP modeling results.
- ***Grid cell averaging sensitivity –*** For the attainment demonstration, relative reduction factors (RRF) will be calculated using 9-cell (15 km by 15 km) averages. As a sensitivity run, 1-cell (5 km by 5 km), 4-cell (10 km by 10 km) and 16-cell (20 km by 20 km) averages will be examined.

USE OF THE MODEL RESULTS

Attainment Demonstration

The modeling results are anticipated to be used for estimating carrying capacities and demonstrating future attainment of the NAAQS. For the attainment demonstration, the years 2007, 2010, 2014 and 2021 will be simulated with the proposed control measures (the control strategy) for 8-hour ozone NAAQS attainment. Attainment of the revoked 1-hour ozone NAAQS will also be demonstrated for the future year 2010 as a milestone and to show reasonable further progress. The years 2006, 2010, 2015 and 2020 will be simulated to demonstrate the particulate matter NAAQS attainment. In the past the use of the model results for these goals has been contingent upon acceptable base case model performance for the episodes simulated. That is, only episodes for which the model is judged to be operating properly and which meet the model performance acceptance criteria will be used.

Weight-of-evidence discussions will also factor into the attainment demonstration by providing supportive analyses to confirm or compliment the modeling assessment. Examples of the weight-of-evidence considerations may include: trend analyses, sensitivity modeling analyses (e.g., altered emissions scenarios), hot spot grid evaluations, and statistical analyses. Special analyses may also be targeted to problem locations, for example, incorporating the Rubidoux study results.

Relative Reduction Factors

Historically, AQMD developed the carrying capacity and attainment demonstration for ozone based on a set of specific control measures that was projected to achieve the 1-hour ozone NAAQS for all modeled episodes. The USEPA 8-hour ozone guidance (USEPA, 2005) and draft particulate matter guidance (USEPA, 2001b) recommend the use of relative reduction factors (RRFs) as part of the attainment demonstration process, assuming that satisfactory base year model performance is established. The RRF is a non-dimensional factor that incorporates design period monitoring data, using the 3-year average of the design value, directly into the attainment test along with the ratio of future to current year model predictions. The RRF is defined as the ratio of the future daily maximum concentration predicted near a monitor (averaged over multiple days) to the baseline daily maximum concentration predicted near the monitor (averaged over the same days).

The RRF are site specific and will be based on the 9-cell average (15 km by 15 km) for multiple episodes. Areas with severe or higher nonattainment status require a minimum of 15 simulated days. It allows the model to be used in a relative, rather than absolute, sense to reduce uncertainty in the predictions. The use of RRFs also potentially address two problems in model applications that tend to result in underestimation of emission reductions needed to attain standards. The first problem is that modeled episodes usually have ozone concentrations lower than the design value. The second problem is that simulation results have historically exhibited a tendency towards underestimation of observed concentrations. By utilizing monitored data along with model estimations, RRFs address both problems.

However, there may be some limitations in using RRFs, especially for 1-hour ozone. Examples of such situations include:

- Measured ozone concentrations at some sites and for some episodes may differ substantially from design values for those sites. That is, each available ozone episode will not be representative of design value conditions at all sites. In such instances it may not be reasonable to include the non-representative sites in the RRF analysis.
- Model performance typically varies considerably between sites and episodes in a domain. The reported ozone performance measures (such as peak prediction accuracy, bias, and gross error) may not capture this variation. Thus it may not be reasonable to include sites which have poor model performance for a given episode.

Some characteristics of RRFs include the following:
- More robust analysis due to multiple episodes;
- Less reliant on peak concentration performance statistics;
- Allows for episodic, seasonal or annual composite application;
- Can be site specific;
- Directly applied to design values so unusually adverse years weigh heavily;
- Weekend/weekday differences may not be adequately characterized;
- More applicable to 8-hour than 1-hour ozone;
- Not applied for previous AQMPs

Carrying Capacity Estimation

A traditional use of models for planning has been the estimation of carrying capacities for ozone precursors. This is typically achieved by exercising the model with a series of across-the-board precursor emission reductions from the future year baseline, from which an ozone isopleth ("EKMA") diagram is constructed. The metric used for the isopleth diagram can be one of several, such as peak 1-hour or 8-hour ozone concentrations within the modeling domain or subregion, number of grid cells above the standard, or one of many population exposure metrics. Since the carrying capacity for each precursor is based on across-the-board emission changes, rather than source- and location-specific controls as would be specified in a plan, it should only be viewed as an initial estimate for determining the emissions reductions necessary for attainment.

For the 2007 AQMP, ozone isopleth diagrams for the following air quality metrics will be constructed by episode:

- Peak 1-hour ozone concentration for the domain.
- Population exposure for 1-hour ozone concentrations.
- Peak 8-hour ozone concentration for the domain. This information will serve as an indicator of the need for potential additional precursor emission reductions to meet the 8-hour ozone NAAQS.

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