ENVIRON

International Corporation Air Sciences

D R A F T

MODELING PROTOCOL

Development of a CAMx/RAMS/EMS95 Photochemical Modeling System for The San Francisco Bay Area Air Quality Basin

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1. INTRODUCTION

The Bay Area Air Quality Management District (BAAQMD or District) is required to submit a State Implementation Plan (SIP) revision for ozone air quality to the California Air Resources Board (CARB) and to the U.S. Environmental Protection Agency (EPA) in 2004. The updated plan must show that the San Francisco Bay Area (SFBA) attains the 1-hour ozone National Ambient Air Quality Standards (NAAQS) by 2006. The forecast of ambient ozone air quality into the future is achieved through computer modeling.

This document establishes and describes the procedures that will be used to develop a new ozone modeling system and database for the San Francisco Bay Area. A Modeling Protocol such as this is essential whenever ozone modeling is carried out for the purpose of developing emission reduction strategies that may be included in a State Implementation Plan. The requirements for a Modeling Protocol are described in two guidance documents:

> "Guideline for Regulatory Application of the Urban Airshed Model," EPA-450/4-91-013, U.S. Environmental Protection Agency, Office of Air Quality Planning and Standards, Research Triangle Park, NC 27711. July 1991.
>
> "Technical Guidance Document: Photochemical Modeling," California Environmental Protection Agency, Air Resources Board. April 1992.

The Modeling Protocol delineates the objectives, procedures, and expected results of the modeling study and sets up a process for participation of the regulators and stakeholders to avoid potential technical conflicts. Protocol development should be a dynamic process that is modified as new information is acquired. Proposed changes will be reviewed by interested parties and incorporated if approved. The California Clean Air Act (CCAA) requires thatthe Modeling Protocol be approved by both the local District and the CARB. The guidance suggests that at least two review groups be established to review and approve the Modeling Protocol and review the results of the study as they become available. For the Bay Area, the District Board's executive committee will serve as the policy review group, and a Modeling Advisory Committee (MAC), including stakeholders and representatives from other agencies, has been assembled to review the technical aspects of the project.

This Modeling Protocol should be viewed as a "living" document. That is, after the District and MAC have reviewed the initial draft, comments will be compiled and responses developed. The Modeling Protocol will then be revised as necessary and made available to the project participants. If new information necessitates updates to the modeling approach well into the study, the Modeling Protocol will be further revised to reflect the alternative methodology, and resubmitted to the participants for review. The development of the Modeling Protocol is viewed as a joint effort between the contracting Team, the District and the MAC. This Modeling Protocol identifies work being carried out by the CARB to prevent duplication of efforts, and emphasizes the synergy between the District's and CARB's modeling of the Central California Ozone Study (CCOS) episodes and modeling domains.

The remainder of this section provides some background information relevant to the ozone air quality problem in the SFBA, establishes the purpose and objectives of the current study along with an overview of the approach and relationship to the CCOS, provides a schedule for completion of the various tasks and associated deliverables, and lists the study participants. Section 2 discusses the episode selection; Section 3 provides a justification for model selection; and Sections 4 through 8 describe the meteorological modeling approach, emissions modeling approach, photochemical model input data preparation, base year photochemical model performance evaluation, and attainment year modeling.

BACKGROUND

The SFBA was initially classified as a "Moderate" nonattainment area for 1-hour ozone following the passage of the 1990 Clean Air Act Amendments (CAAA). The EPA approved the subsequent SIP for the area and found the area in attainment for ozone in May 1995. However, new violations occurred during the summer of 1995, prompting the EPA to reverse its finding in July 1998 and declare the SFBA as nonattainment. Since this action occurred under Section 172 of the CAAA, the SFBA is now classified as "Other". In March 2001, the EPA disapproved portions of the SFBA SIP, and so now the BAAQMD is required to develop and submit a revised SIP for the region in April 2004. The revised SIP is to demonstrate attainment of the 1-hour ozone standard by 2006.

PURPOSE AND OBJECTIVES OF THIS STUDY

The overall purpose for this study is divided into two distinct goals:

> Immediate and foremost goal:
> Provide the District with technical analysis and photochemical modeling results to support the 2004 SIP revision.
>
> Longer-range goal:
> Provide the District with a modern tool base that can be used to analyze regional ozone problems and inter-basin transport..

The District has identified nine specific contract objectives that must be met for the successful execution of the project. They are:

1. All technical modeling development work is to be completed by July 1, 2003, while all future year analyses, SIP documentation, and transfer/training to be completed by September 2003;
2. The modeling system will meet or exceed the requirements in the Request for Proposals;
3. A new computing platform will be acquired that will meet the requirements of the District staff;
4. All data and software will be installed and functional on the specified computing platform;

5. Meteorological and photochemical simulations will be provided for two CCOS episodes:
   14-15 June, 2000
   30 July – 2 August, 2000
6. Emission inputs and scenario development will be generated using the CARB's EMS-95 setup and input databases;
7. Photochemical modeling will meet or exceed EPA/CARB model performance criteria;
8. Full documentation of all results will be provided as a Technical Support Document to the 2004 ozone SIP;
9. The modeling system and all results will be transferred to the District and personnel will be trained on all aspects of operation and evaluation.

These nine objectives will be met by completing the work in nine individual project task elements, as established by ENVIRON and the District:

TASK 1: Develop Modeling Protocol
TASK 2: Acquire Computing System
TASK 3: Simulate Meteorological Conditions for the 2000 Episodes
TASK 4: Produce Emission Inputs for Years 2000 and 2006
TASK 5: Simulate Base Year Ozone and Evaluate Photochemical Model Performance
TASK 6: Simulate Year 2006 Ozone and Examine Model Sensitivity to Emissions
TASK 7: Simulate Year 2006 SIP Control Strategies and Demonstrate Attainment
TASK 8: Management and Reporting
TASK 9: Transfer Project Computer and Modeling System with Training

Although this project is sponsored by the District, we recognize the importance of working closely with the CARB. We plan to fully engage the CARB technical staff in this effort, thus exploiting the relevant data, methods, and technical expertise at that agency. We have been assured by the CARB technical staff and management that they are enthusiastic to work with us to share CCOS data, methods, and results.

Overview of Approach

The EMS-95/RAMS/CAMx modeling system will be used for this study because it contains all of the technical features necessary to simulate ozone air quality in the SFBA. We believe that this system of models has the highest likelihood of generating SIP-quality photochemical modeling databases for the June 14-15 and July 30-August 2, 2000 CCOS episodes in the Bay Area.

The same EMS-95 emissions processor and input databases as used by the CARB will be used in this project to assure CARB compatibility and acceptability. We believe that this is an essential element of the study. Portions of the emissions database may not be ready from CARB in time to meet the schedule demands of this project, so we will maintain close contact with CARB staff so that we may identify which portions of the inventory we may need to process independently. ENVIRON's subcontractor Alpine Geophysics (AG), one of the developers of EMS-95, will take the lead of the emissions modeling task and work closely with CARB to assure consistency and compatibility with the CARB's emissions development efforts. AG is currently under contract with CARB to develop on-road mobile source VMT estimates for the CCOS domain. AG will provide the EMS-95 system and database for the two CCOS episodes to the District and train them on its use.

The RAMS prognostic meteorological model has been selected for the modeling system because of its demonstrated successful application in the Bay Area in the past, its inclusion of all the technical features necessary for simulating the complex Bay Area meteorology, and its familiarity to the District. The CARB is currently using the MM5 meteorological model for their CCOS modeling. However, we believe that the RAMS model may be superior for simulating the Bay Area meteorology because of its formulation and its flexibility, such as supporting any grid meshing ratio. Subcontractor Dr. Craig Tremback of ATMET is one of the developers of RAMS and will lead this task. He will configure RAMS for optimal high speed performance on the project's computer cluster and train the District on its use.

The CAMx photochemical grid model was selected for the modeling system as it is publicly available, contains all of the technical options needed to simulate ozone in the Bay Area, and contains some superior capabilities to the other state-of-science models. In particular, the CAMx contains several "probing tools", including the decoupled direct method (DDM) of sensitivity evaluation, ozone source apportionment technology (OSAT), and Process Analysis, all of which will increase the likelihood of obtaining a photochemical model base case simulation that fully achieves the model performance objectives. The CAMx modeling will be led by its developers, ENVIRON, who have set up CAMx for numerous ozone SIP modeling databases including Los Angeles. The CAMx modeling domain will be based upon current MM5/CMAQ modeling being undertaken by the CARB. However, we would work with the District and the MAC to refine this domain for the purposes of focusing on the Bay Area ozone problem. ENVIRON will set up and evaluate CAMx for the two CCOS episodes, operate the model for several future year (2006) emission sensitivity tests and the final attainment demonstration, and transfer to and train the District on its use.

Project-Specific Computer and Web/FTP Sites

The District has very specific computer performance goals for operation of simultaneous meteorological and air quality model simulations. As part of the current study, the project team will work with District staff to identify an appropriate Unix/Linux multi-node cluster system, purchase and test the system, install all models and supporting databases, and ultimately deliver the system to District offices near the completion of the project. This system can also be enhanced and expanded as new technology becomes available.

As a key part of the work being carried out by ENVIRON with the BAAQMD staff to develop a 2004 SIP revision, we have engaged the members of the MAC to assist in the technical review and guidance of the project. It was agreed that we would keep all project participants advised of the project through a web site maintained by ENVIRON, and to which we would post new information for the MAC as it is developed. Because this is a project site, and intended to be a resource primarily for those that are expected to make meaningful contributions to the technical review effort, we have provided password protection.

Link: http://www.environ.org/basip2004
Username: basip2004
Password: TBD

Links to small documents such as reports, meeting minutes, summaries, and some plots will be provided via the web site to ease dissemination. However, there will likely be a need to provide larger databases to various participants during the project. In that case, we will also establish a password-protected FTP site for this purpose.

Relationship to CCOS

As noted above, the California Air Resources Board has led an effort spanning several years and expending millions of dollars, to develop a robust and highly credible data base to be used in photochemical modeling in much of California. The CCOS project is beginning to yield results in the form of a very large data set that can be used by those engaged in photochemical modeling. Data was collected for several groups of days ("episodes") in 2000. As discussed elsewhere, a subset of those episodes will be evaluated for use in this study.

Because of the complexities of photochemistry, emissions, and meteorology, it is important that air pollution management decisions be based on the best science and most comprehensive data available. While the CCOS study has moved forward significantly in many areas, the schedule under which that project is being performed is not wholly consistent with that of the BAAQMD or EPA for the 2004 SIP submission. Thus, this study, while drawing upon the CCOS effort wherever possible, will have to pursue certain technical areas on a different schedule. This is expected to affect three key areas of this study. First, as noted previously, the CCOS emissions inventory will not likely be completed in a timely basis for explicit use in this Bay Area study. Second, this study is using the RAMS meteorological model for reasons stated earlier. The CCOS project is likely to use the MM5 meteorological model. If MM5 modeling results are available in a timely fashion, they will be compared to those of the RAMS model and in turn to the meteorological measurements against which the model(s) performance will be judged. Lastly, the CCOS study has not yet determined what photochemical model may be used in that study. We will be using CAMx in this study, again, for the reasons stated above.

Not withstanding the potential for different approaches in some aspects of these studies, the Bay Area study participants and the CCOS sponsors have agreed to share all technical information as both studies proceed, thus minimizing any differences in results that cannot be accounted for in an objective fashion.

Considerations for Bay Area SIP and Pollutant Transport

Pollution does not respect political boundaries. There is documented air mass flow from the Bay Area into inland areas of the State, and vice-versa. The Federal Clean Air Act recognizes such transport and addresses the manner in which up and down-wind areas are interconnected in the regulatory process. This study will provide information that should assist in the regulatory assessment. In addition to air mass and pollutant flow, there are also mobile source emissions that originate within one area but continue as vehicles move to another area. For example, automobiles registered in the San Francisco Bay Area clearly transit outside of that area. The same is true of vehicles registered elsewhere.

Both of these phenomenon will be addressed in this study. Pollutant mass transport will be explicitly addressed because the modeling domain used in this study will extend well beyond the SFBA, thus accounting for such air mass movement within the modeling system. The movement of vehicles will be addressed through the use of complex transportation model output results being used in estimating mobile source emissions. Such transportation models are used by Metropolitan Transportation Commission (MTC) in the San Francisco area, and Sacramento Association of Governments (SACOG) in the Sacramento area.

SCHEDULE AND DELIVERABLES

Figure 1-1 displays a time-line for the completion of each of the nine project tasks. The figure also shows major deliverables, to include task reports at the completion of each (except Task 2, Computer Acquisition), draft and final project reports, and the delivery of the computer system. All technical modeling development work is to be completed by July 1, 2003, while all future year analyses, SIP documentation, and transfer/training to be completed in September 2003.

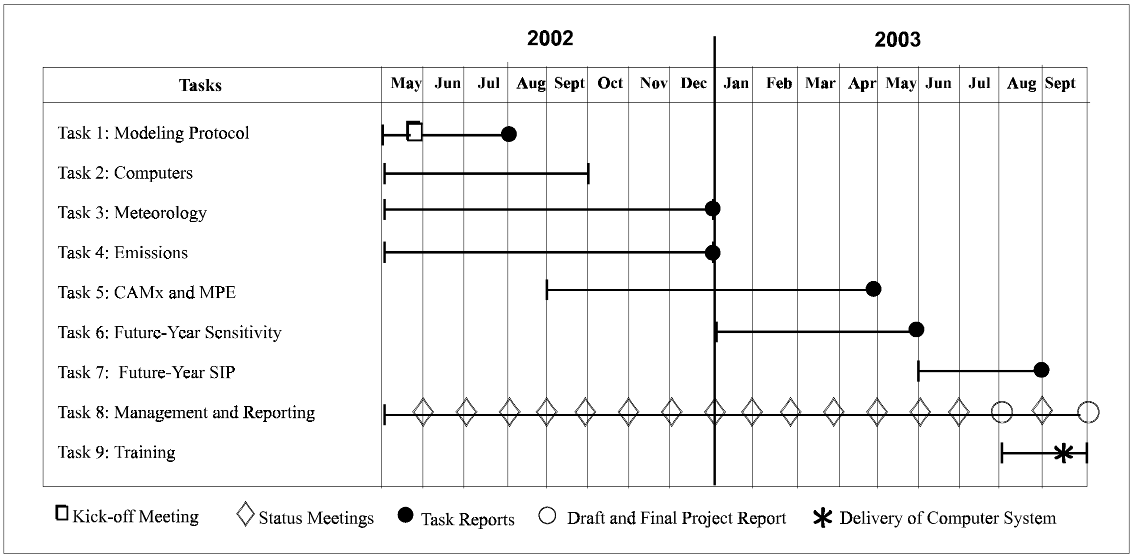

Figure 1-1. Project schedule showing dates for major deliverables.

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Modeling Advisory Committee (MAC)

The District has formed a technical modeling advisory committee for this study. Both the EPA and CARB modeling guidance requires the formation of a “Technical Working Group”. In any study of this type that leads to a SIP development effort, it is important that the technical underpinnings of that SIP be fully examined as they are developed. In this manner, to the extent possible, technical issues can be put aside in the SIP development effort, the focus can be on the many other aspects of this process, and the public can be better assured that the technical community has been rigorous in their review of the work.

The table below lists the current members of the project MAC with their contact information. The MAC includes representatives from other governmental agencies, environmental groups, and industrial stakeholders.

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2. EPISODE SELECTION

State Implementation Plans (SIPs) for ozone require the evaluation of the effectiveness of emission control measures. This is accomplished by simulating the effects of the controls on ambient ozone air quality using three-dimensional air quality models. The air quality models require inputs of time- and spatially-varying emission and meteorological fields. These fields influence significantly the results of these simulations and have the most relevance to the SIP analysis.

The general modeling approach to evaluate control measures is to simulate an episode, a period that exceeded the air quality standard, using emission and meteorological inputs that best approximate the physical conditions of the episode. This simulation defines a reference-case or “base case”. If the model performance of the base case simulation is acceptable, then simulations are performed using emission fields that reflect the changes introduced by the emission control measures. The differences in the two simulations determine the influence of the emission control measures.

Episodes used for this analysis need to be selected carefully so that the analysis has the maximum credibility and generality. The criteria for episode selection are:

- The episode must have included measured ozone concentrations that exceeded the federal ambient air quality standard. The standard for ozone is 120 ppb averaged over one hour. Ozone observations above this maximum are incorporated into the calculation of the ozone “design value”, which is the regulatory measure of ozone levels.

- The episode must be representative of a class of episodes that occur frequently so that the simulation will presumably have greater generality to the analysis of predicted changes in the design value. Incorporating multiple episodes into the analysis would further broaden its generality.

- The episode must have sufficient observations to determine the physical conditions that contribute to the ozone exceedances. Furthermore, the observations must provide data that satisfy model input needs and that can be used to evaluate model performance.

In the year 2000, the Central California Ozone Study (CCOS) collected significant additional air quality and meteorological data, beyond the routine monitoring networks, for use in the analysis and modeling of ozone. The episodes for the 2004 SIP analysis will be selected from this period because the study provides the most extensive air quality database since the 1990 SARMAP field program.

DESCRIPTION OF EPISODES

Periods of high ozone observations during CCOS for the San Francisco Bay Area (SFBA), the San Joaquin Valley (SJV), and the Sacramento Valley (SV) are tabulated below (Fairley, 2001).

			1-hour basin maximum (ppb)			8-hour basin maximum (ppb)		
IOP	**Date**	**Day**	**SJV**	**SV**	**SFBA**	**SJV**	**SV**	**SFBA**
	6/14	Wed	140	102	113	116	85	**101**
	6/15	Thu	139	93	**152***	102	77	**114**
	6/21	Wed	132	**126***	72	106	**102**	59
1	7/23	Sun	115	90	82	89	79	61
1	7/24	Mon	139	110	74	94	86	60
2	7/30	Sun	129	121	82	106	93	56
2	7/31	Mon	118	100	**126***	103	82	**89**
2	8/1	Tue	118	**133***[a]	94	109	**108**	77
2	8/2	Wed	**151***	108	98	112	94	**84**
3	8/14	Mon	111	102	77	84	88	61
	8/21	Mon	94	109	73	83	**100**	62
	9/8	Fri	136	78	65	**117**	69	50
	9/11	Mon	139	95	91	**122**	85	67
	9/13	Wed	**146***	119	96	**125**	94	72
4	9/14	Thu	114	69	42	93	46	38
5	9/17	Sun	125	75	84	99	64	67
5	9/18	Mon	**171***	94	83	**126**	76	67
5	9/19	Tue	**145***	104	100	113	86	76
5	9/20	Wed	128	123	86	111	97	65
5	9/21	Thu	90	53	52	78	44	47
	9/30	Sat	132	117	87	106	**102**	59

* Indicates an episode day for that air basin.
Bold indicates episode for 1-hour max ozone and top 4 for 8-hour average max ozone.
[a] Folsom site not in operation.

In the SFBA only two days, 6/15 and 7/31, exceeded the federal clean air standard with values of 152 ppb and 126 ppb, respectively. Cluster analysis was performed using high ozone observations from 89 episode days between 1989 and 2000. These two 2000 SFBA episodes fell into the cluster in which all but one of the previous SFBA episodes were grouped. This group is characterized by warmer than average SFBA temperatures and by lower than average daytime wind speeds at Bethel Island (Fairley, 2001).

A history of daily maximum observed ozone for inside and outside the SFBA is presented in Figure 2-1. This figure shows that for the SFBA the 6/15 and 7/31 exceedances are isolated events from the relatively clean CCOS period and that the SFBA dailymaxima are correlated with maxima observed outside the SFBA.

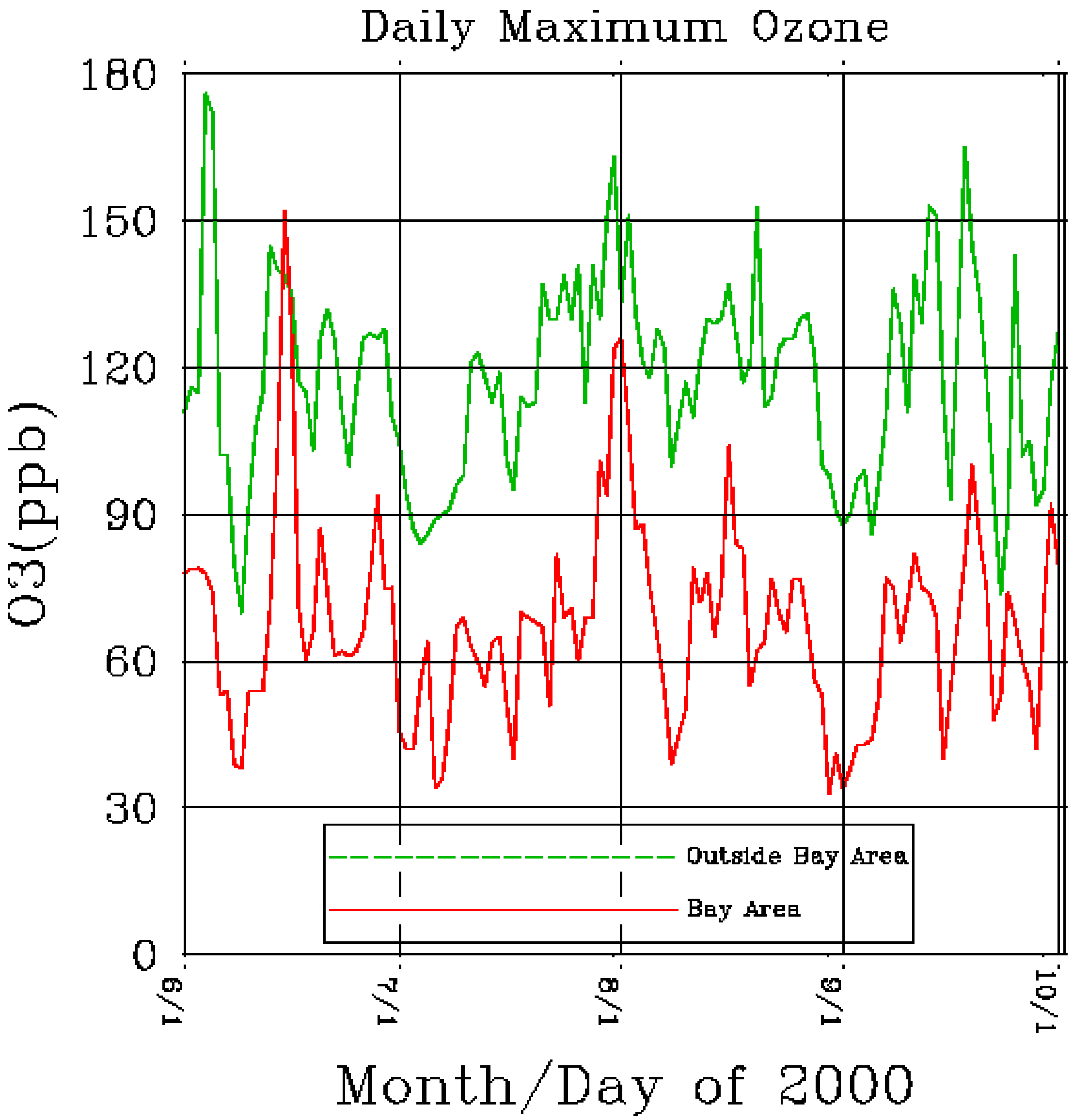


Figure 2-1. Daily maximum for ozone inside and outside the SFBA.

Figures 2-2 and 2-3 present the spatial distribution of maximum ozone for each of the two episodes. The plot of the 6/15 episode shows isolated high ozone values centered at Livermore in the SFBA, clean conditions around Sacramento, and moderate values around Fresno. The plot of the 7/31 episode shows low ozone exceedance values near Livermore, moderate values around Sacramento, and low values around Fresno. The ozone exceedances were shifted more toward the Sacramento area during the 7/31 episode.

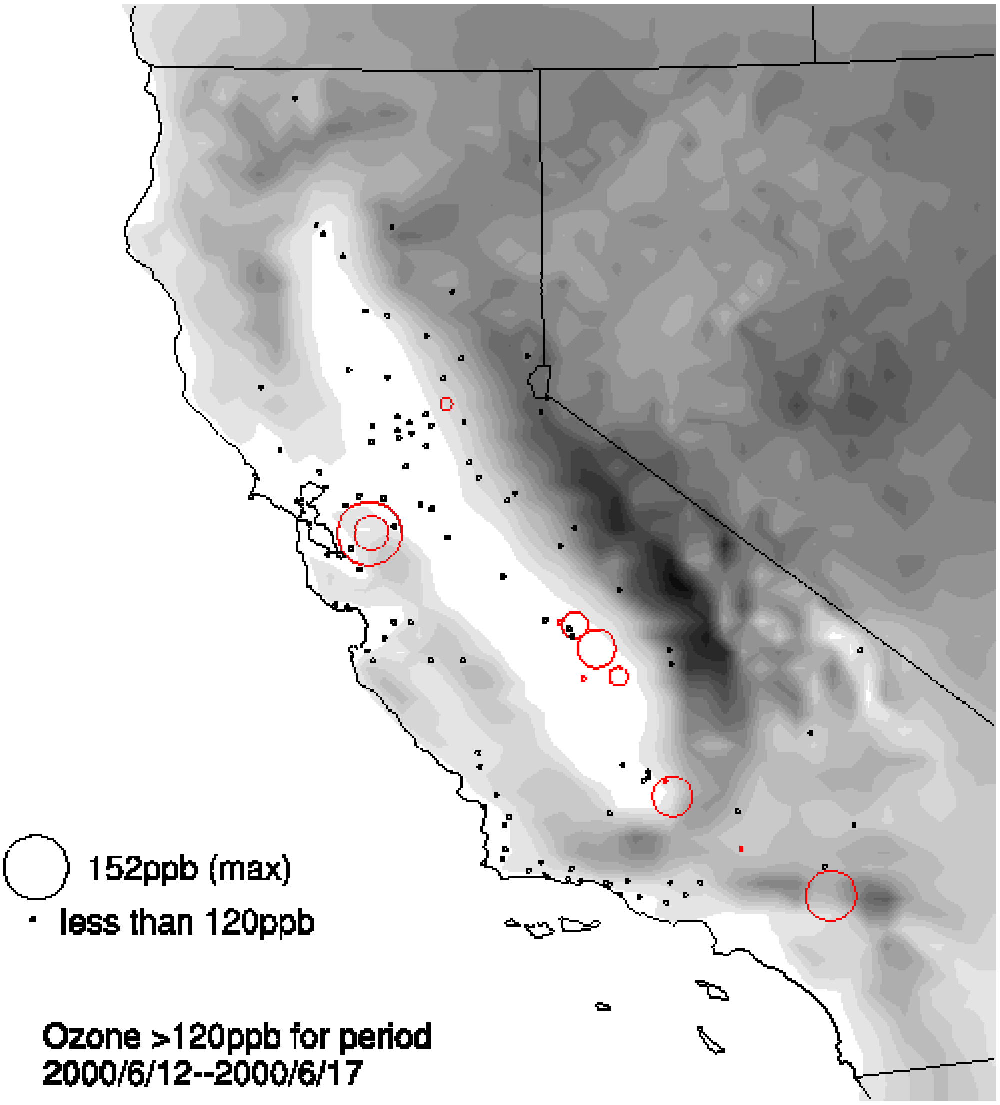


Figure 2-2. Spatial Distribution of ozone values > 120 ppb (red) for the June 15, 2000 episode.

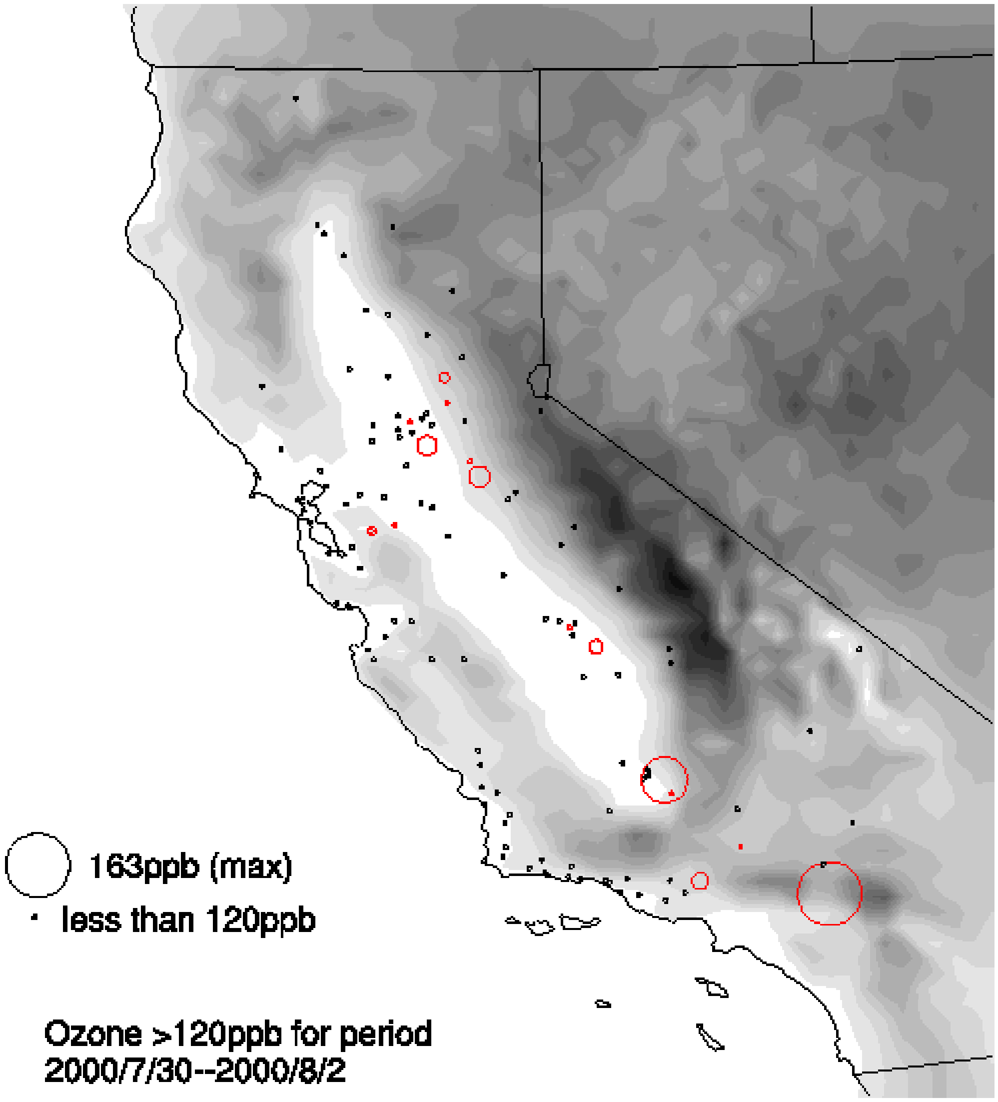


Figure 2-3. Spatial distribution of ozone values > 120 ppb (red) for the July 31, 2000 episode.

Summary of Meteorology

Lehrman et al. (2001) describe the CCOS meteorological conditions and its relationship to ozone values (see also Figure 2-4):

"The relationship between the dispersion of ozone and ozone precursors in California and large-scale synoptic weather patterns is well known. During the summer ozone season, the extension of the eastern Pacific high over the western US effectively blocks the influx of cyclonic weather systems into California from the Gulf of Alaska, and allows the entrenchment of large static air masses which are typically warm, stable, and poorly mixed. The strength and persistence of the resultant boundary layer mixing and transport patterns affects the magnitude and duration of ozone events in Central California. High-pressure ridges and low-pressure troughs in the mid to upper atmosphere are particularly efficient indicators of ozone formation conditions. … Two synoptic scale meteorological parameters, which historically have correlated well with ozone formation and fate in California, are the height of the 500 mb surface and the temperature at the 850 mb level. The time history of 500 mb heights at a fixed location is a general indicator of the behavior of the 500mb surface indicating pressure ridges and troughs. The 850 mb temperature is a measure of large-scale subsidence, which produces stable layers in the atmosphere and limits vertical dispersion of ozone and precursors."

They describe the synoptic conditions leading up to the 6/15 episode:

"The OAK (Oakland) 500 mb height had increased from a low of 5,650 m on June 8 to a maximum of 6,000 m on June 14. During that same period, the OAK 850 mb temperature increased from 7°C on June 8 to a high of 27°C on June 14. As the ridge progressed towards the east-southeast, flow aloft remained from the north throughout the period. This slowly encouraged the onset of offshore flow across the project area during that time. Ozone concentrations increased steadily as the ridge approached with peak ozone values in excess of the Federal and State Standards…"

They also describe conditions for the 7/31 episode:

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

Elevated ozone concentrations persisted in the project area for several days after the IOP, which ended on August 2.

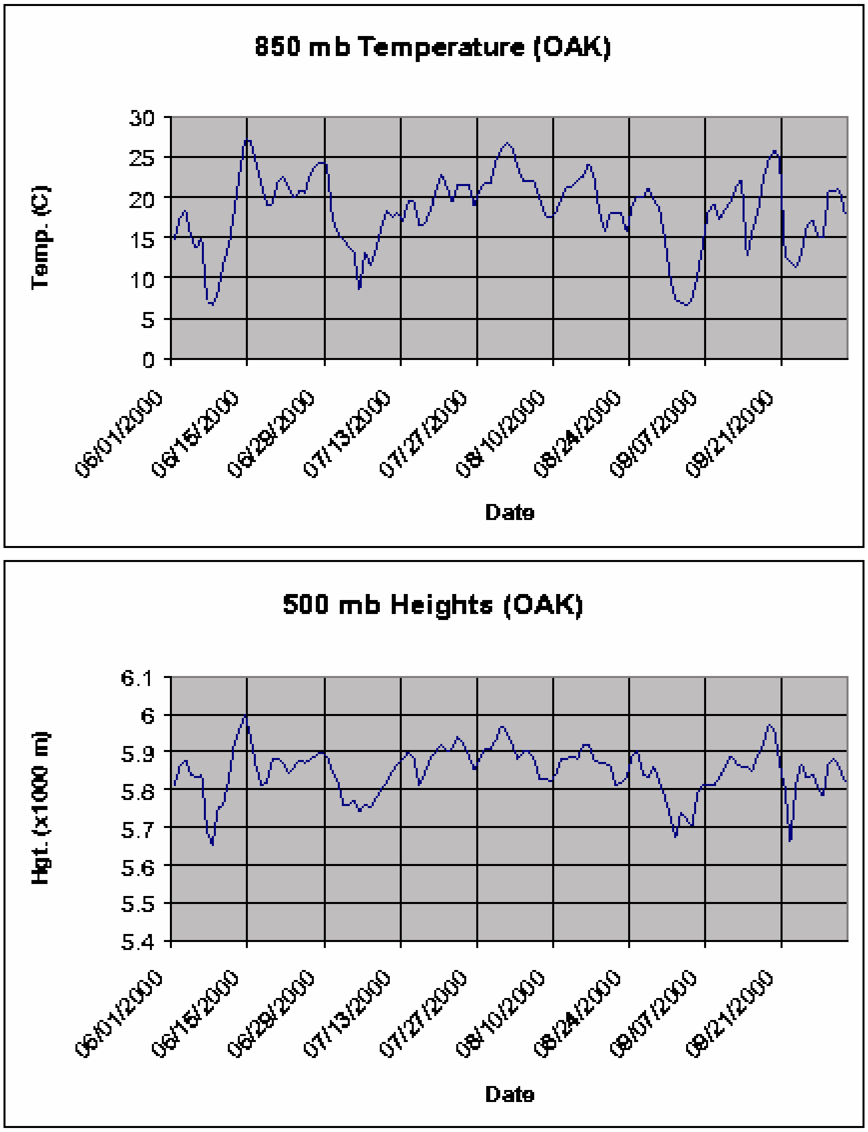


Figure 2-4. Afternoon 850 mb temperature and 500 mb heights measured daily at Oakland NWS station during CCOS 2000 field program (from Lehrman et al., 2001).

DATABASES FOR CANDIDATE EPISODES

Both of the episodes identified as candidates for this study occurred during the CCOS. Most of the data that will be used for SIP modeling and analysis -- for generating model inputs, for model evaluation, and for corroborative studies -- will therefore be derived from the CCOS database. During CCOS, when high ozone episodes were forecast, an intensive operation period (IOP) was launched and additional special field study data were collected. The June episode (6/14-15/2000) occurred outside of an IOP (it was designated a “practice” IOP); the July-August episode (7/30/2000-8/2/2000) was an IOP.

The CCOS data are being archived and made available by the CARB. However, much of the data has not undergone a complete quality assurance analysis and, as such, will require that during the SIP project they be analyzed as they are used.

This section provides a brief overview of the CCOS study and its database. The data available during both of the episode periods, both IOP and non-IOP, are described. A few additional data sources will also be used for producing and evaluating modeling inputs. These sources are identified and briefly described in this section as well.

CCOS Field Study

The CCOS was a large-scale field program involving many sponsors and participants with a research budget of over $8 million for the summer 2000 field measurement campaign. In addition, the CARB and local Air Quality Management Districts (AQMDs) provided substantial in-kind contributions during the measurement campaign. The CARB was responsible on a day-to-day basis for management of the study.

The CCOS field measurement program covered much of northern California, extending north of Redding and including all of central California, the San Francisco Bay Area, and the San Joaquin Valley. A summary report on the CCOS field operations has been completed (DRI, 2001) and is available online: http://www.arb.ca.gov/airways/ccos/docs/ccosv3fdS0.zip. For background information, this section provides a brief overview of the data collected during CCOS. For a more details, the reader should consult the summary report.

According to CARB, all CCOS field observations are currently available from CARB, though not all are in the airways database (http://www.arb.ca.gov/airways/Datamaintenance) and the data formats are not uniform. The level of quality assurance checking conducted for these data is variable; most data have not undergone a complete analysis. To the extent possible, given the time constraints of the project, data will be validated as they are used.

Study Period and Special Measurements

The **primary study period** for CCOS extended from 6 July to 30 September 2000. During this period, continuous surface and upper-air meteorological measurements and surface air-quality measurements were made for ozone (O_3), nitric oxide (NO), oxides of nitrogen (NO_x), reactive oxidized nitrogen NO_y, nitrogen dioxide NO_2, peroxyacetylnitrate (PAN) and peroxyacetylnitrates (PAcN), particulate nitrate NO_3^-, formaldehyde (HCHO), and speciated volatile organic compounds (VOCs) from automated gas chromatography with ion-trap mass spectrometers (three research sites). At regular intervals, speciated VOCs were also available during the primary study period from the Photochemical Assessment Monitoring Stations (PAMS) as discussed briefly below.

During the **intensive operation periods** (IOPs), additional measurement data were collected including instrumented aircraft measurements, speciated VOC at more locations, and radiosonde and ozonesonde measurements. During the month of August only, an ozone

LIDAR was deployed at Livermore, measuring vertical ozone profiles from 50 m to 2000 m with a 200 m-range resolution.

Routine Data

During summer 2000, the CARB and the AQMDs operated over 150 surface-based air quality monitoring stations throughout northern and central California. Many of these sites routinely measured O_3 and NO_x. Carbon monoxide and hydrocarbons were measured at 57 and 11 sites, respectively. Existing PM10 measurements acquired filter samples every sixth day. A few of the PM10 sites had continuous monitors that measured hourly PM10 everyday. A few routine PM2.5 measurements sites were also in operation.

Districts in the Sacramento and San Joaquin Valleys are required to routinely operate photochemical assessment monitoring stations (PAMS) as part of their State Implementation Plan. Each PAMS station measures speciated hydrocarbons and carbonyl compounds, O_3, NO_x, and surface meteorological data. Additionally, each area must monitor upper-air meteorology at one representative site.

An extensive, but uncoordinated, network of surface meteorological monitoring sites is routinely operated by the CARB, BAAQMD, SJVAPCD, SMAQMD, the National Oceanic and Atmospheric Administration (NOAA), the California Irrigation Management Information Service (CIMIS), Interagency Monitoring of PROtected Visual Environments (IMPROVE), the National Weather Service (NWS), Pacific Gas and Electric Company (PG&E), the U.S. Coast Guard, Remote Automated Weather Stations (RAWS), and a few additional agencies. Wind speed and direction, temperature, and relative humidity are the most common measurements. Surface pressure and solar radiation measurements are also common. A few sites measured ultraviolet radiation in the Sacramento and San Joaquin Valleys, and in Santa Barbara County.

The CARB operated two wind profilers (with RASS) in the San Joaquin in Valley, and the San Joaquin Unified APCD and Sacramento Metropolitan AQMD operated one profiler/RASS each as part of their PAMS monitoring program. SJVAPCD also operated a profiler at Tracy during CCOS. Military facilities with operational profilers include Travis AFB,Vandenberg AFB, and the Naval Post Graduate School in Monterey. Radiosonde measurements of winds, temperatures, and humidity aloft are routinely made twice per day at Oakland and, according to military base requirements, at Vandenberg AFB, Edwards AFB, and Pt. Mugu Naval Air Station.

Routine measurements of pollutant emissions from stacks are required for large industrial sources, such as utility boilers. Traffic count data were also routinely collected at many freeway locations in central California.

Finally, polar-orbiting and geostationary satellites collected an enormous amount of radiometric data that yield useful products, including the total ozone column, cloud cover, sea surface temperature, vegetative cover, and surface albedo throughout California.

Field Study Data

The CCOS field measurement program consisted of four categories of supplemental surface measurement sites: Type 0, 1, and 2 sites, described as "supplemental" (S) sites, and "research" (R) sites. The measurements made at each type of supplemental monitoring site are tabulated below. One of the S1 sites was a mobile van operated in the vicinity of Livermore. The carbonyl measurements and the speciated HC measurements at all but the research sites were only collected during the IOPs.

- **Type 0 Sites:**
  - O_3, NO, NO_y
  - wind speed, wind direction
  - temperature, and relative humidity

- **Type 1 Sites:**
  - S0 measurements, plus CO, CO_2, speciated HC, carbonyls

- **Type 2 Sites:**
  - S1 measurements, plus NO_2, PAN

- **Research Sites (3):**
  - S2 measurements, CO, CO_2, NO_y^*, particulate nitrate,
  - light absorption, scattering, actinic flux

Six profilers with RASS were installed and operated during summer 2000 as part of the Central Regional Particulate Air Quality Study (CRPAQS). In addition, nine profilers with RASS and 5 sodars were installed for the CCOS summer 2000 field study. Another sodar was located in the vicinity of the Pittsburgh power plant stacks. During IOPs only, radiosondes and ozonesondes, one in the Sacramento Valley and one in the San Joaquin Valley, were deployed six times per day.

Four instrumented aircraft were used to measure the vertical and horizontal gradients of temperature, humidity, and pollutant concentrations in the study region during CCOS IOPs. These aircraft included two Cessna 172RG and Cessna 182 operated by University of California at Davis (UCD), and a Cessna 182 and Piper Aztec operated by Sonoma Technology, Inc. (STI). One additional aircraft (Twin Otter), flown by the Tennessee Valley Authority (TVA), made measurements in power plant plumes. The TVA data were collected to evaluate the plume-in-grid parameterizations used in air quality models.

Supplemental Data

A number of supplemental data sources exist that may be useful to this study. For example, an on-road vehicle remote sensing special measurement study was conducted by CARB and coordinated with the CCOS study; the CARB also contracted UC Davis to conduct a vehicle traffic count study; and Districts supplied day-specific plant schedules and pollutant profiles, when available. These data will be used for checking the modeling emissions inventory estimates if they are analyzed and available on a schedule that is consistent with the schedule for this project.

Other data sources were independent of CCOS and mostly the result of routine data collection and analysis efforts. These included synoptic-scale meteorological analysis products and multiple satellite data from multiple platforms and sensors. The meteorological analysis products will be used as inputs to the meteorological model; the satellite data yield products that will provide inputs to both the meteorological model and the photochemical model. The meteorological model requirements include surface vegetation amounts, and sea surface temperature; the photochemical model requires total ozone column and surface albedo. These inputs will be derived from satellite data products and/or standard information from the U.S. Geological Survey.

3. MODEL SELECTION

An emissions, meteorological, and photochemical air quality modeling system has been selected that we believe best meets the District's needs in providing high quality modeling databases that can be used for developing the 2004 ozone SIP control plan for the SFBA. This belief is based on the technical features of the selected modeling system and its ability to address the challenges of modeling in the SFBA, the experience and capabilities of the District staff, and the need to maximize the likelihood of a successful model application that achieves the model performance objectives. Specifically, the system we propose comprises the EMS-95 emissions processing model, the RAMS meteorological model, and the CAMx photochemical model.

CHALLENGES OF THE STUDY

There are numerous challenges related to air quality modeling of the Bay Area that will have to be overcome in performing this work effort.

Meteorology: The meteorology of the SFBA and surrounding regions in the CCOS domain is quite complex, and appropriately simulating the effects of micro-climates and flow regimes will be a significant challenge that requires the attention of experts, experienced modelers, and a state-of-science meteorological model:

- Land/sea/bay breezes
- Mountain/valley wind systems in complex terrain
- Role of maritime stratus
- Mesoscale eddies
- Low-level jets

Emissions: Emissions modeling of the Bay Area and central California presents a challenge due to the multitude of diverse sources and the need to remain consistent with theCARB's emissions data and modeling system. Thus, the CARB's emissions modeling system is needed along with full knowledge of how CARB staff generate their emission rate estimates and spatial surrogates:

- On-road mobile sources
- Non-road sources
- Area sources
- Refinery and other industrial sources
- Electrical generating sources
- Biogenic emissions
- Quality assurance and quality control (QA/QC)

Photochemical Modeling: The challenges of the meteorological and emissions modeling of the Bay Area are combined with additional chemical and physical challenges in the photochemical modeling. A state-of-science photochemical grid model with thelatest model sensitivity analysis capabilities will be needed to address this component, along with the use of:

- Multiscale two-way nested grid resolution (e.g., 2/4/12-km)

- Sufficient vertical resolution
- Current chemical mechanisms (CB4, SPARC99)
- Efficient and accurate numerical solvers
- Accurate and mass consistent interface between the meteorological and photochemical grid models

Regulatory Issues: The ultimate objective of the study is to develop a photochemical modeling database that can be used for the year 2004 1-hour ozone control SIP. This SIP must satisfy:

- EPA's SIP guideline documents and requirements including those for photochemical modeling (EPA, 1991)
- CARB's guidance documents including those for photochemical modeling (ARB, 1992)
- Continuous contact with the CARB to assure that the modeling meetsCARB's approval
- Continuous contact with EPA to assure that the modeling is performed to level that leads to an approvable SIP

Strategic Issues: The modeling and computer systems to be set up to address the 2004 1-hour ozone SIP will be applicable to numerous other air quality issues that will be needed in the future:

- The District will be able to use the system to analyze SFBA impacts on downwind areas due to transport
- The modeling system will be directly applicable for addressing 8-hour ozone issues when EPA issues the final 8-hour ozone implementation plan.
- A photochemical model that includes an advanced particulate matter (PM) treatment can be readily adapted to treat fine particulate and visibility issues
- The modeling and computer system will be powerful enough to perform real-time ozone forecasting for the Bay Area.

SELECTED MODELING SYSTEMS

The modeling components selected for the SFBA 2004 SIP revision were specifically identified and requested by the BAAQMD before the study was initiated. All of the models recommended by the District are considered state-of-the-science, and Districtstaff possess a sound experience base for most of the modeling components. All of the selected models have been, or are currently being, used nationally for various ozone, carbon monoxide, and PM SIPs and/or regional regulatory analyses, and thus have been accepted by the EPA and many States for this purpose.

Emissions Model: The processing of episode- and grid-specific emission estimates must use the CARB's emissions data and modeling system, which is based on a California version of the 1995 Emissions Modeling System (EMS-95). Use of any other processing system would likely be unacceptable to CARB and thereby jeopardize the SIP. Furthermore, it would result in inconsistencies with ozone SIP modeling in other areas of the CCOS domain (e.g., San Joaquin Valley) and could produce conflicting results (e.g., inconsistent conformity budgets). Thus, use of EMS-95 is an essential component of the modeling system.

Meteorological Model: Either the RAMS or MM5 prognostic meteorological models would be the most logical choice for this component of the modeling system. Both models arestate-of-science, have a large user community, and are available to all public agencies. We believe that RAMS provides a better treatment of the highly non-hydrostatic processes associated with mesoscale land/sea/lake breeze and planetary boundary layer (PBL)circulations in complex terrain. We have selected RAMS over MM5 because District staff have used this model for several years and so are quite familiar with it, it has demonstrated good performance in the Bay Area, and it provides more flexible grid nesting arrangements (MM5 is limited to a 3:1 ratio).

Photochemical Grid Model: The three logical candidate photochemical grid models for this study include Models-3/CMAQ, CAMx, and UAM-V. The status of UAM-V in terms of public availability is not clear, and its access is strictly guarded. It is also based on legacy (1970-80s) computer code, with very little updating over the past 5-7 years. Thus, UAM-V would not be a good choice. Both CAMx and Models-3/CMAQ are modern codes (1995+) that incorporate state-of-the-science features for allphysio-chemical processes. For this study we have selected CAMx over CMAQ because:

1) CAMx can accept meteorological input fields derived from any meteorological model, while CMAQ is limited to the use of MM5;
2) CAMx supports two-way grid nesting at any nesting ratio (e.g., 2:1, 3:1, 4:1), whereas CMAQ supports only one-way nesting at a ratio of 3:1;
3) CAMx generates hour-averaged concentration fields consistent with measurements, while CMAQ outputs hour-instantaneous fields;
4) CAMx has demonstrated good ozone model performance in southern California, whereas some of the limited CMAQ modeling for California to date (i.e., WRAP) has demonstrated very poor ozone model performance;
5) CAMx has demonstrated successful application in several ozone SIP modeling studies nationally, whereas CMAQ has never been used successfully in an ozone SIP;
6) CAMx supports multi-processing capability to speedexecuation, which is not in the current version of CMAQ;
7) CAMx supports a full suite of probing tools (DDM, OSAT, and Process Analysis) that may be important in insuring that the model is working correctly, whereas CMAQ just supports Process Analysis;
8) the District has a greater familiarity with CAMx and have used it before; and
9) the project team's familiarity with the model will ensure that a working, fully acceptable modeling system will be developed for the two CCOS episodes.

4. METEOROLOGICAL MODELING

The ENVIRON team will use the Regional Atmospheric Modeling System (RAMS) as the prognostic meteorological modeling component of the air quality modeling system and to develop the meteorology for the CCOS episodes (June 14-15 and July 30 – August 2, 2000, plus initialization days). RAMS has been used for this type of simulation for almost 20 years and the application of RAMS by ATMET personnel (which include the original developers of RAMS) will ensure that the District will attain acceptable meteorological simulations. The District has been using RAMS for many years and are familiar with its application. By necessity, the CAMx air quality modeling domain and grid specifications will be based on CARB's current modeling projection configuration, which is a fairly large regional domain on a Lambert Conformal Conic projection. RAMS operates on a Rotated Polar Stereographic projection; thus, an intermediate processor will be used in the RAMS/CAMx modeling system to perform the necessary manipulations of the RAMS output to properly feed into CAMx.

DESCRIPTION OF RAMS

RAMS has many advantages that make it attractive for these types of simulations:

(a) **Non-hydrostatic formulation:** RAMS uses a compressible, time-split non-hydrostatic equation set in its formulation. The predecessor code to the current RAMS started as a non-hydrostatic model more than 20 years ago. Aside from the model's ability to run on arbitrarily high resolutions, our experience has shown a major benefit to the use of this type of non-hydrostatic code even for larger scale simulations. A compressible non-hydrostatic model will adjust much more quickly to the introduction of observations through the initial conditions, boundary conditions, or the 4-dimensional data assimilation schemes.

(b) **Wide range of physical parameterizations:** RAMS is a very general meteorological simulation system that can be applied to a wide range of atmospheric motions ranging from a hemisphere down to the microscale where boundary layer eddies can be resolved. It contains the physical parameterizations necessary to handle these scales and includes a full suite of radiative, convective, microphysical, vegetative, and soil schemes.

(c) **Flexible domain configurations:** RAMS contains a very flexible two-way interaction grid nesting scheme. Any number of nested grids can be specified at any spatial resolution ratios. The nested grids can either be telescoping or have more than one grid that share the same parent grid. If the application warrants, the nested grids may also move in time. Nested grids may be higher resolution in both the horizontal and vertical and run with a user-specified smaller timestep.

(d) **Sophisticated data analysis scheme:** RAMS uses a hybrid isentropic/terrain-following data analysis scheme (ISAN) to prepare the observations for use as the model initial conditions or in the 4-dimensional data assimilation scheme. This type of coordinate system has been shown by NOAA/FSL and others to generate superior data analyses when compared to a standard pressure or height analysis. ISAN also allows a wide range of input observation types including rawindsondes, surface observations, towers, wind profilers, buoys, etc.

(e) **Experience with regional scale simulations:** RAMS has been used for more than 10 years to supply meteorological fields to photochemical models. Among numerous other efforts, RAMS was used for the Lake Michigan Ozone Study program and in the OTAG simulation efforts. We have already encountered and solved the interface issues in linking the RAMS fields to photochemical models, including UAM-V and CAMx.

(f) **Ongoing developments:** RAMS continues to be developed and new features are added frequently. Over the past year, a major development has been to add an option for a new vertical coordinate, similar to the "ETA" coordinate. This allows RAMS to simulate arbitrarily steep topography, in addition to doing extremely high resolution runs (grid spacings of 1 m or less) of flow around buildings and other structures.

RAMS has been developed by a number of groups since its inception, including Colorado State University (CSU) and Mission Research Corporation (MRC). With the changes over the past year, the primary focus of development will be at ATMET and Duke University, although CSU and MRC will still be involved. RAMS is a multipurpose, numerical prediction model that simulates atmospheric circulations ranging in scale from an entire hemisphere down to large eddy simulations (LES) of the planetary boundary layer. It is most frequently used to simulate atmospheric phenomena on the mesoscale (horizontal scales from 2 km to 2000 km) for applications ranging from operational weather forecasting to air quality applications to support of basic research. RAMS has often been successfully used with much higher resolutions to simulate boundary layer eddies (10-100 m grid spacing), individual building simulation (1 m grid spacing), and direct wind tunnel simulation (1 cm grid spacing). RAMS' predecessor codes were developed to perform research in modelingphysiographically-driven weather systems and simulating convective clouds, mesoscale convective systems, cirrus clouds, and precipitating weather systems in general. RAMS' use has continued to increase to more than 140 current RAMS installations in more than 40 different countries. Although RAMS is supported on all UNIX, Linux, and Windows platforms, because of the exceptional price/performance ratios, we are recently focusing on Linux PCs and PC clusters as our primary computational platform.

The current version of RAMS that is released to the general RAMS user community is version 4.3. Version 4.4 will be released shortly, while we anticipate that version 5.0 will be released in late 2002. Along with an upgrade of the RAMS code structure to more modern and safer FORTRAN 90 constructs, during the time frame of this project, the following features will be added to the v5.0 RAMS code:

- Generalized observational-nudging 4DDA scheme
- Urban canopy parameterization
- Antecedent precipitation index scheme for soil moisture initialization
- Several diabatic initialization options
- Use of NDVI datasets to define vegetation characteristics

RAMS CONFIGURATION

We will employ RAMS v4.4 as the control run for the CCOS episode cases of 14-15 June 2000 and 30 July to 2 August 2000. While various aspects of the model configuration may change upon our review of the specific meteorology, observation availability, and air quality characteristics, the following discussion approximates what we anticipate the RAMS configuration will look like.

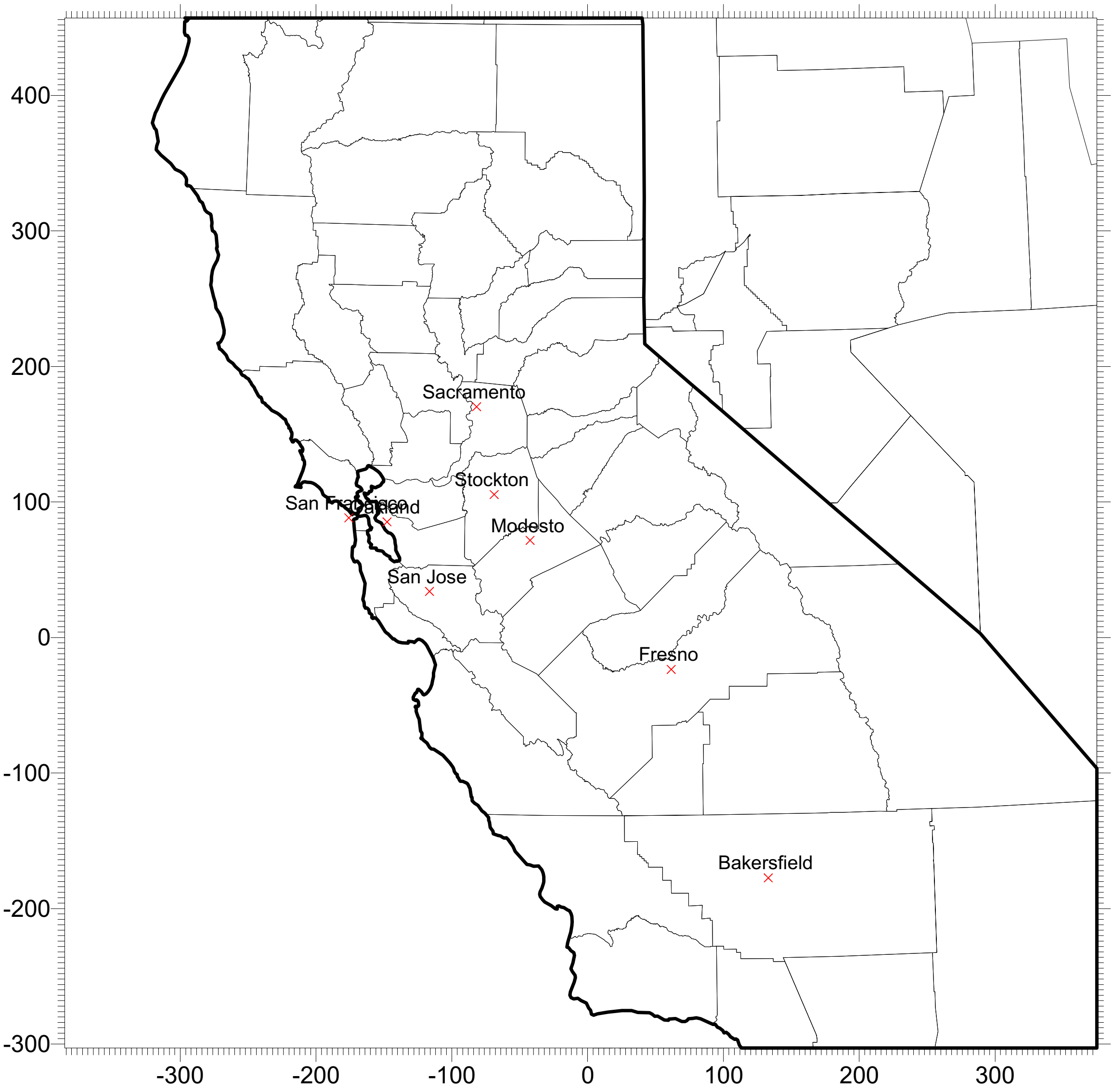
Modeling Grids

For the simulations of the CCOS episodes, the RAMS grids will be configured similarly to previous simulations performed by CARB with MM5. We will primarily use a three grid nested structure with the finest grid at 4 km resolution. However, sensitivity tests using a fourth grid with a 1-2 km resolution over the Bay Area will also be tested to determine the improvements with even higher resolution of the coastlines and topography. Surrounding the finer grids will be a 12 or 16-km nest, which in turn will be nested within a 36-48 km grid to resolve the large scale forcing. Our experience has shown that the meteorological results are greatly enhanced if a significant portion of the synoptic scale is included in the simulation domain, rather than just forced in through the boundary conditions or the four-dimensional data assimilation scheme.

For the vertical structure, RAMS will be configured to run all grids with 41 coordinate levels with the lowest wind and temperature level at about 10 m AGL then smoothly stretching to a maximum of about 1000 m grid spacing. The top of the model will be placed at about 20 km MSL to ensure that the various synoptic scale features such as the sub-tropical jet stream (which is located about tropopause level) are adequately resolved in the simulation domain. Although the upper level jets are not directly important in the low-level transport of ozone and its precursors, the jets do affect the low-level pressure patterns which control the low-level winds.

Care will be taken to closely coordinate the RAMS and CAMx grid resolutions and domain coverages to minimize the impact of interpolation errors and better ensure mass-consistency in the transfer of the meteorological fields from the meteorological model to the photochemical model.

The 4 km CCOS air quality modeling domain is shown in Figure 4-1. While the CARB is performing their modeling on this entire domain at 4 km spacing, we will configure the RAMS grids to cover the focus region (SFBA) at 4 km resolution, with 2 coarser nested grids surrounding it. Figure 4-2 and Table 4-1 depict a likely configuration for the grids. The coarsest grid is 48 km resolution, with grid 2 covering the entire state of California at 12 km spacing. The figure and table also depict an optional grid 4 with ultra-high resolution, which will be employed for sensitivity simulations.



CCAQS 4km Grid
LCP Center: (120.5W, 37N)
Standard Parallels: 30N, 60N
SW Corner: (-385.13, -302.91)
NX x NY: 190 x 190

Figure 4-1. The coverage of the CARB/CCOS air quality modeling domain. Grid spacing over the entire region is 4 km. Map projection is Lambert Conformal.

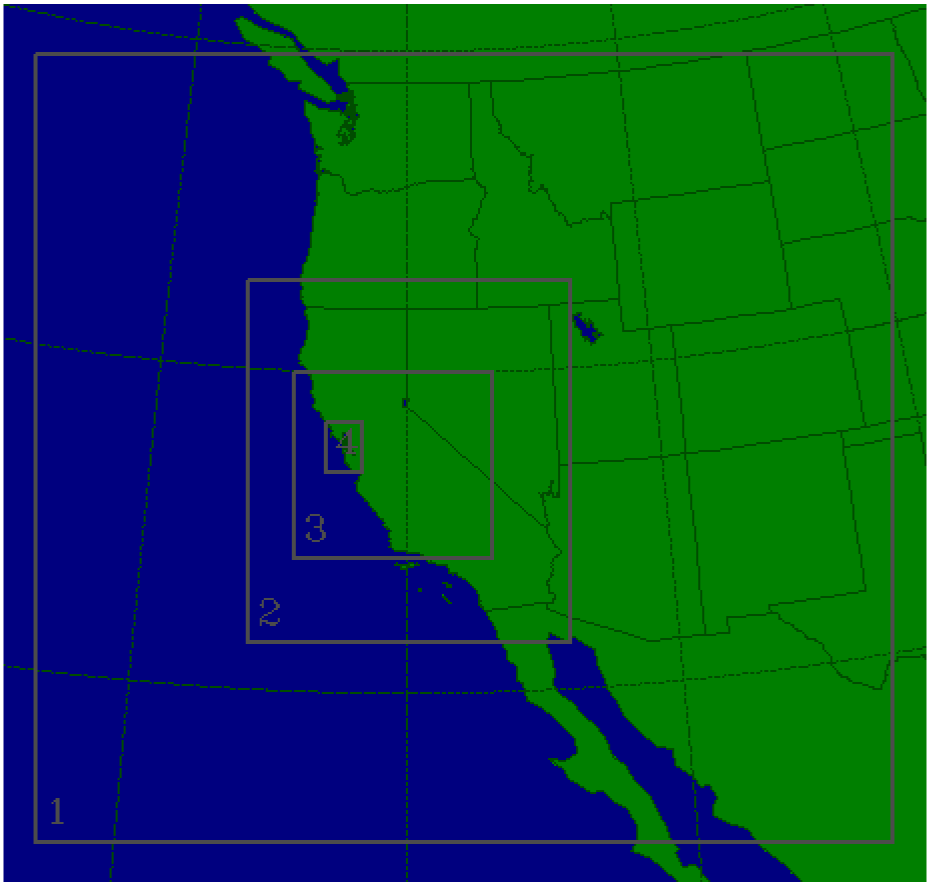


Figure 4-2. Example of the likely configuration for the RAMS rotated polarstereographic modeling grid, which will employ a system of up to four nested grids with successively finer resolution.

Table 4-1. Grid parameters for each of the nested domains shown in Figure 4-2.

Grid	**# of X points**	**# of Y Points**	**Vertical Levels**	**Δx (km)**	**Δy (km)**	**Δz (m) (Lowest)**	**Δt (s)**
1	63	58	41	48	48	10	90
2	77	83	41	16	16	10	45
3	178	174	41	4	4	10	15
4	130	170	41	1	1	10	5.0

Input Data

The input meteorological data for the CCOS episodes will be derived from standard datasets along with the available special observations from the CCOS. The meteorological input data to the meteorological models can be grouped into three categories:

1) **Large scale gridded analyses:** Global analyses of meteorology are available from the National Centers for Environmental Prediction (NCEP). We will use the NCEP/NCAR Reanalysis data. The parameters of wind, temperature, and humidity are analyzed on pressure levels (20 levels extending from 1000 mb up to 10 mb) on a 2.5 degree latitude-longitude grid. These data are archived every 6 hours and serve as a first guess field for the data analysis. We will access this data from the National Center for Atmospheric Research (NCAR).

2) **Standard NWS observations:** The rawinsondes and surface observations reported by the NWS and other national meteorological centers are also archived at NCAR. The rawinsondes are reported every 6 hours and the surface observations are archived every three hours. These data will be accessed for the 6 day period.

3) **Special observations:** Special observations taken during the summer of 2000 from the CCOS monitoring sites will be included in the data analyses and FDDA. These observations included surface observations, wind profilers, rawinsondes, etc. Furthermore, team member Dr. Robert Bornstein has been deeply involved in the development of the Bay Area Mesonet Initiative (BAMI), a program that automates the collection, quality assurance, and consistency of local meteorological data from several networks for public dissemination. To the extent that BAMI data are available during the summer of 2000, and that they do not overlap CCOS databases, we will investigate and consider all observational data for inclusion into the simulations for the two episodes.

The Bay Area Mesoscale Initiative (BAMI) is a consortium between San Jose State University (SJSU), the Naval Postgraduate School (NPS), and the National Weather Service Office in Monterey (NWS) that seeks to enhance the understanding of regional meteorology through establishment of a real-time web-based distribution of meteorological data from mesoscale observational networks. Many agencies already gather such data for different purposes, and BAMI aims to gather and distribute those data. The Cooperative Program for Operational Meteorology, Education, and Training (COMET) in June 1999 thus awarded the consortium funding to use BAMI mesonet data in Limited Area Prediction System (LAPS) for local mesoscale modeling and forecasting. The project has unified the data formats of each constituent network, eliminating non-meteorological information, and provided data in a uniform format for easy processing. The NPS retrieves data from various institutions and SJSU has developed and maintained the BAMI web site (http://meso.met.sjsu.edu/bami), but data are distributed through the Local Data Acquisition and Dissemination (LDAD) system of the Western Region NWS. The LDAD system allows Weather Forecast Offices to collect, check and share local mesonet data, not only within the NWS, but also with local emergency management agencies. BAMI data are also sent to MesoWest, a BAMI-type project for Utah and the western U.S. BAMI data are ingested in the MesoWest data flow to the LDAD system, which makes them available to the entire country in several ways. The simplest is the Forecast Research Laboratory display at http://www-frd.fsl.noaa.gov/mesonet/.

Upon acquisition of the observational data, all NWS, CCOS, and possibly BAMI observational data will be processed with our quality control algorithms. We have developed a QCpackage which consists of three separate schemes: 1) internal consistency checks, 2) "buddy" checks, and 3) "first-guess field" checks.

The internal consistency checks consist of basic sanity and range checking of the observational data along with the physical constraints of hydrostatic balance. Rawindsondes are also checked for lapse rate and wind shear realism. The buddy checks will compare a station's value with that of its neighboring stations. The checks versus the first-guess fields will compare an observation against the large scale gridded pressure data analyses. At any of these three stages, observational data values can be flagged as missing, bad, suspect, or corrected.

After the input meteorological observational data has been quality-controlled, it will be combined with the large-scale gridded analyses to produce a complete data analysis for RAMS initial conditions and the 4-dimensional data assimilation scheme. RAMS/ISAN (Isentropic Analysis package) will be used for the analysis. ISAN is a hybrid isentropic/terrain-following height coordinate scheme which uses a Barnes-type objective analysis algorithm.

Other types of input data which describe the surface characteristics are also necessary for the execution of RAMS. We already possess archives of high-resolution topography, land use, and NDVI for the entire domain. These datasets are global and have about a1 km resolution.

RAMS Physics and FDDA Configuration

We expect that RAMS will be configured with the following physical and numerical options for the CCOS runs:

- Mellor-Yamada type diffusion coefficients with prognostic turbulent kinetic energy
- Long and short wave radiative parameterizations
- Prognostic soil temperature and moisture model
- Prognostic vegetation parameterization
- Explicit and parameterized precipitation
- Four-dimensional data assimilation (analysis and observational nudging)

The four-dimensional data assimilation (FDDA) scheme which has been used in the past by RAMS for these types of simulations has been termed in the meteorological literature as "analysis nudging". However, in certain circumstances, "observational nudging" has some advantages. With the new observational nudging scheme that has been implemented in RAMS, we will have the ability to exercise and test the sensitivity to both types of FDDA schemes.

OUTPUT AND EVALUATION

RAMS will be set to output the simulation results every hour. A complete set of fields will be output for all model grids, including u, v, w wind components, temperature, pressure, cloud variables, precipitation, and eddy diffusion coefficients (or turbulent kinetic energy). The RAMS output files will be converted to CAMx-ready files for use in the photochemical model.

The RAMS Evaluation and Visualization Utilities (REVU) package will be supplied as part of the overall system. For graphical depictions of the meteorological fields, REVU uses NCAR Graphics to generate plots which can then be converted to various other formats such as Postscript, GIF, etc. In addition, we will also install RINGI (RAMS Interactive NCAR Graphics Interface) as part of the system. RINGI is a Graphical User Interface based on TCL/TK, built on top of the REVU package, which provides a convenient, interactive way to look at the raw RAMS output files with the standard REVU NCAR Graphics plots. REVU also has the ability to convert RAMS output files to Vis5D or GrADS format if desired.

For the model's statistical performance, we will use a recently developed, generalized statistical package designed by MRC and ATMET which we termed REVU-GS. Based on the RAMS/REVU code, REVU-GS is compatible with the RAMS input observation files and the raw RAMS output files. The package can produce graphics and tables of various statistical measures for any number of times and levels during a simulation, enabling both spatial and temporal verification. Among the statistical parameters that can be calculated by the REVU-GS package are:

- Root mean square error (RMSE)
- Mean absolute error
- Relative error
- Bias
- Root mean square vector error (RMSVE)
- Correlation coefficient

Sensitivity Simulations

Numerous sensitivity runs of each case will be performed to demonstrate model integrity, sensitivity to resolution, physics, 4DDA, use of special observations, etc. The exact structure of these sensitivity simulations will be discussed with District and the MAC. We will begin with a three-grid control case simulation using RAMS v4.4. These results will then be compared to the new v5.0. We expect the v5.0 results to be similar or better than v4.4, as completed tests have shown in other situations. Additional tests will then be made with v5.0, testing the effect of resolution on the Bay Area with the added 1 km grid 4, along with testing of the new FDDA schemes.

Additional RAMS simulations will likely be required after initial air quality simulation results have been reviewed. The results will be reviewed by the Internal Technical Review Team and the District.

DELIVERABLES

The deliverables for this task are as follows:

- A report on the development, configuration, and evaluations of the meteorological simulations of the two CCOS episodes. The report will be posted to the Contractor-maintained web site.

- The meteorological modeling system comprised of all the software components mentioned above. The software components are:
    a) RAMS, including the ISAN component
    b) Quality control package
    c) REVU and REVU-GS
    d) RINGI
    e) RAMS Grid Configurator
    f) Any supporting components for data conversion
    g) GrADS
    h) Vis5D
    i) NCAR Graphics
    j) RAMS to CAMx converter

5. EMISSIONS MODELING

In order to effectively conduct air quality modeling for the Bay Area SIP revision, it is necessary to develop temporally and spatially resolved emission estimates that are suitable for input to the photochemical model. Emissions are broadly categorized into major stationary or point sources, area sources, on-road mobile sources, and biogenics. In addition, there are many subcategories that comprise the point and area sources. In the following section, we describe the emissions model that will be used in this study. We also describe where the emissions data will be obtained and how they will be used to develop base case and future year emissions estimates.

EMS-95

In order to remain compatible with on-going activities at the CARB, we will use the 1995 Emissions Modeling System, or EMS-95 (Dickson and Oliver, 1991; Dickson et al., 1992; Bruckman and Oliver, 1993; Wilkinson et al., 1994; Janssen, 1998), to prepare the spatially and temporally resolved emissions estimates for the point and area sources. EMS-95 is the emissions modeling system that is currently used by the CARB. Though EMS-95 is capable of preparing biogenics and on-road mobile source emissions estimates, the CARB uses separate systems to prepare these estimates.

For biogenics, the CARB uses the Biogenic Emission Inventory Geographic Information System, or BEIGIS (CARB, 2001). For on-road mobile sources, the CARB is in the process of developing new, statewide emissions estimates under a GIS framework. For both on-road mobile sources and biogenics, we will use the spatially and temporally resolved estimates of volatile organic compounds (VOC), oxides of nitrogen (NO_x), and carbon monoxide (CO) prepared by the CARB for use in the current study. However, we will use EMS-95 to chemically speciate the VOC component of the biogenics and on-road mobile sources into the individual VOC species needed by the air quality model's chemical mechanism. Further, we will use EMS-95 to reformat the emissions estimates for input to CAMx.

To expedite the application of EMS-95 for the current study, the CARB will provide a copy of its working version of EMS-95 on CD-ROM to the project team. This will help ensure that we remain compatible with on-going CARB activities.

Emissions for the CCOS Period

The CARB will provide emissions estimates for the entire CCOS domain, shown in the previous section as Figure 3-1. The major stationary (point) source inventory for the study domain will contain actual stack coordinates and will include year 2000 ozone season day estimates of VOC, NO_x, and CO for each process of the inventoried facilities. The inventory will include the required elements in the format described in Appendix A (Section A-1). The area source inventory will include year 2000, county-wide ozone season day estimates of VOC, NO_x, and CO for each area source category. The inventory will include the required elements in the format described in Appendix A (Section A-2). EMS-95 will be used to process the major stationary source and area source inventories into gridded, speciated, hourly emissions estimates suitable for input to CAMx.

The CARB will also provide gridded, hourly biogenic emissions of isoprene and monoterpenes, at a minimum, for the CCOS domain for each day of the episodes. The CARB may also elect to estimate biogenic emissions of other volatile organic compounds (OVOCs) and nitric oxide (NO). In the event that it does so, we will make provisions to accommodate the biogenic OVOC and NO emissions estimates. The inventory will include the required information as described in Appendix A (Section A-3).

Finally, the CARB will provide gridded, hourly on-road mobile source emissions of total organic gases (TOG), CO, and NO_x for the CCOS domain for each day of the episodes. The inventory will include the required information as described in Appendix A (Section A-4). EMS-95 routines will be used to speciate the biogenic and on-road mobilesource inventory.

Day-Specific Emissions Data

The potential exists that the CARB will supply day-specific emissions estimates for selected facilities and area source categories. If day-specific point source emissions estimates are supplied, the day-specific point source emissions will include the required data described in Appendix A (Section A-5). If day-specific area source emissions estimates are supplied, the day-specific area source emissions will include the required data described in Appendix A (Section A-6).

ON-ROAD EMISSIONS FROM EMFAC

EMFAC2001 version 2.08 is the current model used by the CARB to estimate new on-road mobile source emissions factors for California (CARB, 2002). The EMFAC2001 model supercedes EMFAC2000, which was released in November 2000. As part of the CARB's effort, it will develop gridded, hourly day-specific emissions estimates of TOG, NO_x, and CO for the episodes to be modeled for the Bay Area SIP revision.

Because the CARB plans to modify EMFAC2001 to support changes to heavy heavy-duty diesel emissions factors, among others, it will be necessary to track these revisions and their potential impact on the on-road mobile source inventory. If the CARB indeed does revise EMFAC2001, the project team will decide with the District how best to proceed with integrating these changes into the air quality modeling inventory.

BIOGENICS

As previously stated, the CARB will provide gridded, hourly day-specific biogenic emissions estimates of isoprene and monoterpenes for the episodes to be modeled for the Bay Area SIP revision. However, the CARB does not intend, to the best of our knowledge, to provide estimates of biogenic OVOCs and NO. Biogenic OVOCs comprise around twenty percent of some biogenic inventories and are known to affect air quality modeling predictions (e.g.

Hanna et al., 2002). Furthermore, biogenic NO has been shown to impact the efficacy of anthropogenic emissions control strategies (e.g. Wilkinson and Russell, 2002).

It is unclear how the project sponsors want to proceed regarding the exclusion of biogenic NO and OVOCs from the air quality modeling inventory. Therefore, this issue should be discussed among the project team before a final air quality modeling inventory is constructed.

OTHER EMISSIONS DATA

Other emissions-related data are required in order to prepare emissions estimates that are suitable for input to CAMx. These data include the following:

- Area source spatial surrogates;
- Cross references between area source categories and their spatial surrogates;
- VOC-to-TOG conversion factors by source category;
- Chemical mechanism-specific hydrocarbon speciation profiles; and
- Cross references between source categories and their hydrocarbon speciation profiles.

The area source spatial surrogates are used to spatially allocate the county-wide area source emissions estimates to individual grid cells. The CARB will supply these data per the file format described in Appendix A (Section A-7).

The area source spatial surrogates cross reference data maps each area source category to a specific spatial surrogate. The CARB will supply these data per the file format described in Appendix A (Section A-8).

The VOC-to-TOG conversion factors convert VOC emissions estimates to TOG emissions estimates by source category. These conversion factors are applied to the VOC emissions estimates so that the hydrocarbon speciation profiles, which are typically based on TOG, can be applied. The CARB will supply these data per the file format described in Appendix A (Section A-9).

The chemical mechanism hydrocarbon speciation profiles are used to split the TOG emissions estimates into the individual hydrocarbon components that are modeled within the chemistry processes of CAMx. The CARB will provide hydrocarbon speciation profiles for both the CB-IV and SPARC99 chemical mechanisms per the file format described in Appendix A (Section A-10).

The hydrocarbon speciation profile cross reference data maps an area source category or source classification code (SCC) to a chemical mechanism hydrocarbon speciation profile. The CARB will provide this cross reference per the file format described in Appendix A (Section A-11).

FUTURE YEAR PROJECTION METHODS

Figure 5-1 shows an overview of how air quality modeling emissions inventories are created. In the first step, the base case emissions estimates and data are used to create a historical episode, the "base case" air quality modeling inventory. The base case air quality modeling inventory is used to demonstrate that CAMx can adequately reproduce observed air quality.

In step two, the base case emissions estimates and data are grown and controlled to a future year, the future year emissions estimates and data. In the third step, the future year emissions estimates and data are processed by the emissions model to create the future year airquality modeling inventory. The future year air quality modeling inventory is used in CAMx to establish the baseline air quality field. The baseline air quality field is then used to determine what additional emissions controls, if any, are needed to reach attainment. In the fourth step, additional emissions controls are applied, if necessary, to the future year emissions estimates and data to create the future year air quality modeling controlled inventory. The future year air quality modeling controlled inventory is then used by CAMx to determine if attainment of an air quality metric is reached.

Currently the CARB is developing the base case emissions data and portions of the base case air quality modeling inventory (i.e., biogenics and on-road mobile source emissions estimates). The CARB will develop the state-wide growth and control estimates that are needed to project the base case emissions estimates and data to the future year emissions estimates and data. We will then apply EMS-95 to the future year emissions estimates and data to create the future year air quality modeling inventory for the point and area sources. For the biogenics and on-road mobile sources, the CARB will provide future year gridded, hourly emissions estimates.

In coordination with the BAAQMD, the project team will develop the emissions control strategies specific to the SFBA. We will apply those strategies to the future year emissions estimates and data to develop the future year air quality modeling controlled inventory. Though the development of the future year air quality modeling inventory and the future year air quality modeling controlled inventory is an iterative process, we will be limited by project resources in how many air quality modeling inventories can be created.

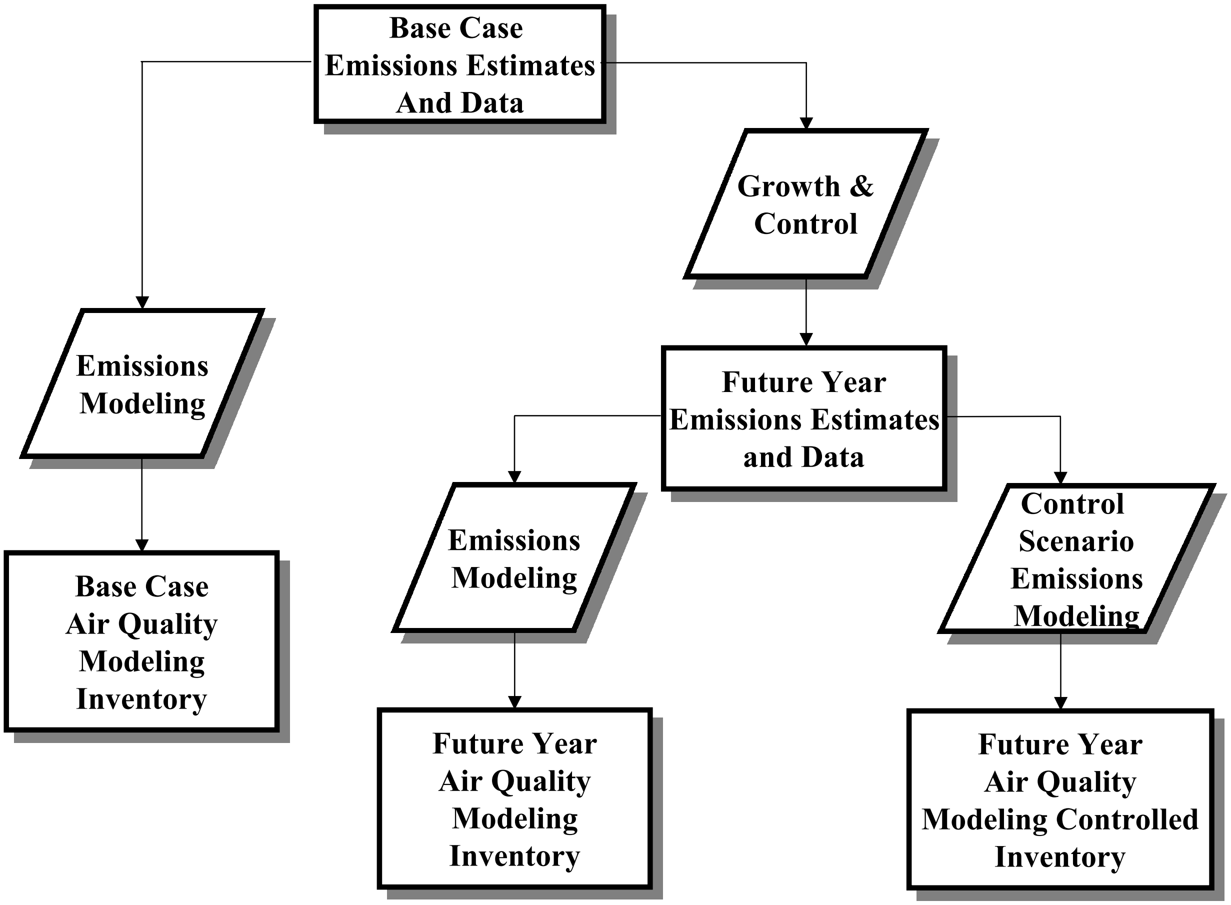


Figure 5-1. Overview of the air quality modeling emissions inventory development.

DELIVERABLES

The deliverables for this task are as follows:

- A report on the development of the base case, future base, and future controlled modeling inventories. The report will be posted to the Contractor-maintained web site.

- The emissions modeling system comprised of all the software components and databases mentioned above. The software components are:
    a) EMS-95 and supporting software systems
    b) CARB models (EMFAC and BEIGIS)
    c) Raw CARB inventories
    d) Ancillary supporting data (surrogates, cross-reference files, etc.)
    e) Processed model-ready inventories used in CAMx
    f) Any supporting components for data conversion

6. CAMx INPUT DATA PREPARATION

Several data preparation tasks are required to provide CAMx with various inputs that define the meteorology, emissions, initial and boundary conditions, surface characteristics, and photochemical conditions of the atmosphere. The bulk of work associated with meteorology and emissions is described in previous sections. However, some additional processing is needed for these components just before the air quality model is run. This section begins with a discussion on the air quality modeling grid specification; it is critical to define the grid system extent and resolution before the development of most of the CAMx input fieldscan begin. This section then goes on to describe the procedures to develop and/or format the various input files for CAMx, and finally lists the model options that will be invoked in the base and diagnostic simulations.

CAMx DOMAIN AND GRID SPECIFICATIONS

The spatial domain (or volume) on which Eulerian models operate is defined as a three-dimensional grid, which is used to discretize the environment into averages contained within many small grid cell volumes. The modeling grid should be defined with sufficient size and resolution to capture all of the significant physical processes that affect pollutant concentration patterns. Obviously a balance must be struck between grid size and resolution, both because of resource constraints (budget, schedule, and computing power), and because of limitations inherent in all Eulerian models to characterize physical phenomena at small scales (< 1 km horizontally).

Therefore, an important step in the design of an ozone modeling system is specifying the extent of the domain and resolution of the grid. By necessity, the air quality modeling domain and grid specifications for this study will be based on CARB's current emissions and air quality modeling projection configuration, but the specific domain extent, nesting configuration, and resolution will be adjusted to maximize the focus of the simulations on the SFBA ozone problem. The CARB is currently undertaking simulations of the CCOS episodes using MM5 with SAQM and CMAQ, which together with EMS-95 are applied on a very large regional domain on a Lambert Conformal Conic projection all at a 4-km resolution (see Figure 4-1). The RAMS model to be used in this study operates on a Rotated Polar Stereographic projection, and so the RAMSCAMx processor will provide the link that performs the necessary manipulations of the RAMS output to properly feed into CAMx on the CCOS Lambert projection. Clearly, the definition of the RAMS polarstereographic grid and the CAMx Lambert grid will need to be closely coordinated to minimize distortions between the two projections.

In Figure 6-1 we submit a preliminary suggestion for the arrangement of the various CAMx nested grids. Since the emissions inventory will be provided for the CCOS domain shown in Figure 4-1, the outermost CAMx grid is limited to the CCOS extent and thus covers the CCOS grid identically. However, while the CCOS grid resolution is 4 km over the entire area, the CAMx grid cell resolution for the outer domain will be set to match the RAMS resolution of 12 km (see Figure 4-2). This resolution is sufficient to capture the influences of regional air quality from the various rural areas outside of central California on the fringe of the CCOS

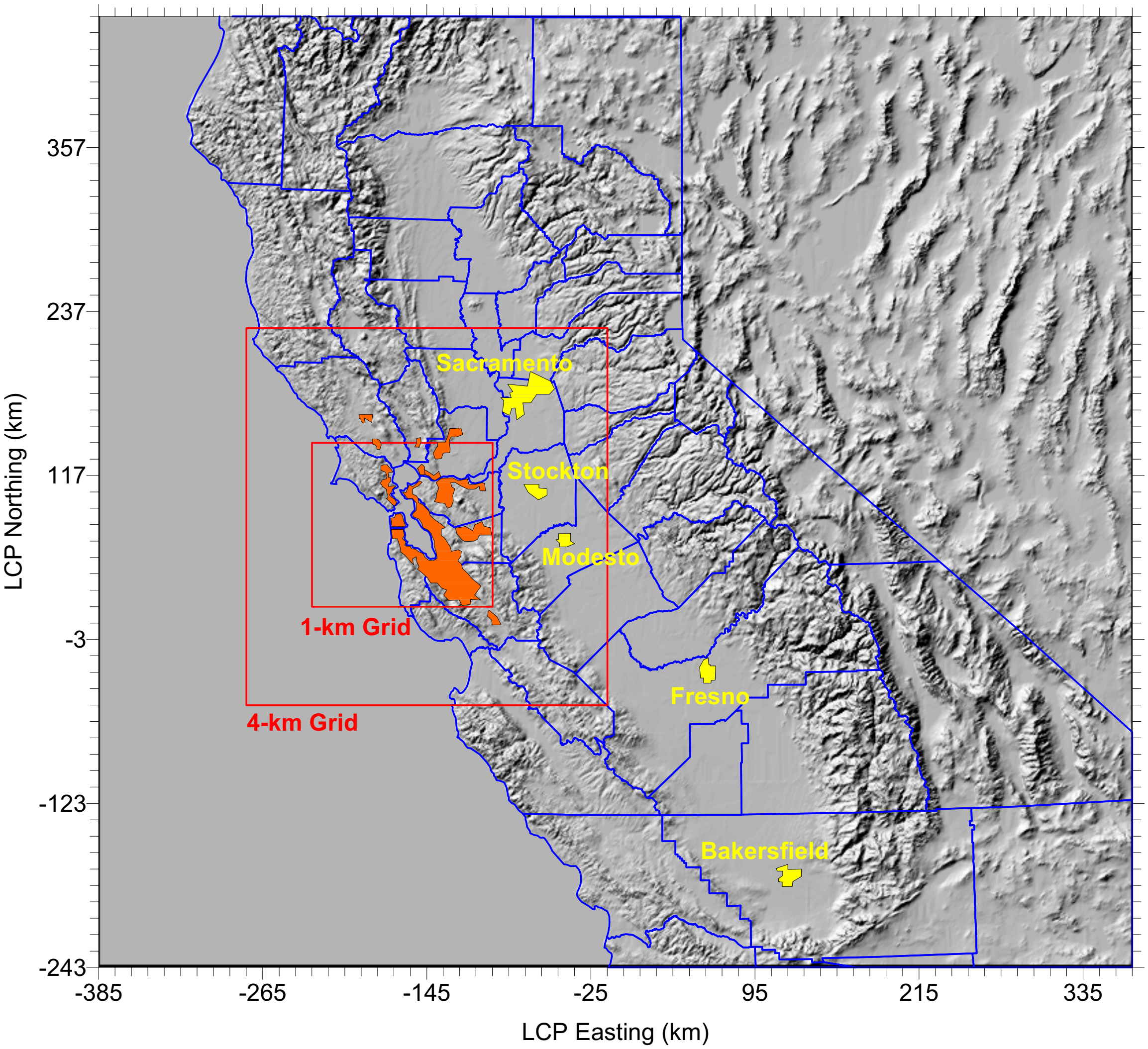


Figure 6-1. Example of the 12/4/1-km CAMx nested grid system covering central California. This domain aligns onto the CCOS 4-km modeling grid.

grid. A simple grid cell aggregation step will be necessary to process 4-km emission inputs to the 12-km grid inputs.

The primary inner nest shown in Figure 6-1 will cover the urbanized areas of central California at a grid resolution of 4 km. The 4-km CAMx nest will exactly overlay a subset of the CCOS grid, so gridded emissions data will simply be “windowed out” for this intermediate grid. This grid will also be consistent with the extent of the RAMS 4-km grid. The 4-km CAMx nest will be used for most of the CAMx developmental/diagnostic simulations.

Finally, a small high-resolution nest will cover the urbanized portion of the immediate SFBA for some sensitivity tests. The resolution is expected to be on the order of 1 km, and will be consistent with the extent of the RAMS high-resolution grid 4 (Figure 4-2). Gridded emission estimates (area, on-road, biogenics, etc.) will need to be reprocessed to this resolution using new spatial surrogates if we are to investigate the full potential effects of such a fine resolution grid. Point sources would not need to be reprocessed as those inputs are not dependent upon model resolution.

In the vertical, CAMx will resolve the atmosphere into 10 to 15 layers up to ~4 km above the surface. CAMx operates in a terrain-following coordinate system, and can match the layer structure of any meteorological model providing three-dimensional gridded input fields. In this case, CAMx will be configured to match a subset of RAMS layers between the ground and about 4 km. CAMx will exactly match every RAMS layer within ~1 km of the surface; aloft, CAMx will span multiple RAMS layers. Sensitivity tests to layer structure will be undertaken to test the model’s response to vertical resolution.

EMISSIONS PROCESSING

While emission files are generated by EMS-95 in model-ready format, there are some final steps to perform before CAMx can be run. First, EMS-95 provides separate gridded surface emission files for each major source category that is processed (i.e., biogenic, area, on-road mobile, etc.). These must be “merged” into a single all-encompassing gridded emissions input file using readily available and standard software tools. Second, the emission files at 4-km resolution must be processed to the various CAMx nested grids. For the outer 12-km grid, the emissions in each 4 km cell will be simply aggregated to the nine overlying 12-km cells and a new file written. For the smaller CAMx 4-km grid, the emissions within a subset of the emissions grid will be simply extracted to a new file. Both aggregation and windowing are accomplished using a single emissions manipulation program developed by ENVIRON. If the 1-km CAMx grid is utilized without any emissions processing at that resolution, CAMx will automatically map the 4-km emissions to the 1-km grid internally.

Third, large NOx elevated point sources must be selected for the CAMx Plume-in-Grid (PiG) treatment. Point sources will be chosen for the PiG treatment based on aminimum threshold daily NOx emissions rate that yields a few hundred PiG sources in the modeling domain. We propose to apply a lower NOx threshold for sources in and around the focus SFBA (e.g., ~5 tons per day), and higher thresholds in the remainder of California (e.g., ~10 tons per day). We will prepare a list of major NOx emitters selected for PiG treatment and review the list with the District and the MAC prior to any simulations with the PiG module invoked.

METEOROLOGICAL PROCESSING

Raw output from the RAMS meteorological model needs to be converted to formats and variables used by CAMx specifically. ENVIRON has authored widely used RAMS and MM5 translation software to complete this task. The software includes the ability to interpolate data from the native map projections used by the meteorological models to any projection to be specified for air quality model (CAMx may be applied on Lambert Conformal, Polar Stereographic, or UTM projections, or in geodetic latitude/longitude). The meteorological translation software will provide an important component of the District's unified RAMS/CAMx modeling system.

CAMx requires meteorological input data for the parameters described in Table 6-1.

Table 6-1. CAMx meteorological input data requirements.

CAMx Input Parameter	**Description**
Layer interface height (m)	3-D gridded time-varying layer heights for the start and end of each hour
Winds (m/s)	3-D gridded wind vectors (u,v) for the start and end of each hour
Temperature (K)	3-D gridded temperature and 2-D gridded surface temperature for the start and end of each hour
Pressure (mb)	3-D gridded pressure for the start and end of each hour
Vertical Diffusivity (m^2/s)	3-D gridded vertical exchange coefficients for each hour
Water Vapor (ppm)	3-D gridded water vapor mixing ratio for each hour
Cloud Cover	3-D gridded cloud cover for each hour
Rainfall Rate (in/hr)	2-D gridded rainfall rate for each hour

All of these input data will be derived from the RAMS results. RAMS output fields will be translated to CAMx-ready inputs using ENVIRON's RAMSCAMx translation software. This program performs several functions:

1. Extracts data from the RAMS grids to the corresponding CAMx grids; in this study, the extraction will include a mass-weighted interpolation from the RAMS polar stereographic grid to the CAMx Lambertian grid, with appropriate rotation of vector (wind) variables.
2. Performs mass-weighted vertical aggregation of data for CAMx layers that span multiple RAMS layers.
3. Diagnoses key variables that are not directly output by RAMS (e.g., vertical diffusion coefficients and cloud information).

The RAMSCAMx program has been written to carefully preserve the consistency of the predicted wind, temperature and pressure fields output by RAMS. This is the key to preparing mass-consistent inputs for CAMx, and therefore for obtaining high quality performance from CAMx.

The data prepared by RAMSCAMx will be directly input to CAMx. Vertical diffusivities (Kv) are an important input to the CAMx simulation since they determine the rate and depth of mixing in the planetary boundary layer (PBL) and above. In general, our experience has been that diffusivities from meteorological models require careful examination before they are used in air quality modeling. This may be because the air quality model results are much more sensitive to diffusivities than the meteorological model results. We will evaluate the CAMx diffusion inputs by comparing the Kv values taken directly from RAMS with several diagnostic calculation approaches, and by analyzing available sounding data from profilers and rawinsondes. Sensitivity simulations will be undertaken with the various Kv fields. Based on prior experience, we will likely apply minimum diffusivity values between layers 1 and 2 to ensure that nocturnal stability near the surface is not over-stated. The minimum value used will depend upon landuse (e.g., urban, forest, agricultural, water, etc.) to represent different impacts of mechanical mixing and surface heat input (e.g., urban heat island effect).

DEVELOPMENT OF ANCILLARY INPUTS

The preparation of ancillary inputs files include initial/boundary conditions, land use distribution for all grids, chemistry parameters, albedo/haze/ozone fields, photolysis rates.

Initial and Boundary Conditions

The initial conditions (ICs) are the pollutant concentrations specified throughout the modeling domain at the start of the simulation. Boundary conditions (BCs) are the pollutant concentrations specified at the perimeter of the modeling domain. One of the reasons for performing regional scale modeling rather than urban scale modeling is to minimize the importance of ICs and BCs. Using a large regional domain moves the boundaries far away (in distance and transport time) from the study area. Including several “spin-up” days prior to the episode period allows time for the influence of initial conditions to be removed.

As a starting point, the initial and boundary concentrations currently specified by CARB in their CCOS modeling effort will be utilized for CAMx; the CCOS approach will be reviewed and discussed with CARB modeling staff. In any event, sensitivity runs to investigate the contribution of the boundaries to ozone in the focus area will be undertaken. Relatively clean initial conditions are expected to be removed via the addition of a three-day model spinup period before each modeling episode (thus the modeling simulation will extent over **June 11-15** and **July 27 to August 2**). The role of initial and boundary conditions may be investigated further by utilizing several of the CAMx “Probing Tools” as well, depending upon available resources and schedule.

Surface Characteristics (Landuse)

CAMx requires gridded landuse data to characterize surface boundary conditions, such as roughness, deposition parameters, albedo, vegetative distribution, and water/land boundaries. The land cover categories utilized by CAMx are based on the 11 category system established in RADM, which are parallel with SAQM and UAM-V.

Land use inputs will be developed from three possible sources: (1) emission surrogates used in emissions processing; (2) high-resolution (~200 m pixel) landuse/landcover data that is freely availble from the USGS in 1:250,000 scale quad maps; and/or (3) any additional high-quality land use data available from local Bay Area planning or other governmental agencies.

ENVIRON and Alpine Geophysics have both developed and possess software to convert raw land cover data to model-ready input variables and formats. These include both Fortran-based systems, and GIS/Arc-Info capabilities. The latter would be crucial if local SFBA data were to be made available to the project.

Chemistry Data

Three input files define the chemistry used in CAMx.

Chemistry Parameters: The chemistry parameters file selects which chemical mechanism to use and specifies the rate constants for the thermochemical reactions. CAMx will be run with the most up-to-date version of the Carbon Bond 4 mechanism (CB4) which is referred to as mechanism 3 in CAMx. Mechanism 3 is the CB4 mechanism with updated radical termination reactions and updated isoprene mechanism as used for the OTAG modeling. Alternatively, CAMx may also be run with the SAPRC99 mechanism, if emission input files are supplied with SAPRC speciation.

Photolysis Rates: The photolysis rates file determines the rates for chemical reactions in the mechanism that are driven by sunlight. The photolysis rates file will be prepared using version 4 of the TUV radiative transfer model developed at NCAR. The rates file is essentially a very large multi-dimensional lookup table that define the variation of 6 photolysis reactions over zenith angle, altitude, surface UV albedo, haze turbidity, and total vertically integrated ozone column density.

Albedo/Haze/Ozone File: The albedo/haze/ozone file specifies how these parameters vary in time and space for the CAMx simulation. The photolysis rates and albedo/haze/ozone files must be coordinated to function together correctly. The surface albedo will be calculated based on the gridded landuse data. The stratospheric ozone column data will be based on available satellite data from http://www.cpc.ncep.noaa.gov. Since there may not be a source of regionally specific haze data for the study area, constant haze turbidity representative of rural areas will be assumed over the entire grid. The CCOS database will be reviewed to identify any source of data that may allow for a more robust manner in setting haze turbidity values.

CAMx MODEL OPTIONS

CAMx has several user-selectable options that are specified for each simulation through the CAMx control file. Most of these options follow naturally from other choices about model inputs. There are three optional inputs that must be decided for this project: the advection scheme, the plume-in-grid scheme and the chemistry solver. The recommended choices for these options are discussed below. See the CAMx User's Guide (ENVIRON, 2002) for more details on these options. The selection for each option will be decided at the stage of thebase case model performance evaluation and then held fixed for the remainder of the project.

Advection scheme: CAMx has three optional methods for calculating horizontal advection (the movement of pollutants due to horizontal winds) called Smolarkiewicz, Bott and Piecewise Parabolic Method (PPM). The Smolarkiewicz scheme has been used for many years, and was used in many previous studies in California with SAQM and UAM. The Smolarkiewicz scheme has been criticized for causing too much artificial diffusion of pollutants, tending to "smear out" features and artificially overstate transport. The Bott and PPM schemes are newer and have less artificial diffusion than the Smolarkiewicz scheme. The PPM scheme will be used for this study. Sensitivity to other options may be examined in diagnostic tests for the base case.

Plume-in-Grid: CAMx includes an optional sub-grid scale plume model that can be used to represent the dispersion and chemistry of major NOx point source plumes close to the source. We will use the Plume-in-Grid (PIG) sub-model for major NOx sources (i.e., point sources with episode average NOx emissions greater than 5-10 tons per day). Sensitivity to no PIG treatment may be examined in diagnostic tests for the base case.

Chemistry Solver: Starting with version 3 of CAMx there are two options for the numerical solution scheme for the gas phase chemistry. The first option is the CMC fast solver that has been used in every prior version of CAMx. The second option is an IEH solver. The CMC solver is fast and more accurate than most chemistry solvers used in current ozone models. The IEH solver is even more accurate than the CMC solver but significantly slower. The CMC solver will be used for this study. Sensitivity to using the IEH solver may be examined in diagnostic tests for the base case.

7. BASE YEAR MODEL PERFORMANCE EVALUATION

For the base year modeling CAMx will be run for the two CCOS 2000 episodes and the performance of the model will be evaluated against available air quality data. The purpose of the evaluation is to build confidence in the model's reliability as an ozone prediction tool. The proposed evaluation plan will follow the procedures recommended in the EPA and CARB guidance documents for 1-hour ozone (EPA, 1991; CARB, 1992), and new draft guidance for 8-hour ozone (EPA, 1999).

APPROACH TO MODEL PERFORMANCE EVALUATION

It is first important to establish a framework for assessing whether the photochemical modeling system performs with sufficient reliability to justify its use in developing ozone control strategies. The framework for assessing the model's reliability consists of the following principals, which are based on EPA's draft 8-hour modeling guidance:

- **The Model Should be Viewed as a System.** When we refer to evaluating a "model" we include not only the CAMx photochemical model, but its various companion preprocessor models, the supporting aerometric and emissions database, and all other related analytical and numerical procedures used to produce modeling results.

- **Model Acceptance is a Continuing Process of Non-Rejection.** Over-reliance on explicit or implied model "acceptance" criteria should be avoided, including EPA's performance goals (EPA, 1991). Models should be accepted gradually as a consequence of successive non-rejections, and confidence builds as the model undergoes a number of different applications (hopefully involving stressful performance testing) without encountering major or fatal flaws that cause the model to be rejected.

- **Criteria for Judging Model Performance Must Remain Flexible.** This approach recognizes the several new elements introduced to SFBA regional application including the use of the latest local-regional emissions data sets and models.

- **Previous Experience is Used as a Guide for Judging Model Acceptability.** Interpretation of the CAMx modeling results for the episode, against the backdrop of previous modeling experience, will aid in identifying potential performance problems and suggest whether the model should be tested further or rejected.

Incorporating these principals into an operational philosophy for judging model performance, we suggest the following approach for assessing the reliability of the CAMx for control strategy development. The model should produce peak unpaired ozone estimation accuracy, overall bias, and gross error statistics within the approximate ranges of±15-20%, ±5-15%, and 30-35%, respectively, as recommended by EPA (EPA, 1991). If the model's performance is better than all of these ranges, the base case would not be rejected unless evidence from any supplemental diagnostic or sensitivity simulations suggest unusual or aberrant behavior.

If the base case fails any one of the above general ranges, it would become necessary to explain why the performance is poorer than commonly achieved in similar applications and whether the problems will compromise the evaluation of emission control strategies. Otherwise, the particular base case in question should be declared inadequate. This outcome would result in one of several courses of action: (a) diagnose the causes of poor performance and rectify such problems, or (b) eliminate the poor-performing episode from use in strategy development and/or identify an alternative episode for substitution in the study.

GRAPHICAL AND STATISTICAL EVALUATION

The evaluation of performance for the 2000 CCOS episodes would be carried out in two sequential phases, beginning with the simplest comparisons of modeled and observed ground-level ozone concentrations, and progressing to potentially more illuminating analyses if necessary (e.g., examination of precursor and product species, comparisons of pollutant ratios and groupings). The procedures outlined in the draft 8-hour modeling guidance provides six means by which to establish acceptable model performance:

1. Inspection of computer generated graphics.
2. Calculation of ozone statistical metrics.
3. Comparison of predicted and observed precursor emissions or species concentrations.
4. Comparison of observed and predicted ratios of indicator species.
5. Comparison of predicted source category contribution factors with estimates obtained using observational models.
6. Retrospective analyses in which air quality differences predicted by the model are compared with observed trends.

Sufficient fulfillment of these six points requires the availability of comprehensive measurement data on ozone and precursors from an extensive monitoring network. This may not be feasible in all cases, particularly in regards to precursor measurements. It is also quite possible that the list given above will change with the release of final guidance by EPA. Therefore, our proposed approach will consist of a blend of those points above and the three basic model performance steps outlined below. To the extent possible, each of the performance procedures described by EPA’s 8-hour guidance will be addressed, and at a minimum, an explanation of why certain components cannot be fulfilled will be provided (e.g., insufficient observational data).

Initial screening of the CAMx base case ozone predictions will be performed for the modeling episodes in an attempt to identify obviously flawed model simulations and to implement improvements to the model input files in a logical, defensible manner. If the screening phase suggests that no obvious flaws or compensating errors exist in the simulation(s), then one progresses to the operational evaluation. The screening evaluation will employ ozone performance statistics and plots. Graphical displays will be generated using a combination of several common software packages that the ENVIRON team possess in-house, most of which are readily accessible to the project sponsors. These software packages include the Microsoft Excel, Surfer, and publicly-available PAVE. Examples of the types of graphical displays to be considered for each base case include:

- Ozone time series plots;
- Ground-level ozone isopleths;
- Ozone concentration scatterplots;
- Bias and error statistics stratified by sub-region and by time (day of episode).

Experience in photochemical modeling is the best basis upon which to identify obviously flawed simulation results. Efforts to improve photochemical model performance, where necessary and warranted (i.e., to reduce the discrepancies between model estimates and observations), should be based on sound scientific principles. A "curve-fitting" or "tuning" activity is to be avoided. The following principals should govern the model performance improvement process (to the fullest extent possible given the project schedule):

- Any significant changes to the model or its inputs must be documented;
- Any significant changes to the model or its inputs must be supported by scientific evidence; analysis of new data, or by re-analysis of the existing data where errors or misjudgments may have occurred; and
- All significant changes to the model or its inputs should be reviewed by the MAC.

If the initial examination of the CAMx ozone results does not reveal obvious flaws, the formal operational evaluation follows. This activity consists of three steps: (1) evaluation of ozone precursors; (2) evaluation of ozone and precursors against aircraft data; and (3) sensitivity/diagnostic simulations. First, the graphical and statistical evaluation utilized in the screening evaluation for ozone will be generated for NOx and VOC to the extent possible (usually speciated VOC samples are taken over much longer periods at a few sites, so statistics based on the small population set are not particularly useful). Should any obvious flaws be detected, the model diagnosis and performance improvement efforts may be needed to fully identify and correct (if possible) the noted problems. Second, the ozone, NOx, and VOC predictions will be examined aloft by comparing to available aircraft data, and this is described in more detail below, as are the diagnostic and sensitivity simulations.

PERFORMANCE EVALUATION AGAINST AIRCRAFT DATA

The air quality and meteorological data compiled from standard and special study networks such as CCOS can be used in “stand-alone” analyses such as developing conceptual models for ozone formation. They are also valuable for improving photochemical modeling studies to provide more reliable air quality plans. Aircraft data are of particular value because they provide data away from the fixed surface monitoring network (i.e., aloft and between surface sites) and so can be useful in evaluating boundary conditions, individual pollutant plumes, and transport of regional sources to urban areas of interest.

ENVIRON has used aircraft data in several model performance evaluations in Texas. We have developed comparison methodologies and software that take into account the different temporal and spatial scales represented by aircraft data and photochemical model results.

As stated in Section 2, four instrumented aircraft were used to measure the vertical and horizontal gradients of temperature, humidity, and pollutant concentrations in the study region during CCOS IOPs. These aircraft included a Cessna 172RG and Cessna 182 operated by University of California at Davis (UCD), and a Cessna 182 and Piper Aztec operated by Sonoma Technology, Inc. (STI). One additional aircraft (Twin Otter), flown by the Tennessee Valley Authority (TVA), made measurements in power plant plumes. The TVA data were collected to evaluate the plume-in-grid parameterizations used in air quality models.

Aircraft data will be procured from the CARB for the specific episodes addressed in this modeling study. These will be used to directly evaluate model performance for ozone and precursors along the flight trajectory paths. Such analyses provide insight into placement of urban and industrial plumes, height of the well-mixed boundary layer, and chemical production aloft (if product species were measured).

Another use for aircraft data is to provide information on setting lateral and top boundary conditions for remote areas such as over the ocean where no routinely available measurements are made. If aircraft flights were not conducted in remote areas during the modeling episodes, we will evaluate whether the data from other flights could be used to set boundary conditions, e.g., similar meteorological/transport conditions, etc.

DIAGNOSTIC AND SENSITIVITY SIMULATIONS

Objectives

A limited number of diagnostic simulations will be performed to help understand and possibly improve base case model performance. In addition, sensitivity tests will be performed to diagnose model sensitivity to changes in key inputs. These tests are an important component of the base case model evaluation process. In general, diagnostic and sensitivity analyses serve to:

- Reveal model responses that are inconsistent with expectations or other model responses.
- Identify what parameters (or inputs) dominate (or do not dominate) model results.
- Examine the relationship between uncertainties in model inputs and model outputs (error propagation through the model).
- Identify alternate base cases that offer similar model performance and therefore identify potential compensating errors.
- Provide guidance for model refinement and data collection programs.

The exact sensitivity simulations that will be needed can only be assessed after the initial model evaluations are performed.

Tests That Are Not Recommended

With the advent of more sophisticated nested regional ozone models (such as CAMx) a number of sensitivity runs that were historically carried out with the UAM and other models are no longer needed or appropriate. These tests include zero-emission, zero initial condition, zero boundary condition runs and modified wind field tests such as halving the wind speeds.

Physically unrealistic tests such as these can produce misleading results that are difficult to interpret. For the zero emission and zero IC/BC sensitivity tests, more can be learned from looking at sensitivity to alternate (but physically possible) inputs. Ad-hoc modifications to wind fields external to meteorological models like RAMS and MM5 are not recommended because they destroy consistency among the meteorological inputs (e.g., winds that are physically unrelated to pressures and temperatures). Other types of meteorological experiments are potentially more useful, such as alternate vertical eddy diffusivities or alternate vertical grid structures.

Recommended Tests

Sensitivity experiments will be considered as part of the performance evaluation analysis as appropriate. The potential need for and nature of these simulations will be discussed with the District, CARB, and MAC representatives. Up to 10 sensitivity/diagnostic CAMx simulations are planned.

Potential diagnostic runs include:

- Boundary conditions, sensitivity to the use of more or less polluted boundary conditions.
- Biogenic emissions, evaluate sensitivity to uncertainties in biogenic emissions levels.
- PiG treatment, to check ozone sensitivity to the implementation of this submodel.
- Advection scheme, impact of this model option on performance.
- Meteorology, specific diagnostic tests identified during the preparation of the meteorological inputs such as: alternate vertical diffusion coefficients; impacts of clouds on photolysis rates; effects of grid resolution (horizontal and vertical); and effects of alternative meteorological realization from varying nudging strengths and/or various model options.

Potential sensitivity runs include:

- Sensitivity to modified initial and boundary concentrations, as they may have an effect on assumptions in extrapolating to future year conditions.
- Sensitivity to reductions/increases in total anthropogenic VOC and/or NOx emissions.
- Sensitivity to reductions/increases in anthropogenic VOC and/or NOx emissions from specific source categories.
- Sensitivity to reductions/increases in anthropogenic VOC and/or NOx emissions from specific source regions (e.g., distant or local).

Use of CAMx Probing Tools for Diagnostic Evaluation

CAMx provides several “extensions” to the basic chemical/dispersion model, referred to as “probing tools”, that provide information concerning source apportionment and the relative importance of various physical and chemical processes. These tools include the Ozone Source Apportionment Technology (OSAT and derivatives), Process Analysis (PA), and the Decoupled Direct Method of tracking sensitivity coefficients (DDM, similar to a source apportionment of emissions). All of these are described in the CAMx User’s Guide for version 3.10.

For diagnostic purposes, the most useful tool is PA, as this provides a wealth of information concerning the rates of change in ozone relative to transport and chemical processes. Reviewing this information can lead to insights into model performance and NOx/VOC-limited chemical kinetics in user-specified portions of the domain. OSAT and DDM are typically used for assessing source apportionment for purposes of designing control strategy scenarios, and both can be used in a diagnostic manner to assess the relative importance of various sources. In this way, the user may be able to discover if a particular source area/category is having a stronger or weaker influence on ozone in key receptor areas than conceptually expected, and then undertake an investigation to determine if that signal is appropriate or not.

Depending on project resources and schedule, use of these probing tools will be considered in the diagnostic evaluation of the CAMx Base Case simulations.

CORROBORATIVE ANALYSES

Recently, emphasis has been continuously placed upon utilizing independent air quality and/or emissions analyses to corroborate the findings of air quality model simulations. Draft 8-hour ozone and PM modeling guidance from EPA now stress the need to evaluate air quality model performance and estimated source attribution against such independent examinations in “weight of evidence” analyses, which are used to support or refute the signals obtained from the simulations. The most useful and varied corroborative examinations are available to an air quality modeling study when it is coordinated with a multi-faceted field study program.

Fortunately, the data analyses planned for the CCOS period could provide ample benefits to this modeling study. The study team and District staff will monitor the progress of the CCOS data analysis projects through spring of 2003 and note any particular analyses that could help explain model performance or guide control strategy development. Depending on available project resources and schedule at the time, the most relevant of these will be considered for corroborative model evaluation. Particularly relevant and useful analyses would include NOx/VOC limited chemistry, Chemical Mass Balance (CMB) modeling for hydrocarbons, any retrospective trends analyses for NOx, VOC and ozone, and Blanchard’s MAPPER results for sites in and around the SFBA.

DELIVERABLES

The deliverables for this task are as follows:

- A report on the development, configuration, and evaluations of the air quality simulations of the two CCOS episodes. The report will be posted to the Contractor-maintained web site.
- The base year air quality modeling system comprised of all the databases and software components developed to support the model performance evaluation.

8. FUTURE/ATTAINMENT YEAR OZONE MODELING

The ozone model developed under this protocol will be used for evaluating the effectiveness of future emissions control scenarios for the SFBA. The methods used for this activity will be consistent with current 1-hour (EPA, 1991; 1996) and evolving 8-hour guidance (EPA, 1999). The selection and development of control strategies will be carried out under the direction of the District and the MAC.

The CAMx future-year baseline simulations will be helpful in assessing the extent to which further emissions reductions are needed in the region to provide for attainment of the 1-hour ozone NAAQS in the SFBA. The strictest test for attainment is the “deterministic” approach, in which all grid cells within the regulated area show 1-hour ozone concentrations below 124 ppb for a given package of control measures. However, numerical models are an imperfect representation of reality, with over and under prediction biases and limited precision. Furthermore, the chosen episode(s) may be characterized by ozone levels that are higher or lower than the current design value. Recognizing this, the EPA promotes the use of “weight of evidence” analyses to support the conclusion that a set of selected control measures do provide, by all available evidence, attainment of the ozone NAAQS.

In particular, EPA has developed a methodology called “design value scaling” for using model estimates in conjunction with recent air quality data to estimate whether the ozone standard will be attained by a specific future year. Briefly, the current ozone design value is scaled by the model predicted change in ozone levels between the base and future years. If this scaled design value continues to exceed the standard, then additional emission reductions are needed. The control strategy developed by this design value scaling can form the basis for an ozone attainment demonstration. Other types of analyses (e.g., emissions and air quality trends, emission shortfall calculations) can also be included in a weight of evidence argument to support a particular control strategy, as described in the previous section. Since this modeling protocol deals with photochemical ozone modeling, this section focuses on the modeling aspects of an attainment demonstration rather than weight of evidence arguments.

FUTURE YEAR BASE CASE OZONE

A future year of 2006 will be used in this study as that is the new attainment date for the SFBA, according to the 2001 EPA partial disapproval of the previous SIP submission. A future year base case will be prepared by adjusting specific model inputs to reflect expected changes between the base (2000) and future (2006) years. The only model inputs that may be changed for the future year are the emissions, initial conditions and boundary conditions.

The future year baseline emissions inventory will be developed by applying source-category specific growth and control factors applied to the 2000 base year inventory. This process is described in Section 5 of this protocol. The initial conditions will be set to relatively clean conditions and allowed to be removed over the course of a three-day model spin up period prior to the days of interest of each episode. Therefore, initial conditions for the future year will remain unchanged from base year values. It is anticipated that the base year boundary conditions will be set to relatively clean values for remote regions over the Pacific Ocean, near the California-Oregon border, and over Nevada, and that these inputs will have little impact on model results for the SFBA. Therefore, it is expected that these boundary conditions will also be unchanged between the base year and future year values.

However, boundary conditions for the southern boundary, which crosses along the mountains separating the San Joaquin Valley and the South Coast Air Basin, will characterize the urban air flux from southern California. The southern boundary conditions will therefore require future year projection adjustments above the background concentrations assumed for the other boundaries. These adjustment will be estimated from information obtained from the CARB and the South Coast Air Quality Management District.

The results from the future year base case will be analyzed to determine the level and types of additional controls (if necessary) to ensure that the SFBA reaches attainment of the 1-hour ozone NAAQS. Numerous analyses will be considered for this purpose, subject to time and budget constraints, to include:

- NOx/VOC Matrix runs: The future year base case will be rerun with incremental NOx and VOC emission reductions applied uniformly "across-the-board" (by category and over space and time). The emission reductions will range from 0% to 50% in increments of 10%. The resulting peak 1-hour ozone values at 2 to 3 sites will be plotted as in an "Ekma" diagram to help determine the most efficient route (NOx or VOC) to attainment. The sites for plotting will be selected by the District, but should include those historically exceeding the standard (such as Livermore, Gilroy, and Los Gatos).

- Probing Tools: The CAMx OSAT or DDM extensions will be utilized to provide source attribution analyses for the future year base case. These tools provide estimates on the fraction of ozone produced from emissions stratified by source category and geographic area (e.g., on-road mobile in the north bay counties) and indicate whether that ozone is produced from NOx- or VOC-limited chemistry. The OSAT "Ozone Tool" is an Excel-based postprocessor that allows for a complete analysis of the relative contributions from all sources/areas at user-selected sites within the domain (see ENVIRON, 2002).

- Emission Sensitivity Tests: As described in the previous section, numerous sensitivity tests may be carried out with specific emission sectors reduced. These tests would use the results from the matrix and/or probing tool applications listed above to test the effects of targeted emission controls. Results will help to shape the selection of SIP control measures.

FUTURE YEAR CONTROL/ATTAINMENT OZONE

This District will be responsible to develop the specific emission control measures needed to demonstrate attainment for the 2004 SIP revision. The selection of which sectors to focus on, and what level reduction to reasonably apply, will be guided in part by the modeling analyses described above. Several modeling iterations will likely be necessary with various control packages and contingencies. The goal of the future year control runs will be to show that simulated ozone is reduced to below 124 ppb over the entire SFBA. Additionally, design value scaling will be employed to demonstrate the relative reduction of the current ozone design value to below 124 ppb.

DELIVERABLES

The deliverables for this task are as follows:

- A report on the development and evaluations of the future year base case, sensitivity, and control strategy air quality simulations of the two CCOS episodes. The report will be posted to the Contractor-maintained web site.

- The future year base and control/attainment air quality modeling databases.

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Appendix A

EMS-95 Emissions Dataset Formats

Section A-1. Point Source Data File Formats

EMS-95 will be used in the Bay Area SIP revision air quality modeling study. Therefore, the following data file formats are specific to the EMS-95 emissions modeling system. The ASCII data files that are required by EMS-95 are record based. Each record is constructed of one or more variables in a predefined format. Each variable has a name, type, and description. Examples of each file that is required by EMS-95 are provided in Appendix D. The following definitions apply to all emissions data file formats that are presented in the protocol (note that units are supplied where necessary in each of the data file formats):

```
>      VARIABLE    -- the name of the EMS-95 variable
>      TYPE        -- the variable declaration
                      I = integer up to FORMAT in length
                      A = character up to FORMAT in length
                      R = real number up to FORMAT in length (real numbers of
                          type w.d are identified but can take any form up to
                          FORMAT in length [w = total width; d = number of
                          positions left of the decimal])
>      FORMAT      -- number of positions the variable has in each record of the data
                      file
>      DESCRIPTION -- brief description of the meaning of each VARIABLE
>      REQUIRED    -- is this a required field?
                      Y = yes, the data is required for proper operation
                      N = no, the data is not required
                      D = it is desirable to have the data, but it is not required
                          for proper operation
```

Of note, all numeric variables must be right justified in their fields, and all character variables must be left justified in their fields.

Also note, that in all cases where stid is required, a value of “6” must be supplied since “6” is the FIPS state identifier for California. The FIPS county identifiers, cyid, for California are as follows:

FIPS Id	Name	FIPS Id	Name	FIPS Id	Name	FIPS Id	Name	FIPS Id	Name	FIPS Id	Name
1	Alameda	21	Glenn	41	Marin	61	Placer	81	San Mateo	101	Sutter
3	Alpine	23	Humboldt	43	Mariposa	63	Plumas	83	Santa Barbara	103	Tehama
5	Amador	25	Imperial	45	Mendocino	65	Riverside	85	Santa Clara	105	Trinity
7	Butte	27	Inyo	47	Merced	67	Sacramento	87	Santa Cruz	107	Tulare
9	Calaveras	29	Kern	49	Modoc	69	San Benito	89	Shasta	109	Tuolumne
11	Colusa	31	Kings	51	Mono	71	San Bernardino	91	Sierra	111	Ventura
13	Contra Costa	33	Lake	53	Monterey	73	San Diego	93	Siskiyou	113	Yolo
15	Del Norte	35	Lassen	55	Napa	75	San Francisco	95	Solano	115	Yuba
17	El Dorado	37	Los Angeles	57	Nevada	77	San Joaquin	97	Sonoma		
19	Fresno	39	Madera	59	Orange	79	San Luis Obispo	99	Stanislaus		

EMS-95 requires five foundation data files for the stationary source emissions data: facility.pt; stack.pt; device.pt; process.pt; and emission.pt.

facility.pt

```
variable type format description                                           required
-------- ---- ------ ----------------------------------------------------- --------
stid       I  2.     FIPS state                                            Y
cyid       I  3.     FIPS county code                                      Y
fcid       A  15.    facility ID                                           Y
```

sic	A	4.	standard industrial classification	D
utmx	R	9.	UTM easting (meters)	Y
utmy	R	9.	UTM northing (meters)	Y
utmz	I	2.	UTM zone	Y
name	A	40.	facility name	D

If the UTM coordinates are not supplied, the facility will be placed in the center of the county for purposes of modeling. If the UTM coordinates are supplied and a spatial check reveals that the source is outside of the county, the facility is again placed in the center of the county for purposes of modeling. In either case, EMS-95 flags the facility as incorrectly located.

stack.pt

variable	type	format	description	required
stid	I	2.	FIPS state code	Y
cyid	I	3.	FIPS county code	Y
fcid	A	15.	facility ID	Y
stkid	A	12.	stack ID	Y
diam	R	8.	inside stack diameter (feet)	Y
heit	R	7.	stack height above ground surface (feet)	Y
temp	R	7.	stack exit temperature (°F)	Y
veloc	R	7.	stack exit velocity (feet/second)	D
flow	R	10.	stack exit flow rate (actual cubic feet/minute)	Y
utmx	R	9.	UTM easting (meters)	D
utmy	R	9.	UTM northing (meters)	D
elev	R	9.	elevation of stack base from mean sea level (feet)	N

If the UTM coordinates are not supplied, the stack will be placed at the coordinates specified for the facility in the facility.pt data file for purposes of modeling. If the UTM coordinates are supplied and a spatial check reveals that the stack is outside of the county, the stack is placed at the coordinates specified for the facility in the facility.pt data file for purposes of modeling. In either case, EMS-95 flags the stack as incorrectly located.

Stack parameters are very critical to the placement of emissions in the vertical air quality modeling domain. It may surprise some that incorrect parameters are sometimes the single largest source of error in the emissions and subsequent air quality modeling, and in some instances, call into question the results of an entire air quality modeling study. EMS-95 will generate a report of suspect stack parameters that will be returned to the ARB for resolution.

device.pt

variable	type	format	description	required
stid	I	2.	FIPS state code	Y
cyid	I	3.	FIPS county code	Y
fcid	A	15.	facility ID	Y
stkid	A	12.	stack ID	Y
dvid	A	12.	device ID	Y
sic	A	4.	standard industrial classification	D
dec	R	5.	fractional December throughput	D
jan	R	5.	fractional January throughput	D
feb	R	5.	fractional February throughput	D
mar	R	5.	fractional March throughput	D
apr	R	5.	fractional April throughput	D
may	R	5.	fractional May throughput	D
jun	R	5.	fractional June throughput	D

jul	R	5.	fractional July throughput	D
aug	R	5.	fractional August throughput	D
sep	R	5.	fractional September throughput	D
oct	R	5.	fractional October throughput	D
nov	R	5.	fractional November throughput	D
win	R	3.	winter throughput (Dec - Feb) (%)	D
spr	R	3.	spring throughput (Mar - May) (%)	D
sum	R	3.	summer throughput (Jun - Aug) (%)	D
fal	R	3.	fall throughput (Sep - Nov) (%)	D
hours	I	2.	code value for hourly operation	Y
days	I	2.	code value for daily operation	Y
weeks	I	2.	weeks of operation per year (weeks/year)	D
dayyear	I	3.	days of operation per year (days/year)	D
houryear	I	4.	hours of operation per year (hours/year)	D

The data in device.pt are used to temporalize the emissions estimates (i.e. allocate average ozone season day emissions estimates into hour-by-hour bins for use in air quality modeling). The hierarchy for how EMS-95 computes the temporalization factors is beyond the scope of this document, though, the reader is referred to Wilkinson et al. (1994) for a full description of how the temporalization factors are estimated. However, if no temporalization data are supplied, EMS-95 will treat the source as if it emits twenty-four hours per day, 365 days per year. Of final note, the *hours* and *days* fields are code values that are used to lookup the actual hours of operation during the day and actual days of operation per week. That is, a value of 8 for *hours* refers to coded value eight in the appropriate lookup table. The value in the lookup table indicates that the source operates from 7:00 AM to 3:00 PM local time and does not operate at any other time during the day.

process.pt

variable	type	format	description	required
stid	I	2.	FIPS state code	Y
cyid	I	3.	FIPS county code	Y
fcid	A	15.	facility ID	Y
stkid	A	12.	stack ID	Y
dvid	A	12.	device ID	Y
prid	A	12.	process ID	Y
scc	A	8.	source classification code	Y
prrt	R	13.	annual process rate (SCC units/year)	N
prun	A	15.	optional process rate units if different from SCC	N

EMS-95 uses the SCC to select an appropriate VOC speciation profile. If no SCC is supplied, EMS-95 selects the default VOC speciation profile that in all likelihood does not represent the actual VOC emissions profile from the source.

emission.pt

variable	type	format	description	required
stid	I	2.	FIPS state code	Y
cyid	I	3.	FIPS county code	Y
fcid	A	15.	facility ID	Y
stkid	A	12.	stack ID	Y
dvid	A	12.	device ID	Y
prid	A	12.	process ID	Y
polid	A	5.	pollutant ID	Y
acef	R	13.	actual emission factor (tons/SCC units)	N

alef	R	13.	allowable emission factor (tons/SCC units)	N
acee	R	13.	actual emissions (tons/temporal basis)	Y
alee	R	13.	allowable emissions (tons)	N
estt	A	2.	temporal basis (AA, AD)	Y
pcec	A	5.	primary control equipment	N
scec	A	5.	secondary control equipment	N
ceef	R	7.4	control equipment efficiency (%)	N

The *polid* field will contain one of the following: CO, NOX, VOC, TOG, or ROG. The definitions of VOC, TOG, and ROG are provided in Appendix G. The *estt* field will contain AD for average weekday emissions, which describes average ozone season weekday emissions.

Section A-2. Area Source Data File Formats

EMS-95 requires two foundation data files for the area source emissions data: area.ar; and areatprl.ar.

areatprl.ar

variable	type	format	description	required
stid	I	2.	FIPS state code	Y
cyid	I	3.	FIPS county code	Y
asct	A	15.	area source category	Y
prrt	R	13.	annual process rate (process units/year)	N
acun	A	15.	activity units	N
dec	R	5.	fractional December throughput	D
jan	R	5.	fractional January throughput	D
feb	R	5.	fractional February throughput	D
mar	R	5.	fractional March throughput	D
apr	R	5.	fractional April throughput	D
may	R	5.	fractional May throughput	D
jun	R	5.	fractional June throughput	D
jul	R	5.	fractional July throughput	D
aug	R	5.	fractional August throughput	D
sep	R	5.	fractional September throughput	D
oct	R	5.	fractional October throughput	D
nov	R	5.	fractional November throughput	D
win	R	3.	winter throughput (Dec – Feb) (%)	D
spr	R	3.	spring throughput (Mar – May) (%)	D
sum	R	3.	summer throughput (Jun – Aug) (%)	D
fal	R	3.	fall throughput (Sep – Nov) (%)	D
hours	I	2.	code value for hourly operation	Y
days	I	2.	code value for daily operation	Y
weeks	I	2.	weeks of operation per year (weeks/year)	D
dayyear	I	3.	days of operation per year (days/year)	D
houryear	I	4.	hours of operation per year (hours/year)	D

The data in areatprl.ar are used to temporalize the area source emissions estimates (i.e. allocate average ozone season day emissions estimates into hour-by-hour bins for use in air quality modeling). The hierarchy for how EMS-95 computes the temporalization factors is beyond the scope of this document, though, the reader is referred to Wilkinson et al. (1994) for a full description of how the temporalization factors are estimated. However, if no temporalization data are supplied, EMS-95 will treat the area source as if it emits twenty-four hours per day, 365 days per year. Of final note, the *hours* and *days* fields are code values that are used to lookup the actual hours of operation during the day and actual days of operation per week. That is, a value of 8 for *hours* refers to coded value eight in the appropriate lookup table. The value in the lookup table indicates that the source operates from 7:00 AM to 3:00 PM local time and does not operate at any other time during the day.

area.ar

variable	type	format	description	required
stid	I	2.	FIPS state code	Y
cyid	I	3.	FIPS county code	Y
asct	A	15.	area source category	Y
polid	A	5.	pollutant ID	Y
acef	R	13.	actual emission factor (tons/process unit)	N
alef	R	13.	allowable emission factor (tons/proc.unit)	N

acee	R	13.	actual emissions (tons/temporal basis)	Y
alee	R	13.	allowable emissions (tons)	N
pcec	A	5.	primary control equipment	N
scec	A	5.	secondary control equipment	N
ceef	R	7.4	control equipment efficiency (%)	N
estt	A	2.	temporal basis (AA or AD)	Y

The *polid* field will contain one of the following values: CO, NOX, VOC, TOG, or ROG. The definitions of VOC, TOG, and ROG are provided in Appendix G. The *estt* field will contain AD for average weekday emissions, which describes average ozone season weekday emissions.

Section A-3. Day-specific Biogenic Emissions Estimates

Biogenic emissions estimates will be supplied for each day in each episode.

biodayspec.bi

variable	type	format	description	required
stid	I	2.	FIPS state code	D
cyid	I	3.	FIPS county code	D
asct	A	15.	area source category (always BI)	Y
icell	I	4.	east-west grid cell number in the domain	Y
jcell	I	4.	north-south grid cell number in the domain	Y
polid	A	5.	pollutant ID	Y
adjest01	R	13.	emissions of *polid* in hour 0000-0100 (ug/hr)	Y
adjest02	R	13.	emissions of *polid* in hour 0100-0200 (ug/hr)	Y
adjest03	R	13.	emissions of *polid* in hour 0200-0300 (ug/hr)	Y
adjest04	R	13.	emissions of *polid* in hour 0300-0400 (ug/hr)	Y
adjest05	R	13.	emissions of *polid* in hour 0400-0500 (ug/hr)	Y
adjest06	R	13.	emissions of *polid* in hour 0500-0600 (ug/hr)	Y
adjest07	R	13.	emissions of *polid* in hour 0600-0700 (ug/hr)	Y
adjest08	R	13.	emissions of *polid* in hour 0700-0800 (ug/hr)	Y
adjest09	R	13.	emissions of *polid* in hour 0800-0900 (ug/hr)	Y
adjest10	R	13.	emissions of *polid* in hour 0900-1000 (ug/hr)	Y
adjest11	R	13.	emissions of *polid* in hour 1000-1100 (ug/hr)	Y
adjest12	R	13.	emissions of *polid* in hour 1100-1200 (ug/hr)	Y
adjest13	R	13.	emissions of *polid* in hour 1200-1300 (ug/hr)	Y
adjest14	R	13.	emissions of *polid* in hour 1300-1400 (ug/hr)	Y
adjest15	R	13.	emissions of *polid* in hour 1400-1500 (ug/hr)	Y
adjest16	R	13.	emissions of *polid* in hour 1500-1600 (ug/hr)	Y
adjest17	R	13.	emissions of *polid* in hour 1600-1700 (ug/hr)	Y
adjest18	R	13.	emissions of *polid* in hour 1700-1800 (ug/hr)	Y
adjest19	R	13.	emissions of *polid* in hour 1800-1900 (ug/hr)	Y
adjest20	R	13.	emissions of *polid* in hour 1900-2000 (ug/hr)	Y
adjest21	R	13.	emissions of *polid* in hour 2000-2100 (ug/hr)	Y
adjest22	R	13.	emissions of *polid* in hour 2100-2200 (ug/hr)	Y
adjest23	R	13.	emissions of *polid* in hour 2200-2300 (ug/hr)	Y
adjest24	R	13.	emissions of *polid* in hour 2300-2400 (ug/hr)	Y

The *polid* field will contain one of the following values: ISOP, TERP, OVOC, or NO.

Section A-4. Day-specific On-road Mobile Source Emissions Estimates

On-road mobile source emissions estimates will be supplied for each day of each episode.

mobdayspec.mo

```
variable type format description                                           required
-------- ---- ------ ----------------------------------------------------- --------
stid       I  2.     FIPS state code                                       D
cyid       I  3.     FIPS county code                                      D
areatype   I  1.     area type designation for roadway                     D
                     0 – rural roadway
                     1 – urban roadway
factype    I  1.     facility type designation for roadway                 D
                     1 – principal arterial, interstate
                     2 – principal arterial, freeways and expressways
                     4 – principal arterial, other
                     5 – collector
                     6 – minor arterial
                     7 – major collector
                     8 – minor collector
                     9 – local roadway
vtype      A  5.     vehicle type                                          Y
                     LDA  - passenger cars
                     LDT1 – type one light duty trucks
                     LDT2 – type two light duty trucks
                     MDV  - medium-duty trucks
                     LHD1 – type one light heavy-duty trucks
                     LHD2 – type two light heavy-duty trucks
                     MHD  - medium heavy-duty trucks
                     HHD  - heavy heavy-duty trucks
                     LHV  - line haul vehicles
                     UBUS – urban buses
                     MCY  - motorcycles
                     SBUS – school buses
                     MH   - motor homes
mvprocess  A  3.     motor vehicle process                                 Y
                     EX – exhaust emissions
                     EV – evaporative emissions
techtype   I  1.     technology type                                       Y
                     1 – non-catalyst gasoline
                     2 – catalyst gasoline
                     3 - diesel
icell      I  4.     east-west grid cell number in the domain              Y
jcell      I  4.     north-south grid cell number in the domain            Y
polid      A  5.     pollutant ID                                          Y
ee01       R  13.    emissions of polid in hour 0000-0100 (g/hr)           Y
ee02       R  13.    emissions of polid in hour 0100-0200 (g/hr)           Y
ee03       R  13.    emissions of polid in hour 0200-0300 (g/hr)           Y
ee04       R  13.    emissions of polid in hour 0300-0400 (g/hr)           Y
ee05       R  13.    emissions of polid in hour 0400-0500 (g/hr)           Y
ee06       R  13.    emissions of polid in hour 0500-0600 (g/hr)           Y
ee07       R  13.    emissions of polid in hour 0600-0700 (g/hr)           Y
ee08       R  13.    emissions of polid in hour 0700-0800 (g/hr)           Y
ee09       R  13.    emissions of polid in hour 0800-0900 (g/hr)           Y
ee10       R  13.    emissions of polid in hour 0900-1000 (g/hr)           Y
ee11       R  13.    emissions of polid in hour 1000-1100 (g/hr)           Y
ee12       R  13.    emissions of polid in hour 1100-1200 (g/hr)           Y
ee13       R  13.    emissions of polid in hour 1200-1300 (g/hr)           Y
ee14       R  13.    emissions of polid in hour 1300-1400 (g/hr)           Y
ee15       R  13.    emissions of polid in hour 1400-1500 (g/hr)           Y
ee16       R  13.    emissions of polid in hour 1500-1600 (g/hr)           Y
ee17       R  13.    emissions of polid in hour 1600-1700 (g/hr)           Y
ee18       R  13.    emissions of polid in hour 1700-1800 (g/hr)           Y
ee19       R  13.    emissions of polid in hour 1800-1900 (g/hr)           Y
ee20       R  13.    emissions of polid in hour 1900-2000 (g/hr)           Y
```

ee21	R	13.	emissions of *polid* in hour 2000-2100 (g/hr)	Y
ee22	R	13.	emissions of *polid* in hour 2100-2200 (g/hr)	Y
ee23	R	13.	emissions of *polid* in hour 2200-2300 (g/hr)	Y
ee24	R	13.	emissions of *polid* in hour 2300-2400 (g/hr)	Y

The *polid* field will contain one of the following values: CO, NOX, or TOG. The definition of TOG is provided in Appendix G.

Section A-5. Day-specific Point Source Emissions Estimates

pdayspec.pt

variable	type	format	description	required
stid	I	2.	FIPS state code	Y
cyid	I	3.	FIPS county code	Y
fcid	A	15.	facility ID	Y
stkid	A	12.	stack ID	Y
dvid	A	12.	device ID	Y
prid	A	12.	process ID	Y
polid	A	5.	pollutant ID	Y
dydy	A	8.	day of the emissions estimates (MM/DD/YY)	Y
tmzn	A	3.	time zone of the data PST – Pacific Standard Time	Y
dy01	R	13.	emissions of *polid* in hour 0000-0100 (tons/hr)	Y
dy02	R	13.	emissions of *polid* in hour 0100-0200 (tons/hr)	Y
dy03	R	13.	emissions of *polid* in hour 0200-0300 (tons/hr)	Y
dy04	R	13.	emissions of *polid* in hour 0300-0400 (tons/hr)	Y
dy05	R	13.	emissions of *polid* in hour 0400-0500 (tons/hr)	Y
dy06	R	13.	emissions of *polid* in hour 0500-0600 (tons/hr)	Y
dy07	R	13.	emissions of *polid* in hour 0600-0700 (tons/hr)	Y
dy08	R	13.	emissions of *polid* in hour 0700-0800 (tons/hr)	Y
dy09	R	13.	emissions of *polid* in hour 0800-0900 (tons/hr)	Y
dy10	R	13.	emissions of *polid* in hour 0900-1000 (tons/hr)	Y
dy11	R	13.	emissions of *polid* in hour 1000-1100 (tons/hr)	Y
dy12	R	13.	emissions of *polid* in hour 1100-1200 (tons/hr)	Y
dy13	R	13.	emissions of *polid* in hour 1200-1300 (tons/hr)	Y
dy14	R	13.	emissions of *polid* in hour 1300-1400 (tons/hr)	Y
dy15	R	13.	emissions of *polid* in hour 1400-1500 (tons/hr)	Y
dy16	R	13.	emissions of *polid* in hour 1500-1600 (tons/hr)	Y
dy17	R	13.	emissions of *polid* in hour 1600-1700 (tons/hr)	Y
dy18	R	13.	emissions of *polid* in hour 1700-1800 (tons/hr)	Y
dy19	R	13.	emissions of *polid* in hour 1800-1900 (tons/hr)	Y
dy20	R	13.	emissions of *polid* in hour 1900-2000 (tons/hr)	Y
dy21	R	13.	emissions of *polid* in hour 2000-2100 (tons/hr)	Y
dy22	R	13.	emissions of *polid* in hour 2100-2200 (tons/hr)	Y
dy23	R	13.	emissions of *polid* in hour 2200-2300 (tons/hr)	Y
dy24	R	13.	emissions of *polid* in hour 2300-2400 (tons/hr)	Y

Note that the identifiers ***stid, cyid, fcid, stkid, dvid, prid,*** and ***polid*** must match the same key identifiers on a record-by-record basis in the file ***emission.pt*** for the day-specific emissions estimates to replace average ozone season day emissions estimates. If no match is found, EMS-95 appends the day-specific records to the emissions estimates and issues a warning to this effect.

The *polid* field will contain one of the following values: CO, NOX, VOC, TOG, or ROG. The definitions of VOC, TOG, and ROG are provided in Appendix G.

Section A-6. Day-specific Area Source Emissions Estimates

adayspec.ar

variable	type	format	description	required
stid	I	2.	FIPS state code	Y
cyid	I	3.	FIPS county code	Y
asct	A	15.	area source category	Y
polid	A	5.	pollutant ID	Y
dydy	A	8.	day of the emissions estimates (MM/DD/YY)	Y
tmzn	A	3.	time zone of the data PST – Pacific Standard Time	Y
dy01	R	13.	emissions of *polid* in hour 0000-0100 (tons/hr)	Y
dy02	R	13.	emissions of *polid* in hour 0100-0200 (tons/hr)	Y
dy03	R	13.	emissions of *polid* in hour 0200-0300 (tons/hr)	Y
dy04	R	13.	emissions of *polid* in hour 0300-0400 (tons/hr)	Y
dy05	R	13.	emissions of *polid* in hour 0400-0500 (tons/hr)	Y
dy06	R	13.	emissions of *polid* in hour 0500-0600 (tons/hr)	Y
dy07	R	13.	emissions of *polid* in hour 0600-0700 (tons/hr)	Y
dy08	R	13.	emissions of *polid* in hour 0700-0800 (tons/hr)	Y
dy09	R	13.	emissions of *polid* in hour 0800-0900 (tons/hr)	Y
dy10	R	13.	emissions of *polid* in hour 0900-1000 (tons/hr)	Y
dy11	R	13.	emissions of *polid* in hour 1000-1100 (tons/hr)	Y
dy12	R	13.	emissions of *polid* in hour 1100-1200 (tons/hr)	Y
dy13	R	13.	emissions of *polid* in hour 1200-1300 (tons/hr)	Y
dy14	R	13.	emissions of *polid* in hour 1300-1400 (tons/hr)	Y
dy15	R	13.	emissions of *polid* in hour 1400-1500 (tons/hr)	Y
dy16	R	13.	emissions of *polid* in hour 1500-1600 (tons/hr)	Y
dy17	R	13.	emissions of *polid* in hour 1600-1700 (tons/hr)	Y
dy18	R	13.	emissions of *polid* in hour 1700-1800 (tons/hr)	Y
dy19	R	13.	emissions of *polid* in hour 1800-1900 (tons/hr)	Y
dy20	R	13.	emissions of *polid* in hour 1900-2000 (tons/hr)	Y
dy21	R	13.	emissions of *polid* in hour 2000-2100 (tons/hr)	Y
dy22	R	13.	emissions of *polid* in hour 2100-2200 (tons/hr)	Y
dy23	R	13.	emissions of *polid* in hour 2200-2300 (tons/hr)	Y
dy24	R	13.	emissions of *polid* in hour 2300-2400 (tons/hr)	Y

Note that the identifiers ***stid, cyid, asct,*** and ***polid*** must match the same key identifiers on a record-by-record basis in the file ***area.ar*** for the day-specific emissions estimates to replace average ozone season day emissions estimates. If no match is found, EMS-95 appends the day-specific records to the emissions estimates and issues a warning to this effect.

The *polid* field will contain one of the following values: CO, NOX, VOC, TOG, or ROG. The definitions of VOC, TOG, and ROG are provided in Appendix G.

Section A-7. Definitions of the Various Forms of Organic Gas And Organic Compounds

Nonmethane Hydrocarbons (NMHC)
Nonmethane Organic Gas (NMOG)
Reactive Organic Gas (ROG)
Total Hydrocarbons (THC)
Total Organic Compounds (TOC)
Total Organic Gas (TOG)
Volatile Organic Compounds (VOC)

TOC: By definition, TOC is any carbon containing compound; however, great care must be taken when using this definition because databases like SPECIATE 3.0 define the profiles as TOC but in fact do not contain such compounds as carbon monoxide and carbonic acid yet do contain carbon sulfide.

TOG: TOG is any organic compounds (i.e. carbon containing compounds except carbon monoxide, carbon dioxide, carbonic acid, metallic carbides [e.g. carbon sulfide], and carbonates [e.g. calcium carbonate, ammonium carbonate]).

THC: THC is computed as TOG minus aldehydes where aldehydes are primarily composed of formaldehyde and acetaldehyde.

NMHC: NMHC is defined as THC minus methane.

NMOG: NMOG is defined as TOG minus methane.

VOC: VOC is defined in 40 CFR § 51.10 and in 63 FR 17331, April 19, 1998, as any compound of carbon, excluding carbon monoxide, carbon dioxide, carbonic acid, metallic carbides, and carbonates that participates in atmospheric photochemical reactions. This includes any such organic compound other than the following, which have been determined to have negligible photochemical reactivity:

- methane
- ethane
- methylene chloride (dichloromethane)
- 1,1,1-trichloroethane (methyl chloroform)
- 1,1,2-trichloro-1,2,2-trifluoroethane (CFC-113)
- trichlorofluoromethane (CFC-11)
- dichlorodifluoromethane (CFC-12)
- chlorodifluoromethane (HCFC-22)
- trifluoromethane (HFC-23)
- 1,2-dichloro-1,1,2,2-tetrafluoroethane (CFC-114)
- chloropentafluoroethane (CFC-115)
- 1,1,1-trifluoro-2,2-dichloroethane (HCFC-123)
- 1,1,1,2-tetrafluoroethane (HFC-134a)
- 1,1-dichloro-1-fluoroethane (HCFC-141b)
- 1-chloro-1,1-difluoroethane (HCFC-142b)
- 2-chloro-1,1,1,2-tetrafluoroethane (HCFC-124)

- pentafluoroethane (HFC-125)
- 1,1,2,2-tetrafluoroethane (HFC-134)
- 1,1,1-trifluoroethane (HFC-143a)
- 1,1-difluoroethane (HFC-152a)
- parachlorobenzotrifluoride (PCBTF)
- cyclic, branched, or linear completely methylated siloxanes
- acetone
- perchloroethylene (tetrachloroethylene)
- 3,3-dichloro-1,1,1,2,2-pentafluoropropane (HCFC-225ca)
- 1,3-dichloro-1,1,2,2,3-pentafluoropropane (HCFC-225cb)
- 1,1,1,2,3,4,4,5,5,5-decafluoropentane (HFC 43-10mee)
- difluoromethane (HFC-32)
- ethylfluoride (HFC-161)
- 1,1,1,3,3,3-hexafluoropropane (HFC-236fa)
- 1,1,2,2,3-pentafluoropropane (HFC-245ca)
- 1,1,2,3,3-pentafluoropropane (HFC-245ea)
- 1,1,1,2,3-pentafluoropropane (HFC-245eb)
- 1,1,1,3,3-pentafluoropropane (HFC-245fa)
- 1,1,1,2,3,3-hexafluoropropane (HFC-236ea)
- 1,1,1,3,3-pentafluorobutane (HFC-365mfc)
- chlorofluoromethane (HCF-31)
- 1-chloro-1-fluoroethane (HCFC-151a)
- 1,2-dichloro-1,1,2-trifluoroethane (HCFC-123a)
- 1,1,1,2,2,3,3,4,4-nonafluoro-4-methoxy-butane (C F OCH) 4 9 3
- 2-(difluoromethoxymethyl)-1,1,1,2,3,3,3-heptafluoropropane ((CF) CFCF OCH) 3 2 2 3
- 1-ethoxy-1,1,2,2,3,3,4,4, 4-nonafluorobutane (C F OC H) 4 9 25
- 2-(ethoxydifluoromethyl)-1,1,1,2,3,3,3-heptafluoropropane ((CF) CFCF OC H) 3 2 2 2 5
- methyl acetate and perfluorocarbon compounds which fall into these classes:
  - cylic, branched, or linear, completely fluorinated alkanes
  - cylic, branched, or linear, completely fluorinated ethers with no unsaturations
  - cylic, branched, or linear, completely fluorinated tertiary amines with no
  - unsaturations and
  - sulfur containing perfluorocarbons with no unsaturations and with sulfur bonds only to carbon and fluorine.

In summary, VOC is TOG minus the exempted compounds.

ROG: ROG is VOC plus aldehydes where aldehydes are primarily composed of formaldehyde and acetaldehyde.

Section A-8. Area Source Spatial Surrogates

surrogates.ar

variable	type	format	description	required
stid	I	2.	FIPS state code	Y
cyid	I	3.	FIPS county code	Y
ssc	A	3.	area source spatial surrogate code	Y
icell	I	4.	east-west grid cell number in the domain	Y
jcell	I	4.	north-south grid cell number in the domain	Y
ratio	R	13.	fractional value of *ssc* in *stid, cyid, icell*, and *jcell*	Y

Section A-9. Area Source Category-to-Area Source Spatial Surrogates Cross Reference

asct2surrogates.ar

```
variable type format description                                             required
-------- ---- ------ ------------------------------------------------------ --------
ssc        A  3.     area source spatial surrogate code                      Y
asct       A  15.    area source category                                    Y
```

Section A-10. VOC-to-TOG Conversion Factors By Source Category

voc2tog.sp

variable	type	format	description	required
asct or scc	A	15.	area source category or source classification code	Y
factor	R	13.	factor applied to convert VOC emissions to TOG emissions	Y

Section A-11. Chemical Mechanism-specific Hydrocarbon Speciation Profiles

profile.sp

variable	type	format	description	required
inprf	A	5.	hydrocarbon speciation profile	Y
mech	A	10.	chemical mechanism identifier CBIV – cabon bond version four SAPRC – SAPRC version 1999	Y
mdlspab	A	5.	chemical mechanism model species abbreviation	Y
factor	R	13.	factor to convert emissions of TOG to emissions of *mdlspab*	Y

Note, emissions of NO_X, in grams, are converted to NO and NO_2, in moles, by multiplying NO_X emissions by 0.01957 and 0.00217 respectively. Emissions of CO, in grams, are converted to CO, in moles, by multiplying CO emissions by 0.03571.

Section A-12. Source Category-to-Hydrocarbon Speciation Profile Cross Reference

scc2profile.sp

variable	type	format	description	required
asct or scc	A	15.	area source category or source classification code	Y
inprf	A	5.	hydrocarbon speciation profile	Y