Data Analysis and Modeling Support Studies for the Central California Ozone Study (CCOS) – Plan Update

Prepared for:

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This plan was prepared with extensive input from the CCOS Technical Committee and the Emission Inventory Coordination Group

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1. INTRODUCTION

The Central California Ozone Study (CCOS) is a multi-year program of meteorological and air quality monitoring, emission inventory development, data analysis, and air quality simulation modeling. The goals of CCOS are being met through a process that includes analysis of existing data; execution of a large-scale field study in summer 2000 to acquire a comprehensive database to support modeling and data analysis; analysis of the data collected during the field study; and the development, evaluation, and application of an air quality simulation model for northern and central California. The results of CCOS modeling will provide much of the technical basis for the State Implementation Plan (SIP) updates that are due in 2004 for ozone nonattainment areas of the San Francisco Bay Area, Sacramento Valley and the San Joaquin Valley. CCOS is also intended to provide progressive improvements in the understanding of the relationships among emissions, transport, and ozone standard exceedances in the study area during the decade since the 1990 San Joaquin Valley Air Quality Study (SJVAQS) Atmospheric Utility Signatures, Predictions and Experiments (AUSPEX) and SJVAQS/AUSPEX Regional Model Adaptation Program (SARMAP) modeling. The data analysis and modeling for CCOS is being conducted in three phases over a period of four years. This document provides an update of the data analysis and modeling support studies that were funded in the first two phases and describes additional studies that are recommended by the CCOS Technical Committee in the final phase of data analysis and modeling.

In the initial phase of data analysis, several modeling support studies were carried out concurrently with the summer 2000 field measurement program in order to acquire day-specific emissions and emissions-related activity data, to develop methodologies to spatially and temporally allocate county-wide area source emissions, and to evaluate the plume-in-grid algorithm. Data management and data validation projects and several descriptive and exploratory data analysis projects were also funded among the initial group of data analysis and modeling support studies. The initial analysis of the CCOS data focused on determining the meteorological representativeness of the ozone episodes that were captured during summer 2000 and their suitability for State Implementation Plan (SIP) modeling. The projects in this initial group are labeled Category I projects.

At the conclusion of the summer 2000 field measurement program, the CCOS Technical Committee outlined the data analysis needs for the study and prepared a data analysis plan in December 2000 (see Appendix A). Based upon this plan, a second group of data analysis and modeling support projects were funded. These projects address the regulatory requirements of the SIP process and are focused on the development and assessment of emissions and meteorological inputs for modeling, evaluations of candidate air quality models and chemical mechanisms, and assessments of model setup including initial and boundary conditions. The projects anticipated to be completed in time for their results to be incorporated into the SIP process were placed on the “fast track” for funding. These projects are labeled Category II projects.

Category III projects, which are the primary subject of this document, are intended to corroborate CCOS modeling results, evaluate potential improvements in modeling formulation and execution, integrate and synthesize CCOS results, and update the current conceptual understanding of ozone formation in central and northern California. The CCOS Technical Committee is recommending funding for Category III projects in two groups, Phase 1 and Phase 2. The main distinction between the two groups of projects is their schedule of performance. Integration and synthesis projects, which require results of other studies, are in Phase 2. Similarly, some model development projects involve the evaluation of results from current air quality models. There are fourteen Phase 1 projects with a total estimated budget of $1.04 M and nine projects in Phase 2 with an estimated budget of $1.01M. In addition, three long-term projects, which are labeled Category IV projects, are described in this update.

The update to the CCOS data analysis plan is summarized in Table 1, which lists the projects in Category I through Category IV. The current and original (i.e., December 2000 plan) project numbers and budget estimates are given in the table so that changes from the initial plan can be identified. Brief summaries of Categories I and II projects are given in Section 2. Sections 3 through 5 provide a prospectus for each project in Category III and IV. The project descriptions include a statement of the problem and technical objectives, suggested scope of work and potential methods and approaches, expected benefits, and estimated project costs.

1.1 Overview of Central California Ozone Study

The goals of CCOS are to: 1) obtain suitable aerometric and emission databases to update, evaluate, and improve model applications for representing urban and regional-scale ozone episodes in central and northern California to meet the regulatory requirements for the state and federal 1-hour and pending federal 8-hour ozone standards; 2) determine the contributions of transported and locally generated ozone and the relative benefits of volatile organic compound (VOC) and oxides of nitrogen (NOx) emission controls in upwind and downwind areas; and 3) assess the relative contributions of ozone generated from emissions in one air basin to federal and state exceedances in neighboring air basins. The modeling domain for CCOS covers all of central California and most of northern California, extending from the Pacific Ocean to east of the Sierra Nevada and from Redding to the Mojave Desert. The selection of this study area reflects the regional nature of ozone exceedances, increasing urbanization of traditionally rural areas, and a need to include all of the major flow features that affect air quality in the modeling domain.

The Central California Ozone Study (CCOS) involves many sponsors and participants. Three entities are involved in the overall management of the Study. The San Joaquin Valleywide Air Pollution Study Agency, a joint powers agency (JPA) formed by the nine counties in the Valley, directs the fund-raising and contracting aspects of the Study. A Policy Committee comprised of four voting blocks: State, local, and federal government, and the private sector, provides guidance on the Study objectives and funding levels. The Policy Committee approves all proposal requests, contracts and reports. A Technical Committee (TC) parallels the Policy Committee in membership and provides overall technical guidance on proposal requests, direction and progress of work, contract work statements, and reviews of all technical reports produced from the study.

The CCOS field measurement program was conducted during a four-month period from 06/01/00 to 10/02/00. During this study period, a network of upper-air and surface meteorological monitoring stations supplemented the existing routine meteorological and air quality monitoring network. Supplemental air quality measurements were phased in during June and early July and continued through 09/21/00, and were phased out over a period extending into October. Additional measurements were made during meteorological scenarios that were conducive to high ambient ozone concentrations. These periods of intensive measurements were known as intensive operating periods, or IOPs. IOP measurements were made on 07/23 - 07/24 (IOP #1), 07/30 - 08/02 (IOP #2), 08/14 (IOP #3), 09/14 (IOP #4), and 09/17 - 09/21 (IOP #5). In addition, additional boundary condition flights were made during 09/30 - 10/2. The CCOS field measurement program was conducted in conjunction with the California Regional PM10/PM2.5 Air Quality Study (CRPAQS), a major study of the origin, nature and extent of excessive levels of fine particles in central California.

Summary of Field Operations - CCOS Volume III (Fujita el al., 2001), documents the meteorological and air quality conditions during the summer 2000 ozone season and during individual IOPs, describes the daily forecasting and making-decision protocols for launching IOPs, and documents the parameters that were measured, locations, measurement methods, times, and levels of data capture. This document is available at the following web site: http://www.arb.ca.gov/airways/ccos/ccos.htm. The Field Study Plan - CCOS Volume I (Fujita et al., 1999 - version 1, 06/11/99; version 2, 09/07/99; and version 3, 11/24/99) and the Field Operations Plan - CCOS Volume II (Fujita et al., 2000 - version 1, 04/28/00; and version 2, 05/31/00) are also available at this web site.

1.2 CCOS Data Analysis and Modeling Objectives

The CCOS data analysis efforts are guided by the following series of questions. These questions are relevant to the development of specific analyses that are needed to support planning efforts to achieve relevant federal and state ozone standards.

1. How do the ozone episodes during CCOS and the year 2000 ozone season compare with previous years in terms of meteorology and pollutant levels in central California?
   a. To what extent does each CCOS ozone episode display characteristics desired for modeling and control strategy development for each central California air basin?
   b. How many of each basin's key episode types (in terms of severity, geographical distribution, and transport patterns) are represented among the CCOS episodes?
   c. Are the data collected during each CCOS episode adequate for modeling?

2. How can the spatial and temporal variations in aerometric variables and dynamics of atmospheric processes be characterized to aid in preparing model inputs and in evaluating the performance of the modeling systems that will be used in SIP planning?

3. What progress has been made in improving ozone-related air quality over the last decade?
   a. Is the progress toward lower ambient ozone levels statistically significant for peak ozone concentrations (1-hour and 8-hour) and numbers of hours over the 1-hour standard?

b. To what extent can annual variations in meteorological conditions affect year-to-year trends in the peak ozone concentrations and numbers of exceedances of the standard? Are meteorology-adjusted ozone trends significant? What are the margins of ozone standard exceedances within the CCOS domain in relation to the magnitude of the effect of variable meteorological conditions on ozone trends?

c. Are there meteorological cycles that occur over multiple years that can affect long-term ozone trends? If so, what is the nature of those conditions and what is the prognosis for the period from 2003-2005 and 2005-2010?

d. What differences exist between the urban and rural sites in the 1-hour and 8-hour averaged ozone trends?

e. Where data are adequate, what are the corresponding VOC and NOx trends?

4. Were the 1990 and 1999 emissions inventories (by source category) that were used in the 1994 SIP modeling over- or underestimated?

   a. To what extent were emissions reductions (by source category) realized? Did these reductions correspond with the reduction targets specified in the 1994 SIP?

   b. Are changes in the emissions inventory between 1990 and 1999 consistent with precursor concentration trends?

   c. Where air quality objectives are not met, is it possible to distinguish between falling short of meeting control targets and underestimating growth? If unanticipated growth occurred, can the sectors experiencing growth be identified?

5. Have there been changes since 1990 in which precursor is limiting with respect to ozone formation at various urban, rural, and peak monitors?

   a. Are changes consistent in this determination between the use of a photochemical modeling approach and other analytical approaches such as use of MAPPER?

6. To what extent are upwind emissions sources and the degree of control (or lack of control) imposed on them responsible for ozone changes observed?

7. Is there evidence to suggest that reductions of precursors made over the last decade are taking a path nearly parallel or sharply oblique to ozone isopleths when viewing these reductions using an ozone response surface?

   a. Given emissions projections, can one anticipate that it is possible to favorably alter (i.e., render more effective, in terms of ozone reduction per unit cost of emissions reduction) the trajectory of movement along an ozone response surface for regions (and thus local monitors) that are not now compliant with the standard?

   b. Can precursor reductions be tailored to maximize ozone reduction? Thus, NOx emissions reductions would be favored where they will provide maximum benefit, and VOC emissions reductions would be favored where these reductions will provide maximum benefit.

These questions are reconciled with the CCOS data analysis plan in Table 2. The table indicates which questions are addressed by each of the data analysis and modeling support projects and provides an overview of how resources are distributed among the each the above questions and project category.

Table 1
CCOS Data Analysis and Modeling Support Projects

Project Number Revised	Project Number original	Project Category	Projects	Investigator	Funding (x1000) Revised	Funding (x1000) Original	Status	Estimated Start Date	Estimated Completion Date or Duration
CATEGORY I. COMPLETED OR ON-GOING PROJECTS									
I-1	I-1	P&D	Validation of CCOS Data	DRI	$120	$120	Funded	-	3/03
I-2	I-2	EI	Biogenic Emissions Model Expansion	UC-Ext.	$80	$80	Funded	-	completed
I-3	I-3	EI	Point and Area Source Emissions Update	UCD,STI	$100	$100	Funded	-	completed
I-4	I-4	EI	Area Source Surrogates	STI	$150	$150	Funded	-	completed
I-5	I-5	EI	Source Sampling of Power Plants	UCR	$39	$39	Funded	-	completed
I-6	I-6	EI	Day-Specific Traffic Count Data (CRPAQS-$325K, total $600K)	UCD	$275	$275	Funded	-	completed
I-7	I-7	DA	Characterization of CCOS Episodes - Phase 1	T&B	$110	$110	Funded	-	completed
I-8	I-8	DA	Advanced Data Analysis - Phase 1	UCD	$115	$115	Funded	-	4/03
I-9	I-9	MD&E	Enhancement of Plume-in-Grid Modeling in Central California	EPRI	$143	$143	Funded	-	12/03
			SUBTOTAL		$1,132	$1,132			
CATEGORY II. SHORT-TERM STUDIES TO SUPPORT SIP PROCESS									
II-1	II-1	P&D	Completion of Project Planning for CCOS	DRI	$70	$70	Funded	-	6/03
II-2		P&D	PAN and NO2 Data Processing	CE-CERT	$8		Funded	-	3/03
II-3	III-16	P&D	Database Development for CCOS	Capitol Data	$238	$250	Funded	-	9/03
II-4	II-10	EI	Analysis of Remote Sensing Data	UCB	$60	$60	Funded	-	9/03
II-5	II-11	EI	Analysis of VOC Data	UCB	$50	$50	Funded	-	9/03
II-6		EI	Emission Inventory Technical Support	Alpine	$57		Funded	-	12/04
II-7		DA	Analysis of Elevated NOx Plumes (CEC/EPRI-$140K)	TVA			Funded	-	12/03
II-8	II-2	DA	Characterize of Summertime 2000 Measurement Period in Central California - Phase 2	T&B	$100	$100	Funded	-	12/03
II-9	II-8	DA	Evaluation of Pollutant Transport (Episode and Seasonal)	ARB	in-kind	in-kind	in-kind	4/03	9/03
II-10	II-6	MD&E	Characterization of Atmospheric Processes and Improve Boundary Layer & Mixing Depth Calculations (Met and Air Quality Models) (NOAA-$250K)	NOAA			Funded	-	9/03
II-11	II-7	MD&E	Evaluation of CMAQ and CAMx in the CCOS Domain with Process	UCR	$120	$120	Funded	-	9/03
II-12	II-9	MD&E	Evaluation of Deposition Algorithm and Soil NOx	ARB	in-kind	in-kind	in-kind	4/03	9/03
II-13		MD&E	Modification of the SAQM and its Meteorological Preprocessor for the CCOS Modeling Domain	Environ	$15		Funded		9/03
II-14	III-1	I&S	Summary of Air Quality Studies Conducted in Central California and a Commentary on Selected Issues - Phase 1	Envair	$30		Funded	-	12/03
			SUBTOTAL		$748	$650			

Table 1 (Continued)
CCOS Data Analysis and Modeling Support Projects

Project Number Revised	Project Number original	Project Category	Projects	Investigator	Funding (x1000) Revised	Funding (x1000) Original	Status	Estimated Start Date	Estimated Completion Date or Duration	Priority
CATEGORY III. UNCOMMITTED CCOS PROJECTS PHASE I										
III-1	III-3	EI	Emissions Inventory Evaluation and Reconciliation		$160	$70	Uncommitted			
III-2	III-4	EI	Review of Emission Estimation and Projection Methodology		$100	$100	Uncommitted			
III-3	III-8	EI	Ground Truth New Roadway Network		$40	$40	Uncommitted			
III-4	III-9	EI	Development of CEFS Control Rule Profiles		in-kind	$200	Uncommitted			
III-5		EI	Emissions Processing for Modeling	UCR	$20					
III-7	II-3	DA	Advanced Data Analysis - Phase 1	UC	$65	$250	Pending			
III-8	II-4	DA	Corroborative Data Analysis	Envair/UCR	$80	$80	Augmentation			
III-9	II-5	DA	Multivariate Trend Analysis	RFP	$75	$50	RFP	5/03		
III-10	II-12	MD&E	Link Data Analysis and Modeling Efforts		$100	$100	Uncommitted			
III-11a	III-10	MD&E	Improve Mass Conservation Module (Met and AQ Models) - Phase 1		$100	$300	Uncommitted			
III-12	III-13	MD&E	Improve Aloft Model Performance		$150	$150	Uncommitted			
III-13a		MD&E	Long-Term Seasonal Modeling - Phase 1		$100		Uncommitted			
III-14		MD&E	Web Access of Modeling Results		$20		Uncommitted			
III-15		MD&E	Cloud Effects		$30		Uncommitted			
			Contingency		$200	$200	Uncommitted			
			TOTAL		$1,240	$1,540				
CATEGORY III. UNCOMMITTED CCOS PROJECTS PHASE II										
III-6	III-5	EI	Refinement of Stack Parameters		$40	$40	Uncommitted			
III-11b	III-10	MD&E	Improve Mass Conservation Module (Met and AQ Models) - Phase 2		$200	$300	Uncommitted			
III-13b		MD&E	Long-Term Seasonal Modeling (Phase 2)		$200					
III-16	III-2	MD&E	Extend Previous Analysis Effort		$150	$150	Uncommitted			
III-17	III-11	MD&E	Conduct Uncertainty Analysis and Suggest Improvements		$100	$200	Uncommitted			
III-18	III-1	I&S	Summary of Air Quality Studies Conducted in Central California and a Commentary on Selected Issues - Phase 2		$80	$110	Uncommitted			
III-19	III-14	I&S	Refine Conceptual Model from CCOS Results (Concluding Element and Final Report)		$150	$150	Uncommitted			
III-20	III-15	I&S	Integration of Findings of CCOS and CRPAQS		$60	$60	Uncommitted			
III-21		I&S	Preparation and Publication of CCOS Summary Document		$30		Uncommitted			
			TOTAL		$1,010	$1,010				
CATEGORY IV. ADDITIONAL LONG-TERM PROJECTS										
IV-1		EI	Day-of-Week Variations in Emissions of Ozone Precursor		$350		Uncommitted			
IV-2		DA, MD&E	Enhancement of Existing Air Quality and Meteorological Monitoring for Data Analysis and Modeling		$10,000	$10,000	Uncommitted			
IV-3		MD&E	Deposition Studies		$3,500	$3,500	Uncommitted			
			TOTAL		$13,850	$13,500				

Footnote for Table 1

<u>Project Category</u>

P&D	Planning and Database
EI	Emission Inventory Development and Evaluation
MD&E	Model Development and Evaluation
DA	Data Analysis
I&S	Integration and Synthesis

Table 2
Distribution of Funded and Uncommitted CCOS Data Analysis and Modeling Support Projects by Topic

Questions and Issue	Category I	Category II	Category III	Category IV
1 Characterization of CCOS episodes and summer 2000 ozone season				
a. Suitability of CCOS ozone episodes for modeling	**I-7**			
b. Representativeness of CCOS episodes	**I-7**			
c. Adequacy of CCOS data for modeling	**I-1, I-7, I-8**	**II-2, II-3**		
2 Characterization of aerometric measurement and dynamics of atmospheric process		**II-10, II-12**		
3 Progress over last decade in reducing ambient ozone				
a. Ozone trends	**I-7**		III-7	
b. Met-adjusted ozone trends			III-9	
c. Multi-year meteorological cycles		**II-8**		
d. Urban versus rural ozone trends		**II-8**		
e. Ozone precursor trends	**I-7**	**II-8**		
4 Quality of Emissions Estimation and Projections	**I-2, I-3, I-4,I-5, I-6, I-8**	**II-4, II-5, II-6**	III-2,III-3,III-4, III-6	IV-1
a. Verification of emission reduction projections in 1994 SIP			III-2	
b. Emissions and ambient air quality reconciliation between 1990 and 1999.		**II-8**	III-1	
c. Emissions projections versus growth			III-2	
5 Trends in sensitivity of ozone formation to precursor concentrations				
a. Corroboration of model results of precursor sensitivity with data analysis	**I-8**	**II-11**	III-7, III-8	
6 Effect of upwind emission sources		**II-7, II-9**		
7 Analysis of ozone isopleths				
a. Reconciliation of emissoin projections with ozone isopleths			III-8	
b. Evalaution of effect of alternative control strategies			III-8	
Planning		**II-1**		IV-2
Model evaluation and setup	**I-9**	**II-11, II-12, II-13**	III-5, III-10, III-11, III-12, III-13, III-14, III-15	IV-3
Integration and Synthesis		**II-14**	III-18, III-19, III-20, III-21	

Note: Projects in bold are funded projects and those in regular text are uncommitted.

2. SUMMARY OF CCOS CATEGORY I AND II DATA ANALYSIS AND MODELING SUPPORT PROJECTS

This section summarizes the objectives and scope of work for the projects that have been funded during the first two phases of CCOS data analysis and modeling. The following summaries are grouped according to the following areas: 1) planning and database; 2) emission inventory development and evaluation; 3) model development and evaluation; 4) data analysis; and 5) integrations and synthesis. The investigators conducting the work are indicated at the end of each project description.

2.1 Planning and Database

2.1.1 Validation of CCOS Data (Project I-1)

This project provides Level 2 validation of the meteorological and air quality data collected during the period June 1 through September 30, 2000 as assembled by the CCOS Database Manager and as previously validated to Level 1 by each reporting contractor. Level 2 applies consistency tests based on known physical relationships between variables to the assembled data. These tests fall into three categories: detection of extreme values; consistency between redundant measurements and co-pollutants; and examination of temporal and spatial variations. CCOS supplemental data collected by DRI will be resubmitted, if necessary, to reflect adjustments that may be required as a result of the data validation. Validation results that indicate problems with other data sets will be forwarded to appropriate measurement groups for review and possible adjustment to their data. Contractor: Desert Research Institute

2.1.2 Completion of Project Planning for CCOS (Project II-1)

DRI will review the sources of uncertainty related to air quality modeling and develop work statements for projects to address these uncertainties. Project deliverables will consist of an integrated set of projects to improve the reliability of the CCOS modeling results by addressing deficiencies in the input data for modeling and by providing corroboration of modeling results through data analysis. DRI will define the problems and project objectives, estimate the significance of the problems to the overall uncertainty of the CCOS modeling results, describe potential methods and approaches, and estimate project costs. The benefits of the proposed projects will be evaluated with respect to the goals and technical objectives of CCOS and rationale will be developed for focusing available resources on the projects with the greatest potential to reduce the uncertainties associated with the CCOS air quality modeling results. Contractor: Desert Research Institute

2.1.3 PAN and NO_2 Data Processing (Project II-2)

CE-CERT built eight analyzers to measure nitrogen dioxide (NO_2) and peroxyacetyl nitrate (PAN) for use in the CCOS 2000 summer measurement study. There were two problems that were difficult to resolve during the initial data validation: the shifting of retention times due to changes in the temperature of the shelter and a sinusoidal response due to the pulsing of the liquid luminol pump. Since each 1-minute chromatogram was stored in the analyzer's computer CE-CERT was able to manually calculate the PAN peak height to determine concentrations. This approach is laborious and was carried out only for the intensive days. A program will be written and executed in EXCEL to correct NO_2 and PAN chromatographic peak areas for retention time and baseline drifts. EXCEL will be programmed to select peak retention times for both NO_2 and PAN during all periods when valid data was collected from the NO_2/PAN GCs during the CCOS summer study. The sinusoidal background response will be calculated for each peak elution and subtracted from the peak integration. At the same time, any PAN response interferences due to tailing of the NO_2 peak will be subtracted out. This would also allow PAN to be determined for all injections and for the entire field measurement program duration. The results will be compared to the manually derived PAN concentrations and the method further refined if necessary. The refined data will be submitted as EXCEL spreadsheets as done previously. If funding allows, data for the CRPAQS study period will be similarly corrected. This is of secondary importance, however, since the instruments were upgraded between CCCOS and CRPAQS study periods and PAN concentrations are often below the detection limit in the winter. Contractor: CE-CERT

2.1.4 Database Development for CCOS (Project II-3)

Capital DataWorks has been the primary database development contractor for the Central California Ozone Study Data Management System. This database processes and stores all related CCOS and supplemental data. The purpose of this contract is to develop several applications for the database system to facilitate dissemination and review of the database. A parameter query application addresses requests for data in various groupings (flat files) as needed by researchers. The application is being developed around standard output datasets for various groups of parameters, such as, surface continuous meteorological, upper level wind, upper level virtual temperature, upper level meteorological, surface continuous gaseous air quality, and upper level air quality. A process is being developed to update existing database records with newly corrected/invalidated data based on these same files. Plotting applications are being developed for generating internal consistency plots involving single station and external consistency plots involving multiple monitoring sites. Support is being developed to provide data retrieval per user input to improve online data access and the user interface. The contractor will add version control to the database queries for the parameter grouping file creation and extraction process. The CCOS production database server, "Genesis", will be tuned to maximize throughput. This will include database optimization and a detailed audit of the database and re-indexing all tables. The contractor is developing draft formats for study parameter groupings and continuing the development of CCOS reference data elements to support incoming data and QA processing. Supplemental data are being formatted for database submittal. Functional and technical maintenance documents will be developed for the quality assurance, reference data maintenance, data retrieval, query catalog and administration modules and related scripts. These documents will explain the various setup and configuration information to ensure proper application function. The technical maintenance document will be used to help staff add to existing program functionality and proper configuration.

2.2 Emission Inventory Development and Evaluation

Most of the emission inventory data necessary for CCOS modeling are being provided by public agencies as in-kind contributions to the CCOS study. However, there are some critical elements of the CCOS emission inventory that the agencies do not have sufficient resources or expertise. In general, these needs relate to the spatial and temporal distribution of emissions from motor vehicles and other area sources. The emission inventory elements supported by CCOS are listed below.

2.2.1 Biogenic Emission Model Expansion (Project I-2)

Biogenic emissions are calculated using BEIGIS, the ARB's geographic information system (GIS) model for estimating biogenic hydrocarbon emissions. The major input databases needed to run BEIGIS currently exist, but several require validation. The first database requiring field validation is the spatial distribution and identification of vegetation species in natural areas as defined by the Gap Analysis Project (GAP). The second is a 1-kilometer resolution leaf area index (LAI) database developed from satellite imagery. Validation of the GAP and LAI databases is critical as these are the primary input databases used in estimating the green leaf mass and spatial distribution of dominant plant species in the CCOS domain. This project will conduct field validation of the GAP and LAI databases at a number of sites in the CCOS study area. Contractor: University of California Extension

2.2.2 Point and Area Source Emissions Update (Project I-3)

This project is to provide assistance to small districts in the CCOS domain to review and update their point and area source emission inventories. Student from UCD made site visits to point sources within the nine air quality management districts in the Sacramento Air Basin emitting 10 tons or more per year of any criteria pollutant. Process rates and other information were obtained for each facility and the information updated in ARB emission inventory data system. Work on area sources included review of existing emission estimation methodologies and suggested improvements. STI applied improved methods to derived updated county-wide area source emissions. Contractor: University of California Davis and Sonoma Technology Inc.

2.2.3 Area Source Surrogates (Project I-4)

In this project, Sonoma Technology, Inc. will develop base year and future year gridding surrogates for spatially distributing area source and off-road emission source categories. The spatial allocation factors will be used to geographically distribute emissions throughout the Central California Ozone Study (CCOS) domain at a spatial resolution of 1 x 1 km covering all of California from Shasta to Kern County. Spatial allocation factors for area and off-road mobile sources will be developed for the years 2000, 2005, 2010, and 2020 using various sources of data that are representative of the spatial distribution of emissions activity. These data are referred to as surrogates and commonly include demographic and socioeconomic data and land cover/land use data. STI will review existing area and off-road mobile source surrogate assignments and use new and innovative methodologies similar to those used in the 1997 South Coast Ozone Study (SCOS97) to assign surrogates to emissions sources. Additionally, STI will review and recommend improvements to existing temporal distributions (hourly, daily, seasonal) of emissions activity for all area and off-road sources. In order to complete this project, local data will be acquired to develop area source surrogates that are more applicable to specific areas of the CCOS domain. Contractor: Sonoma Technology, Inc.

2.2.4 Source Sampling of Power Plants (Project I-5)

CE-CERT was contracted to perform stack testing at up to five stationary gas-fired combustion power generation facilities. CE-CERT was able to complete testing at two of the facilities before the onset of the California energy crisis, which impaired access to additional facilites. Results of the testing include flow rates, temperatures, and moisture content of effluent streams as well as emission concentrations and mass flow rates of CO, CO2, NO, NO2, PM10, aldehydes, and ketones, chlorinated hydrocarbons, and C1-C4 hydrocarbons. Contractor: University of California Riverside College of Engineering Center for Environmental Research and Technology (CE-CERT)

2.2.5 Day-Specific Traffic Count Information (Project I-6)

As part of CCOS, observed traffic data are being used in conjunction with travel demand model information to obtain more accurate hourly estimates of traffic volumes. Improved hourly estimates of traffic are required because travel demand models typically produce volumes in blocks of time, some as long as the 24 hours. The purpose of this project is to estimate hourly allocation factors for CCOS applying a disaggregation method that makes use of observed traffic data to predict the hourly allocation of traffic volumes for links in travel demand network. Contractor: University of California, Davis

2.2.6 Analysis of Remote Sensing Data (Project II-4)

During the Central California Ozone Study (CCOS) field measurement program in summer 2000, ARB's Mobile Source Operations Division conducted a remote sensing field study of vehicle emissions at sites in the San Francisco Bay Area, Sacramento, and the San Joaquin Valley. Exhaust emissions of CO, HC, and NOx were measured in the exhaust plumes of about 200,000 individual vehicles as they drove by the remote sensors. This large dataset of remote sensing measurements will be analyzed in this research to determine average vehicle emission factors for CO, HC, and NOx. Separate results will be presented for the Bay Area, Sacramento, and the San Joaquin Valley. The emission factors will be combined with fuel consumption estimates resolved to the county level to estimate on-road vehicle emissions. Changes in vehicle emissions in central California between 1990 and 2000 will also be assessed. Contractor: University of California Berkeley

2.2.7 Analysis of VOC Data (Project II-5)

A series of highway tunnel experiments has been conducted in the San Francisco Bay Area to characterize vehicle emissions. Measurements of speciated VOC concentrations have been collected at the Caldecott tunnel, which is located on highway 24 between Alameda and Contra Costa Counties. Speciated VOC measurements are available for 1991 (Zielinska and

Fung, 1992), 1994-97 (Kirchstetter et al., 1999), and 1999 and 2001 (Kean et al., unpublished data, analyzed by Technical Services Division of BAAQMD). In 1994 and later years, additional air samples were collected to determine concentrations of aldehydes and ketones. In conjunction with the tunnel experiments conducted in summers 1995, 1996, 1999, and 2001, service station samples of liquid gasoline were collected in Berkeley. All major brands, including both regular and premium grades of gasoline, were sampled. In summer 2001, additional service station samples were collected in Sacramento. Kohler and coworkers at Chevron Research and Technology Company in Richmond, CA analyzed all but the most recent liquid gasoline samples for detailed composition (ca. 200 compounds) using GC/FID. Similar analyses are currently underway for the summer 2001 gasoline samples. The goal of this research is to describe the chemical composition of motor vehicle-related VOC emissions in central California. In the intervening decade since the last large-scale field study in 1990, major changes have been made to the properties of gasoline, so updated VOC composition profiles are needed. The chemical composition profiles that will be developed in this research are essential inputs for both grid-based photochemical modeling and receptor-oriented source apportionment studies. Contractor: University of California Berkeley

2.2.8 Emission Inventory Technical Support (Project II-6)

The goals of this project are: 1) create gridded, hourly on-road mobile source emissions estimates of PM, CO, NOx, and TOG which are representative of an ozone season episode and a winter episode for the base year 2000; 2) provide a cost and schedule estimate to create more refined PM estimates (i.e. EC, OC, SO2, SO4, NH3, Na, Ca, K, Mg, and other PM in lieu of a total PM estimate); and 3) transfer data and estimation software to the ARB and provide necessary training so that ARB staff can generate additional on-road mobile source emissions estimates using other data sets. Contractor: Alpine Geophysics

2.3 Data Analysis

2.3.1 Characterization of CCOS Episodes – Phase 1 (Project I-7)

T&B Systems will characterize the meteorology and air quality during the CCOS field study. In the initial phase of this work, which has been completed, T&B and their subcontractors evaluated the meteorological representativeness of the CCOS modeling episodes and utilized routine ambient data to identify where and when ozone formation is limited by the availability of radical species or NOx. Contractor: T&B Systems

2.3.2 Advance Data Analysis - First Phase (Project I-8)

A consortium of investigators within the University of California System and the Desert Research Institute will perform detailed analyses of the CCOS measurements to validate key features of the database that will be used to drive air quality simulations. These analyses include evaluation of mobile source emissions using remote sensing data, comparisons of the proportions of species derived from ambient and emission inventory data, VOC source apportionment using Chemical Mass Balance receptor modeling, evaluation of photolysis parameters, and statistical analysis of species that may be used to infer VOC or NOx limitation with respect to formation of ozone. Additional analyses are currently under consideration. These include: evaluation of additional observation-based methods (OBMs) that require speciated VOC data obtained from GC/MS instruments at research sites during CCOS 2000, comparison of rates of O_3 change obtained from data analysis to predictions of photochemical air quality models, use of Principal Component Analysis to study underlying mechanisms of ozone days and formulate explanations for observed trends and patterns, and exploration of statistical analysis methods for evaluating and ranking observation based methods according to their ability to capture ozone mechanisms. Contractor: University of California and Desert Research Institute

2.3.3 Analysis of Elevated NOx Plumes (Project II-7)

As part of the CCOS field study, the Tennessee Valley Authority (TVA) Atmospheric Sciences staff made measurements with an instrumented aircraft downwind of the Moss Landing and Pittsburg gas-fired power plants. A twin engine de Havilland Twin Otter Aircraft was equipped with 6 TEI instruments, 4 for the measurement of various nitrogen oxides, one for "fast" ozone measurements, and one for ambient CO measurements. A LiCor instrument for CO_2 was on board, along with a TSI 3-wavelength nephelometer, a solar radiation device, and probes for temperature, relative humidity, (GPS) position, and (pressure) altitude. Samples of hydrocarbons were taken in canisters and bags were filled for post-flight collection on DNPH cartridges and analysis for carbonyl compounds. The objectives of this study are to map detailed ozone, precursor, and products in power plant plumes and in regional airmasses from the measurements obtained during the study, evaluate plume models and to assess the impact of elevated NOx plumes on downwind ozone concentrations.

2.3.4 Characterization of Summer 2000 Measurement Period in Central California - Second Phase (Project II-8)

The analyses performed during phase I will be expanded by utilizing the full CCOS database. This phase will also include an historic perspective of the long-term meteorological cyclic pattern in relation to air quality in central California during 1980-2002. Long-term trends in ozone concentrations (maximum 1-hour and 8-hour) and its precursors will be characterized within the CCOS domain for the summer ozone seasons from 1980 to 2002. In addition, the trends in the timing of peak 1-hour and 8-hour ozone concentrations will be examined. Available data from Photochemical Assessment Monitoring Stations (PAMS) will be used to establish VOC trends. If appropriate, carbon monoxide data will be used as a partial surrogate for nonmethane organic compounds during the early years during which VOC data are not available. T&B will quantify the changes in ozone, ozone precursors, and oxidation products between 1990 and 2000 using the data from the SJVAQS/AUSPEX and CCOS field studies. Changes that will be examined include organic and nitrogen speciation, VOC/NOx ratios, photochemical reactivity of organic compounds, and extent of reaction. T&B will also summarize and interpret relevant results and findings from past studies that provide insight into the patterns of change in ozone concentrations with changes in emissions. Contractor: T&B Systems

2.3.5 Evaluation of Pollutant Transport (Episode and Seasonal) (Project II-9)

Various modeling simulations will be conducted to study the transport of ozone and its precursors within an air basin as well as between air basins in the CCOS domain with the selected SIP model. This modeling effort will be done using in-kind staff resources. Contractor (In-kind)

2.4 Model Development and Evaluation

2.4.1 Enhancement and Application of Plume-in-Grid Modeling in Central California (Project I-9)

The objectives of this project are to improve and evaluate a state-of-the-science reactive plume sub-model and embed it into a three-dimensional photochemical model and to evaluate the performance of the plume sub-model with data collected during the CCOS field study. This sub-model must be fully documented, have an open source code, and be available for use in the development of State Implementation Plans. These objectives will be accomplished by upgrading existing plume algorithms to account for plume downwash and to establish the importance of accounting for asymmetry when plumes are dispersed vertically. A photochemical grid model which includes EPRI's advanced plume treatment and other plume treatments will be set up for application in the CCOS domain for the periods that included power plant plume measurements. Differences obtained in simulated ground level ozone concentrations will be studied to understand how options in modeling the role of point source plumes influence predicted ozone levels. The findings will be analyzed by working with other experts involved and interested in CCOS, to recommend an optimal approach for treating plumes in the CCOS region.

2.4.2 Characterization of Atmospheric Processes and Improvement of Boundary Layer & Mixing Depth Calculations (Project II-10)

During the CCOS 2002 field program, extensive observations were collected in central California to document high ozone episodes and the meteorology that is associated with them. In addition, research grade meteorological observations were taken. The purpose of this study is to evaluate and optimize the available meteorological model by analyzing and using observations. This assessment will be quantitative and will focus on specific meteorological conditions that can adversely impact ozone concentrations. NOAA will prepare detailed analyses of the meteorological observations for three IOP's, documenting the timing, strength, horizontal and vertical structure of the sea-breeze, Carquinez Straight flow splitting, nocturnal jet, eddies (Schultz, Fresno, Bakersfield), up-slope/down-slope flows, and mixing depths. Quantitative measures or definitions of each of these phenomena will be developed. MM5 simulations will be run for the three case studies with and without the use of the Four Dimensional Data Assimilation. NOAA will prepare detailed comparisons of the model simulations and observations for the three case studies and investigate how the meteorological flow features may be affecting air quality. In particular, the roles of each of the flow features of Task 2 on the transport of ozone and its precursors will be documented. Contractor: NOAA

2.4.3 Evaluation of CMAQ, SAQM and CAMx in the CCOS Domain with Process Analysis (Project II-11)

The University of California Riverside (UCR) will perform a comprehensive comparison of the U.S. EPA's Community Multiscale Air Quality (CMAQ) model, ENVIRON Corporation's Comprehensive Air Quality Model with extensions (CAMx), and the Air Resources Board's SARMAP Air Quality Model (SAQM) using process analysis and a model performance evaluation against ambient data. The process analysis comparison will focus on developing an understanding of how O_3 production and reactivity are represented in each of the models. This will include a detailed mass budget analysis of reactions of VOC, generation of free radicals (HOx) and conversion of reactive NOx to inert forms of oxidized nitrogen (NOz). The process analysis comparison of the three models will be useful as a quality assurance procedure in that it will verify that chemical budgets are being simulated within expected bounds. It will also be useful for characterizing differences among the three models in the budgets of VOC, HOx, NOx and O_3. These differences will provide explanations for differences in predicted O_3 concentrations and for differences in the sensitivity of O_3 to reductions in VOC and NOx precursors. Model simulations will also be performed with the CB4 and SAPRC99 photochemical mechanisms, and the process analysis will be used to identify differences in O_3 production and the budgets of VOC, HOx and NOy for both models and both mechanisms. All three models will be applied for two episodes during the CCOS 2000 field study: July 30 to August 2 and September 17 to 20. Simulations will also be performed for several VOC and NOx precursor reduction strategies. The number and type of model simulations will be determined in consultation with CARB, TC and UCR staff. The process analysis will also be applied to the model to simulate precursor reduction strategies to provide an explanation of the O_3 response in each of the models. Contractor: University of California Riverside

2.4.4 Evaluation of Deposition Algorithm and Soil NOx (Project II-12)

During the California Ozone Deposition Experiment (CODE) in 1991, aircraft and tower-based flux measurements were taken over different types of San Joaquin crops, irrigated and non-irragated fields, and over dry grass. Modeled ozone deposition onto the ground will be evaluated against the data collected during the 1991 Study in the San Joaquin Valley. In addition, estimate NOx emission from soils (mostly from agricultural soil) will be evaluated using the field data collected in the San Joaquin Valley during the summer of 1995. Estimates will be derived of the spatially resolved soil NOx emissions and incorporated into the CCOS gridded emission inventory. Estimated deposition velocity for ozone will be evaluated against the 1991 study. This study will be accomplished using in-kind staff resources. Contractor: In-kind

2.4.5 Modification of the SAQM and its Meteorological Preprocessor for the CCOS Modeling Domain (Project II-13)

The ARB plans to compare the SARMAP Air Quality Model (SAQM) to other models for the CCOS modeling grid. This will require changing the number of horizontal grid cells and vertical layers from previous simulations on the SARMAP modeling domain. The ability to change the number of vertical layers needs to be checked because SAQM has always been run with 15 layers and some sensitivity tests with different number of layers produced results that were difficult to interpret. This project would review and modify the SAQM model and its meteorological preprocessing program to ensure that the number of vertical layers can be adjusted throughout the existing user interface program. In addition, the way the layers are matched and combined from MM5 to SAQM will be reviewed. The objective of this project is to review computer codes for correct numerical operation. Contractor: Environ

2.5 Integration and Synthesis

2.5.1 Summary of Air Quality Studies Conducted in Central California and a Commentary on Selected Issues - Phase1 (Project II-14)

Past attainment plans for ozone nonattainment areas in central California and elsewhere have been consistently overly optimistic in their projections for attainment. Possible problems associated with previous projections may include (but are not limited to) inaccurate emissions inventories for base case and future projections, poor characterization of boundary conditions, incorrect representation of chemical and meteorological processes, and emissions controls that were less effective than expected. An understanding of the key factors that contributed to inaccurate projections for attainment is required prior to preparing the next SIP update. This project evaluates and reconciles the technical basis for the projections of attainment of the ozone standard in prior SIPs for each of the ozone nonattainment areas in the CCOS study domain, reconciles these projections with actual trends in ozone, and identifies the key factors and assumptions that contributed to the inaccurate ozone attainment projections. The contractor will evaluate the 1994 SIP process (and previous SIPs if necessary) to determine why the ozone attainment projections were inaccurate. The contractor will evaluate the suitability of the air quality and meteorological models and databases used in the 1994 SIP and compare them with those available currently. The contractor will evaluate the modeling episodes including boundary conditions and determine their representativeness for the projection of ozone trends. The contractor will evaluate the accuracy of previous emission estimates, compare projected emissions with updated emissions using current methodology for estimating emissions, identify the major uncertainties and if appropriate suggest improvements. They will review the expected efficacy vs. the actual benefits of emission control equipment or strategies. Contractor: Envair

3. CATEGORY III PROJECTS – PHASE 1

This section explains the technical objectives for proposed Phase 1 Category III projects and describes their scope of work and estimates the costs and benefits. Thirteen Phase 1 projects with a total estimated budget of $1.04 M. The Air Resources Board will complete one additional phase 1 project using in-kind resources.

3.1 Emission Inventory Development and Evaluation

3.1.1 Emissions Inventory Evaluation and Reconciliation (Project III-1)

Uncertainties in precursor emissions are largely viewed as potentially one of the weaker links in the air quality modeling process. These uncertainties are not well characterized because most emission estimates are based upon models, engineering analyses and limited test data rather than on systematic measurements of actual or ”real-world” emissions. Approaches for evaluating emission inventories that have been applied in prior studies include reconciliation with ambient data and other data such as remote sensing and on-road tunnel measurements. On-going CCOS data analysis projects that apply such methods include ambient source apportionment by receptor modeling (Project I-8), spatial and temporal comparisons of ambient and emission inventory pollutant ratios (e.g., CO/NOx and VOC/NOx) (Project I-8), fuel-based inventory based on regional gasoline sales and fleet-averaged, fuel-based emission factors from remote sensing measurements (Project I-8 and II-6), comparisons of long-term trends in ambient pollutant concentrations and concentration ratios with emission inventory trends (III-3), and comparison of weekday differences in ambient and corresponding emission inventory data (III-3). The results of these studies need to be integrated and compared to analogous analyses using model predictions as input data in place of ambient data and additional model performance evaluations that evaluate the consistencies between model output and ambient data for each of the CCOS modeling episodes.

<u>Technical Objectives</u>

The objectives of this study are to conduct performance evaluations of the CCOS modeling outputs that are relevant to evaluating the uncertainties and potential biases in the emission inventory. The contractor will integrate and synthesize similar evaluations from other CCOS data analysis studies, review biases that are indicated among the different approaches and make general and specific conclusions regarding the reliability of the CCOS emissions inventory base on the weight of the evidence.

<u>Scope Of Work</u>

The scope of work for this project includes the following three tasks:

Task 1. Integrate and synthesize the results from CCOS data analysis and modeling support studies I-8, II-6, III-3 that reconcile the emissions inventory with ambient or other data.

Task 2. Compare and reconcile the spatial and temporal patterns in predicted VOC/NOx and CO/NOx ratios with corresponding ratios from PAMS and CCOS supplemental monitoring sites.

Task 3. Compare and reconcile the spatial and temporal pattern in the predicted levels of lumped VOC species with the corresponding ambient data.

Task 4. Using the source composition profiles from an existing receptor modeling study for CCOS, apply the VOC speciation predicted by the CCOS modeling to the Chemical Mass Balance receptor model for the grid cells with corresponding ambient speciation. This calculation should be made for specific chemical species and not lumped species.

Task 5. Draw appropriate conclusions regarding potential biases and uncertainties that may exist in the CCOS emissions inventory based on the previous tasks. Contrast these conclusions with similar analyses conducted during the 1990 SARMAP modeling and significant changes that have occurred during the decade of the 1990s in the methodologies used to estimate emissions.

Task 6. Prepare a final report documenting the findings and conclusions of the study.

<u>Expected Results And Benefits</u>

This study will provide an improved assessment of the emission inventory and its uncertainties and will result in better estimates of the temporal and spatial variability and the effects of meteorology on the emissions.

<u>Estimated Cost:</u> Not exceed $130,000

<u>Schedule:</u> Nine months are allocated for completion of this project and three months for review and preparation of the final report.

3.1.2 Evaluate the Quality of Emission Estimation and Projections (Project III-2)

Photochemical air quality modeling systems are the fundamental analytical tools that are used in the management of air quality to relate precursor emissions to ozone air quality. Estimating the spatial, temporal, and chemical nature of precursor emissions is viewed as a major source of uncertainty in this modeling process. The compilation of day-specific, temporally and spatially resolved emissions inventories for modeling purposes requires extraordinary effort involving many parts with varying degrees of complexity. The methodologies that are used to derive estimates for various categories of emissions are based upon guidance documents, handbooks, manuals, and other documentation. The implementation of these methods requires specific datasets such as emissions and activity factors, spatial and temporal allocation surrogates, and growth and emission control parameters that are appropriate for the CCOS modeling domain. The quality and suitability of these factors and parameters have not been assessed in many cases and are not well documented. Moreover, limitations impose by approximations and assumptions of the methods result in unknown level of uncertainties for many emission estimates.

Biases and inconsistencies in the CCOS emissions inventory are being evaluated using several "top-down" approaches. CCOS data analysis project III-7 will integrate the findings and conclusions from these "top-down" evaluations with operational evaluations of CCOS model outputs against ambient data. While these analyses are potentially useful for identifying potential biases in the emission inventory, they do not address the underlying causes for the discrepancies. A critical review of the methodologies and databases that were used to compile the emission inventory would provide a useful complement to the "top-down" evaluations in identifying and prioritizing the components of the inventory needing further development.

Technical Objectives

The primary objectives of the project are to critically review the technical basis, assumptions, and limitations in the methodologies and input data that are used to estimate and spatially and temporally disaggregate, and forecast emissions in the CCOS modeling domain. Detailed sensitivity analysis of emissions models and methodologies are beyond the scope of this project and are not intended. Nevertheless, a thorough evaluation of input data and assumptions can be useful in identifying potential biases and uncertainties associated with major components of the emissions inventory. For example, some data in the current CCOS modeling emissions inventory are based on the 1990 census data rather than the 2000 census data.

Scope Of Work

The project will consist of the following tasks:

Task 1. Document the methods and associated factors and parameters used to estimate VOC and NOx emissions in the CCOS modeling domain and evaluate the quality, completeness, and suitability of the data used to estimate emissions. For each emissions category, summarize the technical basis for the methodology, assumptions and limitations. Summarize relevant evaluations that have been conducted, particularly studies that assess the sensitivity of the emission estimations with variations in input data.

Task 2. Document the speciation profiles used to apportion total VOC to individual species. Compare these speciation profiles to suitable alternative profiles and reconcile and evaluate differences. Assess uncertainties in the profiles due to measurement method and variations among sources within major source categories. Identify major differences in the speciation for source and ambient data due to variations in analytical methods and assess the implications for modeling.

Task 3. Document the methods used to spatially and temporally (diurnal and day-of-week) disaggregate total VOC and NOx emissions and evaluate the suitability of the parameters that are used.

Task 4. Prepare a final report summarizing the finding and conclusions of the previous tasks and place them in context with the findings from CCOS data analysis Project III-7.

Expected Results And Benefits:

This project will provide a single comprehensive documentation of the method and databases used to derive the emissions inventories for CCOS modeling, and identify limitations and weakness in the "bottom-up" methods for estimating emission which can be reconciled with "top-down" evaluations of the CCOS emissions inventory.

Estimated Cost: $100,000

Schedule: Nine months

3.1.3 Ground Truth New Roadway Network (Project III-3)

In California, local transportation agencies (e.g. COGs, or Councils of Governments) develop, for conformity/traffic planning, their own GIS-based traffic networks. These constitute local, independent roadway pieces. Most of the old COG networks used the State Plane Network, consisting of about 8 east-west map strips in California, converted to the Lambert system. This likely resulted in some map distortion. Another question as to the correct geographic positioning of these networks arises because some old methods were based on digitizing from street maps; consequently there is much uncertainty as to whether traffic nodes in these networks are in fact where they should be. CALTRANS (California Transportation Department) has developed its own statewide roadway network, also GIS-based.

Under an existing CCOS contract, ARB has collected data from the local networks, based on their different routines and different map projections, and pieced together a new Integrated Transportation Network (ITN), combining them under the same roadway network overlays. Where there were no data, or no local networks, the contractor used CALTRANS data. The resulting network is thus based on various different independent pieces using different routines and map projections, filled in and pieced together using CALTRANS data. There have evidently been no ground investigations of critical node locations. However, there is certainty on the part of ARB roadway experts that errors exist, leading to inaccuracies in spatial assignment of mobile emissions used for modeling. Part of ARB's new ITN is being used for CCOS modeling. The problem and focus of this proposed project is how to best and most efficiently examine the accuracy of the ITN using observations and empirical data from sensitive nodes (intersections, roadway sections).

Technical Objectives

The primary technical objective is to conduct ground surveys of critical nodes and roadway segments in ARB's Integrated Transportation Network to examine the accuracy of their spatial coordinates. The focus will be on obtaining precise spatial coordinates of critical nodes with sufficient geographical representation to verify or refine New Roadway Network data. In certain of the most critical nodes, the study might be enhanced with observations of the temporal variability of vehicle miles traveled (VMT) and vehicle speed distributions.

Scope Of Work

Initially, appropriate COG's should be contacted for information on roadway portions that have already been verified by observational data. These include the Sacramento COG, San Diego and Monterey.

Next, select specific nodes and roadway segments for ground truth studies. This might be done by first identifying several sub-regions within the overall network to obtain a good geographical representation of areas with highest total VMT. Within sub-regions, specific nodes and segments might also be selected based on relative traffic volumes. Since every county has its own traffic demand model, selection of measurement locations should be made in collaboration with local COG's and with CALTRANS, as well as with the ARB.

After selecting the most sensitive nodes (intersections, major roadways), this project would consist essentially of establishing accurate coordinates (e.g. latitude/longitude) of specific network components, using GPS methods to track vehicles for example, and bringing them into a common coordinate system. Acquired data will be used to examine the accuracy of existing spatial roadway data and to upgrade the New Roadway Network using GIS methods.

Suggested tasks to be completed during this study are:

Task 1 – Develop ground-truth test methods and methods for upgrading the existing Roadway Network based on acquired field data.

Task 2 – Identify and acquire existing ground truth information, such as exists for the Sacramento COG and possibly others.

Task 3 – Identify critical nodes and road segments for study.

Task 4 – Conduct surveys to obtain precise spatial coordinates.

Task 5 – Use field data to upgrade spatial data in the New Roadway Network.

Expected Results And Benefits

Presently, the accuracy of the Integrated Transportation Network is estimated to be no greater than 1km. Per a visual comparison with other, non-verified GIS coverages (e.g. Tiger/Line county boundaries and CalTrans CALIB data), the accuracy of the ITN appears to vary regionally. For example, many northern and central California regions in the ITN appear to fall within the 1km level of accuracy whereas some Southern California, and Central Coast regions in the CCOS modeling domain exhibit spatial differences of around 10km (e.g. Los Angeles and Santa Barbara). Because verified data are not available for use as an absolute reference, the actual accuracy of the network is unknown since comparisons may be affected by additive or compensating errors.

Due to the dominant status of mobile source emissions in urban areas, significant improvements to urban-area model performance may result if large spatial errors in urban mobile source emissions are corrected. At a minimum, this project will provide greater confidence in the spatial allocation of mobile source emissions.

Estimated Cost

Compared to other projects proposed for CCOS funding, this one would be relatively inexpensive. The funding allocation estimated by ARB was $40K. A more detailed cost analysis should probably be prepared before the project goes forward.

Duration Of The Project

This project should be completed within a 3 to 6 month period.

3.1.4 Development of CEFS Control Rule Profiles (Project III-4)

The California Emission Forecasting System (CEFS) is used to develop the projected stationary source emissions for the CCOS modeling domain. The control assumptions used to develop the baseline forecasts are critical in developing projected modeling inventories that are accurate. For this reason, an up-to-date and comprehensive control rule data set is needed which represents all local district rules that have been promulgated in the CCOS domain. The CEFS system currently contains rule-specific control information for several of the larger air quality management and air pollution control districts in the state (e.g. South Coast AQMD, Bay Area AQMD, San Joaquin Valley APCD, Ventura County APCD). The SJVAPCD completed an extensive study (under contract with Arons Air Quality Services -- completed April 2000) to assess control efficiencies, rule penetration, and rule effectiveness for all locally adopted ROG and NOx rules. To date, most of the districts in the CCOS domain have not been studied to develop similar control data sets.

Technical Objectives

The objective of this study is to determine whether all State and local control measures that are needed to effect emission reductions have been adopted and to assess the degree of implementation of these control measures.

Scope Of Work

With the assistance of local District staff, identify the state and local control measures that have been implemented since the adoption of the 1994 SIP and those scheduled for implementation prior to 2005 and 2010, and the projected emission reductions and years in which the reductions are effective. For control measures with significant emission reductions, determine specific changes in emission rate and/or activity factors that are responsible for the emissions reductions and the assumptions upon which they are based. Summarize available information regarding the degree of implementation of these control measures and any independent evaluations of control measure effectiveness or quantitative reconciliation of expected and actual emission reductions.

Estimated Cost**:** $100,000

Schedule: Six months

3.1.5 Emissions Processing for Modeling (Project III-5)

The University of California Riverside (UCR) is performing a comprehensive comparison of the U.S. EPA's Community Multiscale Air Quality (CMAQ) model, ENVIRON Corporation's Comprehensive Air Quality Model with extensions (CAMx), and the Air Resources Board's SARMAP. The objective of this project is to process the preliminary CCOS spatially and temporally resolved modeling emission inventory for input into the three alternative air quality models.

3.2 Data Analysis

3.2.1 Advanced Data Analysis – Phase 2 (Project III-7)

This work would be the second phase of an existing data analysis project by a consortium of investigators within the University of California System and the Desert Research Institute to perform a detailed analysis of the CCOS measurements to validate key features of the database that will be used to drive air quality simulations. Data analyses that are being conducted during phase 1 include evaluation of mobile source emissions using remote sensing data, comparisons of the proportions of species derived from ambient and emission inventory data, VOC source apportionment using Chemical Mass Balance receptor modeling, evaluation of photolysis parameters, and statistical analysis of species that may be used to infer VOC or NOx limitation with respect to formation of ozone.

A proposal has been received for the second phase and is currently under review. Additional analyses that are proposed by the investigators include, evaluation of additional observation-based methods (OBMs) that require speciated VOC data obtained from GC/MS instruments at research sites during CCOS 2000, comparison of rates of O3 change obtained from data analysis to predictions of photochemical air quality models, use of Principal Component Analysis to study underlying mechanisms of ozone days and formulate explanations for observed trends and patterns, and exploration of statistical analysis methods for evaluating and ranking observation based methods according to their ability to capture ozone mechanisms.

3.2.2 Corroborative Data Analysis (Project III-8)

Although air quality simulation modeling (AQSM) will be used to address the CCOS goals, past experience has demonstrated the need for thorough operational and diagnostic evaluations and corroborative data analysis to assess the reliability of outputs from each part of the modeling system (i.e., emissions, meteorological, and air quality models). In recognition of model uncertainties, a variety of "observation-based methods" (OBM) have been developed to infer important relationships between ozone, its precursors, and the sources of these precursors. These methods are driven principally by observed data as opposed to AQSMs that are driven by emission estimates and meteorology. OBMs include receptor models, regression and transport characterization techniques, ambient pollutant ratios, multivariate trend analysis, indicator species and semi-empirical based models. OBMs are used to assess emission inventories, infer NOx or VOC control preferences, and to assess the contribution of transport of ozone and its precursors to ozone exceedances in downwind areas. These methods provide an independent evaluation of the accuracy of emission-based model predictions. However, these methods are not without their own limitations and uncertainties, and as a result are best used in conjunction with emission-based models. The diagnostic feature of observation-based methods complement the prognostic capabilities of emission-based models.

Technical Objectives

In this study, observations and appropriate results of the CCOS air quality modeling will be corroborated using observation-based methods that treat AQSM-predicted parameters in the same manner as observational data. This project will require outputs from the CCOS air quality modeling and are not expected to commence until mid-2003. This project will be an augmentation and extension of existing work (Project I-7 and I-8).

Scope Of Work

The sensitivity of ozone to VOC and NOx will be determine throughout the CCOS domain by applying CCOS AQSM-predicted parameters to the following three observation-based methods. The “Photochemical Indicator Method” (Sillman, 1995) uses observed ratios of specific chemical species, such as H2O2/HNO3, to characterize the regime of precursor limitation. The “Observation-Based Model” (Cardelino and Chameides, 1995) uses air quality observation to derive a photochemical box model that infers ozone production sensitivity to precursors on the basis of Carter’s Relative Incremental Reactivity factors. Compare these OBM results to corresponding results that will be obtained through existing data analysis efforts using measured ambient data. The MAPPER method uses ambient measurements in tandem with O3-NOx relationships expected from smog chamber experiments to derive the “extent of reaction” (Johnson and Quigley, 1989; Blanchard et al., 1999).

Expected Results And Benefits

The results of this project will provide an independent evaluation of the accuracy of emission-based model predictions and thus reduce the level of uncertainty associated with these predictions and improve the characterization of ozone precursor relationships. The results of this project are intended to provide a more credible basis for development of ozone attainment plans.

Estimated Cost: $80,000

Duration Of Project: Twelve months

References

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Cardelino, C.A., and W.L. Chameides, (1995). An observation-based model for analyzing ozone precursor relationships in the urban atmosphere. J. Air Waste Manage. Assoc., 45, 161-180.

3.2.3 Multivariate Trend Analysis (Project III-9)

It is well known that meteorological parameters influence ozone concentration. The factors include solar radiation and cloud cover, mixing height, average and maximum temperature aloft (500-mb height, 850-mb temperature) and surface temperature, relative humidity, the vertical temperature structure (atmospheric lapse rate or stability), surface wind speed, upper-air winds (long-range transport) and synoptic-scale weather patterns. Interannual variations in meterological conditions mask long-term trends in ozone levels. Day-to-day variations mask day-of-week differences in ozone levels and the impact of interbasin transport. After coordination with existing efforts, this project seeks to understand and account for these variations to more accurately characterize the long-term variations in ozone with changes in precursor emissions.

Some work on CCOS meteorology has been done and additional effort is on-going. The SJVAPSA awarded a contract to T&B Systems to characterize the meteorology and air quality during the CCOS field study. In the initial phase of this work, which has been completed, T&B and their subcontractors evaluated the meteorological representativeness of the CCOS modeling episodes and utilized routine ambient data to identify where and when ozone formation is limited by the availability of radical species or NOx. These initial analyses will be expanded in the next phase of T&B's study by utilizing the full CCOS data base. This phase will also include a historic perspective of the long-term meteorological cyclic pattern in relation to air quality in central California during 1980-2002. Long-term trends in ozone (maximum 1-hour and 8-hour) and its precursors will be characterized within the CCOS domain for the summer ozone seasons from 1980 to 2002. In addition to concentration, the trends in the timing of peak 1-hour and 8-hour ozone concentrations will be examined. Available data from Photochemical Assessment Monitoring Stations (PAMS) will be used to establish VOC trends. If appropriate, carbon monoxide data will be used as a partial surrogate for nonmethane organic compounds during the early years during which VOC data are not available. T&B will quantify the changes in ozone, ozone precursors, and oxidation products between 1990 and 2000 using the data from the SJVAQS/AUSPEX and CCOS field studies. Changes that will be examined include organic and nitrogen speciation, VOC/NOx ratios, photochemical reactivity of organic compounds, and extent of reaction. T&B will also summarize and interpret relevant results and findings from past studies that provide insight into the patterns of change in ozone concentrations with changes in emissions.

<u>Technical Objectives</u>

This project is coordinated with past and on-going efforts and is focused on multivariate trends analysis to addresses the following objectives.

- Characterize the meteorology-adjusted changes that have occurred in ambient ozone and precursor concentrations in central California between 1990 and 2002 (pending data availability), and reconcile the ambient trends with corresponding trends in VOC and NOx emissions.

- Classify ozone episodes by meteorological condition and transport potential.

- Characterize day-of-week variations in peak ozone levels relative to corresponding variations in ambient VOC and NOx.

These objectives are to be meet by updating similar analyses that have been conducted in the past and by complementing or expanding data analysis efforts that are currently underway.

Scope of Work

The scope of work for this project includes the following three tasks.

Task 1. Multivariate analysis of air quality trends and effects of meteorological variations on the temporal and spatial variability of pollutant concentrations

Based on a review of existing ozone forecasting methods and protocols in current practice within the CCOS domain, identify the physical and chemical variables that influence ozone concentrations in the domain. Supplement the air quality data used in the previous tasks with appropriate meteorological data and other predictor variables. Use appropriate statistical methods to establish the quantitative relationship between peak ambient ozone concentrations and the predictor variables, and evaluate the performance of the statistical model by randomly selecting a portion of the data set for independent evaluation. Correlation methods to be considered include, but are not limited to, the criteria approach, classification and regression tree analysis (CART), and parametric regression analysis (Cox and Chu, 1993, an EPA-recommended method). The contractor should evaluate both multi-linear regression and curvilinear regression. Curvilinear regression may be valuable for including NOx or VOC in the trend analysis because it may capture the non-linear relationships of ozone and predictor variables better than multi-linear regression. Apply the same approach to observations and model predictions. Generate regression equations or other statistical results from each set and compare predictive capabilities. Determine the effect of uncertainties on the statistical results by appropriate methods. Use the results to apply meteorological adjustments to and estimate uncertainties for ozone trends for the years 1990 to 2002.

Task 2. Classification of ozone episodes by meteorological condition and transport potential

Past attempts to classify high ozone days in the CCOS region are summarized in Fujita et al, 1999, Chapter 2. As part of the CCOS planning effort (Fujita et al. 1999, "CCOS Field Study Plan, Version 3, 11/24/99"), a subjective classification method (inspection of weather charts) for all 1996-1998 ozone season days and a cluster analysis of selected high ozone days during those three seasons were performed. In the latter analysis, differences in a few meteorological variables were statistically significant among three ozone clusters identified. As part of the current T&B contract, ozone episodes will be classified according to upper air weather maps, and statistical analyses will be used to determine if meteorology alone can distinguish between the different ozone-based classifications. In this new task, the contractor will attempt to classify high ozone days that exceed a selected threshold during the period from 1996 to 2001 by meteorological scenario determined by analysis of synoptic and mesoscale meteorological parameters.

To complement previous work and the existing T&B effort, the contractor shall evaluate several corroborative methods to classify ozone episodes into meteorological and potential transport scenarios. This evaluation may include, but is not limited to: cluster analysis performed on ozone concentrations (e.g., Fairley and Demandel 1996; Fujita et al. 1999) and/or performed on selected meteorological parameters; empirical orthogonal functions analysis (including principle components analysis) applied to ozone concentrations (e.g., Ludwig et al. 1995) and to windfields (e.g., Green 1992); backtrajectory classification (e.g., Ashbaugh et al. 1983; Stoeckenius et al. 1994; Green and Gebhart 1997); and CART analysis. The contractor shall justify selection of two methods as most promising for the CCOS region. Perform the classification using those two methods. For each air basin, classify episodes according to transport potential. Evaluate the representativeness of the CCOS episode days for investigating pollutant transport scenarios in different regions of the CCOS domain.

Task 3. Day-of-week variations in peak ozone levels relative to corresponding variations in ambient VOC and NOx

It is well documented that ozone levels in many urban areas are higher on weekends relative to weekdays despite the fact that NOx, and to a lesser extent, VOC emissions are lower on weekends (Altshuler et al, 1995). This effect was limited to coastal areas of the CCOS domain during the 1980's, but has become more noticeable in urban areas of the central valley during the 1990s (Marr and Harley, 2002). In addition, the effect has become more pronounced on Sundays in recent years. Past analyses have documented trends in the magnitude and spatial extent of the weekend ozone effect but have not fully examined the underlying cause of the effect.

This task will summarize and update existing analysis of the day-of-the-week variations in ozone and ozone precursors in the CCOS domain using VOC data from the Photochemical Assessment Monitoring Stations. The analysis should focus on day-of-week changes in the diurnal variations in NO, NOx, and VOC concentrations and VOC/NOx ratios during the 1995-2001 period and the effect of these variations on the extent of ozone inhibition and rate of ozone accumulation. Similar analysis may be extended to earlier period using routine CO data if correlations between VOC and CO can be established. The weekend ozone effect are typically observed in areas that are VOC limited with respect to ozone formation. The degree of the NOx disbenefit that may result from lower weekend NOx levels could be a function of the extent of reaction. Therefore weekday variations in ratios of ozone to potential ozone (e.g., O_3 + NO_2) should be examined in relation to corresponding variation in VOC/NOx ratios. Develop a conceptual explanation of the evolution of the magnitude and spatial extent of the weekend ozone effect in the CCOS domain. Characterize the day-of-week variations in ozone and ozone precursor during CCOS episodes that include weekends and determine whether these variations are consistent with this general conceptual explanation. Evaluate the consistency in the spatial and temporal variations in ambient VOC/NOx ratios and speciation of VOCs and oxides of nitrogen with corresponding values derived from emission inventory data. Identify and, to the extent possible, quantify discrepancies between ambient and emission inventory data.

Task 4. Reporting

Prepare progress reports in accordance with contract requirements and submit a draft and revised final report summarizing the study results, findings, and conclusions. Prepare and submit a manuscript for publication in a peer-reviewed journal.

Expected Results and Benefits

Provides better understanding of the meteorological uncertainties associated with long-term ozone and ozone precursor trends and their implications for ozone attainment.

Estimated Cost**:** $75,000

Schedule**:** 12 months

References

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3.3 Model Development and Evaluation

3.3.1 Link Data Analysis and Modeling Efforts (Project III-10)

Past modeling efforts in central California have required compromises in model resolution, both spatially and temporally, due to computational limitations and regulatory deadlines. These compromises in model resolution may mask important features that might lead to a better understanding of atmospheric dynamics and transport, and ozone formation and distribution. While improvements have been made in model formulation and computing capability, many of the same limitations may pose unnecessary constraints on model performance.

Technical Objectives

This project would identify specific cases of significant discrepancies between model predictions and observations and develop a hypothesis of their cause. Examples include discrepancies in the gradient of ozone concentrations from source to receptor. Model setup will be appropriately modified (e.g., grid resolution, temporal resolution) to determine effect of the modifications on model predictions and reconcile the differences with air quality and meteorological data. These analyses and simulations will be compared to determine consistencies in the conclusion derived from modeling versus data analyses and the implications of limitations in both modeling and data analysis.

Scope Of Work

In order to link data analysis and modeling efforts, the contractor will determine the important physical and chemical variables that influence ozone concentrations in the CCOS domain. The contractor will review data analysis results and investigate from observations the details of meteorological parameters and determine the spatial and temporal resolution. The contractor will make suggestions on the model setting (e.g, horizontal and vertical grid spacing and time spacing) to capture the details in observation that may affect ozone formation and accumulation.

Specific cases of significant discrepancies between model predictions and observations will be identified and a hypothesis for their causes will be developed. Examples include potential discrepancies in the gradient of ozone concentrations from source to receptor, the rate of change in mixing heights, and rate of change in the concentrations of short-lived species. Model setup will be appropriately modified (e.g., better grid resolution and greater temporal resolution than one hour) to determine the effect of the modifications on model predictions and reconcile the differences with air quality and meteorological data. The contractor will formulate the implications of their analysis for ozone formation and its abatement.

Expected Results And Benefits

Results of data analysis may provide useful guidance in selecting modeling setup and parameterizations in order to improve modeling of atmospheric and chemical processes associated with the formation, accumulation and transport of ozone in the CCOS modeling domain. The results of this study will result in better optimization between computational requirements and accuracy of modeling results.

Estimated Cost**:** $100,000

Duration Of Project: Twelve months

3.3.2 Improve Mass Conservation Module (Meteorological and Air Quality Models) (Project III-11)

The mathematical structure of certain algorithms in atmospheric, dispersion and air quality models has assumptions and simplifications that can lead to incomplete treatment of mass conservation. One of the main problems in atmospheric models is incomplete treatment of the continuity equation that consequently induces mass inconsistency of species in some of the photochemical and other chemical models. The incomplete treatment of air density and wind fields is actually similar, since individual continuity equations for every species have pseudo-source/sink terms. An additional problem arises for air quality modeling applied to regional and mesoscale domains since the inflow of total air mass is supplied by large-scale models that generally have incompressibility and hydrostatic assumptions with governing equations in a non-conservative form. These are very important issues since air quality models require strictly mass-consistent atmospheric input to ensure mass conservation of trace gases. Practical solutions that introduce mass adjustment terms in some or all components of the modeling system (atmospheric, dispersion, and chemical modules) occasionally introduce large mass corrections that can bring large errors, bias, and artificial compensating effects when applied to SIP models. This project will focus on analysis of the effects of the mass adjustment terms in each of the modeling components and suggest efficient ways of minimizing the use of the mass adjustment terms that are relevant to SIP modeling.

Technical Objectives

In principle, a fully-coupled meteorological-chemical model (Seaman 1995) would avoid most of the mass inconsistency effects. A meteorological model needs to be fully incompressible with governing equations in the conservative form and using a coordinate system that fully preserves mass. In this case, all meteorological parameters should be available at the finite time steps needed for the air quality model.

Since most air quality models currently use meteorological models that are not fully conserving mass, various correction terms to account for mass consistency have been developed. In photochemical models the mass consistency error is corrected by advecting a reference quantity (calibration gas) together with the trace species concentration. The concentration of this calibration gas is then used to correct the interpolated concentration of the trace species. Some of the commonly used mass correction schemes are based on the following principles:

- The approximation of mass inconsistency considers only the local tendency term in the continuity equation.

- Use of the continuity equation without any approximation. The mass-correction term is then estimated from the finite-difference approximation of the local tendency term.

- Application of a two-step time-splitting method by solving the continuity equation with zero source terms separately from the mass-correction step. This leads to the most accurate mass-corrected concentration of species.

It is also important to understand the additional assumptions and approximations in air quality computations that lead to errors and uncertainties in the estimated concentrations. These include:

- Inaccuracies due to temporal interpolation of the velocity and density fields that are used in chemistry transport models.

- Choice of time-independent vertical coordinates that do not allow full conservation of mass.

- Assumptions and simplifications in the treatment of the atmospheric dynamics such as incompressibility, hydrostatic approximation, non-divergent flow, and the Boussinesq approximation that affect the full treatment of mass conservation through the continuity equation.

- Assumptions and simplifications of the treatment of topography in the atmospheric models that eventually lead to erroneous computations of the pressure and density fields.

- Treatment of dry and wet deposition processes and their effect on mass conservation.

- Interaction of trace species with the earth's surface and their detrainment in the free atmosphere.

- Chemical transformation mechanisms that are not fully incorporated in the treatment of the mass conservation.

The purpose of this study is to evaluate the mass-correction algorithms that are being used in the CCOS air-quality modeling program. The analysis should quantify the effects of mass-correction terms and possible inconsistencies in other components of the air quality models. The study should propose more effective and accurate ways of improving or fully incorporating treatment of mass conservation.

<u>Scope Of Work</u>

The study should consists of the following main components:

- A review of the air quality modeling efforts performed for the CCOS study so far.

- A critical analysis of atmospheric models used to drive photochemical and other air quality models. The analysis should include treatment of the mass conservation and errors in the mass conservation algorithm that are caused by selection of the coordinate system and framework, incomplete continuity equation, presentation of topography, approximations in the numerical solution of the model equations, and other relevant factors.

- A critical analysis of the air quality models used for the CCOS study with an emphasis on the photochemical models. The analysis should include model structure, assumptions, and approximations.

- An examination of mass correction/adjustment procedures used in the air quality models. The study should reveal to what extent this mass-correction terms induce mass imbalance as artificial sinks and/or sources of emission and consequently lead to bias or compensating errors in the SIP models.

- This project will suggest the optimum use of the mass conservation algorithms and alternative ways that can minimize or substitute their use.

- The study should provide a cost-benefit analysis of using various levels of mass conservation treatment (from simple mass correction terms to a full treatment of the mass conservation) with a special emphasis on the photochemical models used and to be used in the CCOS program.

- The final step of the study should include sensitivity tests of various schemes for mass conservation treatment on the final predictions of pollutant concentrations by air quality models.

<u>Expected Results And Benefits</u>

The main results from the study will be:

- A comprehensive analysis of the algorithms used for mass conservation treatment and corrections that are required by the air quality models.

- A valuable critical evaluation and inter-comparison of various mass conservation techniques and their effect on air quality model predictions.

- Estimates of air quality model uncertainties and errors due to incomplete treatment of the mass conservation.

The main benefits of the project will include:

- Suggestions for the optimum use of the mass correction terms and innovative ways of minimizing their use.

- The study results will improve the accuracy of the SIP models as well as will have bearing on the development and modification of air quality models in general.

Schedule

The study will be completed in two phases. The first phase of four-month duration should include a critical evaluation of the models and mass-conservation treatment algorithms. The second phase taking up to eight-months will include sensitivity tests using a selected air quality model used in the CCOS study and recommendations for the optimum treatment in the air quality models and their implementation in the SIP models.

Estimated Cost

This project will be funded in two phases, $100,000 for Phase 1 and $200,000 for Phase 2.

References

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Chang, J. S., S. Jin, Y. Li, M. Beauharnois, C.-H. Lu, H.-C. Huang, S Tanrikulu, and J. DaMassa, 1997: The SARMAP air quality model. Fin. Rep., SJVAQS/AUSPEX, Regional Modeling Adaptation Project, 53 pp.

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3.3.3 Improve Aloft Model Performance (Project III-12)

A review of previous California air quality studies shows that models have not done well in predicting ozone aloft. For example, in the San Joaquin Valley, Thuillier and Ranzieri (1995, 1997a,b) have described evaluation of the SARMAP (San Joaquin Valley Air Quality Study and Atmospheric Utility Signatures, Predictions and Experiments Regional Model Adaptation Program) effort. They conclude that, in general, the model represented the relative magnitude and distribution of ozone, it tended to underestimated surface ozone as well as ozone and ozone precursors aloft and overestimated surface ozone at night. Modeled boundary conditions also significantly departed from concentrations measured aloft by aircraft.

The CCOS measurements can support many independent approaches to evaluate and corroborate model results and uncertainties, including those applicable to this ozone aloft problem, as discussed in the CCOS Conceptual Plan (Fujita et al, 1999). This is an opportunity to understand relevant model deficiencies and improve model performance.

Technical Objectives

Technical objectives for this project are:

- Diagnostic evaluation of model performance in predicting ozone aloft. The evaluation should include both atmospheric and photochemical modules of the modeling system and the interaction between them.

- Investigation into the reasons for model-measurement discrepancies during CCOS. The investigation should focus on major components of the modeling system such as:
  - Inaccuracy of initial and boundary conditions
  - Insufficient model horizontal, and especially vertical resolution
  - Uncertainty in the computation of mixing depth and treatment of turbulence aloft
  - Problems in predicting accurate moisture and cloud parameters
  - Problems in treating radiation effects in cloudy and clear sky atmosphere
  - Inaccuracy of predicting local circulations in complex terrain

- Recommendations on improving model performance (both atmospheric and photochemical models) in predicting ozone aloft

- Recommendations on improving measurements aloft (aircraft, balloon, remote sensing) to provide more accurate initial and boundary conditions for modeling and the model evaluation

Scope of Work

Other approaches might be considered, but the following is proposed:

Prepare a summary of past documentation of poor model performance of ozone aloft, not only in California, but also in large modeling-measurement air quality studies conducted around the country in the last decade or so. Then the basic approach is to then find the times when CCOS model predictions of ozone aloft depart significantly from measured ozone aloft, develop hypothesis for the cause of the departures, perform sensitivity studies to characterize the effects of changing parameters, and make recommendations to improve model performance. Sensitivity studies should include estimates of the extent to which inaccuracy of the predicted meteorology causes discrepancies and errors in predicting ozone aloft. Some diagnostic evaluation of modeling is already expected as part of the CCOS modeling effort. This could serve as a starting point to identify departures between modeling and measurement.

The study should cover a wide range of spatial and temporal scales of interests. The spatial scales should cover regional to urban scales, while the temporal should consider diurnal effects that are relevant for accurate prediction of elevated ozone.

The following is a task-level statement of work to be completed during this study:

Task 1 – Summarize what is known about past inconsistencies between model prediction of ozone aloft and measurement of ozone aloft.

Task 2 – Using the CCOS modeling results, identify all model-measurement discrepancies, classify them into different types, and summarize any new problems. Compare CCOS results to past modeling performance.

Task 3 – Using the CCOS modeling results, perform an investigation of each type of discrepancy. Develop working hypothesis of sources of the discrepancies.

Task 4 – Perform sensitivity analyses to see the impact of different parameters on improving model performance.

Task 5 – Documentation and Reporting

Expected Benefit and Results

An improvement in model performance in predicting ozone concentrations aloft is expected. This would give better estimates of inter-basin transport, currently the single best method to estimate the impact of upwind emissions on downwind concentrations. Furthermore, transport is known to occur at night when radiative cooling can cause de-coupling of the flow aloft in some areas (e.g., the San Joaquin Valley nocturnal jet). Better predictions can lead to greater confidence by local district personnel in model predictions of transport would help ARB negotiate inter-basin issues. The expected results will also provide an excellent basis for the future real-time forecasting of ozone on short and long-time scales.

Estimated Cost: $150K.

Schedule**:** 15 months, the last 6-9 months after CCOS modeling is completed.

References

Chang, J. (1997) The SARMAP Air Quality Model (SAQM) – Prepared for the San Joaquin Valley Air Quality Study Agency.

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3.3.4 Long-Term Seasonal Modeling (Project III-13)

The implication of the state 1-hour ozone standard and the new federal 8-hour ozone standard is that they require a reappraisal of past strategies that have focused primarily on addressing the urban/suburban ozone problem to one that considers the problem in a more regional context. Current practice for air quality planning involves modeling one or two high-ozone episodes of three to four days. However, there are about three times as many exceedances of the 8-hour ozone standard than the 1-hour standard in most part of the CCOS modeling domain. Because ozone formation is a nonlinear process with respect to its precursors, VOC and NOx, different control strategies may be required to address the 1-hour and 8-hour ozone standards. Evaluating appropriate strategies to address the 8-hour standard will require modeling over significantly longer time periods that the CCOS episodes.

Technical Objectives

A comprehensive air quality modeling system will be used to simulate the summer 2000 season in Central California. The objective is to determine how emission control requirements may differ in space and time within Central California for the current 1-hour, 120 ppb ozone standard, and the new 8-hour, 80 ppb ozone standard.

Scope of Work

This project involves analyses of meteorological, emissions, and air quality measurements made during CCOS and defining day-specific model inputs for the summer season. Model performance will be evaluated using the CCOS data set and diagnostic tools. The sensitivity of air pollutants to local vs. upwind sources of emissions will be quantified. Products of our research, achieved through modeling and extensive analyses, will be suggestions for strategies that effectively improve the air quality throughout the region.

Task 1 - Develop Modeling Protocol. Prepare a modeling protocol that describes the objectives, project schedule, input data preparation methods, modeling and analysis tools, performance evaluation, and plans for interpretation and dissemination of the results.

Task 2 – Install Computing System. Ascertain the required computing requirements and acquire and install a high-performance computing system to enable air quality modeling need for this project.

Task 3 – Prepare Model Input Data. Prepare or obtain from the ARB temporally- and spatially-resolved input data for boundary conditions, source emission rates, and meteorological conditions across the modeling domain. Where necessary and applicable, use field measurements from CCOS in developing the necessary input data. It is anticipated that the meteorological modeling will be conducted by researches at NOAA under separate funding. While ARB will provide summer 2000 emissions inputs for CCOS episodes, it will be necessary to make adjustments to emission estimates on a day-by-day basis to account for variations in temperature, which in turn influences evaporative and biogenic VOC emissions.

Task 4 – Conduct Air Quality Modeling. Select an air quality model and chemical mechanism with input from ARB. Conduct episodic modeling in order to provide a basis for compoarison for the seasonal modeling. Run seasonal modeling for the summer 2000 season and evaluate model performance.

Task 5 – Analysis of Model Results. In addition to the operational evaluation of model results in Task 4, apply state-of-the-science analytical tools to study in detail the responses of air pollutants to precursor emissions. Potential approaches include Direct Decoupled Method, Process Analysis, and various corroborative analyses. Quantify and diagnose the response in ozone levels to precursor emissions for different subregions of the modeling domain, on weekdays versus weekends, for a wide range of meteorological conditions including stagnation, recirculation and inter-basin transport.

Task 6 – Deliverables. Prepare a final report documenting the objectives, methods and results. In addition, prepare and submit a manuscript for publication in a suitable peer-reviewed journal.

Expected Benefits

This project addresses the efficacy of emission control programs in meeting the 1-hour versus 8-hour ozone standards and the effects of transport on peak 1-hour versus 8-hour ozone levels in downwind areas.

Estimated Cost: This project will be split-funded with $100K allocated during Phase 1 and $200,000 in Phase 2.

Schedule**:** 36 months

3.3.5 Website Access to Modeling Results (Project III-14)

The benefits of Internet access to data from large field projects is well established by previous air quality studies similar to CCOS. More efficient and flexible dissemination of modeling results will the facilitate review of preliminary results by study sponsors and the CCOS Technical Committee. The SIP planning process will benefit from more timely distribution and analysis of the CCOS modeling results.

Technical Objectives

This project establishes a website to disseminate CCOS modeling results and provide access to post-processing software for generating selective outputs of model results. Internet access to meteorological and air quality results from all CCOS simulations would be placed and maintained on the ARB website.

Scope of Work

Coordinate with ARB website personnel and the ARB Modeling and Meteorology Branch to place all CCOS modeling results on the ARB website for public dissemination. Establish the website and provide technical support to ARB staff in maintaining the web site. Add new modeling results as they becomes available and preserve the original form of the model results but also offer a standardized form across the modeled results.

Expected Benefit and Results

Personnel from local districts and research organizations can have immediate access to modeling results. More extensive evaluation of modeling results by a variety of different organizations is possible, leading to more constructive feedback on the SIP modeling exercise.

Estimated Cost: $30 K

Schedule: 12 months, the last 9 after CCOS modeling is completed.

3.3.6 Cloud Effect in Modeling (Project III-15)

Meteorological modeling for SARMAP (San Joaquin Valley Air Quality Study and Atmospheric Utility Signatures, Predictions and Experiments Regional Model Adaptation Program) overestimated cloud cover. Consequently, the cloud module was turned off in the SARMAP meteorological modeling. This did not affect the results of these simulations because no clouds were present during any of the SARMAP episodes. However, clouds were present during some of the CCOS episodes, and their effects will need to be addressed. Also, there is interest in meteorological adjustments of long term ozone trends, and to support the requirements of seasonal modeling (Project III-18) for summer 2000, where some cloudy days did occur in 2000. In addition, some summer monsoon days, with a potential for clouds, can exacerbate ozone in the southern SJV, where southerly flow may reduces the outflow over the Tehachapi Mountains. Finally, the cooling effect of nearby clouds may influence mesoscale flows so as to impact the transport and/or formation of ozone in and around areas that are otherwise sunny. For all these reasons, improved treatment of clouds in the MM5 meteorological model can be important.

Technical Objectives

This project will evaluate the presence of clouds during CCOS episodes and estimate the likely implications of ignoring the actual presence of clouds on ozone predictions and transport.

Scope of Work

The contractor will test and evaluate MM5 for simulating clouds and identify deficiencies in the cloud module and suggests improvements. Inputs for the MM5 simulations will be supplied by the ARB. Determine which summer 2000 days were cloudy, anywhere in the CCOS domain. Determine on which of these days clouds may have had impacts to ozone formations, and identify those potential impacts. Work with ARB to run sensitivity tests on a few selected days, with and without the cloud module.

Expected Benefit and Results

An improvement is expected in seasonal modeling results, and in the treatment of cloudy days in assessing long term meteorologically adjusted ozone trends. A better understanding of the effects of monsoonal flow in the southern SJV may result.

Estimated Cost**:** $80 K.

Schedule: 15 months, the last 6 months after CCOS modeling is completed.

4. CATEGORY III PROJECTS – PHASE 2

This section explains the technical objectives for proposed Phase 2 Category III projects and describes their scope of work and estimates the costs and benefits. Seven Phase 2 projects are recommended with a total estimated budget of $0.61 M. Two additional projects totaling $0.4 M are continuations of Phase 1 projects.

4.1 Emission Inventory Development and Evaluation

4.1.1 Refine Stack Parameters (Project III-6)

Stack Parameter data (stack exit velocity, exit temperature, flow rate, pollutant emission rates, physical parameters) are archived at ARB in CEIDARS (California Emissions Inventory Development and Reporting System), the ARB emissions database. CEIDARS is in turn accessed for specific applications. The CEFS (California Emissions Forecasting System), for example, accesses CEIDARS to generate base year Emissions Inventories for specific domains and, from that, to forecast and back-cast Emissions Inventories based on projected economic and demographic changes and on projected emission control penetration. CEIDARS is also the basis for emissions input data files used for CCOS modeling. Emissions data is entered into CEIDARS at the District level, either directly through batch loading or on-line, or indirectly through written reports that are subsequently entered by ARB staff, with corresponding QA reports returned to the districts. There is presently no QA screening to check data for reasonability, other than very broad flagging criteria that are used only to establish deviations from extremely broad boundaries to identify only the most obvious errors. These broad boundaries are insufficient for assigning default stack parameters, or for the more refined error flagging essential to accurate modeling.

There are many reasons for imprecise or uncertain stack data, not all associated with source or District-level input. There may be imprecise definitions of what constitutes a stack, and standards and definitions may differ from District to District. Stack data are not always easy to find for smaller stacks. (ARB asks all districts to provide stack information on any stack over 49 feet and 25 t/year of any criteria pollutant emission.) In some cases, facility coordinates have been used for all processes within a single facility. Steam generators and Internal Combustion engines, because of their ubiquitousness within large facilities, have been assigned stack status and are thus prime candidates for development of default parameters described below. Some of the stack parameter uncertainty may be a result of insufficient District-level time and labor resources, or insufficient expertise on the part of small reporting operators with respect to air pollution and test methods and procedures for stack parameter measurement and reporting.

The result is possible shortcomings with respect to stack parameter data completeness and accuracy. Also, preparation of gridded emissions inventories with present resources can result in many stacks that are not important to the specific application, e.g. CCOS emissions data files. The issues, which require refinement of CEIDARS stack data to resolve, are:

Some of the stacks may be too small to matter.

Some of the “stacks” may not be stacks.

Entered values may be null values, or unreasonable values.

To address these issues, ARB needs to be able to screen stack data archived in CEIDARS and identify stacks with data that are good or invalid/missing, and stacks that are significant (with respect to type and quantity of emissions) and stacks that are not significant. In the case of invalid/missing data, a method for defining and substituting default values could add to the completeness of stack emissions inventories used in CCOS and other modeling applications. Such a default paramaterization method should be based on rigorous statistical analyses of existing valid stack data. Associated software should include safeguards to protect the database from inappropriate use that could compromise data integrity.

Technical Objectives

Technical objectives for this project are to develop screening criteria for stack data in CEIDARS, default stack parameter values for defined source types in CEIDARS, and develop and implement modular software, for use with CEIDARS, to screen stack data, identify erroneous or missing stack parameters, and replace as appropriate with default values.

Scope Of Work

The following is one approach, as suggested by an ARB scientist who has researched the problem in detail. Other approaches might be considered.

1. Do a clean-up and analysis of existing CEIDARS stack data, with the following considerations:

a. Exclude obviously erroneous data, and establish overall distribution (quartiles/deciles/percentiles/median/max/min/mean) for stack data both for the entire data set, and for SCC (Source Classification Code)-SIC (Standard Industrial Classification) groupings (or SCC only). Look for clusters in the distributions for all of the parameters and emissions.

b. In cases where a given SCC seems to break into subgroups based upon emissions or a given parameter value, establish sub-grouped SCC-SIC-parameter value classes, or something similar.

c. Establish sub-groupings based upon region of the state, to see if stack parameters vary by region within the state.

d. Do categorical statistical correlation analysis to see of there is a correlation between SCC-SIC category and stack parameter numeric value (and other analyses, such as cluster analysis, etc.). In some cases, a multivariate approach may be required.

e. Group similar SCC's together to attempt to create a more robust/larger data set and then repeat categorical correlation, and other analyses.

f. Do basic regression analyses to look for relationships between various parameters, including stack height/diameter/velocity/flow/temperature versus emissions, or some type of process throughput for the entire data set, and then compare to single SCC's or grouped SCC's (or SCC+SIC).

g. Try to establish internal relationships between the stack parameters, both in terms of regression and ranges.

2. Prioritize by SCC code and emissions by the amount of perceived "problem" parameter entries, and determine the stack groupings that need to be focused on first.

3. Based upon the results from steps 1 and 2, perform surveys to determine “standard” installations for any given SCC-SIC grouping. This should include a literature search and consultations with Air Quality Districts, EPA, industry trade groups, and equipment manufacturers and installers. These may vary by facility size and may need to consider various ranges of process throughput. Results should include clear and precise numeric values and ranges, with ample documentation. Definitions of standard grouping parameterizations should be additionally validated through field ground truth surveys of a statistically representative sample of facilities.

4. Compare results from step 1 with results from step 3. Establish confidence levels in the default assignments, which will need to be provided to users of any data that has been impacted by the default assignments.

5. If the confidence levels in step 4 are sufficient to warrant it, on an SCC-SIC grouping basis, write code into CEIDARS that incorporates the statistically-based, and survey-based default assignments. This code should produce flagged reports back to the district, and would allow users of the data to select to override the existing CEIDARS stack parameter data (or supplement it with additional fields) with the input default data. By having a confidence level rating (say 1 for lowest, and 5 for highest), modelers could, for example, choose to only default if the confidence level is at level 5, and discard any stacks that cannot be assigned defaults with that level of confidence.

Default data could also be used to rate existing stack parameters according to how well it compares with the default values according to a similar confidence rating. This would allow modelers to decide if they need to examine certain data that differs from the typical (default) data for that SCC-SIC-emissions level.

Along with the confidence levels, modelers and District personnel will need to know how the defaults were arrived at, so ample on-line documentation will be essential.

Code developed for default paramaterization of stack data in CEIDARS should be written with the intent of minimizing modification of existing data. This could be done by writing new fields into CEIDARS, or by creating default data externally, with options for using default data when creating domain-specific Emissions Inventories.

6. The final report for this project should be well documented, as should be any computer code for CEIDARS that is written, so that ARB staff could update the default assignments as conditions change, or as additional data becomes available. Documentation should clearly describe methods used to maintain the integrity of original stack data.

The following is a task-by-task statement of work to be completed during this study:

Task 1 – Initial Assessment and Cleanup of CEIDARS Stack Data

Task 2 – Statistical Analysis of Stack Data in CEIDARS

Task 3 – Literature Review (including communication with other agencies and manufacturers).

Task 4 – Specification of Source Groupings and Associated Stack Default Parameters

Task 5 – Software Development and Testing

Task 6 – Documentation and Reporting

Expected Results And Benefits

The expected benefit to the CCOS program might best be estimated by considering the total ozone precursor emissions (NO_x and ROG) that might be affected by uncertainties in associated stack parameterization, as a percentage of all precursor emissions in the CCOS study area. The attached table shows annual average daily emissions (t/day) for all stationary sources that could be coded as stacks, average daily emissions from all sources, and the corresponding percentages of total precursor emissions that are from stationary stack sources. Overall, within the CCOS study area, Stationary sources account for about 19% of all NO_x emissions and about 25% of all ROG emissions. This of course includes major stationary sources such as power plant stacks for which stack parameters encoded in CEIDARS have high certainty. The greatest uncertainties with respect to stack parameters coded in CEIDARS are likely to be associated with mid-size to small stacks, with lower individual emissions. The actual percentage of emissions that are likely to be affected by the proposed project is probably less than indicated by the attached table, perhaps 5% to 10% of all emissions.

In addition to its benefits for ozone modeling for CCOS, the proposed project also has great potential benefit for increasingly important toxics modeling, especially hot spots modeling which is significant on a very local basis and highly sensitive to the paramaterization of nearby stationary stack sources.

Estimated Cost: $100K.

Duration Of The Project:

The study should be completed in a 6 to 9 month period. Sufficient time should be allowed to ensure adequate development and validation of sensitive modular software to be used with CEIDARS.

NOx (t/day)	San Francisco Bay	Mountain Counties	North Central	Sacramento Valley	San Joaquin Valley	Total
	Air Basin					
Stationary Source Emissions	61.46	6.16	20.36	31.18	180.96	300.12
Total Emissions	553.6	60.75	81.99	292.61	602.15	1591.1
Percent NOx Emissions from Stationary Sources	11.1	10.1	24.8	10.7	30.1	18.9
ROG (t/day)						
Stationary Source Emissions	313.36	7.05	14.27	47.12	96.34	478.14
Total Emissions	939.28	107.31	82.21	291.66	507.97	1928.43
Percent ROG Emissions from Stationary Sources	33.4	6.6	17.4	16.2	19.0	24.8

4.2 Model Development and Evaluation

4.2.1 Improve Mass Conservation Module (Meteorological and Air Quality Models) – Phase 2 (Project III-11b)

See Page 3-14 for description of both Phases 1 and 2 of this project.

4.2.2 Long-Term Seasonal Modeling – Phase 2 (Project III-13b)

See Page 3-20 for description of both Phases 1 and 2 of this project.

4.2.3 Extend Previous Analysis Effort (Project III-16)

The Central California Ozone Study (CCOS) is the latest milestone in the developing understanding of the physical and chemical processes that govern the formation, accumulation and transport of ozone in central California. Prior to CCOS, much of the existing conceptual understanding of the ozone problem in the central California was based on the field measurements, data analysis, and modeling associated with the San Joaquin Valley Air Quality Study/Atmospheric Utilities, Signatures, Predictions, and Experiments (SJVAQS/AUSPEX). In the intervening decade since the completion of SJVAQS/AUSPEX, data analysis and modeling methods have continued to develop and improve. These latest data analysis and modeling approaches are being applied to the CCOS database. This project seeks to apply some of these tools to the SJVAQS/AUSPEX data to determine whether such reanalysis of the data confirms the original analysis or yields new insights.

Technical Objectives

This objective of this project is to identify analyses that were applied to the CCOS data that were not applied to the 1990 SJVAQS/AUSPEX data, perform selective reanalysis of the 1990 database and to reconcile the findings of the new analyses with previous relevant conclusions.

Methods And Approach

The contractor will reanalyze the 1990 database using current data analysis methods. A retrospective analysis of the previous efforts will be made to identify previous data analysis that can be updated using methods that have been developed since SJVAQS/AUSPEX. The contractor will utilize products from CCOS data analysis and modeling to revisit prior ozone episodes to examine the applicability of SIP modeling to the full range of episode types identified in the characterization process for all air pollution precursors and products. The project will include an examination of the representativeness of the episodes used for SIP modeling based on meteorology and air quality considerations and an identify deficiencies in the previous SIP modeling efforts.

Expected Results And Benefits

An examination of data from both CCOS and SJVAQS/AUSPEX using common data analysis methods may provide additional insights into the evolution of the region's ozone problem in the past decade. Changes in spatial distributions of peak ozone levels in response to changing precursor concentrations must be reconciled with changes in estimated emissions in order to understand the consequence of past emission control programs.

Estimated Cost: Not to exceed $150,000.

Schedule: Six months

References

California's 1994 State Implementation Plan for Ozone, http://www.arb.ca.gov/sip/sip.htm

California's State Implementation Plan, http://www.arb.ca.gov/sip/siprev1.htm

California's 1994 State Implementation Plan for Ozone, Volume IV, The "Local Emission Control Plans and Attainment Demonstrations" for six California nonattainment areas include the nature of the regional ozone problem, the status of the local plan, a summary of the ozone attainment strategy and Board actions, http://www.arb.ca.gov/sip/sipvol4.htm

4.2.4 Conduct Uncertainty Analysis and Suggest Improvements (Project III-17)

Air quality models are developed using experimental data from the laboratory, in environmental chambers, or in the field, and they require a great amount of input data for their operation. There is always error and uncertainty associated with these measurements. The reliability of model predictions can be assessed if the uncertainty distributions of the model parameters can be determined. It may be possible to use a probabilistic model to estimate the plus and minus uncertainties on results from the SIP modeling exercise.

The importance of uncertainty in an air quality model depends upon how sensitive an important prediction is to the uncertain process. Thus a coupled sensitivity and uncertainty analysis is required to assess the reliability of model predictions. If investigators could understand which experimental and/or input data uncertainties are most sensitive and which are negligible, they might be able to focus this combined sensitivity/uncertainty analysis on the largest source(s) of model output uncertainty.

One possible sensitivity analysis tool is the decoupled direct method (Dunker, 1984; McCroskey and McRae, 1987) was first applied to the simulation of atmospheric chemical mechanisms. These have been applied to estimate the "error bounds" of model predictions from the product of the uncertainty of a model parameter (or input) and the sensitivity of ozone mixing ratios (or other parameters; Gao et al., 1995; Russell et al., 1995). More recently the decoupled direct method has been implemented in 3-d air quality models (Mendoza-Dominguez and Russell, 2000; Mendoza-Dominguez, et al. 2000) and it could be modified to provide a coupled sensitivity and uncertainty analysis. Another possible method is the Monte Carlo approach. It has the advantage in that it has been applied to process studies, meteorological and 3-d air quality models (Sathya et al., 2001a; 2001b; 2001c)

Technical Objectives

This project will review existing methods and ongoing work for estimating uncertainty within models and model inputs relative to simulation outputs that estimate how ozone concentrations respond to precursor reduction. As a result an uncertainty estimation routine will be developed and incorporated into the SIP model to place uncertainty estimates on simulation results.

Scope of Work

In order to perform the modeling uncertainty analysis the contractor will perform the following tasks.

Task 1. Review existing methods, such as the decoupled direct method, Monte Carlo and other current work for estimating sensitivity and uncertainty within air quality models and their input data.

Task 2. Review methods for linking sensitivity and uncertainty to provide estimates of the "error bounds" on model predictions.

Task 3. Develop combined uncertainty/sensitivity routine for SIP air quality model.

Task 4. Incorporate uncertainty/sensitivity routine into SIP model and perform test simulations.

Expected Results and Benefits

The uncertainty analysis should help understand whether estimates of emission reductions are within the “noise” of the SIP model, or should be considered as reflective of real responses to emission changes. Probability estimates may be applied to bound SIP simulation results.

Estimated Cost: $300,000

Schedule: 12 months

References

Dunker, A.M. (1984) The decoupled direct method for calculating sensitivity coefficients in chemical kinetics, J. Chem. Phys., 81 , 2385-2393.

Gao, D., W.R. Stockwell and J. B. Milford, First Order Sensitivity and Uncertainty Analysis for a Regional Scale Gas-Phase Chemical Mechanism, J. Geophys. Res., 100, 23153-23166, 1995.

Gao, D., W.R. Stockwell and J.B. Milford, Global Uncertainty Analysis of a Regional Scale Gas-Phase Chemical Mechanism, J. Geophys. Res., 101, 9107-9119, 1996.

McCroskey, P.S., and G.J. McRae (1987) Documentation for the Direct Decoupled Sensitivity Analysis Method--DDM, Department of Chemical Engineering, Carnegie Mellon University, Pittsburgh, PA.

Russell, A., J.B. Milford, M.S. Bergin, S. McBride, L. McNair, Y. Yang, W.R. Stockwell and B. Croes, Urban Ozone Control and Atmospheric Reactivity of Organic Gases, Science, 269, 491-495, 1995.

Sathya, V., A.G. Russell, S.Perego, M.Junier, A.Clappier and H. Van Den Bergh (2001a): "Photochemical grid model uncertainty estimates derived from Monte-Carlo analysis of a mesoscale meteorlogical model", (submitted)

Sathya, V., A.G. Russell and H. Van Den Bergh, (2001b) "Correlations among the uncertainty perturbations in meteorological inputs and their influence on Monte-Carlo uncertainty analysis of a Photochemical grid model", (submitted)

Sathya, V., A.G. Russell and H.Van Den Bergh (2001c) "Impact of meteorological input uncertainties on the effectiveness of emission controls designed with a photochemical grid model", (submitted)

Mendoza-Dominguez, A.; Russell, A.G.: (2000) "Iterative Inverse Modeling and Direct Sensitivity Analysis of a Photochemical Air Quality Model," Environ. Sci. Technol. 34, 4974-4981.

Mendoza-Dominguez, A.; Wilkinson, J.G.; Yang, Y.-J.; Russell, A.G.: (2000) "Modeling and Direct Sensitivity Analysis of Biogenic Emissions Impacts on Regional Ozone Formation in the Mexico-U.S. Border Area," J. of the Air & Waste Management Association. 50, 21-31.

4.3 Integration and Synthesis

4.3.1 Summary of Air Quality Studies Conducted in Central California and a Commentary on Selected Issues – Phase 2 (Project III-18)

The Clean Air Act, as amended in 1990, required an attainment plan for each ozone nonattainment area classified as serious, severe or extreme. Nonattainment areas were assigned a statutory deadline for achieving the national 1-hour ozone standard. Serious areas were required to attain the standard by the end of 1999, severe areas by 2005 or 2007 (depending on their peak ozone level), and extreme areas by 2010. In the Central California Ozone Study (CCOS) study region, both the Sacramento Metropolitan area and the San Joaquin Valley were designated serious ozone nonattainment areas. California's 1994 State Implementation Plan (SIP) contained commitments to adopt additional control measures and projected attainment in Sacramento and the San Joaquin Valley by the statutory deadlines. A number of large air quality studies have been conducted over the past twenty years such as SARMAP, SJVAQS, AUSPEX, SAQS to acquire the data necessary to develop ozone abatement strategies and demonstrate ozone attainment. When it was clear that the standard would not be attained by 1999, the ozone attainment status was redesignated for both areas from serious to severe. As for the Bay Area, its attainment status has flip-flopped from attainment in May 1995 to nonattainment in July 1998. The currently deadline for attainment of the national ozone standard in the Bay Areas is 2006.

Past attainment plans for ozone nonattainment areas in central California and elsewhere were consistently overly optimistic in their projections for attainment. Possible problems associated with previous projections may include (but are not limited to) inaccurate emissions inventories for base case and future projections, poor characterization of boundary conditions, incorrect representation of chemical and meteorological processes, emissions controls that were less effective than expected. An understanding of the key factors that contributed to inaccurate projections for attainment is required prior to preparing the next SIP update.

<u>Technical Objectives</u>

This project evaluates and reconciles the technical basis for the projections of attainment of the ozone standard in prior SIPs for each of the ozone nonattainment areas in the CCOS study domain, reconciles these projections with actual trends in ozone, and identifies the key factors and assumptions that contributed to the inaccurate ozone attainment projections.

<u>Scope Of Work</u>

The contractor will evaluate the 1994 SIP process (and previous SIPS if necessary) to determine why the ozone attainment projections were inaccurate. The contractor will evaluate the suitability of the air quality and meteorological models and databases used in the 1994 SIP and compare them with those available currently The contractor will evaluate the modeling episodes including boundary conditions and determine their representativeness for the projection of ozone trends. The contractor will evaluate the accuracy of previous emission estimates, compare projected emissions with updated emissions using current methodology for estimating emissions, identify the major uncertainties and if appropriate suggest improvements. They will review the expected efficacy vs. the actual benefits of emission control equipment or strategies.

Expected Results And Benefits

An evaluation of the technical basis for previous projections of attainment in prior SIPs will result. The evaluation will identify the factors that contributed to the inaccurate ozone attainment projections of the 1994 SIP. The factors may include the air quality and meteorological models and databases, modeling episodes and conditions, current emissions and projected emissions. Recommend revisions to the modeling process will result and these can be evaluated and used to improve the modeling in Project III-02.

Estimated Cost: Not to exceed $80,000 (Phase I - $30,000, Total - $110,000)

Duration Of Project: Six months

References

California's 1994 State Implementation Plan for Ozone, http://www.arb.ca.gov/sip/sip.htm

California's State Implementation Plan, http://www.arb.ca.gov/sip/siprev1.htm

2001 Bay Area Plan, http://www.arb.ca.gov/sip/basip01.htm

1999 Bay Area Plan, http://www.arb.ca.gov/sip/BASip.htm

4.3.2 Refine Conceptual Model from CCOS Results (Concluding Element and Final Report) (Project III-19)

Mathematical modeling of air quality is a major component of the Central California Ozone Study (CCOS), and the primary tool for developing and projecting the efficacy of ozone control strategies for the study region. For the modeling system to produce relevant and valid results, it must accurately reproduce the spatial and temporal variations in ozone precursor emissions, the meteorology that affects their transport and dispersion, and the chemical and physical processes that are involved in the formation and removal of ozone.

The data requirements of CCOS were also driven by a need for complementary, independent and corroborative data analysis so that modeling results can be compared to a conceptual understanding of the phenomena replicated by the model. Past conceptual model of ozone formation in central California must be revisited and refined using the results of CCOS. New phenomena, if they are observed, must be conceptualized so that a mathematical model to describe them may be formulated and tested. The formulation, assumptions, and parameters in mathematical modules that will be included in the integrated air quality model must be examined with respect to their consistency with reality.

Technical Objectives

The objectives of this project are to construct an integrated analysis of ozone formation in the CCOS modeling domain and use it to critically assess whether existing meteorological and air quality models can accurately describe the major relevant processes. Information used for photochemical model evaluation

Scope Of Work

The conceptual model is a qualitative compilation and description of the physical and chemical processes that govern the formation of ozone. The contractor will derive a conceptual model of ozone formation for central California using the quantitative information derived from descriptive and statistical analyses of the CCOS meteorological and air quality data. Elements of the conceptual model include surface and aloft transport processes that affect interbasin transport of air pollutants, emissions and concentrations of ozone precursors and fluxes of air pollutants between air basins, and the sensitivity of ozone to its precursors throughout the modeling domain under varying meteorological conditions. This newly derived conceptual model will be compared and reconciled with the conceptual model that was derived from the 1990 SJVAQS/AUSPEX study.

Using the new conceptual model, critically review the output from the CCOS meteorological and air quality modeling and assess the suitability of these models. Assess the accuracy of emission inputs and the ability of modeling system to properly simulate transport, vertical mixing and gas-phase chemistry. Identify key knowledge gaps and specific areas for improvements of meteorological and air quality models.

Expected Results And Benefits:

This project will enhance our understanding of ozone formation in Central California (Bay Area, Sacramento, SJV) by integrating and synthesizing existing knowledge of chemical and transport processes with the enhanced understanding derived from CCOS data analysis and modeling studies. The results of this study will help to establish a level of confidences in the use of model predictions of ozone and associated precursors control strategies.

Estimated Cost: $150,000

Schedule: nine months

References:

Fujita, E., R. Keislar, W. Stockwell, S. Tanrikulu, A. Ranzieri, H. Moosmuller, D. DuBois, D. Koracin, B. Zielinska, 1999: Central California Ozone Study, Volume I, Conceptual Program Plan, Version 3. Prepared for the California Air Resources Board by Desert Research Institute, Reno, NV, November 24, 1999.

Pun, B.K., J. Louis, C. Seigneur, A Conceptual Model for Ozone Formation in the San Joaquin Valley, Document Number CP049-1-98. Prepared for Technical and Ecological Services, Pacific Gas and Electric Company, 3400 Crow Canyon Rd., San Ramon, CA 94583. Prepared by Atmospheric and Environmental Research, Inc., 2682 Bishop Drive, Suite 120, San Ramon, CA 94583, 15 December 1998.

Pun, B.K., J. Louis, P. Pai, C. Seigneur, S. Altshuler, and G. Franco (2000). Ozone Formation in California's San Joaquin Valley: A Critical Assessment of Modeling and Data Needs. *J. Air & Waste Manage. Assoc.* **50**:961-971.

Sillman, S. (1999). The relation between ozone, NOx and hydrocarbons in urban and polluted rural environments. Atmos. Environ. 33, 1821-1845.

4.3.3 Integration of Findings of CCOS and CRPAQS (Project III-20)

The California Regional PM10/PM2.5 Air Quality Study (CRPAQS) The CRPAQS programmatic goal is to provide additional and more comprehensive information than is currently available to explain the nature and causes of particulate concentrations and visibility impairment in and around central California. The CRPAQS field study will consist of a long-term campaign from 12/1/1999 through 1/31/2001, a winter intensive study within the period of 11/15/2000 through 1/31/2001, and a fall intensive study within the period of 9/1/2000 through 10/31/2000. Several experiments will be conducted during the summer period of 7/1/98 through 8/31/98.

Technical Objectives

After completing CCOS data analysis go back and apply the same analysis to 1990 data base. Identify the analyses that were applied to the CCOS data that were not applied to the 1990 data. Compare the results of the data analysis and determine if anything has changed

Methods And Approach

The contractor will simulate the 1990 database using current models and methods. A retrospective analysis of the previous efforts will be made and evaluation is to include (but are not limited to) emissions (including biogenic) and their speciation, model boundary conditions, chemistry mechanism and meteorology as they were used in the 1994 SIP analysis. They will examine suggested improvements and alternatives in the modeling process that result from the evaluation on Project III-01 and any additional improvements to the modeling process developed by the contractor. The contractor will utilize products from CCOS data analysis and modeling to revisit prior ozone episodes to examine the applicability of SIP modeling to the full range of episode types identified in the characterization process for all air pollution precursors and products. The project will include an examination of the representativeness of the episodes used for SIP modeling based on meteorology and air quality considerations and an identify deficiencies in the previous SIP modeling efforts The contractor will identify possible new modeling improvements, including new modeling episodes if appropriate.

Expected Results And Benefits

An understanding of the key factors that contributed to the consistently overly optimistic SIP attainment plans for ozone, in particular the 1994 SIP, will be identified. The simulations of the 1990 database using current models will identify potential model or database problems and evaluate the uncertainty of the future simulated ozone trends. New alternative modeling procedures will increase the accuracy of model forecasted ozone trends and improve the probability of attaining ozone abatement goals.

Estimated Cost: Not to exceed $150,000.

Schedule: Six months

4.3.4 Preparation and Publication of CCOS Results for Policy Makers and Public (Project III-21)

The CCOS data analysis and modeling will generate large volumes of technical results that must be synthesized and summarized for the scientific and stakeholder communities, policy and decision makers and the general public. The contract will provide for preparation of two summary documents. One document will provide an overview of CCOS and summarize the major scientific findings and conclusions. The second document will be a more concise summary of the policy-relevant findings and conclusions from the study. These summaries will be patterned after similar documents prepared at the end of SJVAQS/AUSPEX and SOS.

Estimated Cost: $30,000

5. CATEGORY IV PROJECTS

5.1 Day-of-Week Variations in Emissions of Ozone Precursor in the CCOS Domain (Project IV-1)

Observations show that the ambient concentrations of NOx and, to a lesser extent, VOC are lower on weekends than weekdays in urban areas. These differences arise from day-of-week variations in the temporal and spatial patterns of VOC and NOx emissions. Results of past studies in central California and elsewhere indicate that air quality on Sundays is significantly different from weekdays and Saturdays. It has been postulated that observed weekend effect arise from day-of-week variations in precursor emissions coupled with the complex interactions of physical and chemical processes. The two primary CCOS episodes of interest for modeling begin on a Sunday and the preceding Saturday would be included as a “ramp-up” day. Because the spatial and temporal patterns of precursor emissions are significantly different on Saturday and Sunday relative to a typical weekday, it is essential that day-of-week variations in emissions be accurately reflected in the CCOS modeling emissions inventory.

As part of the 1997 Southern California Ozone Study (SCOS97), the ARB sponsored a study to determine day-of-week variations in traffic patterns, construction activity and use of recreational vehicles, lawn and garden equipment, and barbeques. The findings and conclusions from this study and other relevant studies should be examined to ascertain whether the CCOS emissions inventory adequately accounts for day-of-week variations in VOC and NOx emissions and to identify specific improvements to the emission inventory that may be necessary.

Technical Objectives

This study will evaluate the accuracy and validity of the CCOS emission inventory with respect to spatial and temporal patterns that exist in VOC and NOx emissions on typical summer weekdays, Saturdays and Sundays) based upon a review of relevant studies. If necessary, data will be collected to derive appropriate adjustments to the CCOS emission inventory to properly account for day-of-week variations in VOC and NOx emissions from major sources of emissions.

Scope Of Work

This project will be conducted in two phases: an assessment phase and a data collection phase. In the assessment phase, the contractor will review relevant information regarding day-of-week variations in emissions related activity and evaluate the accuracy of day-of-week variations in the CCOS emission inventory. In the second phase, the contractor will identify and, if necessary, collect the data to derive appropriate adjustments to the CCOS emission inventory.

Task 1 - Assessment of the accuracy of day-of-week variations in the CCOS emissions inventory. Review the basis for day-of-week variations in the CCOS modeling emissions inventory VOC and NOx emissions. Reconcile these methods and data with

Task 2 – Collect activity data to derive day-of-week variations in emissions for major source categories. Include activity dairy for households of daily vehicle trips using onboard data loggers. Supplemental traffic counts near monitoring stations. Surveys of lawn and garden equipment use, construction activity, reacreational vehicle use.

Estimated Cost

Phase 1 - $ 75,000

Phase 2 - $350,000

Schedule

Four months for Phase 1 and 18 months for Phase 2.

5.2 Enhancement of Existing Air Quality and Meteorological Monitoring for Data Analysis and Modeling (Project IV-2)

This project will evaluate the adequacy of existing air quality and meteorological monitoring in the CCOS domain to support air quality modeling for any day during the ozone season. Key input variables and data necessary for model performance evaluations will be identified and the minimal and optimum spatial and temporal resolutions will be specified.

5.3 Deposition Studies (Project IV-3)

The role of dry deposition in removing important chemical species is not well quantified in the CCOS domain. Some work has been done on ozone (Pun et al. 1998), but ozone precursor dry deposition rates have not been the subject of as much investigation. During the California Ozone Deposition Experiment (CODE) in 1991, aircraft and tower-based flux measurements were taken over different types of San Joaquin crops, irrigated and non-irragated fields, and over dry grass. Results are briefly summarized in Pun et al. (1998) and include estimates of ozone deposition velocities of 0.7-1.0 cm/s (Pederson et al. 1995). Vertical fluxes (deposition rates) can be calculated if a vertical gradient is known (assumed or measured). Order of magnitude calculations by Pun et al. show that dry deposition can be a few percent (~3-5%) of the total ozone budget in the San Joaquin Valley. Dry deposition may play a more significant role in the budget of important ozone precursors, NO and NO2, but even less is known about these deposition rates compared to ozone.

Reasons for further flux and deposition measurements during the CCOS study, with its expanded geographic scope, include:

- Further consideration of NO sources. While NO was not considered to be a problem at three sites reported on by Pederson et al. (1995), Mahrt et al. (1995) found that rapid titration of O_3 by NO did affect aircraft-based ozone surface flux measurments. Controlled experiments that employ a spatially diverse array of NOx monitors upwind or surrounding a flux measurement site could help quantify this effect.

- Further consideration of relative humidity effects. The Sacramento River Delta region and coastal regions are part of the CCOS domain. Ozone is not highly water soluble, but McLaughlin and Taylor (1981) report that ozone deposition to plants can increase by a factor of 2-3 when relatively humidity changes from 35% to 75%. Based on this, Mahrt et al. (1995) suggest that ozone deposition may show a more complex spatial and/or temporal pattern than heat and moisture fluxes. Deposition studies for CCOS could include measurement of ozone fluxes over more varied types of terrain within the CCOS study area, including the higher humidity areas of delta or the coastal areas. Desjardins et al. (1995) report that aircraft flux measurements compared well with tower-based flux measurement at two instrumented vineyard sites during CODE. Aircraft could be used to expand the diversity of sites measured.

- Precurser deposition rates. Fluxes of NOx and VOC were not measured during CODE.

Scope of Work

Specify the equations, assumptions, input data, and uncertainties for a deposition model. From the examination of micrometeorological data and vertical flux measurements, determine the extent to which these equations represent reality, and the degree to which assumptions are satisfied. Derive and present dery deposition rates for O3, NO, and NOx for representative terrain types in the CCOS region. Evaluate the effects of input data uncertainties on these deposition estimates.

Expected Results and Benefits:

It is expected that better estimates of dry deposition will improve model treatment of species mass balance, and improve numerical estimates of ozone concentration, and more accurately represent the impacts of longer range, overnight transport where dry deposition rates more have time to affect species concentration.

Estimated Cost: $1.4 million

Schedule: 3 years

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