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SOUTHERN CALIFORNIA AIR QUALITY STUDY (SCAQS)

SUGGESTED PROGRAM PLAN

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Prepared for review and comment purposes by

Sonoma Technology Inc. (STI) and Desert Research Institute (DRI) with extensive input from the California Air Resources Board (ARB) and other potential sponsors and members of the technical community

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This plan has been prepared by the above contractors and represents their recommendations based upon the information available to them. It has not been approved by ARB or any of the other sponsors and does not represent the policy or intent of ARB or any of the other sponsors. This draft plan serves as a starting point for discussion and to make potential sponsors aware of ways in which they can usefully participate.

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ABSTRACT

This program plan outlines a suggested measurement and management approach and reviews the technical background for the Southern California Air Quality Study (SCAQS). SCAQS will be a multi-year, integrated, cooperative study which will be funded by many different government agencies, industry groups, and individual corporate sponsors. This plan has been prepared with the input of the sponsors and potential participants and represents a composite of their ideas.

The overall goal of SCAQS is to develop a comprehensive and properly archived air quality and meteorological data base for the South Coast Air Basin that can be used to test, evaluate, and improve elements of air quality simulation models for oxidants, PM-10, fine particles, toxic air contaminants, and acidic species. In addition, SCAQS will address specific technical questions regarding the emission, transport, transformation, and deposition of pollutants.

The study is planned to take place in 1987 during six weeks in early summer and four weeks in late fall. Extensive routine measurements and special studies will take place on about 19 days during the study. Most of the monitoring will take place at existing air quality monitoring sites. Airborne, meteorological, and tracer measurements are planned at additional locations.

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Several parts of the plan were prepared by members of the STI or DRI Staff and by STI consultants. In addition, members of the Technical Advisory Group for the project have contributed ideas and text to the plan as well as provided continuing review of the planning effort.

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1. INTRODUCTION

1.1 BACKGROUND AND ISSUES

In recent years in California, the mix and spatial distribution of pollutant emissions have changed substantially, and several new classes of pollutants have gained the public's attention. In the next few years, many difficult regulatory issues relating to these changes will confront the California Air Resources Board (ARB). Resolution of these issues and development of effective control strategies to ameliorate California's air quality problems will require a better understanding of the relationships among the sources, receptors, and effects of the pollutants in question. This understanding can only be developed through measurement, data analysis, and modeling in an iterative fashion. Design and evaluation of alternative control strategies must be done using models which embody our best understanding of the above relationships.

This program plan outlines the first steps in a measurement, analysis, and modeling strategy which can ultimately provide the ARB with tools necessary to make effective regulatory decisions. This study, the Southern California Air Quality Study (SCAQS), addresses the following issues: ozone (O_3), NO_2 and the roles of nitrogen oxides (NO_x), PM-10, fine particles, visibility,² toxic substances, and atmospheric acidity. The first five issues are addressed in depth, and adequate information should result from this project for the development and testing of descriptive and prognostic models. Understanding of the latter two issues will be greatly improved by this study, but this project alone will not necessarily provide the information required to develop and test prognostic models.

Although similar problems are faced by most California air basins, the focus of this study will be the South Coast Air Basin (SOCAB) since that is where the problems are most severe. Also, the SOCAB is one of the most well documented and intensively researched airsheds in the world.

Since the scope of the project is beyond the resources of the ARB alone, and since the results of the study could affect the actions of both government and industry, the SCAQS has been designed as a cooperative project. Coordinated sponsorship by both government and industry should help assure adequate funding to meet the goals of the study. In addition, development of a protocol which is satisfactory to the parties affected by the results should minimize conflict about technical issues during the regulatory process.

SCAQS is designed to meet the goals and objectives agreed upon by the ARB and other potential sponsors. This study plan is the result of an open planning process which entailed extensive consultation with the modeling and measurement communities. The resulting design is an attempt to satisfy the needs expressed by the technical community to meet the stated objectives. The scope is quite large, and there obviously will be changes as the design evolves. This document represents a starting point from which the final design will be constructed. Feedback from potential sponsoring agencies and data users regarding their relative priorities and levels of resources will be used to refine the design. A mailing list including most of the people and organizations who have been involved in the planning process to date is included in Appendix A.

SCAQS data will be used to test and evaluate models which predict or describe the ambient distribution of pollutants. These models, in turn, will be used to develop and assess control strategies. The relationship between the SCAQS measurements and their ultimate use in developing control strategies is shown schematically in Figure 1-1. The primary focus of SCAQS is to provide measurements which relate source emissions to ambient pollutant spatial and temporal distributions. SCAQS will also include some source and effects related measurements and a data analysis component.

The development and use of models can be a controversial subject because the model results have direct implications in terms of controls. To minimize controversy and to expedite the measurements, SCAQS is designed to focus on measurements and data analysis but not directly to include modeling efforts. This modeling will be performed by the sponsors at a later date. Since SCAQS must serve the needs of the modelers, however, extensive input has been solicited from the modeling community during the SCAQS design phase, and a mechanism has been established for the modeling community to have direct input to the ongoing design of SCAQS.

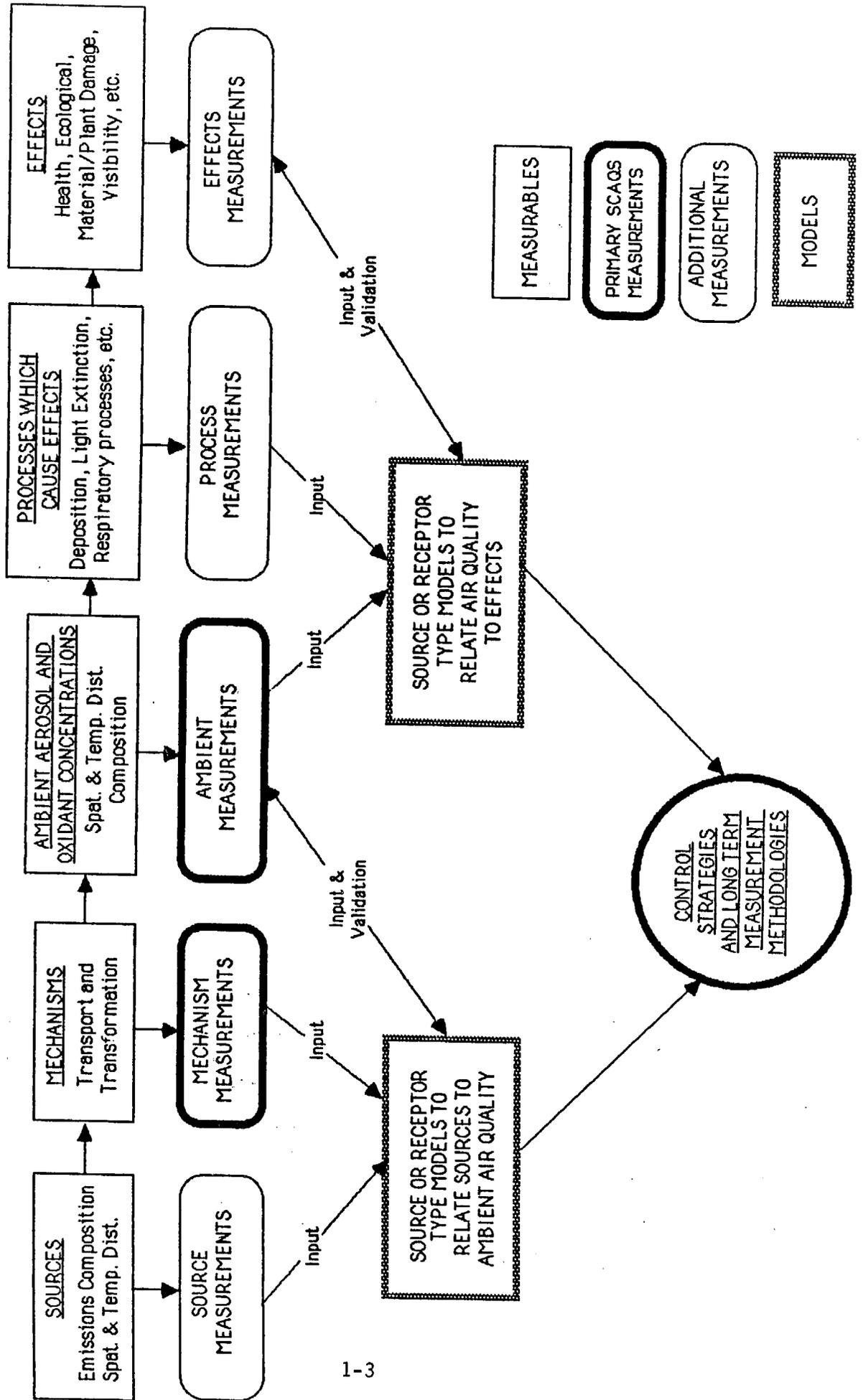
1.2 STUDY GOALS

The overall goals of the study are:

1. to develop a comprehensive and properly archived air quality and meteorological data base for the South Coast Air Basin which can be used to test, evaluate, and improve elements of air quality simulation models for oxidants, NO_2 , PM-10, fine particles, visibility, toxic substances, and acidic species. The data base should be adequate:
 - to test models proposed for the design of attainment strategies for PM-10, ozone, and NO_2 ; and
 - to clarify the hydrocarbon/ NO_x / O_3 relationships so that ozone prediction models can be improved and new strategies to meet federal "reasonable efforts" requirements can be developed and tested;
2. to evaluate measurement methods for PM-10, fine particles, acidic species, and important nitrogen and carbon species; and
3. to enhance our understanding of the relationships between emissions and the spatial and temporal distributions of pollutants so that air quality simulation models and, ultimately, air quality management strategies can be improved.

The data obtained by meeting these goals should be of utility in the development and testing of air quality models of known accuracy, precision, and validity which can be used to design and evaluate the effect of proposed attainment strategies for O_3 , NO_x , PM-10, and selected toxic substances.

Figure 1-1.
 RELATIONSHIP BETWEEN MEASUREMENTS,
 MODELS AND CONTROL STRATEGIES



1.3 TECHNICAL OBJECTIVES

To meet the goals stated in Section 1.2, a set of program objectives has been defined. Each of these objectives can be accomplished by addressing specific technical issues. The SCAQS objectives and their related technical issues are listed in this section. The origins and importance of the issues are discussed in Section 2.

The primary goal of SCAQS is to develop a data base for use by modelers. Although modeling per se is not a part of SCAQS, the modeling community has been surveyed to determine the objectives of some of the groups which will use the SCAQS data. A summary of these objectives is presented to put SCAQS in perspective.

For most modeling activities, knowledge of the physical and chemical characteristics of the emissions from the major source types is required. For many of the source types in the South Coast Basin, the chemical and physical properties of particulate and hydrocarbon emissions are not well known. To improve our knowledge of these properties, some emissions characterization studies are being designed which will be complementary to and coordinated with SCAQS. The objectives of these studies are also presented in this section.

1.3.1 SCAQS Objectives and Issues

Objective 1

Obtain a data base representative of the study area and sampling periods, with specified precision, accuracy, and validity, which can be used to develop, evaluate, and test episodic source and receptor models for O_3 , NO_2 , PM-10, fine particles, and atmospheric optical properties and annual average models for PM-10.

Issues to be addressed:

Data should be obtained which can be used to:

describe the spatial, temporal, and size distributions, and physical and chemical characteristics of suspended particles less than 10 μ m diameter;

describe the spatial and temporal distribution of O_3 and O_3 precursors including important intermediate species such as OH, HO_2 , NO_3 , H_2O_2 , and products such as HNO_3 and PAN.

refine the South Coast Air Basin emission inventory for the spatial and temporal distributions of particle, hydrocarbon, NO_x , and SO_x emissions for the study period;

describe the spatial distribution of selected toxic substances;

describe the three-dimensional distributions of wind, temperature, relative humidity and cloud cover in the study area;

describe the initial pollutant spatial distribution and the pollutant concentrations at the boundaries of the SOCAB for the study days;

determine the relationship between the hydrocarbon/NO_x ratios in ambient air and their ratios in current emissions inventories;

determine the organic composition of selected samples of source and receptor region aerosols;

determine the contribution of toxic metals to atmospheric aerosols in source and receptor areas as a function of size; and

determine the spatial distribution of nitrogen species. Perform a nitrogen mass balance across the basin, accounting for total nitrogen species through transformations and deposition.

Objective 2

Identify the characteristics of emissions from specific sources or source types for use in receptor modeling of both gases and aerosols with emphasis on sources of organic and toxic emissions.

Issues to be addressed:

Determine which chemical and physical properties of source emissions are most useful for source attribution of receptor concentrations.

Estimate the changes in the ratios of chemical species as a function of source-receptor travel time, interactions with other species, and meteorological conditions.

Quantify the uncertainty of source attribution by receptor models as a function of the chemical and physical properties used to characterize sources. Select the optimal properties for routine source profile measurements.

Determine the percentages of the PM-10 and fine particles which are primary and secondary. Assess the relative contributions of natural and anthropogenic sources to PM-10 concentrations.

Objective 3

Assess the dependence of particle and O₃ formation and removal mechanisms upon selected meteorological and precursor variables.

Issues to be addressed:

Assess the importance of water in the vapor and liquid phases for the formation of aerosol in the SOCAB.

Assess the role of aromatic hydrocarbons in the formation of particles and as an ozone precursor.

Assess the formation rates of nitric acid and aerosol nitrate as a function of: (1) the presence of liquid water, (2) altitude, (3) UV intensity, and (4) the presence of O_3 .

Estimate the rate of ozone removal at surfaces as a function of time of day and atmospheric stability.

Objective 4

Assess how the spatial and temporal distributions of particles, O_3 , O_3 precursors, and NO_x depend upon emission height and selected meteorological variables.

Issues to be addressed:

Assess the relative contribution of elevated and ground based emissions to ground level O_3 , NO_x , PM-10, and fine particle concentrations, with emphasis on the influence of elevated source emissions of NO_x on wintertime NO_2 and summertime ozone concentrations.

Assess the importance of various mechanisms for day-to-day carryover of pollutants.

Assess the effects of high temperatures upon evaporative emissions and thus on ambient concentrations of hydrocarbon species.

Objective 5

Quantify the contributions of aerosols in an upwind source region and in an eastern basin receptor region to atmospheric acidity, mutagenicity, and visibility degradation.

Issues to be addressed:

Determine the species contributing to total acidity (aerosol and gas) in source and receptor regions, and estimate the contribution of aerosol and gaseous components to total acidity and to dry deposition.

Determine the relative contributions of primary and secondary aerosol species to visibility degradation in each region.

Assess the mutagenicity of PM-10 and PM-2.5 in each region.

Objective 6

Evaluate the validity of methods of measuring PM-10, fine particles, and precursor species in quantifying atmospheric constituents as they exist in the atmosphere during sampling.

Issues to be addressed:

Determine the concentrations of liquid water in particles in source and receptor areas as a function of relative humidity (RH) and particle size. Assess the change in mass as a function of size when particles are collected on substrates and analyzed under non-ambient environmental conditions.

Determine the concentration of particulate organic matter in source and receptor areas as a function of particle size and ambient temperature. Assess the change in mass as a function of particle size, ambient temperature, and ambient pressure when particles are collected on substrates for subsequent laboratory analyses.

Determine the relationship between measurement values obtained at a single station and volume-averages over grid sizes used in prognostic air quality models.

Compare and evaluate various methods for the measurement of nitric acid and other nitrogen species and determine their accuracy, precision, and validity under a range of environmental conditions.

Compare and evaluate various methods for the measurement of carbonaceous species and determine their accuracy, precision, and validity under a number of environmental conditions.

1.3.2 Modeling Considerations

The modeling community has been surveyed to determine the proposed and suggested uses of the SCAQS data. A Model Working Group (MWG) has been established to provide technical input to the SCAQS design process in order to ensure that the measurement protocols are consistent with the requirements of the modeling community. The expected objectives of future modeling efforts include the following:

Sensitivity Testing

Performing model sensitivity tests to identify the sensitivity of model results to uncertainties in the model input data in order to refine the design of the SCAQS measurements.

Model Mechanisms Evaluation

Evaluating the physical and chemical bases for air quality models which describe photochemical and aerosol processes in the SOGAB.

Issues to be addressed:

Evaluate objective and fundamental methods of estimating three-dimensional wind fields.

Evaluate chemical and physical mechanisms for O_3 and aerosol formation.

Quantify the uncertainties in model results which are caused by:
(1) measurement uncertainties of the model input data and parameters,
(2) deviations from model assumptions, and (3) the stochastic nature of the atmosphere.

Compare the ability of alternative mathematical models to represent atmospheric and chemical mechanisms.

Overall Model Performance Evaluations; Performance Comparisons

Testing the performance of air quality models in predicting concentrations of PM-10, ozone, and important precursor and intermediate species as a function of space and time.

Issues to be addressed:

Identify common measures of performance applicable to all models.

Compare model results with corresponding measurements in space and time for each model tested.

Compare performance measures among air quality models.

1.3.3 Emissions Considerations

An Emissions Working Group (EWG) has been established as part of the SCAQS planning process. This group is developing the program plan for an emissions inventory which will be a part of SCAQS and for emissions characterization studies which will be coordinated with SCAQS. The objective of the inventory effort is included in SCAQS Objective 1. The objective and some of the related issues for the characterization studies are outlined below.

Emissions Characterization Objective

Improve the "characterization" of primary emissions of particles and hydrocarbon gases from all major source types in the South Coast Air Basin. Use this information to improve the SCAQS emissions inventory.

Issues to be addressed:

Characterize the emissions at equilibrium in the ambient air as well as in the stack or tailpipe.

Identify the chemical and physical properties of primary hydrocarbons and particles from specific source types.

Properly account for primary soot.

Include all significant categories of natural and anthropogenic sources.

1.4 OVERVIEW OF STUDY AND GUIDE TO PROGRAM PLAN

The study will include the following elements:

- a project management and coordination activity;
- planning and preparation;
- instrumentation intercomparison and evaluation studies;
- a six week summer and a four week winter field measurement program and associated quality assurance activities;

- an emissions inventory assessment and update for the study period;
- data archiving and distribution;
- data analysis and coordination activities;
- complementary emissions characterization studies for important source types; and
- reports and presentations.

We expect that complementary model development and evaluation activities will be funded independently by some of the sponsors. This program plan describes the study elements listed above with the exception of the instrument intercomparison studies. These studies are being planned separately and will be completed before the SCAQS measurements start.

The SCAQS field measurement program will take place during early to mid summer and early winter periods. During each study period, three to five, two-day to three-day periods will be studied intensively, for a total of 16-19 "intensive study" days.

The field study will include the following elements:

- a network of existing routine air quality monitoring stations (type "C" sites);
- nine monitoring stations located along typical air trajectories which will measure aerosols and gases routinely on "intensive study" days (type "B" sites). Type "B" sites typically will be collocated with type "C" sites. Type "B" measurements will be made by techniques of known precision and accuracy. Type "B" measurements will be more extensive and have better time resolution than type "C" measurements. Nine type "B" sites will be operated in the summer period and five during the winter period;
- one research station each in a source and receptor region in the summer and one station in a source region in the winter (type "A" sites). These stations will be collocated with type "B" sites and will be the base of operations for cooperating investigators. Type "A" measurements will be more sophisticated and experimental than the type "B" measurements;
- a network of meteorological measurements at the surface and aloft to be operated on intensive study days;
- routine upper-air pollutant and lidar measurements to be made by aircraft on intensive study days;
- complementary measurements of selected toxic substances to be made by ARB at selected sites;

- complementary physical and chemical measurements of fog and clouds on intensive study days;
- "special" studies on selected intensive study days - including multiple tracer studies and studies of spatial representativeness;
- assembly and archiving of complementary data from existing data sources; and
- a quality assurance program including independent systems and performance audits.

Between and after the study periods, selected aerosol measurements will be continued at the type "B" sites to obtain data suitable for the calculation of annual averages.

The study will consist of a number of closely coordinated projects funded by several co-sponsors including the ARB, the Environmental Protection Agency (EPA), the South Coast Air Quality Management District (SCAQMD), and various industry groups or individual corporate sponsors. The sponsors will oversee and provide guidance to the project through a Management Advisory Group (MAG). The project will be coordinated by one or more contractors who will be funded by the ARB. The management contractor will prepare a final protocol which, to the maximum extent feasible, is satisfactory to all of the members of the MAG, and the project will be conducted according to that protocol. The ARB will also fund a data manager who will assemble, archive, and distribute to participants all data obtained as part of the study. Agreement to abide by a data management and exchange protocol will be a condition of participation in the study.

Details of the program plan are outlined in the subsequent sections. Discussions of prior studies in the SOCAB, the data needs of various types of models, and the existing data resources in the SOCAB are presented in Section 2. Details of the suggested project measurements and emissions assessments are presented in Section 3, and the approach to quality assurance is discussed in Section 4. The data management activities and protocol are outlined in Section 5. Data analysis and complementary modeling activities are discussed in Section 6, and a suggested program management structure is described in Section 7. Cost estimates, contracts which will be required, and the potential contributions of various sponsors are discussed in Section 8.

The preparation of this plan is an iterative process, and the structure of the program will continue to evolve. This third version of the SCAQS program plan incorporates additions, corrections, and changes in scope which resulted from review of the two previous versions by ARB, potential sponsors, and the scientific community.

2. CURRENT KNOWLEDGE AND INFORMATION NEEDS

2.1 AIR QUALITY MANAGEMENT PLAN

The South Coast Air Basin (SOCAB) comprises 6600 square miles of the non-desert portions of Los Angeles, San Bernardino, Riverside and Orange Counties. Its population of approximately 10.5 million inhabitants is expected to increase to 13 million by the year 2000. This will be accompanied by a 31% increase in the number of dwellings and a 33% increase in employment. It is expected that 10.1 million on-road vehicles in the Basin will travel 234.3 million miles per day by the year 2000 (SCAQMD, 1982). The tremendous growth predicted over the next two decades reflects the even more rapid growth which has occurred since 1950. This growth has been accompanied by deterioration of air quality. Without careful planning and appropriate emissions controls, air quality could become even worse in the future.

The South Coast Air Quality Management District (SCAQMD) is charged with the responsibility for determining compliance with California state and federal air quality standards, proposing plans to attain those standards when they are exceeded, and for implementing those plans to the greatest extent possible. To these ends, the SCAQMD operates a network of sampling sites, illustrated in Figure 2-1, which measure ambient concentrations of carbon monoxide (CO), ozone (O₃), sulfur dioxide (SO₂), nitrogen dioxide (NO₂), total suspended particulate (TSP) matter, and suspended particulate lead. Table 2-1 presents the federal primary and secondary and California state standards for different atmospheric pollutants along with the number of sites and number of days in 1982 which exceeded these standards (Hoggan et al. 1983). The most recent data for 1983 (ARB, 1983a, b and Hoggan et al. 1984) and earlier years are consistent with the number of exceedance cases indicated in Table 2-1. It is evident that the South Coast Air Basin was in violation of every standard, except that for SO₂, at nearly every one of its sampling sites during 1982. Results for 1983, 1984, 1985 and beyond are not expected to change significantly without changes in emissions. There is an obvious need to undertake measures to reduce ambient concentrations of carbon monoxide, nitrogen dioxide, ozone, and suspended particulate matter.

The Air Quality Maintenance Plan (AQMP) (SCAQMD, 1982) proposes several control measures which would be implemented between now and the year 2000. SCAQMD (1982) estimates that these "Short Range Control Tactics" will cost approximately \$800 million to implement, most of which will be borne by petroleum refineries, electric utilities, and motor vehicle manufacturers. The emissions reductions are in addition to control measures which had been mandated prior to the Plan. The largest emission reductions by the year 2000 will result from the following additional control measures:

- Major CO reductions will result from more frequent tuneups to manufacturers' specifications; low emission, high fuel economy vehicles for local government; bicycling improvements; ride sharing; modified work schedules; home goods delivery; traffic signal synchronization; electric, methanol-powered and dual-fueled vehicles; and more stringent emissions controls on in-use and new vehicles.
- Major SO₂ reductions will result from flue gas desulfurization on fluid-cracking units, electric utility boiler modifications,

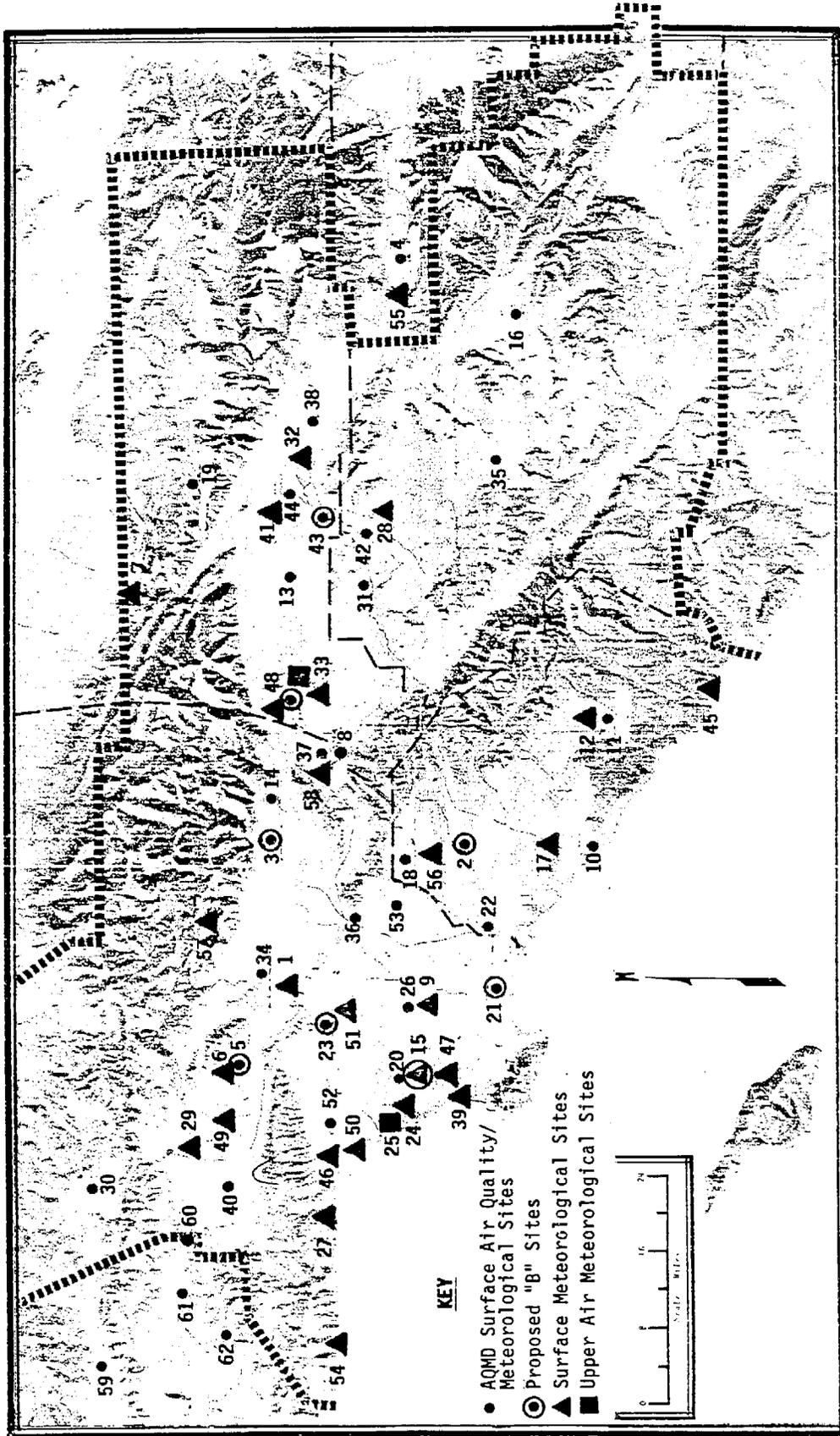


Figure 2-1. Existing Air Quality and Meteorological Monitoring Sites in the South Coast Air Basin. (Site codes are listed in Table 2-3.)

Table 2-1. Federal and California State Standards with Number of Sites^(d) Exceeding them in 1982.

Pollutant	Federal Primary Standard	No. of Sites in Violation	Range in No. of Violation Days per site ^(e)	Federal Secondary Standard	No. of Sites in Violation	Range in No. of Violation Days per site ^(e)	California State Standard	No. of Sites in Violation	Range in No. of Violation Days per site ^(e)
Ozone	0.12 ppm (1 hr)	32	1 to 121	0.12 ppm (1 hr)	32	1 to 121	0.10 ppm (1 hr) ^(a)	33	2 to 160
Carbon Monoxide	9.0 ppm (8 hr)	13	2 to 50	9.0 ppm (8 hr)	13	2 to 50	9.0 ppm (8 hr)	13	2 to 47
	35.0 ppm (1 hr)	0	0	35.0 ppm (1 hr)	0	0	20.0 ppm (1 hr)	6	1 to 7
Nitrogen Dioxide	0.05 ppm (aaa) ^(f)	9	NA ^(c)	0.05 ppm (aaa)	9	NA	--	--	--
	--	--	--	--	--	--	0.25 ppm (1 hr)	11	1 to 8
Sulfur Dioxide	0.03 ppm (aaa)	0	0	0.03 ppm (aaa)	0	0	--	--	--
	0.14 ppm (24 hr)	0	0	--	--	--	0.05 ppm (24 hr)	0	0
Sulfate	--	--	--	--	--	--	25 ug/m ³ (24 hr)	14	1 to 3
Lead	1.5 ug/m ³ (calendar qtr.)	1 ^(b)	1 ^(b)	1.5 ug/m ³ (calendar qtr.)	1 ^(b)	1 ^(b)	1.5 ug/m ³ (per 30 days)	2 ^(b)	1 to 3 ^(b)
TSP	75 ug/m ³ (aga) ^(g)	14	NA	60 ug/m ³ (aga)	18	NA	60 ug/m ³ (aga)	18	NA
	260 ug/m ³ (24 hr)	4	1 to 2	150 ug/m ³ (24 hr)	23	1 to 22	100 ug/m ³ (24 hr)	26	2 to 37
PM-10	50-65 ug/m ³ (aaa)	--	--	--	--	--	30 ug/m ³ (aga)	--	--
	150-250 ug/m ³ (24 hr)	--	--	--	--	--	50 ug/m ³ (24 hr)	--	--

(a) Oxidant instead of ozone

(b) Number of quarters instead of number of days

(c) NA - not applicable for annual average

(d) Out of a total of 35 sites for 0, 3, 27 sites for CO, 24 sites for SO₂, and 27 sites for TSP, lead, and sulfate.

(e) Only sites exceeding the standard at least once are included.

(f) aaa = annual arithmetic average

(g) aga = annual geometric average

weatherproofing of existing homes, insulation standards for new homes, and greater reliance on wind energy.

- Major primary particulate reductions will result from paving roads and vehicular emissions controls.
- Major nitrogen oxides (NO_x) reductions will result from controls on stationary internal combustion engines, truck freight consolidation terminals, additional emissions controls on in-use and new motor vehicles, introduction of electric vehicles, electrification of railroad line haul operations, emissions standards for off-road heavy duty equipment, and improved home insulation.
- Major reactive organic species reductions will result from controls on thermally enhanced oil recovery and wood furniture finishes, changes in aerosol spray can contents and other consumer solvents, ride sharing, modified work schedules, reduction of the number of aircraft engines involved in idle and taxi operations, further controls on in-use and new vehicles, methanol fleet conversion, emissions standards for new boats and pleasure craft, and new source review.

When these measures are implemented, it is anticipated that the SCAQMD will continue to be in compliance with the federal SO₂ standard and will attain the federal NO₂ standard. Though attainment of the CO standard is not predicted by the AQMP analysis, this standard is exceeded at only a few sites, and the proposed emissions reductions bring the total to within 1.5% of the emissions estimated for CO attainment.

However, the reductions in precursor gas and primary particle emissions are insufficient to predict attainment of the ozone and suspended particulate matter standards. Additional controls with existing technology are problematic, and the AQMP is not expected to yield attainment of these standards by the year 2000.

The AQMP is a living document which is constantly being changed in response to new information and new standards: "...both the AQMP and the 1982 Revision are interim reports which represent the most complete information which could be gathered within the time and resources available....New approaches and new ways of assessing the problems are required if the region is to meet its air quality goals without serious economic and social disruption." (SCAQMD, 1982). The SCAQS will provide these new ways of assessing problems if the objectives stated in Section 1 can be met.

2.2 AIR POLLUTION CHARACTERISTICS OF THE SOUTH COAST AIR BASIN

The key components of air pollution are emissions, transport and transformation, and receptor concentrations. This subsection provides a brief summary of knowledge about these components in the South Coast Air Basin. Emphasis is given to effects of these components on particulate matter and ozone concentrations at receptors. Effects on atmospheric acidity, toxic substances, and visibility are inextricably related to the concerns about ozone and suspended particulate matter.

2.2.1 Emissions

Table 2-2 presents the SOCAB emissions classified into five categories as compiled from the 1979 emissions inventory (ARB, 1982; Grisinger et al. 1982). The AQMP is based on these emissions. However, it is likely that several of these categories have since changed as the result of the implementation of controls on various sources and fuel switching (from oil to natural gas) in the utility industry. Total emissions from the state of California are given for comparison.

The first observation from this table is that the SOCAB contained a large fraction of all emissions in the state during 1979, ranging from 25% to 35% for all species except primary particles. Furthermore, this large fraction of total state emissions was confined to only 4% of the state's land area and is roughly comparable with the area's 44% of the state population. The largest emitters of both reactive organic gases (ROG) and nitrogen oxides in 1979 were on-road vehicles. Light duty passenger vehicles and light and medium duty trucks were the largest contributors within this source category, though heavy duty diesel trucks were significant NO_x emitters. Solvent use was a major emitter of reactive organic gases, with architectural coatings, other surface coatings, and domestic uses being its major sources. Fuel combustion was also a major NO_x emitter, with the electric utilities being the highest contributor within this category. The large total organic gas (TOG) emission rate derived largely from solid waste landfills. Primary particle emissions were relatively low compared to the rest of the state, owing to the low amount of agricultural tilling taking place in the SOCAB during 1979. Tilling, re-suspended road dust, and light duty passenger vehicle emissions were the major primary particle emitters, with diesel trucks and mineral processing also of significance.

While Table 2-2 shows some slight seasonal deviations in these Basin-wide emission rates, these changes are typically within the measurement uncertainty of the inventory process. Seasonal differences are related primarily to weather conditions, with higher fuel consumption in the wintertime for heating. Reactive organic emissions are higher in the summer owing to the use of paints in construction. The increased CO and particulate emissions from fuel combustion in the winter are somewhat offset by negligible winter emissions from the unplanned fires which take place intermittently during the hot summer months. Thus, while the aggregate emission rates do not vary appreciable over the year, the temporal and spatial detail of these emissions varies significantly. Figures 2-2 and 2-3 show the gridded emissions of TOG, CO, NO_x , SO_x , and TSP from surface and elevated point sources. These figures illustrate the spatial complexity of emissions in the SOCAB. They represent 1982 emissions projections from the 1979 data of Table 2-2. The vertical scales of each figure are unequal, so comparisons among Figure 2-2, Figure 2-3, and Table 2-2 must be qualitative. Nevertheless, several inferences can be made. Surface emissions of TOG, CO, and NO_x have similar spatial distributions. These emissions are highest near the center of the Basin and taper off near the coastal areas and toward the eastern extremes. Table 2-2 implies that the major sources of these species are on-road vehicles. Surface SO_x emissions are most concentrated near and south of the Palos Verdes

Table 2-2. 1979 Emission Rates^(a) in the South Coast Air Basin Compared to Those of California (Emission rates in tons/day based on one year of emissions)

Emissions Source Categories	Location	Total Organic Gases (TOG)	Reactive Organic Gases (ROG)	Carbon Monoxide (CO)	Nitrogen Oxides (NO _x)	Sulfur Oxides (SO _x)	Total Emitted Particles (TEP)
Fuel Combustion	SOCAB	55.3	26.2	110.2	371.6	114.1	32.7
	Calif.	149.8	74.5	370.0	1168.5	559.1	121.1
Waste Burning	SOCAB	0.3	0.1	1.5	0.3	3.4	0.4
	Calif.	99.1	45.7	931.4	5.6	7.3	100.5
Solvent Use	SOCAB	371.8	340.0	0.3	0.5	0.0	2.7
	Calif.	863.7	787.3	0.3	0.5	0.0	2.8
Petroleum Processing, Transfer & Storage	SOCAB	466.3	179.8	15.5	13.2	57.0	3.1
	Calif.	1432.6	863.8	109.0	28.0	117.0	14.4
Industrial Processes	SOCAB	26.6	22.3	171.1	9.9	16.0	32.6
	Calif.	122.1	86.5	506.8	28.9	124.0	188.6
Misc. Processes	SOCAB	1888.3	122.3	289.3	10.3	0.5	445.5
	Calif.	3052.2	447.9	555.8	61.7	4.7	4855.8
On-Road Vehicles	SOCAB	806.5	753.7	5747.0	723.2	47.7	82.5
	Calif.	1911.2	1786.5	13034.9	1824.9	110.7	201.0
Other Mobile Sources	SOCAB	74.7	71.1	431.8	109.0	25.8	7.1
	Calif.	311.4	299.5	1632.3	2252.4	189.6	249.6
All Sources (annual)	SOCAB	3689.8	1515.6	6766.6	1238.1	264.5	606.6
	Calif.	7942.1	4391.6	17140.3	3545.7	1001.7	5532.8
All Sources (summer weekday)	SOCAB		1697.0	6430.0	1335.0	274.2	660.0
All Sources (winter weekday)	SOCAB		1560.0	6830.0	1359.0	314.0	559.0
Uncertainty ^(b)	SOCAB		+10%	+16%	+11%	+9%	+19%

(a) Data from ARB (1982) and Grisinger et al. (1982). TOG and ROG in equivalent weights of CH₄, NO_x in equivalent weights of NO₂, SO_x in equivalent weights of SO₂, and TEP contain all particles less than 50 um.

(b) Composite relative uncertainty of total emissions derived from subjective estimates for individual source type emissions which range from +15% to +100%. Uncertainties are much higher for size and time-resolved emissions rates.

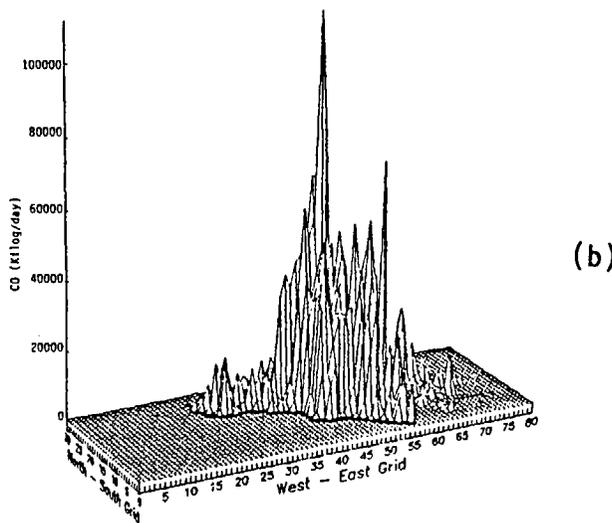
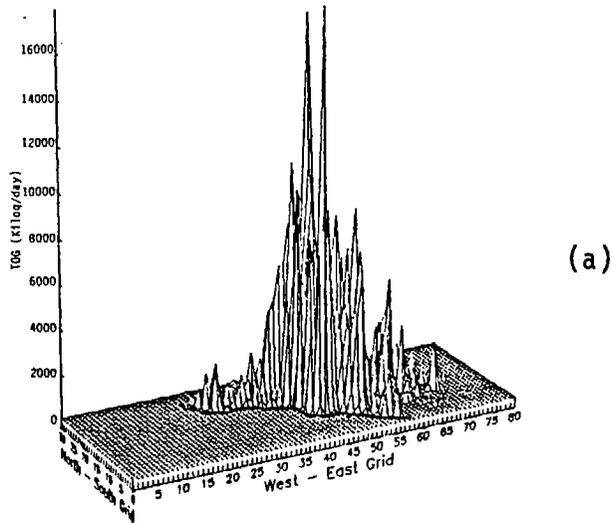


Figure 2-2. Spatial Pattern of Surface Emissions (<10 m AGL) in the South Coast Air Basin. These Data are 1982 Projections from the 1979 Emission Inventory for TOG (a), CO (b), NO_x (c), SO_x (d), and TSP (e) (personal communications with Ed Yotter of ARB, 1986).

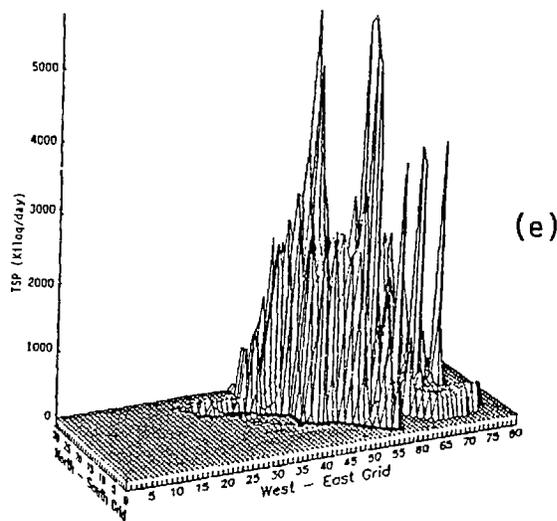
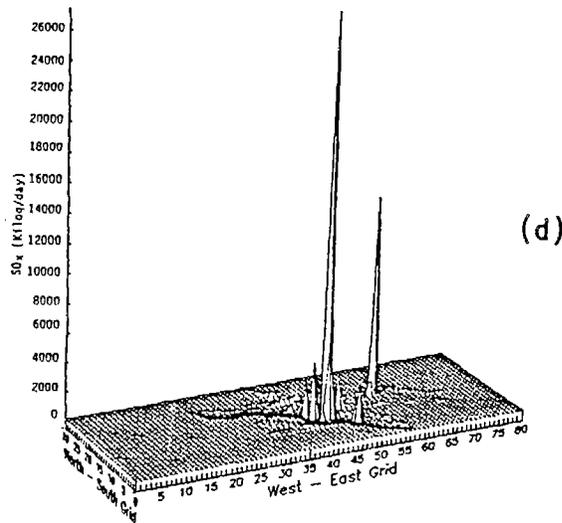
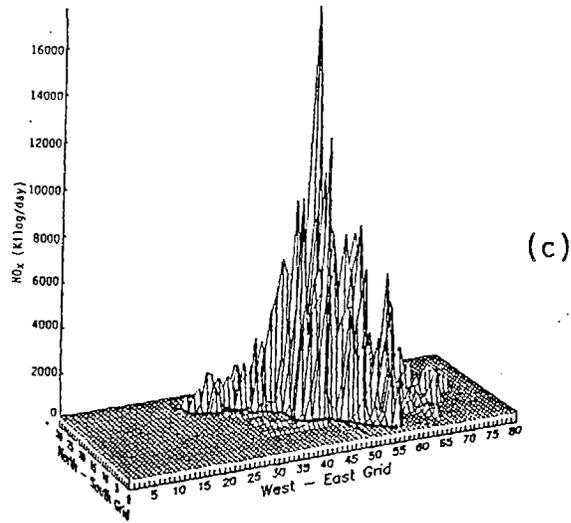


Figure 2-2. (Continued)

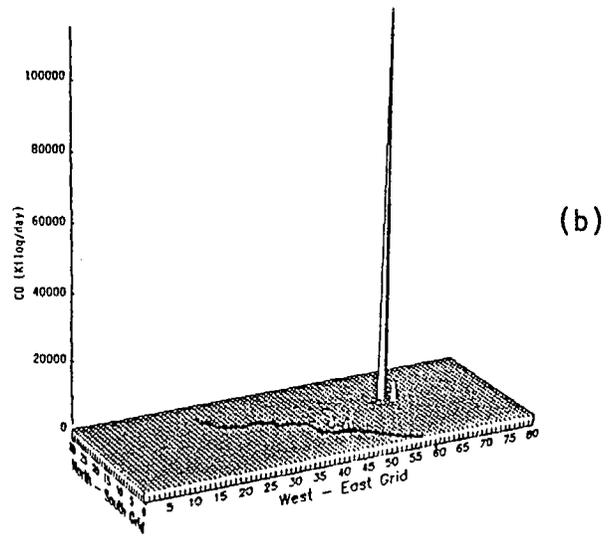
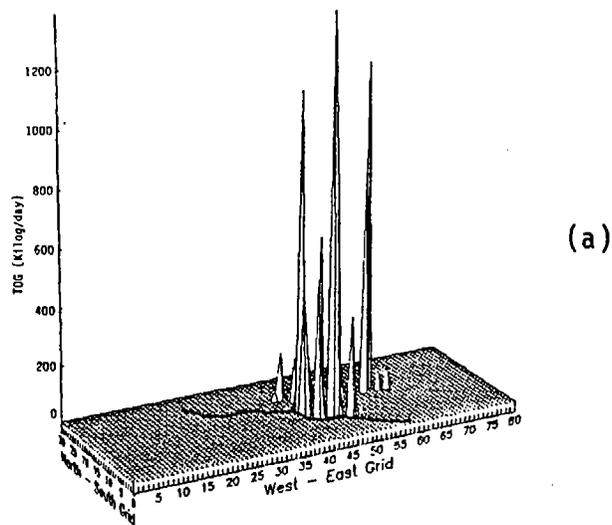


Figure 2-3. Spatial Pattern of Elevated Emissions (>10 m AGL) in the South Coast Air Basin. These Data are 1982 Projections from the 1979 Emission Inventory for TOG (a), CO (b), NO_x (c), SO_x (d), and TSP (e) (personal communication with ED Yotter of ARB, 1986).

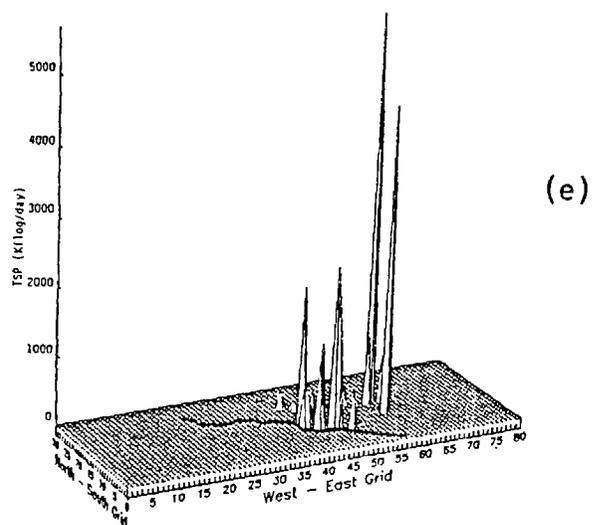
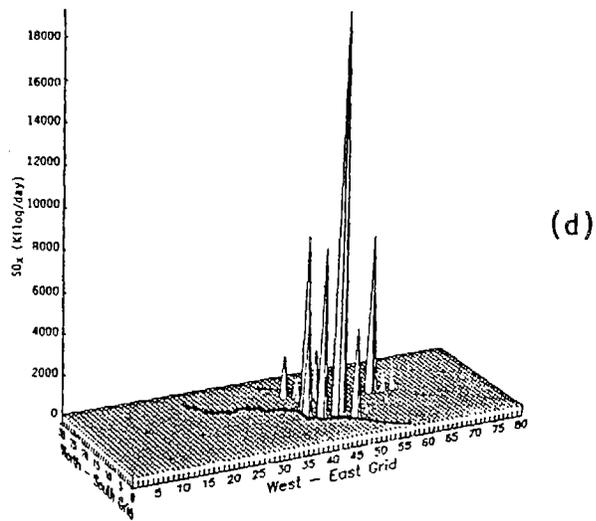
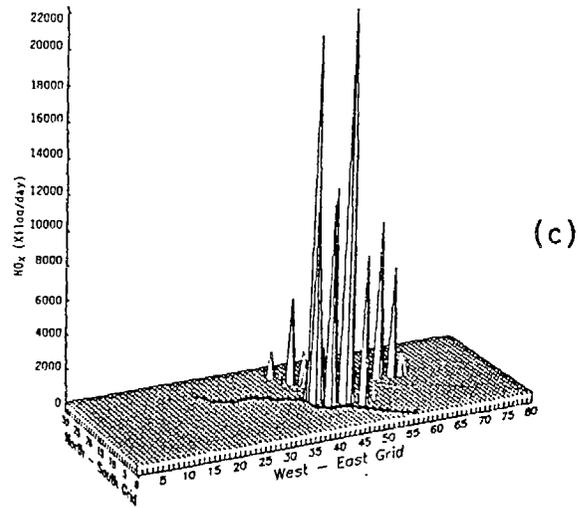


Figure 2-3. (Continued)

peninsula. Table 2-2 implies that petroleum transfer and storage and low-level combustion of sulfur-containing fuels take place in these grid squares. Surface particulate emissions are more uniformly distributed throughout the Basin with several large peaks which are probably attributable to some of the "miscellaneous processes" listed in Table 2-2. The downtown particle peak corresponds to similar patterns on the T_{OG}, CO, and NO_x plots and can probably be attributed to re-suspended road dust. The East Basin peaks could be attributable to agricultural tilling.

The peaks for all pollutant emissions in Figure 2-3 originate from the same point sources, and they are relatively few. Grisinger et al. (1982) list these sources and their location in order of emission rate. These elevated emitters are concentrated along the middle and southern coast with a few located in the east Basin. NO_x appears to be the most widely distributed elevated source, and many of its isolated appearances probably result from natural gas combustion which is accompanied by few other pollutant emissions. The elevated emissions of suspended particulate matter are more isolated in space than are the surface emissions, but their emissions rates are comparable to or greater than the surface rates in corresponding grid squares.

The temporal variations in pollutant emissions are not well documented. Though Grisinger et al. (1982) provide diurnal patterns for on-road vehicle emissions which show peaks during the morning and evening rush hours and lower than average emissions at night, these patterns are inferred rather than measured. SCAQMD receives daily NO_x emission rates from large stationary sources, but these are not formally incorporated into the inventory process. The ambient concentration changes observed during the 1984 Olympics by Davidson and Cassmassi (1985) indicate that temporal emission distributions may have an important effect on the products of those emissions.

The ARB and SCAQMD emissions inventory for the South Coast Air Basin is one of the best of its type in existence. Nevertheless, it contains uncertainties which derive from errors in the vast amount of acquired data, emission factors which are not derived from the specific emissions sources, and variable or undocumented process rates. The emission rates reported in Table 2-2 reflect activities as they were in 1979. Even though the SCAQMD (1982) has made projections into 1987, these projections are no substitute for a re-assessment of the emitting sources during the year of concern.

The 1979 inventory may not even present an entirely accurate picture for that year. Emission rates from stationary sources which exceed 10 tons/year are updated with each inventory revision from approximately 65,000 permits filed by 10,000 companies. Emissions from smaller sources are not routinely re-estimated, and these can account for more than 50% of the reactive organic gas emissions from stationary sources.

Grisinger et al. (1982) provide semi-quantitative estimates of the uncertainty of emission rates for the 1979 inventory, and the Basin-wide estimates recorded in Table 2-2 are tolerable for most assessment purposes. The individual emissions category uncertainties, however, range from 15% to 100% (these coefficients of variation are one standard deviation centered on the average emission rate estimate). Uncertainties for ROG rates from major emission categories such as surface coatings and gasoline hot soak and

evaporation are especially large (30% to 40%). Uncertainties associated with smaller spatial scales and time intervals probably are much higher than these estimates.

One specific concern involves the uncertainty of the ratio of reactive hydrocarbons to nitrogen oxides (NO_x) emissions which is used in the EKMA modeling (Liu, 1982) for the AQMP. The Basin-wide ratio for these emissions is approximately 3.5 while ambient measurements in the downtown area yield an average ratio of 10.3. (The ROG/NO_x ratio is based on volumetric concentrations of these gases. The mass emission rates in Table 2-2 must be converted by a factor equal to the ratio of their molecular weights.) This inconsistency can be explained by (1) inaccurate ROG or NO_x emission rates, (2) ROG and NO_x chemical reactions in the atmosphere, including different deposition rates, or (3) inaccurate measurements of ambient ROG and NO_x . Oliver and Peoples (1985) re-examined the 1979 inventory with respect to hydrocarbon and NO_x emissions from stationary and off-road mobile sources. They found some evidence of double counting, missing sources, and inconsistent use of emissions factors. Their corrections to the 1979 inventory amounted to 0.2%, 1.0%, and -3.0% adjustments to the Basin-wide rates for TOG , ROG , and NO_x , respectively, being emitted by stationary and off-road mobile sources. However, the relative adjustments within specific source categories were larger.

The total emitted particulate emissions in Table 2-2 are also highly uncertain and not necessarily applicable to the existing state and proposed federal standards for size-specific particulate matter. Size distributions for several primary emissions sources have been measured in the SOGAB (Taback et al., 1979) which can be applied to the TEP values to apportion these emissions among size ranges, but these size specific inventories have not been generated.

Grisinger et al. (1982) also call attention to the need to add ammonia emissions, better hydrocarbon profiles, and chemical speciation of emitted particulate matter (including hazardous substances) to the inventory. Ammonia is needed because of its potential involvement in the secondary fraction of PM_{10} . The hydrocarbon profiles are needed to separate ROG into reactivity categories. Several of these categories have been proposed and compared (e.g. Trijonis et al., 1978a) and others have been defined for air quality modeling. These hydrocarbon profiles can also be combined with other properties of the emissions to apportion ambient concentrations to their sources (e.g. Mayrsohn and Crabtree, 1976, Mayrsohn et al. 1977; Feigley and Jeffries, 1979). Chemical speciation of particulate matter is also necessary to apportion sources (e.g. Friedlander, 1973) and because of the roles of certain species on sulfur oxidation and atmospheric acidity. Abatement of toxic material concentrations will also require chemical-specific inventories for these species. Though Taback et al. (1979), Parungo et al. (1980), Rodes and Holland (1981), Dzubay et al. (1979), Miller et al. (1972), and Oliver and Peoples (1985) have made several chemically specific measurements of source emissions in the SOGAB, no comprehensive data of the important components are yet available for any SOGAB source category.

2.2.2 Transport, Transformation, and Deposition

Transport, transformation and deposition are treated together because of the large effects which meteorological conditions have on the movement and changes of pollutants. These phenomena have been, and continue to be, subjects

of intensive research on which volumes have been written. The intent here is to identify the subject areas of importance for particle and oxidant concentrations in the South Coast Air Basin. The data acquired in SCAQS will be used to elucidate these transport and transformation phenomena.

Southern California is in the semi-permanent high pressure zone of the eastern Pacific. It experiences hot summers, and the sparse rainfall occurs mostly during winter. Frequent and persistent temperature inversions are caused by subsidence of descending air warmed by compression settling over the cool, moist marine air. These inversions often occur during periods of maximum solar radiation (SCAQMD, 1982). Relative humidities can vary, depending on the origin of the air mass. RH typically exceeds 50% throughout the basin, being higher near the coast than farther inland (Smith et al., 1984).

As illustrated in Figure 2-1, the SOCAB is surrounded on the north, east, and west by mountains, some of which rise above 10,000 feet. The Basin opens to the Pacific Ocean on the southwest. The topography of the Basin combined with the land/sea interface introduces important mesoscale effects which are superimposed on the synoptic weather patterns.

Figures 2-4 and 2-5 from Smith et al. (1972) illustrate the diurnal evolution of surface flow patterns in the SOCAB for summer and winter months respectively. Similar patterns were found by Keith and Selik (1977). In the summertime, the sea breeze is strong during the day and there is a weak land-mountain breeze at night. Because of the high summer temperatures, the land temperature does not usually fall below the water temperature at night, and the nocturnal winds are slow and weak. The opposite is true during the winter, when the mountain-land breeze at night yields strong ventilation, and a mild sea breeze is only established late in the day when temperatures approach their maxima.

The predominant trajectories are from the west and south during summer mornings, switching to predominantly westerly flows by the late afternoon and early evening. These summertime trajectories become difficult to discern at night owing to the generally stagnant conditions. As shown in Figure 2-5, the prevailing wintertime trajectories are from the east and north at night, switching to westerly trajectories by late afternoon. In both cases, there is strong propensity for the transport of emissions from the western and southern parts of the SOCAB to the eastern and northern parts, with this propensity being higher during the summer months than in the winter months. Aircraft (e.g. Blumenthal et al., 1978; Calvert 1976a, 1976b), tetraon (e.g. Angell et al., 1976), and tracer (e.g. Shair et al., 1982) studies provide results which are qualitatively consistent with the trajectories illustrated in Figures 2-4 and 2-5.

The land/sea breeze circulation can cause air to transfer back and forth between the Basin and the Pacific Ocean. Cass and Shair (1984) estimated that up to 50% of the sulfate measured at Lennox was attributable to backwash of emissions which had been transported to sea on the previous day. During the daytime, emissions from coastal sources are advected inland by the sea breeze. At night, these polluted air masses are swept back toward the coast to await their re-entry to the Basin on the following day. There is ample evidence (e.g. Kauper and Niemann, 1975; 1977), however, that a good portion of these pollutants which pass the coastline can be transported to neighboring air basins.

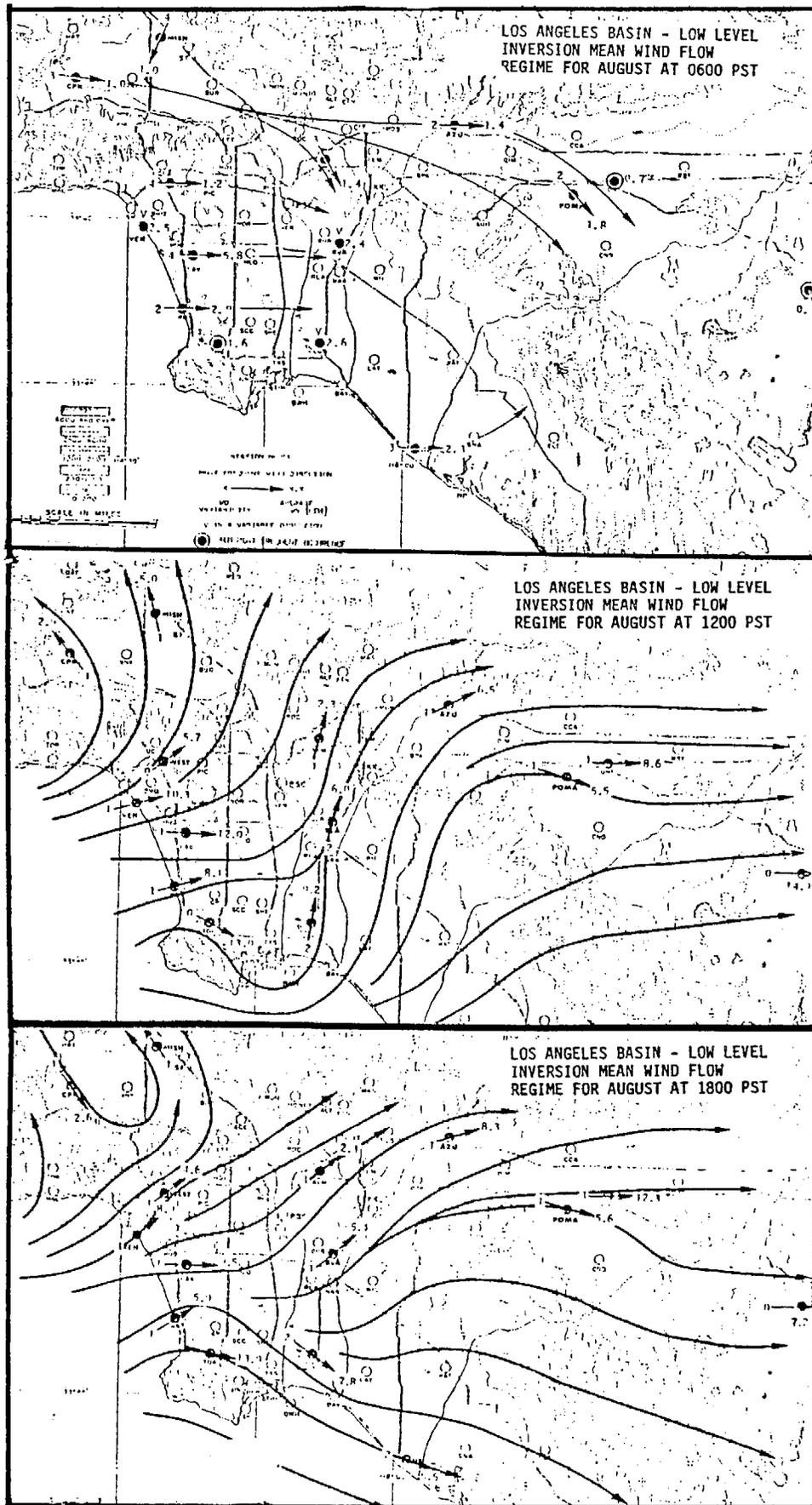


Figure 2-4. Summer Variation in Surface Wind Flow Patterns throughout the Day in the South Coast Air Basin (Smith et al., 1972).

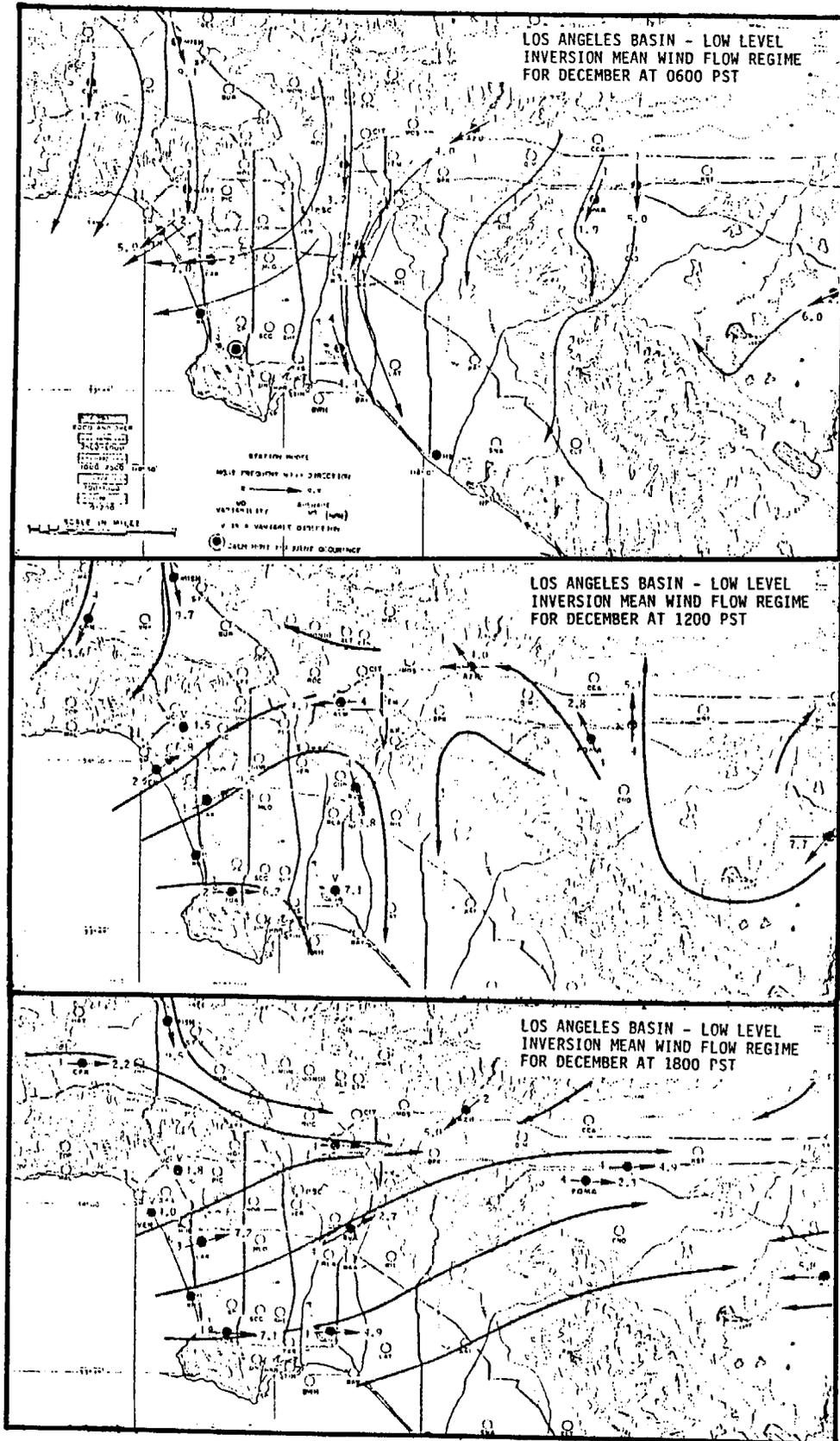


Figure 2-5. Winter Variation in Surface Wind Flow Patterns throughout the Day in the South Coast Air Basin (Smith et al., 1972).

Air from the Basin can exit through a number of routes other than the sea. Smith and Shair (1983) found transport routes through Soledad Canyon, Cajon Pass and San Geronimo Pass when they released tracer gases in the South Coast Air Basin. Smith and Shair (1983) also showed evidence of transport aloft from the San Fernando Valley into eastern Ventura County. Godden and Lague (1983) note, however, that tracer experiments also provide "...circumstantial evidence...that pollutants can be transported both from Ventura County through the Simi Hills and along the coast to West Los Angeles...".

Smith et al. (1984) have made a comprehensive study of air pollution climatologies in California. In addition to the above observations, Smith et al. (1984) note the potential for slope flows and convergence zones in the SOCAB. Slope flows provide a mechanism for the transport of pollutants from below the inversion to above. They occur when the mountains absorb solar radiation and heat the surrounding air, making it more buoyant. Smith et al. (1984) comment that "In areas such as the South Coast Air Basin, this transport mechanism provides one of the more effective methods of removing pollutants from the Basin." This upslope flow can result in high pollutant concentrations at elevated locations. These locations would not normally experience such pollution due to their own local emissions.

Convergence zones occur where terrain and pressure-gradients direct wind flows in opposite directions; the convergence results in an upwelling of air, and a consequent transport of pollutants to higher elevations. These convergence zones can also restrict the transport of pollutants from one basin to another. Smith et al. (1984) plot SOCAB convergence zones at Elsinor (McElroy et al. 1982; Smith and Edinger, 1984), the San Fernando Valley (Edinger and Helvey, 1961), El Mirage, the Coachella Valley, and Ventura.

Several of these meteorological features (upslope flow, convergence zones, marine air intrusions, transport into the stable layer, and plume rise from elevated sources) inject pollutants above the mixed layer. As the mixing depth increases during the day, some of these elevated pollutants can become re-entrained in the mixed layer and advected to ground level.

Smith et al. (1984) comment that "... The primary source of uncertainty in defining meteorological air pollution potential in the state lies in the description of mixing height behavior, particularly in the coastal areas where mixing height changes significantly with distance inland." They believe that SOCAB upper air measurements should be supplemented with additional soundings in the San Bernardino/Riverside area. While these complex meteorological phenomena affecting pollution potential are qualitatively simple, their quantitative description is much more difficult.

In addition to atmospheric movements, temperature, insolation, and relative humidity affect the transformations of precursor gases to ozone and suspended particulate matter. Photochemical transformations are probably the most important of these, and they have been recognized as important since the days of Haagen-Smit in the early 1950s. Ozone plus the sulfate, nitrate and organic fractions of the aerosol are influenced by photochemical processes.

The photochemical influence on ozone formation is well established in the SOCAB in laboratory studies (e.g. Kopczynski et al. 1972), in semi-coherent air parcels sampled with airborne platforms (e.g. Calvert,

1976a, 1976b; Feigley and Jeffries, 1979; Spicer et al. 1983) and at fixed ground stations (e.g. Spicer, 1977; Reynolds et al. 1974; McRae and Seinfeld, 1983; Godden and Lurmann, 1983) which represent SOCAB atmospheres. Measurements in these studies all show a morning buildup (or initial concentration) of NO from fresh emissions, followed a few hours later by a dramatic decrease in NO and peak of NO₂, which is in turn followed by a peak in ozone concentrations in the early to late afternoon (depending on the location of the sampling site). While these qualitative features are well-established and reproducible, the chemistry and physics describing them is not. Dunker et al. (1984), Leone and Seinfeld (1984a, 1984b), and Killus and Whitten (1983) have compared the most recent photochemical reaction mechanisms applied to similar situations. Though all mechanisms exhibit the same qualitative features of reactant and end-product concentrations with time, the peak values and the time of occurrence of those peaks are mechanism dependent. The practical mechanism which is most representative of reality is still open to judgment.

Photochemical sulfate formation in the Los Angeles atmosphere typically follows a diurnal cycle with a daytime maximum rate near 6% per hour (Roberts, 1975; Cass, 1981). Nitrogen dioxide is converted to nitric acid by hydroxyl radicals at rates five to ten times faster than sulfur dioxide is converted to sulfate (Forrest et al., 1981). Nitrogen dioxide is also converted to peroxyacetyl nitrate (PAN), and the proportions depend on the initial ROG/NO_x ratios (Spicer et al. 1983). Though both nitric acid and PAN are gases, nitric acid is also present in liquid particles. The photochemical formation of organic aerosol is less well understood (Pitts et al. 1978; Hidy and Mueller, 1979), but is the subject of much current work. Studies of organic aerosol formation are inconclusive because of the plethora of precursors and the volatilities of their products. Theoretical mechanisms for the photochemical conversion of gases to particles are still in their formative stages.

The differences between inventoried and ambient ROG/NO_x ratios can be explained, at least in part, by these theoretical reaction mechanisms. Haney and Seigneur (1985) re-examined the ambient ROG and NO_x concentrations generated by a recent application of the SAI urban airshed model to the SOCAB which used an initial ROG/NO_x emissions ratio of 2.86. They found that the ROG/NO_x ratios at Anaheim and Downtown L.A. reached values of 7 to 9 during the hours just past noon and dropped to values of 3 to 5 at night. The afternoon values correspond to the period of maximum ozone production, when a large portion of the ambient NO_x is reduced by photochemical reactions. Photochemistry ceases after sunset, allowing the NO_x to be replenished. Calculations for Riverside show ratios ranging from 4.5 to 61.7 because the pollutants have undergone longer photochemical reaction times and ambient NO_x levels are much lower than those at the downtown sites. Haney and Seigneur (1985) conclude that the faster oxidation of NO_x with respect to ROG during photochemical smog formation can account for the difference between inventoried and ambient ROG/NO_x ratios and that neither the inventory nor the ambient measurements are necessarily in error.

Though photochemical transformation processes are of greatest importance for the production of ozone, gases can be transformed into suspended particulate matter by a number of other processes. Husar et al. (1976) show direct evidence of the condensation of gaseous species on solid

or liquid particles. Relative humidity changes affect the water content of aerosols, which have consequences with respect to their size and their propensity to scatter light (Charlson et al. 1969; Covert et al. 1972; Tang et al. 1981). This effect tends to be important at relative humidities above 70% when many dry, ionic particles deliquesce. Sulfate formation rates increase when small particles in solution are present in the atmosphere (Cass, 1975; Dittenhoeffer and dePena, 1978; Gillani and Wilson, 1983; Gillani et al. 1983). Under these conditions, the growth of relatively large particles can be favored (McMurry and Wilson, 1980; Hering and Friedlander, 1982).

Particles can also form in fog and clouds because soluble particles are preferentially activated during the formation of clouds and fog, and ionic species formed in fog or cloud water will become part of these particles when the fog or clouds evaporate. This mechanism has been inferred from models (e.g. Chameides and Davis, 1982; Seigneur and Saxeena, 1984; Young et al. 1983; Jacob and Hoffmann, 1983), from rain chemistry (Lazrus et al. 1983), and cloud measurements (Richards et al., 1983a, 1983b; Daum et al., 1983). Catalysis by trace metals such as manganese and iron may be important in sulfate formation in fog and clouds (Martin, 1983; Young et al., 1983; Jacob and Hoffmann, 1983; Seigneur and Saxeena, 1984; Seigneur et al. 1985). Nitric acid has been shown to be rapidly scavenged by fog or clouds (Levine and Schwartz, 1982).

The non-photochemical particle formation mechanisms may be especially influential at night and during winter periods. Richards (1983) proposes a mechanism in which ozone aloft reacts with NO_x to form nitrate. Richards (1983) speculates that this mechanism may explain the high morning concentrations of large particle nitrate which were observed by Appel et al. (1978). Recent theoretical formulations of these particle formation mechanisms have been developed for incorporation into the comprehensive mathematical models describing the SOCAB (e.g. Russell et al. 1983; Bassett and Seinfeld, 1983; Heisler and Friedlander, 1977; Bassett et al. 1981; Seigneur et al. 1985).

Wet and dry deposition of atmospheric constituents in the SOCAB are not well understood, even though Roberts (1975) estimated that nearly 50% of the sulfur oxides are removed at the ground within the Basin and Morgan and Liljestrang (1980) estimated that the dry deposition of pollutants may exceed wet deposition by an order of magnitude. Most theoretical formulations of deposition describe the flux to the surface as a product of an ambient concentration and a deposition velocity. These deposition velocities are functions of turbulent diffusion near the ground, molecular motions at the ground-air interface, and the reaction of the pollutant with the surface. McRae et al. (1982b) mathematically described the turbulent diffusion mechanisms and found that the deposition rates are extremely sensitive to atmospheric stability. They noted that there are no satisfactory theoretical treatments of mass transfer close to the surface and that field data on pollutant uptake by surfaces are inadequate. Dry deposition samples in the SOCAB have been collected on surrogate surfaces (as summarized in Shikiya et al. 1984), but these are not considered to be accurate estimates of dry deposition fluxes.

2.2.3 Receptor Measurements

Figure 2-1 shows the sampling sites which have been acquiring routine air quality monitoring data in the South Coast Air Basin. Though several of these sites have changed from time to time, the basic network has remained essentially the same since 1965. Ludwig et al. (1983) have examined the spatial distribution of this network with respect to its adequacy in determining ozone standard violations. They found that as few as ten of the SCAQMD stations would provide an accurate estimate of the number of exceedances per site. The coverage of this network is such that coastal, inland, and valley areas are represented. All EPA siting criteria and shelter requirements are complied with at all sites.

Table 2-3 identifies the routine measurements which are made at existing sampling sites in the South Coast Air Basin. Carbon monoxide by non-dispersive infrared spectrophotometry, ozone by ultraviolet photometry, nitrogen oxide and nitrogen oxides by chemiluminescence, sulfur dioxide by pulsed fluorescence, total hydrocarbons by flame ionization detector, and total suspended particulate matter by standard HiVol samplers are measured at most sites. Gas concentrations of one-hour duration are acquired continuously and suspended particle samples of 24-hour duration are acquired on a six-day schedule. Mass, sulfate, nitrate, and lead measurements are made on most of the HiVol samples. Size-classified particulate matter in the 0 to 10 μm size range is currently being collected at 11 sites, as indicated in Table 2-3, using automatic mass flow controlled high volume samplers with Sierra-Anderson 321A size-selective inlets. This monitoring is being performed in anticipation of the promulgation of a new national ambient air quality standard for particulate matter (Federal Register, 1984) and to determine compliance with California's size-selective particulate matter standard. Mass, sulfate and nitrate measurements are currently being made on these samples.

Table 2-3 also shows the distribution of surface meteorological monitoring networks which acquire wind speed, wind direction, temperature, relative humidity, and insolation data. Goodin et al. (1979, 1980) have examined the adequacy of this network for replicating a known surface wind field and have found it adequate when the proper interpolation and adjustment schemes are used. The network is not adequate, however, for determining a three-dimensional wind field.

Ambient air quality data acquired from this network over many years show the following general features taken from the 1982 Summary of Air Quality (SCAQMD, 1983; Hoggan et al. 1983):

- Ozone. Coastal stations experience the lowest concentrations and the lowest number of standard exceedance cases. Concentrations increase sharply from the coastal to the inland valley portions of the Basin. The area with the highest ozone levels extends from the San Fernando Valley through the San Gabriel Valley and into the Riverside-San Bernardino area and adjacent mountains. In 1982, Azusa, Pico Rivera, Los Angeles, and Norco exhibited hourly ozone concentrations in excess of 0.35 ppm. The highest value of 1982 was 0.40 ppm which occurred at the downtown Los Angeles site between noon and 1 p.m. on September 2, 1982. Figures 2-6a, b, c, and d show

Table 2-3. Air Quality and Meteorological Routine Measurements at Existing Sites in the South Coast Region

Site Code	Sampling Site	03	NO/NOx	CO	Gaseous			Pollutants Monitored					Meteorological Measurements				
					SO2	THC(a)	NMHC (b)	TSP	Pb	S04	H1Vo1 NO3	TOF (c)	PM10	Temp	Humidity	WS/WD(d)	Radiation
LOS ANGELES BASIN																	
SURFACE																	
1	Alhambra			X	X												X
2	Anaheim	X	X	X	X												X
3	Azusa	X	X	X	X												X
4	Banning	X	X	X	X												X
5	Burbank	X	X	X	X												X
6	Burbank AP																X
7	Cajon																X
8	Chino	X															X
9	Compton AP																X
10	Costa Mesa	X	X	X	X												X
11	El Toro	X	X	X	X												X
12	El Toro MB																X
13	Fontana	X	X	X	X												X
14	Glendora	X															X
15	Hawthorne AP																X
16	Hemet	X															X
17	John Wayne AP																X
18	La Habra	X	X	X	X												X
19	Lake Gregory	X	X	X	X												X
20	Lennox	X	X	X	X												X
21	Long Beach	X	X	X	X												X
22	Los Alamitos	X	X	X	X												X
23	Los Angeles	X	X	X	X												X
24	LAX																X
26	Lynwood	X	X	X	X												X
27	Malibu																X
28	March AFB																X
29	Mission Hills	X															X
30	Newhall	X															X
31	Norco	X															X
32	Norton AFB																X
33	Ontario AP																X
34	Pasadena	X	X	X	X												X
35	Perris	X	X	X	X												X
36	Pico Rivera	X	X	X	X												X
37	Pomona	X	X	X	X												X
38	Redlands	X	X	X	X												X
39	Redondo Beach Airport																X
40	Reseda	X	X	X	X												X
41	Rialto																X
42	Riverside	X	X	X	X												X
43	Rubidoux	X	X	X	X												X

Table 2-3. (continued)

Site Code	Sampling Site	Pollutants Monitored										Meteorological Measurements						
		03	NO/NOx	CO	S02	Gaseous	THC(a)	MMHC(b)	TSP	Pb	S04	HiVol NO3	TOF(c)	PM10	Temp	Humidity	WS/WD(d)	Radiation
44	San Bernardino	X	X	X	X	X	X	X	X	X	X	X	X				X	
45	San Juan Capistrano																X	X
46	Santa Monica AP													X	X		X	X
47	Torrance AP													X	X		X	X
48	Upland	X	X	X	X	X	X	X	X	X	X	X	X	X	X		X	X
49	Van Nuys													X	X		X	X
50	Venice																X	X
51	Vernon																X	X
52	W. LA	X	X	X	X	X	X	X	X	X	X	X	X				X	X
53	Whittier	X	X	X	X	X	X	X	X	X	X	X	X				X	X
54	Zuma Beach																X	X
55	Beaumont													X	X		X	X
56	Fullerton AP													X	X		X	X
57	Mt. Wilson																X	X
58	Pomona AP																X	X
UPPER AIR																		
25	Loyola-Marymount																X	X
33	Ontario AP	X												X	X			

Table 2-3. (continued)

Site Code	Sampling Site	Pollutants Monitored										Meteorological Measurements				
		03	NO/NOx	Gaseous CO	S02	THC(a)	NMHC (b)	TSP	Pb	S04	H1Vo1 NO3	TOF(c) PM10	Temp	Humidity	WS/WD (d)	Radiation
<u>VENTURA COUNTY</u>																
<u>SURFACE</u>																
	Anacapa Is	X									X					X
	Casitas Pass										X					X
	El Rio	X		X							X					X
	Laguna Peak										X					X
	Ojai	X									X					X
59	Oxnard AP										X					X
	Piru	X									X					X
	Pt. Mugu										X					X
60	Rocketdyne	X									X					X
	San Miguel Is										X					X
	Santa Barbara Is										X					X
	Santa Cruz Is										X					X
	Santa Rosa Is										X					X
61	Simi Valley	X		X	X	X	X	X	X	X	X					X
62	Thousand Oaks										X					X
	Upper Ojai	X		X	X	X	X	X	X	X	X					X
	Ventura	X		X	X	X	X	X	X	X	X					X
<u>UPPER AIR</u>																
	Pt. Mugu															X
	San Nicolas Is														X	X

(a) THC = total hydrocarbon

(b) NMHC = non-methane hydrocarbon

(c) TOF = total benzen extractable organic fraction

(d) WS/WD = wind speed and wind direction

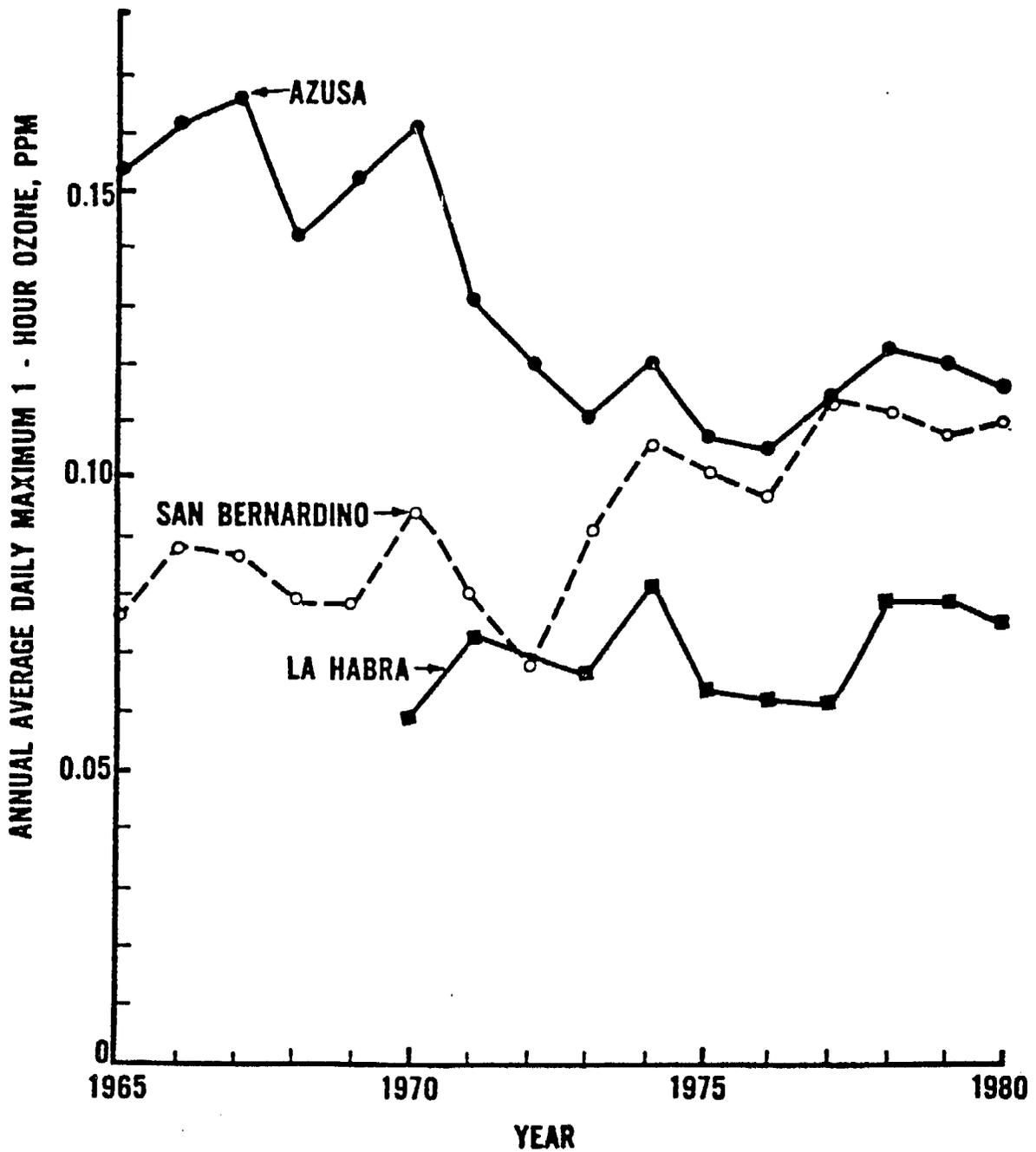


Figure 2-6a. Sixteen Year Trend in the Annual Average of Daily Maximum 1-Hour Ozone Concentration from 1965 to 1980 at Azusa, San Bernardino, and La Habra. (SCAQMD, 1981)

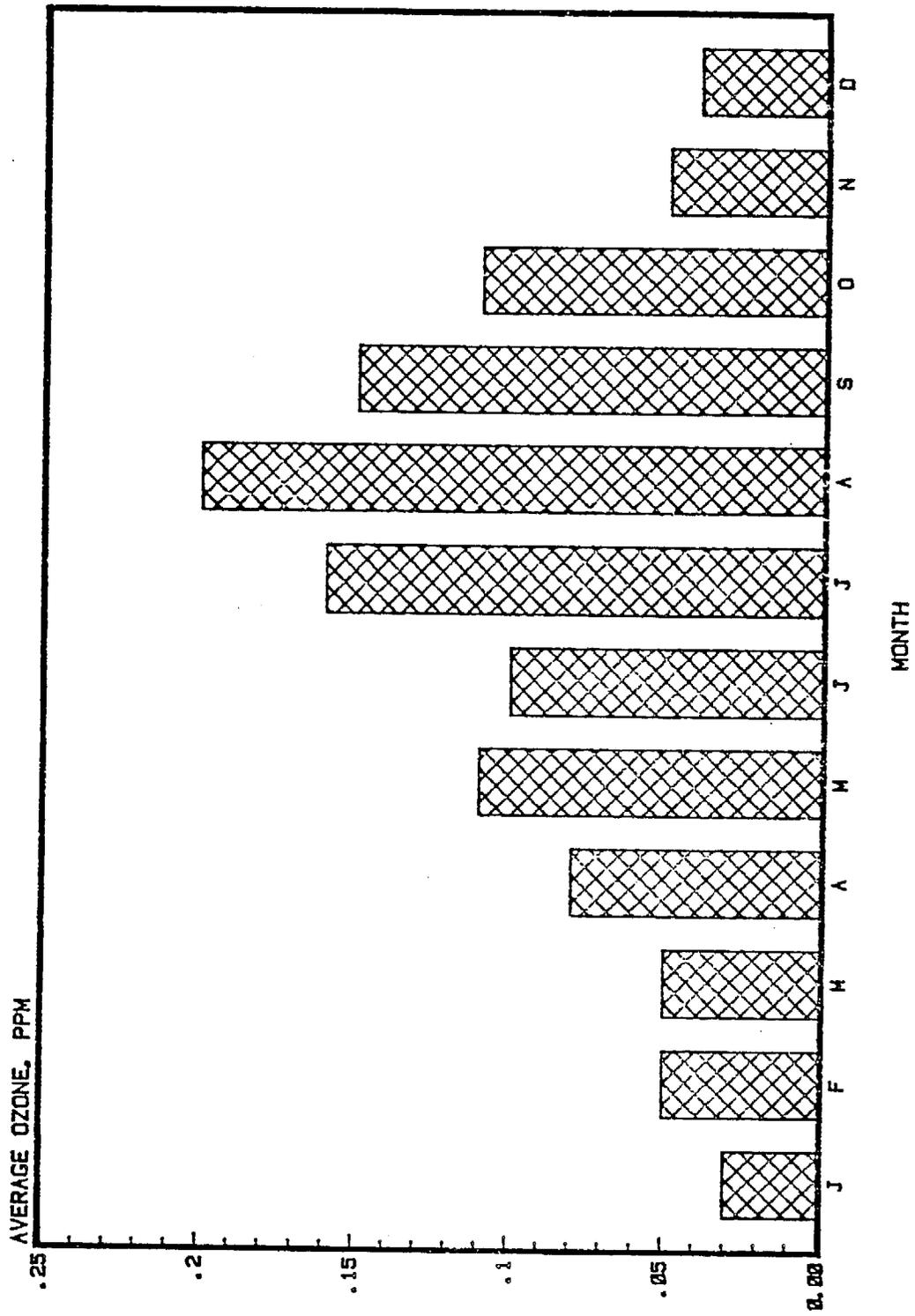


Figure 2-6b. 1982 Ozone Monthly Average of Daily 1-Hour Maximum at Azusa, CA. (Hoggan et al., 1983)

AZUSA (JAN, FEB, DEC, 1982)

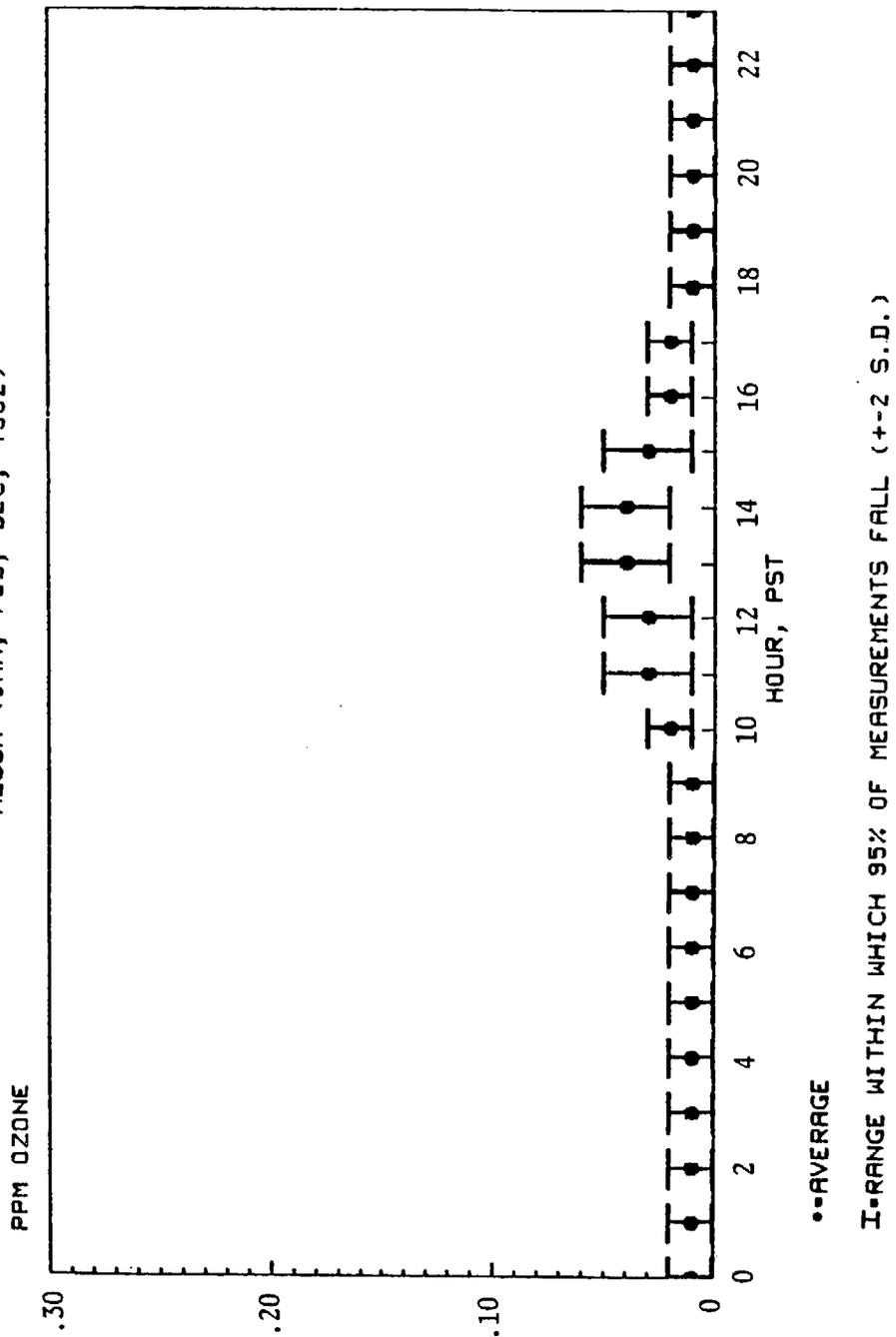


Figure 2-6c. 1982 Winter Average Ozone for Each Hour at Azusa, CA. (Hoggan et al., 1983)

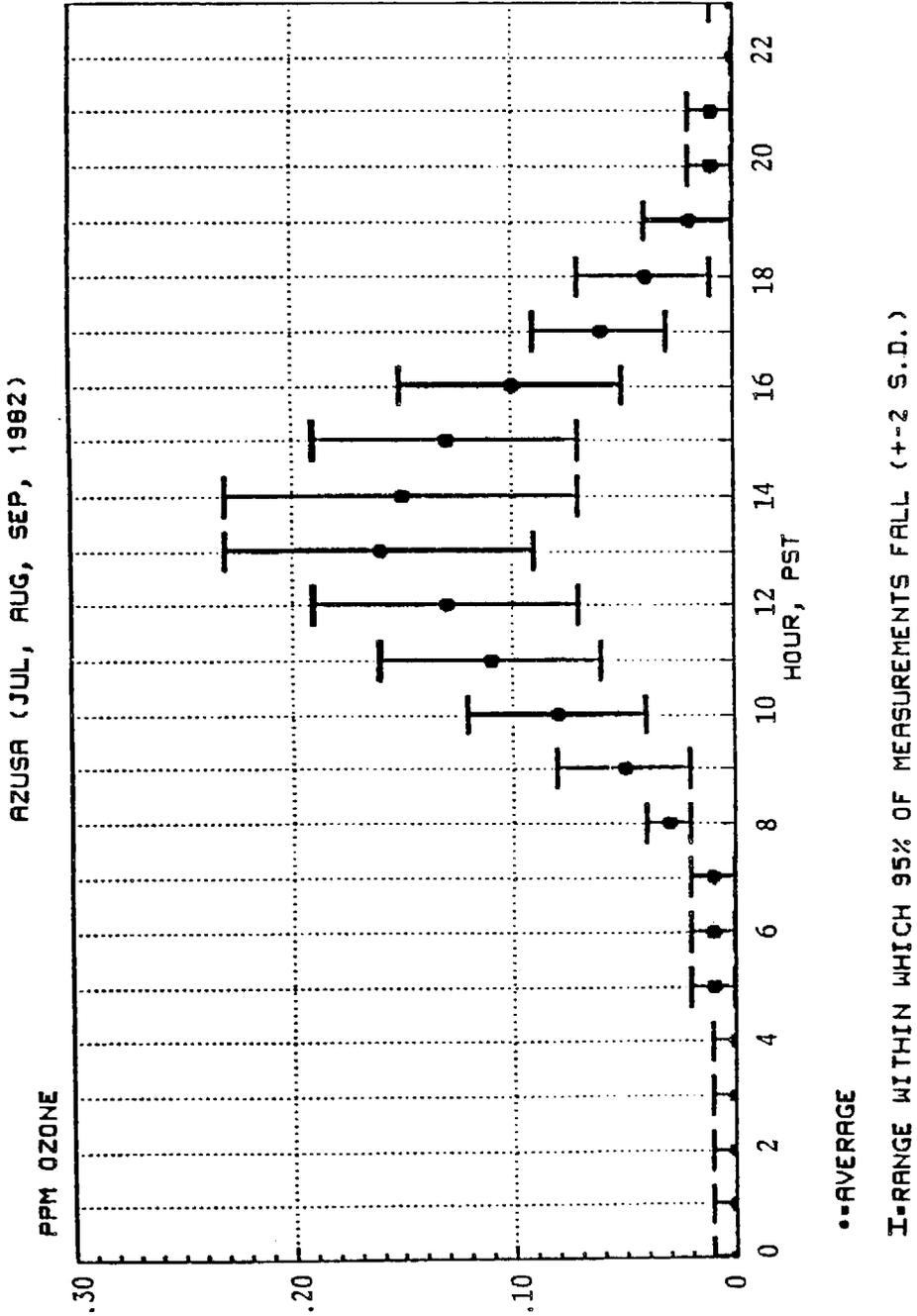


Figure 2-6d. 1982 Summer Average Ozone for Each Hour at Azusa, CA. (Hoggan et al., 1983)

long-term trends, monthly averages, and the diurnal pattern of ozone concentrations at Azusa which are typical of the patterns at most inland sites in the network. Highest ozone dosages tend to occur at elevated sites in the San Gabriel and San Bernardino Mountains. NO values are very low at these sites, and there is little opportunity for the O₃ which reaches them to be scavenged.

- Carbon Monoxide. More than half of the SOCAB stations are in compliance with the CO standard. The highest concentrations are observed during the winter at Lennox, Lynwood, Burbank, and Reseda. The highest one-hour value of 27 ppm in 1982 occurred at Lynwood on December 17, 1982. The diurnal distribution of CO follows the morning and evening rush hours. This pollutant is particularly useful in identifying the presence or absence of motor vehicle emissions at each receptor.
- Sulfur Dioxide. SO₂ concentrations are generally low throughout the Basin, except when the monitor encounters a plume. Daytime concentrations are generally higher than nighttime concentrations. This is consistent with SO₂ emissions from elevated sources being injected above the nighttime mixing layer. For the most part, the presence or absence of this pollutant indicates the influence or absence of nearby elevated source emissions. The maximum twenty-four hour average SO₂ concentration in 1982 was 36 ppb at Lennox on December 7.
- Nitrogen Oxides. Highest concentrations were found in 1982 at Los Angeles, West Los Angeles, Lennox, Long Beach, and Whittier. NO₂ concentrations do not show consistent patterns across the Basin, probably owing to the multitude of possible interactions of this pollutant with other pollutants, nearby emissions, and meteorological variables. The maximum hourly average NO₂ concentration in 1982 was 410 ppb measured at Los Angeles on September 3. This followed closely on the maximum ozone concentration which was measured at the same site on the preceding day.
- Total Suspended Particulate Matter. The highest 24 hour TSP levels are detected in an area extending from the eastern San Gabriel Valley, through the Pomona Valley and into the Riverside-San Bernardino area. Seasonal averages vary from location to location, indicating the multiplicity of factors affecting TSP concentrations. The sulfate, nitrate, and lead fractions of TSP provide some insight into the contributors to these pollutant levels. Sulfate typically comprises 7%-13% of TSP and the highest levels are consistently found downwind of major SO₂ emission sources. Highest sulfate levels generally occur during the late summer under conditions of high humidity, while the lowest concentrations are evident in the winter. Nitrate typically comprises 12%-20% of TSP. Highest levels are experienced in the San Bernardino-Riverside area in the summer and fall. Lead concentrations ranged from

0.3% to 1.1% of TSP in 1982 and are decreasing as lead is phased out of use in the motor vehicle fleet (Hoggan et al. 1978). Highest lead levels in 1982 were found in the densely populated areas of Lennox and Lynwood. In 1982, the highest TSP value of $272 \mu\text{g}/\text{m}^3$ occurred at Fontana on July 16 and the highest daily sulfate value of $37.3 \mu\text{g}/\text{m}^3$ occurred at Lennox on December 7, though most other high values were found in the September/October time-frame. The highest annual average nitrate of $21.3 \mu\text{g}/\text{m}^3$ occurred at Riverside, and the highest monthly average lead level was $1.7 \mu\text{g}/\text{m}^3$ at Lennox in October. The SCAQMD has estimated PM-10 annual averages from 1984 TSP data (Figure 2-7). These averages are likely to exceed $50 \mu\text{g}/\text{m}^3$ at nearly all SOCAB sampling sites, with the sites in the San Bernardino/Riverside areas having the highest values. Measured PM-10 values at seven sites show definite exceedance cases at Downtown L.A. and Rubidoux. In addition, Azusa and Burbank are very likely to be in violation of the annual PM-10 standard. Only Rubidoux exceeded the lower limit ($150 \mu\text{g}/\text{m}^3$) of the proposed 24-hr PM-10 standard with a high concentration of $208 \mu\text{g}/\text{m}^3$.

While most historical monitoring has focused on O_3 , CO , SO_2 , NO_2 , and TSP owing to their regulation by National Ambient Air Quality Standards, it has also been recognized that particulate and gaseous organic material, nitrogenous substances, trace metals, atmospheric mutagens, acid deposition, and visibility are also phenomena of public concern. Both short-term and long-term monitoring programs have been implemented to study these issues. Typical concentrations and ranges for several of these measurements are summarized in Section 3.

A major concern in the interpretation of receptor measurements has been the extent to which these measurements are representative of reality. The limitations of measurement technology have repeatedly clouded the interpretation of data used to elucidate cause and effect relationships between variables.

Oxidant measurements taken in the SOCAB prior to 1974 indicated that the major problem areas were confined to the eastern cities in the Basin, and scrutiny of mid-Basin cities, such as Pasadena, was minimized. Pitts et al. (1976) reexamined the oxidant measurements taken between 1955 and 1974 after applying corrections for different calibrations (buffered and unbuffered KI calibrations were converted to an ultraviolet absorption standard) used in Los Angeles County and other counties of the SOCAB. Their re-interpretation of the corrected data concluded that "...oxidant levels do not increase along a west to east axis across the basin [as was previously believed]....they do increase along a southwest to northeast axis across the basin, which roughly matches the orientation of the prevailing onshore sea breezes." Hydrocarbon interferences with the current ultraviolet absorption ozone measurement method must be considered in interpretation of ozone measurements derived from it.

Winer et al. (1974) have quantified the interference of PAN and several other organic nitrates in the chemiluminescent monitoring of NO_2 . Nitroethane and nitric acid were found to interfere, but only

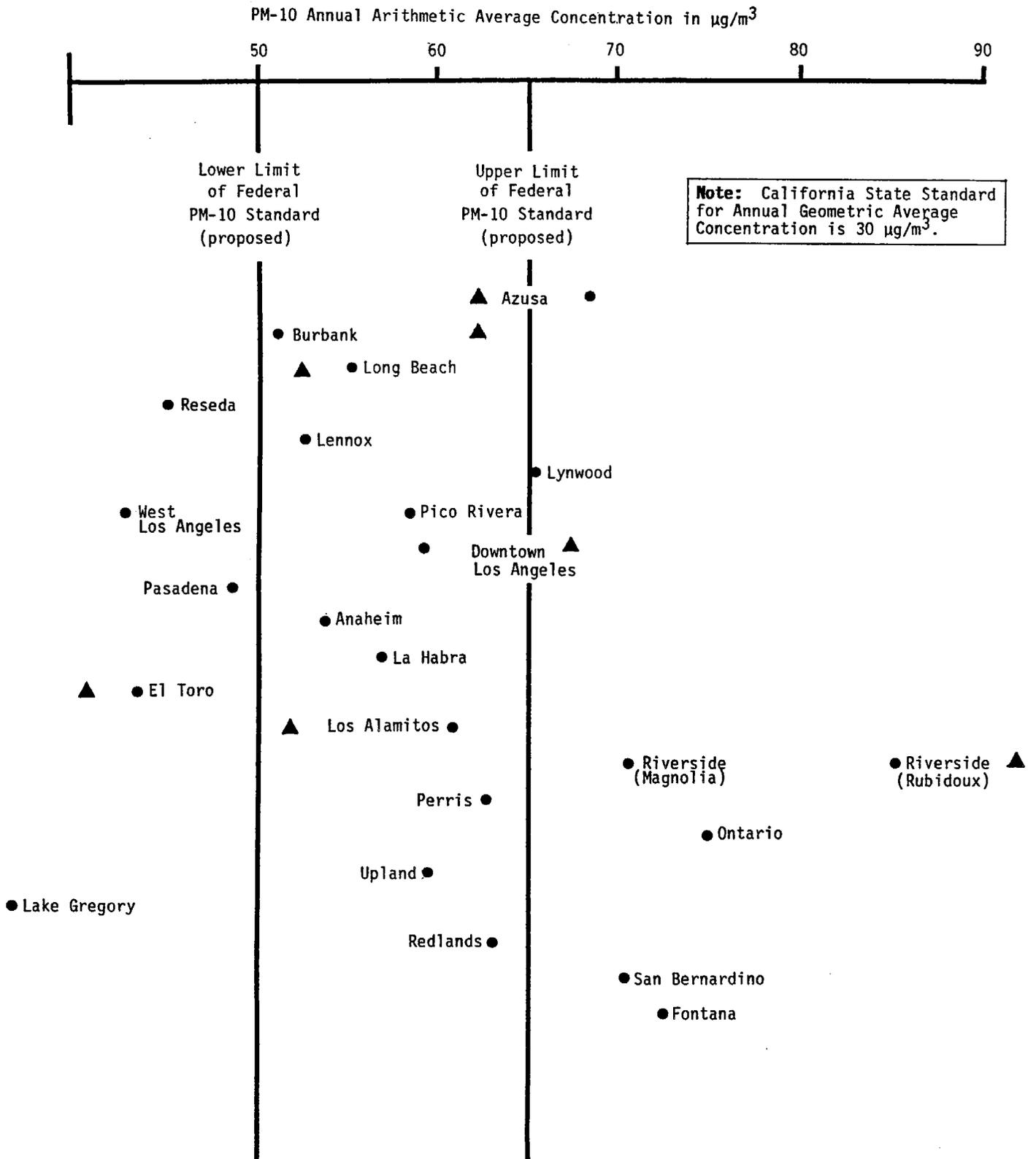


Figure 2-7. Estimated PM-10 Annual Arithmetic Averages (●) from 1984 TSP Data (Based on TSP x 0.59 = PM-10) and Measured PM-10 Annual Averages (▲) from October 1984 to October 1985 (personal communication, Art Davidson, SCAQMD, 1985).

semi-quantitative estimates are given by Winer et al. Grosjean (1983) observed that "On smoggy days...NO₂ can be seriously overestimated if the response of chemiluminescent instruments to PAN and HONO₂ is not taken into account." He found that NO₂ was overestimated by as much as 33%, 56%, and 65% in three different smog episodes. Godden and Lurmann (1983) found that many of their model predictions of NO and NO₂ could easily fall within the range of uncertainties caused by the unknown degree of measurement interference caused by other nitrogenous species. These measurement interferences clearly affect the interpretation of these data and the determination of compliance with standards.

The particle size ranges and chemical composition of routine TSP measurements have been shown to be uncertain. The standard HiVol sampler has a 50% sampling effectiveness between 30 and 50 μm, depending on wind speed and sampler orientation with respect to the wind direction (McFarland et al., 1979). The glass fiber filters used for SOCAB measurements yield higher sulfate and nitrate concentrations than are actually present in the atmosphere (Witz and MacPhee, 1977; Witz and Wendt, 1981; Witz et al. 1982). Spicer (1977) warns that "...some of the extreme particulate nitrate levels recorded in Southern California [in ACHEX] during 1-2 hr afternoon sampling periods may be attributable in part to collection of artifact nitrate." Grosjean (1975) found that the benzene-soluble organic fraction of TSP, which has been measured for years on SOCAB samples, is a variable fraction of the total organic content which is not relatable to any significant phenomena.

These particle measurement concerns have not been abated by the proposed PM-10 reference method. Watson and Rogers (1985) have evaluated the proposed California Method P for PM-10 mass measurement and have semi-quantified the potential effects of different sampler inlets, filter media, flow measurement and control, sample handling and other environmental variables. Each of these variables has a measurable effect on the mass and chemical species concentrations, though not all of these effects are quantifiable in a specific application. The greatest controversy involves the size-selective properties of PM-10 inlets (Rodes et al. 1985; Wedding et al. 1985; McFarland and Ortiz, 1985; Wedding et al. 1986).

A portion of the difference between ROG/NO_x ratios in ambient air and in the emissions inventory may result from the ambient ROG measurements. Liu (1982) compared measured ROG/NO_x ratios acquired for every day of June, 1981, by three different monitoring methods. Several adjustments were applied to the ROG and NO_x values to account for interferences. These average ratios obtained by the different methods ranged from 1.7 to 41, a range which surely includes the 3.5 ratio yielded by the Basin-wide emissions inventory. The ROG/NO_x ratio of 10.3 which was finally selected for EKMA modeling must, therefore, be used with due consideration of its large uncertainty.

These recognized measurement limitations and their effects on the data interpretation apply to routine measurement methods which have been in place for years. Limitations to several of the measurements proposed for SCAQS in Section 3 are only partially known, or are totally unknown, at this time. Past history suggests that a portion of SCAQS resources should be dedicated to the quantification of these measurement limitations, and that the uncertainties derived from this quantification must be integral to the data interpretation process.

2.3 PAST AIR QUALITY STUDIES IN THE SOUTH COAST AIR BASIN

The South Coast Air Basin has probably been subjected to more air pollution analyses than any other location in the world. Much of the generally applicable and fundamental knowledge regarding emissions, air pollution meteorology, air pollution chemistry, and receptor concentrations has been derived from these studies. The combination of outstanding scientific expertise in California universities; interest from local and national industries located in the SOCAB; community concerns about air quality; and cooperation and financial support from local, state, and federal regulatory agencies, has encouraged this high level of productivity. Table 2-4 identifies a fraction of these studies, categorized by specific problem areas. Though this list is far from complete, it conveys the long historical record and the intense scientific interest which are characteristic of air pollution research in the SOCAB.

Most of these studies were of short duration and of small geographical extent. Though they provide evidence of cause-effect relationships among emissions, meteorological, and receptor variables, this evidence is rarely conclusive. These studies have proposed novel measurement, modeling and data interpretation methods, but the modeling efforts have usually had to settle for whatever data were available. The measurements have rarely been coordinated in such a way that they were compatible with each other or with the models. This brief survey of studies leaves the impression that had these projects been coordinated with one another, and had they been designed around a set of common and inclusive objectives, their value would have been substantially increased.

Important field measurement studies which did involve a degree of this coordination were the Pasadena Aerosol Study (Hidy and Friedlander, 1972), the Aerosol Characterization Experiment (Hidy et al. 1975; Hidy and Mueller, 1979), the Three Dimensional Gradient Study (Blumenthal et al. 1978), the Los Angeles Reactive Pollutant Program (Feigley and Jeffries, 1979), the Los Angeles Catalyst Study (Tiao and Hilmer, 1978), and the Air Quality Maintenance Plan (SCAQMD, 1982). Several of these studies are summarized in Appendix B. Each of these studies involved a planned acquisition of data with the goal of using those data for interpretive purposes. Each study resulted in reports and papers which drew generalized conclusions concerning source-receptor relationships, physical and chemical mechanisms, and the potential effects of emissions changes.

Three of these studies are worthy of further scrutiny in the design of the SCAQS:

- The California Aerosol Characterization Experiment (ACHEX), because it is the predecessor to the SCAQS and it resulted in many of the hypotheses to be tested by the SCAQS.
- The Los Angeles Reactive Pollutant Program (LARPP), because it provided extensive data for model development and testing.
- The Final Air Quality Management Plan Analysis (AQMP), because it serves as the basis for proposed emissions reductions in the SOCAB.

Table 2-4. Previous Air Quality Related Studies Undertaken in the South Coast Air Basin

EMISSIONS INVENTORY AND CHARACTERIZATION:

ARB (1982)
Cass et al. (1982a)
Chass and George (1960)
Dzubay et al. (1979)
Grisinger et al. (1982)
Huang and Head (1978)
Mayrsohn and Crabtree (1976)
Mayrsohn et al. (1977)
Oliver and Peoples (1985)
Parungo et al. (1980)
Pitts et al. (1984)
Pueschel et al. (1979)
Richards et al. (1976, 1977)
Rodes and Holland (1981)
Rose et al. (1965)
Taback et al. (1979)
Tombach (1982)

METEOROLOGY, WIND FIELDS AND DISPERSION:

Ackerman (1977)
Angell et al. (1975, 1976)
Blumenthal et al. (1978, 1979)
Cass and Shair (1984)
Chang and Norbeck (1983)
Crane et al. (1977)
Drivas and Shair (1974a, 1974b)
Drivas (1975, 1982)
Edinger (1959)
Edinger and Helvey (1961)
Edinger et al. (1972)
Farber et al. (1982b)
Gloria et al. (1974)
Goodin et al. (1979)
Goodin and Lague (1983)
Hanna (1977)
Hidy et al. (1971)
Hinds (1970)
Husar et al. (1977)
Kauper and Niemann (1975, 1977)
Keith and Selik (1977)
Lissaman (1973)
McElroy et al. (1982)
McRae et al. (1981)
Pack and Angell (1963)
Panofsky (1975)
Reible et al. (1982)
Sackinger et al. (1982)
Schultz and Warner (1982)

Table 2-4. (continued)

Shair et al. (1982)
Shettle (1972)
Smith et al. (1972, 1976, 1984)
Smith and Edinger (1984)
Smith and Shair (1983)
Vaughn and Stankunas (1974)
Wakimoto and Wurtele (1984)
White and Husar (1976)
Zak (1982)
Zeldin and Meisel (1977)

MULTICOMPONENT, SIZE-CLASSIFIED AEROSOL MEASUREMENT AND SOURCE APPORTIONMENT:

Cass (1978a)
Cass and McRae (1981, 1983)
Colucci et al. (1969)
Friedlander (1973)
Gartrell and Friedlander (1975)
Giauque et al. (1974, 1979)
Grisinger (1982b)
Hammerle and Pierson (1975)
Heisler et al. (1973)
Hidy (1972)
Hidy and Friedlander (1972)
Hidy et al. (1974, 1975)
Hidy and Mueller (1979)
Ho et al. (1974)
Hoggan et al. (1978)
Husar et al. (1972, 1976)
Huang et al. (1982, 1983)
Ludwig and Robinson (1968)
Lundgren (1971)
MacPhee and Bockian (1967)
Miller et al. (1972)
Mueller et al. (1972)
Neiburger and Wurtele (1949)
Novakov et al. (1972a, 1972b)
Porch and Ellsaesser (1977)
Saltzman et al. (1985)
Stelson and Seinfeld (1981)
Tiao and Hilmer (1978)
Trijonis et al. (1975a)
Volz (1973)
Wadley et al. (1978)
Whitby et al. (1972)
White et al. (1973)
Witz and Wadley (1983)

VISIBILITY:

Alkezweeny and Lockhart (1972)
Appel et al. (1983)
Barone et al. (1978)
Cass (1979)
Charlson et al. (1968, 1969)

Table 2-4. (continued)

Charlson and Pierrard (1969)
Charlson (1972)
Covert et al. (1972)
Ensor et al. (1972)
Noll et al. (1968)
Pratsinis et al. (1984)
Thielke et al. (1972)
Thomas (1962)
Trijonis (1982a, 1982b)
White and Roberts (1977)

SULFATE AND NITRATE MEASUREMENTS AND RELATIONSHIPS TO SOURCES:

Appel et al. (1977a, 1977b, 1978, 1982)
Baboolal and Farber (1982)
Cass (1975, 1978b, 1981)
Grisinger (1982a)
Grosjean (1982a)
Harker et al. (1977)
Heisler et al. (1980)
Henry and Hidy (1979)
Hering and Friedlander (1982)
Novakov et al. (1972a, 1972b)
Richards (1983)
Roberts and Friedlander (1975)
Russell et al. (1983)
Russell (1985)
White et al. (1978)
Witz and MacPhee (1977)
Witz and Wendt (1981)
Witz et al. (1982)
Zeldin et al. (1983)

CARBONACEOUS, ORGANIC, HYDROCARBON, AND HALOCARBON MEASUREMENTS (including toxic organics):

Altshuller and Bellar (1963)
Altshuller and McPherson (1963)
Altshuller et al. (1966)
Appel et al. (1976, 1977a, 1979)
Brenner et al. (1980)
Cass et al. (1982b)
Cronn et al. (1977)
Duval and Friedlander (1981)
Ellis et al. (1984a, 1984b)
Ellis and Novakov (1982)
Gordon et al. (1968)
Gordon and Bryan (1973)
Gordon (1976)
Gray et al. (1985)
Grosjean and Friedlander (1975)
Grosjean et al. (1983)
Grosjean (1975, 1982b, 1984)
Grosjean and Fung (1984)

Table 2-4. (continued)

Gundel and Novakov (1984)
Hester et al. (1974)
Kotin et al. (1954)
Lonneman et al. (1968)
Madar et al. (1952)
Miguel and Friedlander (1978)
Neligan (1962)
Novakov (1982)
Pitts et al. (1981, 1982, 1985)
Rosen et al. (1982)
Schuetzle et al. (1973, 1975)
Singh et al. (1985)
Wolff et al. (1982)

DETERMINISTIC PHOTOCHEMICAL AND AEROSOL MODELS AND APPLICATIONS:

Feigley (1978)
Godden and Lurmann (1983)
Gutfreund et al. (1981)
Haney and Seigneur (1985)
Heisler and Friedlander (1977)
Killus and Whitten (1983)
Liu and Roth (1973)
Liu and Grisinger (1982a, 1982b)
Liu (1982)
Liu et al. (1982)
Lloyd et al. (1979)
Lurmann et al. (1979, 1982)
Martinez (1971a, 1971b)
Martinez et al. (1983)
McRae et al. (1982a, 1982b)
McRae and Seinfeld (1983)
Renzetti and Bryan (1961)
Reynolds et al. (1973, 1974, 1976, 1978, 1979)
Roth (1972)
Roth et al. (1974, 1983a, 1983b)
Seigneur et al. (1981a, 1981b, 1983a, 1983b, 1983c, 1984, 1985)
Sklarew et al. (1972)
Tesché (1983)
Tiao et al. (1976)
Tesché et al. (1983a, 1983b)
Wayne et al. (1971)

PHOTOCHEMICAL MEASUREMENTS AND EMPIRICAL MODELS:

Altshuller et al. (1971)
Aron and Aron (1978b)
Aron (1980)
Bailey (1975)
Calvert (1976a, 1976b)

Table 2-4. (continued)

Caporaletti et al. (1977)
Chang et al. (1980a)
Chock and Levitt (1976)
Chock et al. (1982)
Chock (1982, 1985)
Coyne and Bingham (1977)
Davidson and Cassmassi (1985)
Decker (1972)
Edinger et al. (1972)
Edinger (1973)
Eldon and Trijonis (1977)
Elkus and Wilson (1977)
Estoque (1968)
Evans (1977)
Farber et al. (1982a)
Feigley and Jeffries (1979)
Fontjin et al. (1970)
Grosjean (1982a)
Grosjean et al. (1983)
Grosjean and Fung (1984)
Hamming and Dickinson (1966)
Hanst et al. (1982)
Harris et al. (1982)
Johnson and Singh (1976)
Kok (1983)
Kopczynski et al. (1972)
Lawrence (1972)
Lea (1968)
Levitt and Chock (1976)
Lin (1982)
Littman et al. (1956)
Ludwig et al. (1981, 1983)
McKee (1976)
Merz et al. (1972)
Miller and Ahrens (1970)
Mosher et al. (1970)
Paskind and Kinosian (1974)
Phadke et al. (1977)
Pitts et al. (1976)
Platt et al. (1980)
Renzetti and Romanovsky (1956)
Reviatt (1978)
Rogers et al. (1956)
Schuck et al. (1966)
Severs (1975)
Simmonds et al. (1974)
Spicer (1977)
Spicer et al. (1983)
Stephens (1968, 1969)
Tiao et al. (1975a, 1976)
Tombach (1982)
Trijonis and Eldon (1978)
Trijonis and Mortimer (1982)

Table 2-4. (continued)

Trijonis et al. (1978b)
Tuazon et al. (1978)
Tuazon et al. (1981)
Winer et al. (1983)
Zafonte et al. (1977)

ATMOSPHERIC ACIDITY:

Brewer et al. (1983)
Broadbent et al. (1985)
Ellis et al. (1984)
Hansen et al. (1982)
Hering et al. (1986)
Hoffmann et al. (1983)
Hoffmann(1984)
Jacob et al. (1985)
Kawamura and Kaplan (1983, 1986)
Kok (1980)
Liljestrang and Morgan (1978, 1981)
Marsh and Bregman (1984)
Morgan and Liljestrang (1980)
Munger et al. (1983)
Richards et al. (1983a, 1983b, 1985)
Riggan et al.(1985)
Seigneur and Saxeena (1984)
Seigneur et al. (1985)
Shikiya et al. (1984)
Tombach and Pettus (1982)
Waldman et al. (1982)
Waldman (1984)
Waldman et al. (1985)
Walker (1985)
Wall et al. (1984)
Yoong (1981)
Young et al. (1983)
Zeldin and Ellis (1984)

EFFECTS OF EMISSIONS CONTROLS:

Atkinson et al. (1983)
Chock et al. (1981)
Costanza and Seinfeld (1982)
Glasson (1981b)
Hamming et al. (1973)
Kauper and Hopper (1965)
Killus et al. (1981)
Leonard et al. (1976)
Oliver et al. (1983)
Pitts et al. (1983)
Roth et al. (1983a, 1983b)
SCAQMD (1982)

Table 2-4. (continued)

Seigneur et al. (1983c)
Tesche and Burton 1978
Tesche et al. (1984)
Trijonis (1972, 1974, 1983)
Trijonis and Arledge (1975)
Trijonis et al. (1978a)

CARBON MONOXIDE AND PRIMARY NITROGEN DIOXIDE:

Aron and Aron (1978a, 1978b)
Chang et al. (1980b)
Colucci and Begeman (1969)
Hamming et al. (1960)
Horie and Mirabella (1982)
Liu and Goodin (1976)
Neuroth (1979)
Pandolfo and Jacobs (1973)
Pandolfo et al. (1976)
Rogers (1958)
Tiao et al. (1975b)
Trijonis et al. (1975b)
Ulbrich (1968)
Witz and Moore (1981)
Witz et al. (1982)

ACHEX was an exploratory study aimed at developing a basic understanding of the sources and compositions of California aerosols. It was successful at describing the size distribution and the major elemental components of the suspended particles. Much was learned about the spatial distribution and composition of the aerosol, and the general sources of particulate matter concentrations were identified. The specific mechanisms for homogeneous and heterogeneous aerosol formation and the composition of the organic component of the aerosol were left as major unresolved issues. The role of water in aerosol formation, composition, and visibility was indicated to be important (Ho et al. 1974), but this role was not defined. The major conclusions of ACHEX were summarized by Hidy and Mueller (1979) as follows:

- the mass concentration of aerosol in California varies widely and is heavily influenced by sulfate, nitrate, and organic carbon formed from gas-phase precursors;
- aerosol concentrations in the eastern part of the SOCAB exhibit marked diurnal variations in concentration and composition. Two-hour average concentrations were substantially higher than 24-hour averages, reaching $450 \mu\text{g}/\text{m}^3$ for mass, $70 \mu\text{g}/\text{m}^3$ for sulfate, $70 \mu\text{g}/\text{m}^3$ for nitrate, and $50 \mu\text{g}/\text{m}^3$ for non-carbonate carbon;
- the multimodal aerosol size distribution was confirmed, with a submicron fraction dominated by aerosol formed from anthropogenic emissions and a supermicron fraction derived from dust and natural sources;
- sulfate, nitrate, and organic species were primarily in the submicron size range. Sulfate was more effective, per unit mass, than any other species in reducing visibility;
- the portion of aerosol attributable to photochemical processes was consistently in the 0.1 to 1.0 μm size range;
- the photochemical mechanism was a major contributor to the formation of sulfate, nitrate, and organic particles. Heterogeneous formation pathways were also inferred to be important;
- ammonia has an important influence on the formation of photochemical aerosol, and these particles may contain a large fraction of water;
- though many sources contribute to the aerosol, sulfate is mainly linked to stationary sources using fuel oil; organic materials result from transportation using gasoline; and nitrates derive from both of these sources;
- more than half of the total suspended particulate material in the SOCAB measured during ACHEX was due to atmospheric chemical reactions. The remaining half was attributed to primary emissions from stationary and transportation sources and background materials such as sea salt and soil dust; and

- the aerosol sources and constituents primarily responsible for visibility reduction varied over the Basin, with sulfate and transportation sources being generally of greatest importance.

ACHEX was a state-of-the-art study for its time. Many of the instruments in common use today were developed for and tested in this study. Since ACHEX, much has been learned via laboratory experiments and field studies regarding the interactions of atmospheric variables, and this knowledge has been incorporated into complex and computationally intensive models which simulate these interactions. In hindsight, and with this additional knowledge, a study to address the issues raised by the above-stated conclusions would be designed quite differently from the ACHEX. This hindsight does not detract from the value provided by measurements and data interpretation provided by these researchers more than a decade ago. Of particular note are the large number of publications and fundamental theories which resulted from the ACHEX. These results are a direct consequence of the participation of a variety of experts, the open planning process and the free data exchange protocols established at its outset. Several subsequent air quality studies have cost more but were less influential because they neglected these important features.

The Los Angeles Reactive Pollutant Program (LARPP) consisted of airborne meteorological and pollutant sampling of coherent air parcels as they moved along a trajectory. Thirty-five days of sampling were conducted between September and November of 1973. Tetroons and tracer releases were used to locate the positions of air parcels, and instrumented helicopters continuously measured ozone, nitrogen oxides, total and non-methane hydrocarbons, carbon monoxide and air temperature. Ground-based lidar and mobile van measurements were also taken. The data were used in the development and testing of the ELSTAR Photochemical Air Quality Simulation Model (Lloyd et al., 1979). This was one of the first studies which involved industrial (Coordinating Research Council), federal (Environmental Protection Agency and the National Oceanic and Atmospheric Administration) and state (Air Resources Board) sponsors. It provided a model for cooperation among different sponsors to achieve common goals.

While the ACHEX and LARPP were primarily research studies which did not focus on pollution control objectives, the AQMP provides a management analysis of current (1979) emissions and air quality levels with the objective of determining those emissions reductions which are required to reduce air quality concentrations by a certain amount. Three analysis methods applied to routine emissions and ambient data were used by SCAQMD:

- Linear rollback (e.g. Barth, 1970; deNevers and Morris, 1973) was used for CO, SO₂ and NO₂. The total emissions in the Basin are to be reduced by the proportional reduction required of the highest non-background concentration to meet the standard.
- Species fractionation rollback was used for suspended particulate matter. Proportional reductions in Basin-wide primary particulate emissions are prescribed for non-sulfate and non-nitrate fractions of TSP in excess of the ambient standard. Proportional reductions in SO₂ and NO_x emissions are prescribed for the sulfate and nitrate fractions of TSP.

- City-specific EKMA (U.S. EPA, 1981) was applied to 27 station days selected from worst-case situations observed in 1977-1980. Trajectory-specific EKMA was applied to 17 of these cases. Individual back trajectories were plotted for each case and only hourly NO_x and hydrocarbon emissions along those trajectories were considered. Assuming that NO_x emissions will be 23% less in 1987 than they were for 1979^x, the necessary reductions in Basin-wide hydrocarbon emissions were calculated. Assumptions and sensitivity analyses results are given by SCAQMD (1982) and are too lengthy to repeat here.

The AQMP conclusions are plagued by great uncertainty. There is still controversy concerning whether or not NO_2 emissions reductions will increase or decrease ozone levels (Glasson, 1981a, 1981b; Chock et al. 1981; Pitts et al. 1983; Roth et al. 1983a). Davidson and Cassmassi (1985) provide convincing empirical evidence that shifting emissions schedules may significantly affect ozone concentrations, an option which has not been considered by the AQMP. Given the likelihood that a large fraction of the suspended particle concentrations may be composed of photochemical aerosol, linear rollback may not be an adequate approximation of the effects of emissions on this variable. The large variability in particle composition from site-to-site also calls into question the assumption that Basin-wide emissions reductions will affect the most highly loaded samples in a linear manner. The AQMP presumes a 23% reduction in NO_x emissions by 1987 and a corresponding reduction in suspended particulate matter, ozone, and NO_2 concentrations during that year. The effectiveness of the methods used to arrive at the proposed control measures are amenable to testing.

Contrasting the ACHEX and LARPP to the AQMP, it is evident that the research and regulatory needs are complementary. While the regulatory process must continue with the information it has, regardless of the imperfection of that information, it can nevertheless identify where more precise information is needed to make effective decisions. Research efforts can then include, and possibly even focus on, those information needs.

2.4 CONTEMPORARY AND FUTURE AIR QUALITY STUDIES IN THE SOCAB

There is an obvious need for further research to address the cause and effect relationships between emissions, meteorology, and ambient concentrations of precursors and products for ozone and suspended particulate matter. Knowledge of the distributions of other pollutants (such as acid species and toxic substances) and of their effects on human health, visibility, and materials, is still sparse in the SOCAB. Basic information on the values attained by these observables and their spatial and temporal distributions is needed before these important relationships can be established. The sources, emission rates, and locations of species other than particulate matter, sulfur dioxide, nitrogen oxides, carbon monoxide, and ozone need to be determined. Little is known about PM-10 in the SOCAB and how it is similar to and differs from TSP. With the advent of a new PM-10 standard, and the necessity to create an implementation plan within nine months of promulgation of that standard (Federal Register, 1985), this information becomes even more topical.

Several air quality studies have recently been completed, are currently taking place, or are in the planning stages, which address measurement and modeling issues which are relevant to SCAQS. Some of these can be used in the design of, or should be made an integral part of, the SCAQS.

- The ARB is currently taking samples of benzene, carbon tetrachloride, chloroform, ethylene dibromide, ethylene dichloride, methyl chloroform, perchloroethylene and trichloroethylene gases in Tedlar bags for gas chromatographic analysis. HiVol samples are also being taken with total chromium, lead, manganese and nickel being measured by X-ray fluorescence. The state-wide network includes the Los Angeles, El Monte, Rubidoux, Long Beach, and Upland sites from the SOCAB.
- The SCAQMD is sponsoring a dichotomous sampler network, run by the California Institute of Technology, to measure PM-10 between August 1985 and August 1986. Carbon, ions and elements will be quantified on the samples. Sampling sites are Burbank, Los Angeles, Lennox, Long Beach, Anaheim, Riverside, and San Nicolas Island. PM-2.5 is being measured at the Los Angeles site.
- The SCAQMD intends to conduct chemical characterization studies of source types suspected of affecting PM-10 concentrations to provide input data for receptor models. One such test may include the characterization of motor vehicle exhaust from a tunnel.
- The SCAQMD is also developing models appropriate for estimating contributions to the annual average PM-10. One of these includes sponsorship of aerosol chemistry development of the SAI urban photochemical model.
- Dr. Glen Cass of the California Institute of Technology has recently completed a 15-day measurement program which acquired four-hour aerosol samples between 11 a.m. and 3 p.m. at Pasadena during the summer of 1984. These fine and coarse samples have been chemically characterized and are accompanied by detailed EAA, OPC, nephelometer, RH, T, HNO₃, NH₃, impactor, and SCAQMD gas data. Though the interpretation of these data is not planned for the near future, their thorough examination prior to SCAQS sampling would answer many of the measurement and data interpretation questions posed in this and subsequent sections.
- Project BASIN (Wakimoto and Wurtele, 1984), which was sponsored by the ARB, provided intensive upper air measurements at numerous sites throughout the SOCAB for three days in August of 1984. Mountain wind stations, additional upper air soundings with four-hour resolution, airborne lidar, tracer release, and acoustic sounder measurements were made simultaneously. Though some of these data are being interpreted by scientists at the California Institute of

Technology and UCLA, a thorough examination prior to SCAQS meteorological and aircraft measurements would help optimize network placement and identify potential difficulties in the measurement processes.

- The Electric Power Research Institute (EPRI) has created a flexible emissions inventorying system covering the entire United States, including the SOCAB (Heisler, 1985). Some of the contents, such as alkaline emissions, nine reactive hydrocarbon classes, and ammonia emissions, are not easily available in other inventories. The inventory system allows rapid updating and regridding for modeling purposes. The current contents are for a base year of 1982, and an update is scheduled for 1987.
- The Southern California Edison Company (SCE) has conducted, and intends to continue, numerous studies in the SOCAB which characterize inorganic and organic components of the aerosol near source dominated as well as photochemically influenced, downwind receptor areas. Over sixty sampling events have been completed at Lennox and Duarte. Inorganic composition has been measured, and detailed organic analyses are being performed on selected samples (Singh et al. 1985).
- SCE released SF₆ from the Ormond Beach Generating Station and took airborne and ground-based tracer and air quality measurements during August, 1985. This study was designed to characterize the chemistry in the plumes of gas and oil powered combustors when coupled with coastal meteorology. The 1985 data are being examined to elucidate the nitrogen chemistry in the plume during periods of elevated ozone concentrations. Additional tracer studies are planned for future years to explore power plant influences on atmospheric acidity. These studies will use soluble tracer species and remote sensing devices.
- SCE is conducting empirical and objective analyses of air quality and meteorological data to relate aerosol concentrations to meteorological regimes. Source apportionment methods are being developed and tested.
- The Coordinating Research Council (CRC) is sponsoring laboratory and field investigations to improve size-selective aerosol sampling. Positive and negative biases in the sampling process are being quantified, and steps are being taken to correct them by researchers at the University of Minnesota.
- CRC is sponsoring investigation of the atmospheric chemistry and aerosol-forming potential of aromatic organic substances via experiments in the California Institute of Technology's outdoor smog chamber. These experiments are intended to:
(1) identify and quantify the gas-phase reaction products and aerosol molecular composition, (2) measure evolution of aerosol size distributions resulting from atmospheric photo-oxidation

of aromatic hydrocarbons in the presence and absence of primary particles, and (3) develop more realistic aromatic gas-phase photochemical reaction mechanisms for air quality models used in the SOCAB.

- CRC is sponsoring the development of a tunable diode laser to measure NO, NO₂, HNO₃, and CH₂O at levels as low as 0.5 ppb. The builder of this instrument, Unisearch Associates, will field test it under polluted conditions typical of those in the SOCAB.
- CRC will sponsor a project in 1986 to develop a vehicle evaporative emissions model which estimates emissions from contemporary motor vehicles over a realistic range of operating and ambient temperature conditions. The model will produce more accurate estimates than current methods because it will include diurnal temperature profiles, individual fuel system component temperatures, control system-use pattern interactions, and weathering of tank fuel. This model is applicable to improvements of ROG emission rates in the SOCAB.
- CRC will sponsor a study in 1986 of the effects of oxygenates used in gasoline blending on evaporative emissions, with emphasis on ethanol and methanol-gasoline blends. A companion study is intended to determine the effects of fuel volatility, dispensed fuel temperature, and initial tank temperatures, dispensed fuel rate, and vehicle fuel system design on the magnitude of vehicle refueling emissions. Results are applicable to improvements of ROG emission rates in the SOCAB.
- The SCAQMD has recently completed a 1983 emissions inventory update for the SOCAB. The ARB is compiling a 1984 point source inventory and a 1985 planning inventory for the National Acid Deposition Program which will include ammonia emissions. The next comprehensive inventory for the SOCAB is scheduled for 1987 with availability by mid-1990. This could be changed to a 1986 inventory for release in 1989.
- The Electric Power Research Institute (EPRI) is studying alternatives to the contrast method for determining light extinction in the atmosphere. The assumptions of visibility measurement methods have been examined and alternatives have been developed to eliminate several of the assumptions which are not met in normal situations. Modifications to the integrating nephelometer which minimize the alteration of suspended particles with respect to water, organic content, and size distribution have been explored. The results of these studies can be applied to visibility measurements in the SOCAB.
- EPRI is examining alternatives for the measurement of the liquid water content of suspended particles and constructing a calibration and audit standard for these methods. These methods are applicable to the quantification of liquid water in the SOCAB aerosol.

- EPRI has developed quality assurance and standard operating procedures as part of its regional air quality studies. These procedures have optimized maintenance and performance test schedules and contain appropriate data forms. They are available to be combined with other procedures for the development of a SCAQS procedures manual.
- The ARB is sponsoring wet and dry deposition measurement networks in the SUCAB during 1986. The purpose is to estimate deposition fluxes in the region and to determine the acidity of fog. An estimate of the dry deposition velocities of sulfur and nitrogen species using the profile method (Businger et al. 1971) is included in these measurements.
- The ARB is sponsoring studies of atmospheric mutagens and the role of nitrogenous pollutants in their formation (e.g. Pitts et al. 1981).

These studies and others can help to provide the technical bases for decisions which must be made in the near and distant future. Their results will be even more valuable if they can be coordinated with each other and can be supplemented with additional emissions, meteorological, and air quality measurements which will allow cause-effect relationships to be established.

2.5 DATA NEEDS FOR MODELS

The approach taken in the design of SCAQS has been to start not with the measurements, but with the data interpretation methods. Methods applicable to the air pollution situation in the South Coast Air Basin, including both source and receptor models, have been identified from the references in Table 2-4. These references were reviewed, and, where appropriate, the creators and users of these methods were contacted to determine which measurements would be needed as input data, to determine parameters, to evaluate, and to estimate the uncertainties of these methods. Both research and regulatory applications were considered. Since most data interpretation approaches have been designed around existing data bases, and since they often contain many assumptions or calculational schemes which act as surrogates for non-existent measurements, the recommendations for additional measurements ranged from "nothing" to "everything measured at every point at all times." When reasonable compromises were made, and when past experience with data interpretation methods, including models, applied to the SUCAB was consulted, several common data needs were identified, irrespective of the data interpretation approach considered.

The most input intensive data interpretation methods are source and receptor models which quantitatively relate ambient concentrations to source emissions. Data which are acquired for these models can also be used for less quantitative data interpretation methods, such as case-studies, statistical summaries, and correlation analysis.

Source models are those which explicitly describe the movement of constituents in the atmosphere and the interactions between them to predict the concentrations of key species at selected receptors which result from source emissions. Receptor models are those which measure numerous variables

at selected receptors and infer the source contributions and transport and transformation mechanisms from those data. The data needs of several of these models specific to the South Coast Air Basin are briefly outlined in the following subsections. These models are extremely complex, and volumes have been written to describe them, their assumptions, their data requirements, and the compromises which have been made to accommodate existing data resources. It is not possible for this planning process to summarize all of the information about these models nor to consider the merits of each. This plan will not select "the model" most appropriate for describing the situation in the SOCAB. Model building is an iterative process which attempts to include those mechanisms and measurements which have the greatest influence on model output. The adequacy of those choices is then tested through focused experiments. The results of those experiments then feed back into the model-building process. The models described here are in evolution even as this is written, and the perceived importance of the data they require will certainly change as new knowledge is gained.

To reiterate: no attempt is made here to prefer one model over another. It is expected that by polling the modeling community, a common set of measurements will be defined which will be of utility to the future development of several modeling approaches and their ultimate use in making pollution control decisions.

2.5.1 Regression on Principal Components (RPCA)

The RPCA establishes an empirical relationship between atmospheric end-products, such as ozone and constituents of PM-10, by determining rotated eigenvectors of correlations among the causative variables. Linear regressions of the dependent variables on these factors are calculated. RPCA was first applied by Henry and Hidy (1979) to routine air quality data from the South Coast Air Basin, and they found photochemical, relative humidity, and dispersion/stagnation components to have varying influences on ambient sulfate levels. Since that application, several other studies have been published (e.g. Henry and Hidy, 1982; Liou et al. 1982; Wolff and Korsog, 1985; Malm, 1985; Chow and Spengler, 1985) which show the potential of this method. Chow (1985) provides the most recent summary of these applications and testing of this method.

The RPCA model produces mathematical factors which must be interpreted as physical factors based on the atmospheric variables included in the analysis. These variables need to be selected such that they will be surrogates for the important physical factors. Past applications of RPCA have been limited because these important variables have not always been available.

The important physical factors which are expected to affect oxidant and PM-10 concentrations in the South Coast Air Basin are: (1) primary and precursor emissions of particulate matter, NO_2 , reactive hydrocarbons and SO_2 , (2) photochemical transformation mechanisms, (3) heterogeneous transformation mechanisms, (4) transport and stagnation, (5) temporal variability of all factors, (6) emissions injection height, and (7) previous day carryover.

The observables which have been deemed important by their users for these RPCA models applied to oxidant and PM-10 concentrations are:

- sequential samples (of four to six hour maximum duration on consecutive days) of size segregated and chemically speciated particulate matter. Important species are geologically-related elements (Al, Si, Fe, Ti), other tracer components (e.g. Pb, Br, V, Ni, Cl, Na, elemental carbon, K), secondary products (e.g. total organic carbon, polar organics, sulfate, nitrate), and in situ liquid water content of the aerosol;
- hourly average oxidant, PAN, speciated reactive hydrocarbons, and NO_x/NO_2 concentrations;
- four to six hourly estimates of mixing depth, ventilation, atmospheric stability, relative humidity, and components of wind direction;
- four to six hourly estimates of fog and cloudwater, when fog exists;
- four to six hourly emission rates in the vicinity of sampling sites, classified by ground-level and elevated injection heights, for primary particulate, reactive hydrocarbons, NO_x , SO_2 . Day of the week variability may be adequate;
- nighttime ozone and PM-10 concentrations off the coast and above the inversion layer; and
- light scattering measurements which correspond with particle and gas measurements.

The RPCA methods require at least fifty (and preferably over one hundred) sets of measurements which cover the entire range of variability expected to occur. It is not yet known whether or not these methods can be used in a predictive mode nor if they will be able to extract better relationships between causative factors and ozone and PM-10 levels because the data required to test them have not been previously available. The results obtained in the cited studies show promise operating on routine data, however.

Several related models, such as objective analysis methods (e.g. Aron and Aron, 1978a, 1978b; Davidson and Cassmassi, 1985), multiple linear regression (e.g. Pratsinis et al. 1984; White and Roberts, 1977) and time series analysis (e.g. Tiao et al. 1975a, 1975b; Trijonis et al. 1975b) make use of the same data as that required for the RPCA model. Watson et al. (1985) observe that a detailed physical explanation of the processes which are likely to affect the atmospheric end-products, and identification of the variables which are likely to be indicative of those processes, is a pre-requisite for a RPCA application. Though Watson et al. (1985) provides such an explanation for factors affecting fine particulate concentrations in the San Joaquin Valley, their analysis is not complete enough to cover the more complex situation in the SUCAB.

2.5.2 Chemical Mass Balance Receptor Model

The chemical mass balance (CMB) receptor model (e.g. Friedlander, 1973) has been used as the basis for control strategies related to total suspended particulate matter (e.g. Cooper et al., 1979). However, the major contributors in these previous applications have been related to primary emitters. Since previous measurements have shown that major contributors to TSP in the SOGAB are of secondary origin, this model may not be directly applicable to the apportionment of these aerosols to sources. Nevertheless, this model is being incorporated into EPA's PM-10 assessment guidelines (personal communication, Tom Pace, U.S. EPA Office of Air Quality Planning and Standards, August, 1985) and has been shown (Watson, 1979) to put an upper limit on the secondary aerosol contribution and to apportion some of the precursors (Mayrsohn and Crabtree, 1976; Tombach, 1982; Feigley and Jeffries, 1979) of secondary aerosol to their sources. If the fractionation among species from various sources as a result of transport and transformation can be measured (e.g. Houck et al. 1982) or estimated (e.g. Duval and Friedlander, 1981), then the CMB might be an appropriate method for apportioning PM-10, and possibly the precursors of ozone, to their sources.

The CMB model consists of solutions to a set of equations which describe receptor concentrations of selected constituents as linear sums of the fraction of each constituent in source emissions times the total mass contribution of that source to the receptor. The receptor concentrations and source compositions are given to the model and the contribution from each source to each atmospheric constituent is calculated. Chow (1985) provides the most recent compilation of past applications while Watson (1979) presents the model assumptions and testing results. Other test results are reported by Currie et al. (1984) and Dzubay et al. (1984).

A recent evaluation of this model sponsored by the Electric Power Research Institute (Harold Javitz, SRI International, personal communication, September, 1985) concludes that although the CMB formulation is adequate for accurately determining many source contributions, even aggregate secondary contributions and the contributions to their precursors, this adequacy is extremely sensitive to the available observables and their random variability. The accuracy of current applications has been controlled more by the inadequacy of source profile measurements than by ambient measurements. There is no set of common source profile measurements in which all emitted species are characterized for all important sources. Chow (1985) and Edgerton (1985) have recently shown the value of including gaseous as well as particulate species measured in both the source and receptor samples. This increases the accuracy and precision of source apportionment and allows the gaseous species to be apportioned to their emitters. Very few current source profile measurements include the gaseous as well as particulate chemical constituents.

Although the CMB model can be applied to single samples of any duration, samples taken over shorter time periods provide more precise results in that they allow a better definition of contributing sources and a more accurate estimate of fractionation factors.

The important input data needs for the chemical mass balance model are:

- receptor particle measurements of key elements (Al, Si, Pb, Br, K, Cl, Na, V, Ni, Fe), ions (SO_4^- , NO_3^- , NH_4^+), organic and inorganic carbon, speciated organic materials, and individual particle characteristics in 0 to 2.5 and 0 or 2.5 to 10 μm size ranges;
- receptor gas measurements of NO_x , SO_2 , CO, reactive and nonreactive hydrocarbons;
- source profiles for power plant, motor vehicle, refinery, resuspended dust, and marine aerosol which include gaseous and particulate observables specified above for all sources; and
- estimates of fractionation factors (after Stafford and Liljestrand, 1984) between source and receptor.

2.5.3 Photochemical and Aerosol Models

Many grid and trajectory models have been proposed for describing the relationships between emissions, transport and transformation, and receptor concentrations. These involve transport and transformation mechanisms. Godden and Lurmann (1983), McRae et al. (1982a), Killus et al., (1985), and U.S. EPA (1981) describe photochemical mechanisms which have been incorporated into deterministic modeling packages. Each of these models has been applied to the June 26 and 27, 1984 smog episode and the O_3 , NO, and NO_2 concentrations have been compared with those at downwind monitoring stations. Though these "model validation" studies are not strictly comparable, the comparisons of model results and ambient measurements are qualitatively equivalent, regardless of the model used. A model/model comparison is not justified based on the individual reports, however, because these applications were never coordinated in such a way that objective performance measures could be calculated. While much emphasis has been placed on model performance (i.e. a one-to-one match in model end-product with a corresponding measurement in place and time), little emphasis has been placed on model diagnostics (i.e. the comparison of intermediate model calculations with measurements of reactive species and independent measurements of transport variables in space and time). Sensitivity and uncertainty analyses (e.g. Seigneur et al., 1981a; Tilden and Seinfeld, 1982) have shown that model end-product values vary substantially, even with small variations in selected input data. The sensitivity of intermediate calculations, and the extent to which input errors compound upon each other, have not yet been compared to real measurements outside of a smog chamber.

Work is underway to better represent other aerosol formation processes in these models (Seigneur et al. 1985, Russell et al. 1983). The ultimate goal is to produce comprehensive treatments which can estimate receptor concentrations of PM-10, ozone, and other constituents with specified accuracy and precision. These are currently the only types of models which are capable of estimating the effects of a hypothetical change in emissions on air quality. Receptor models can only be used when they are applied before and after such an emissions reduction has taken place.

These models require precise definitions of wind fields, initial values of pollutant and precursor concentrations of the atmospheric constituents, reaction rates, vertical and horizontal fluxes into and out of the volume being modeled, temporal and spatial distributions of gaseous and particulate precursor and primary emissions, and deposition rates at surfaces. It is technically impossible to measure all of these variables with the spatial and temporal resolution required of the models; therefore, simplifying assumptions regarding their values are used to estimate them.

The most important measurements which are not currently being made, but which are feasible, are the following:

- emission rates with a three hour minimum time resolution. The photochemical precursors, NO_x , and speciated hydrocarbons, are the most important species. These are needed as input data for photochemical and aerosol models;
- improved speciation for both gaseous and particulate emissions. The same types of measurements should be made on all major source types and should include elements, ions, organic and inorganic carbon, sulfur dioxide, nitrogen oxides, ammonia, carbon monoxide, speciated gaseous and particulate organic species. Exhaust gases should be cooled, diluted and preferably aged prior to sample collection to approximate their compositions in the environment. Aggregate samples of area sources (e.g. motor vehicle emissions) are preferable to measurements of single sources. These measurements should be sufficient to determine ROG/ NO_x ratios for all sources. These speciations are needed both as input data for source models and for receptor models. Ammonia emission rates are also needed for aerosol models;
- accurate wind fields which account for the complex meteorological phenomena described earlier. These are critical to the establishment of effective cause-effect relationships between emissions and receptor concentrations. Additional locations and more frequent upper air measurements are needed to supplement and verify surface measurements;
- boundary and initial concentrations of oxidant and particulate species, and their precursors. These are needed to determine their evolution over a period of time. Of critical importance are the concentrations above the mixed layer during nighttime and morning periods. Concentrations over the ocean are required, and these may be at levels lower than those detected by conventional instruments which have been used previously. Hydrocarbon speciation and free radical concentrations are also needed at various sites to serve as initial concentrations and to verify model predictions throughout a simulated event; and
- intermediate reaction products. These are required to verify that chemical mechanisms are reproducing the multitude of chemical constituents which are actually observed during an episode.

2.6 SUMMARY

It is impossible to do justice to the wealth of information available regarding air quality in the South Coast Air Basin in a survey of this type. The emphasis here has been placed on learning from the past in order to gain from the future. The subsequent parts of this program plan have been influenced by these lessons, which can be summarized as follows.

- The value of simultaneous measurements of emissions, transport, transformation and receptor variables is far greater than the value of any of these measurements acquired at disparate places and times, and the cost effectiveness of simultaneous data collection exceeds that for separate studies.
- The physical and chemical understanding of the atmospheric processes affecting pollutant concentrations in the SOCAB is sufficient to define the observables which need to be measured, their averaging times, and the characteristics of episodes which are conducive to high pollutant concentrations.
- Measurement technology is capable of determining the values of most observables, but each measurement method has a set of assumptions which must be met. Provisions must be made to test those assumptions for each measurement period, and to consider deviations from them in the data interpretation process.
- Potential data interpretation methods, including models, must be identified prior to taking the first measurement and their data requirements must be specified. These requirements include testing as well as input data.

3. MEASUREMENT APPROACH

3.1 PLANNING AND MANAGEMENT

A proposed field measurement scenario for SCAQS is outlined in this Section. Final revisions to the SCAQS measurement plan will be prepared by the SCAQS management contractor when the resources available for the study are more completely defined.

3.1.1 Field Management

The SCAQS field program will be coordinated by a field manager who will perform the following tasks:

- determine the power, space, and logistical needs of all field participants;
- arrange for access to the AQMD sites to be used as type "B" and type "A" sites;
- arrange for additional power and other necessary facilities;
- coordinate the activities of all measurement personnel and provide support as necessary. Type "A" and "B" sites will be operated by a contractor whose activities will be coordinated by the the field manager;
- prepare the field measurement revisions to the program plan;
- coordinate meteorological forecasting activities and provide daily forecasts;
- decide the schedule of intensive sampling days, after consultation with the Project Coordinator and the other participants;
- coordinate the distribution, exposure, labeling, and transportation to the laboratory of all routinely collected samples; and
- document field activities for progress reports.

3.1.2 Planning Activities

The measurement sites and measurements proposed in this plan are tentative and are based on discussions with potential modelers, participants, and sponsors. To assure that the measurements will meet the modelers' and analysts' needs, some preliminary modeling and analysis activities are useful. The following preliminary activities are planned to be performed prior to final selection of measurement sites, flight plans, sampling instrumentation, etc.

- Review or perform new sensitivity studies to evaluate the sensitivity of model results to variations in the spatial and temporal density of the initial and boundary pollutant

concentration measurements. Recommend necessary modifications to the proposed initial and boundary measurements.

- Evaluate the sensitivity of model predictions to the level of hydrocarbon speciation of the input data and to the time resolution of the hydrocarbon data. Recommend optimum sampling times and averaging periods for hydrocarbon samples.
- Evaluate the sensitivity of model predictions to the spatial and temporal density and locations of wind and mixing height measurements. Suggest the best locations for these measurements.
- Evaluate the sensitivity of O_3 and particulate matter models to emissions grid size³ and to the uncertainties in the emissions inventory. Suggest optimum grid size for emissions inventory efforts.
- Review the 15 days of data collected recently by Caltech in Pasadena with systems similar to those suggested in this plan. (See Section 2) In addition, review the PM-10 and fine particle data which will be collected in the next year by Caltech at many of the sites proposed for SCAQS. Assess the adequacy and potential pitfalls of the proposed SCAQS measurement and analysis techniques and sample site locations using these data.

The modeling activities suggested above address the first modeling objective in Section 1.3.2. These activities will be coordinated or performed by the Model Working Group.

3.2 SELECTION OF STUDY PERIODS

The two study periods have been chosen to be representative of the worst oxidant and aerosol periods in the South Coast Air Basin. In addition, these periods allow the documentation of substantially different types of pollutant conditions.

The first study period is proposed for mid-June through July 1987. The first part of this period is typically a period of high humidity in the South Coast Air Basin and should be a period which favors heterogeneous aerosol formation. During June, the percentages of days with low morning stratus clouds and poor afternoon visibility in the inland areas are the highest of any month as indicated in Table 3-1. The highest average TSP concentrations in the Basin typically occur in June, July, and December. The second half of the study period typically experiences the highest concentrations of photochemical pollutants of the year. High ozone concentrations generally occur in the Basin when the 850 mb temperature is greater than 20°C. Figure 3-1 indicates that July includes the most consistent high 850 mb temperatures of the summer. Figure 3-2 indicates that July also experiences consistently high maximum ozone concentrations. During mid to late July, the inland visibility is consistently low (Table 3-1), and there are stratus clouds along the coast about 1/3 of the time. Inland stratus is much less common. Thus, this sampling period should produce periods

Table 3-1. Percentage of Days for 1978-83 with Early Morning Clouds and Low Afternoon Visibility.

	Ceiling (0800 PST)		Visibility (1400 PST)	
	LAX ≤ 1800 ft.	ONT ≤ 1000 ft.	LAX ≤ 6 miles	ONT ≤ 6 miles
May 1 - 15	19%	16%	12%	49%
16 - 31	37	27	20	65
June 1 - 15	40	25	36	75
16 - 30	33	21	12	63
July 1 - 15	27	8	17	44
16 - 31	33	9	33	71
August 1 - 15	40	13	27	55
16 - 31	32	8	18	53
Sept 1 - 15	15	12	31	49
16 - 30	21	3	20	41
Oct 1 - 15	36	12	37	51
16 - 31	18	9	33	44

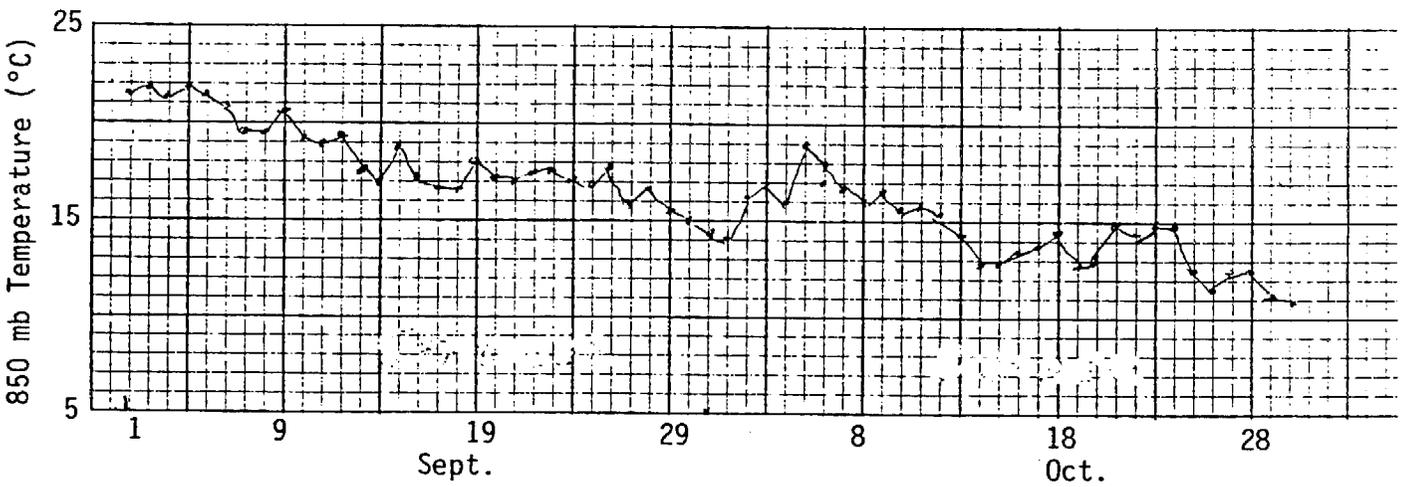
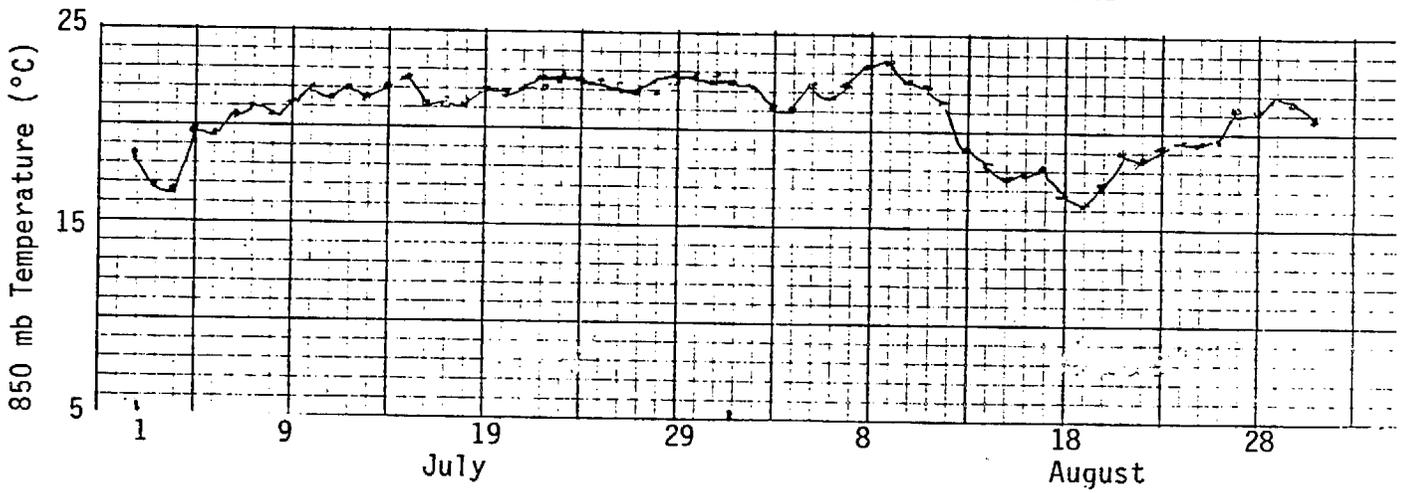
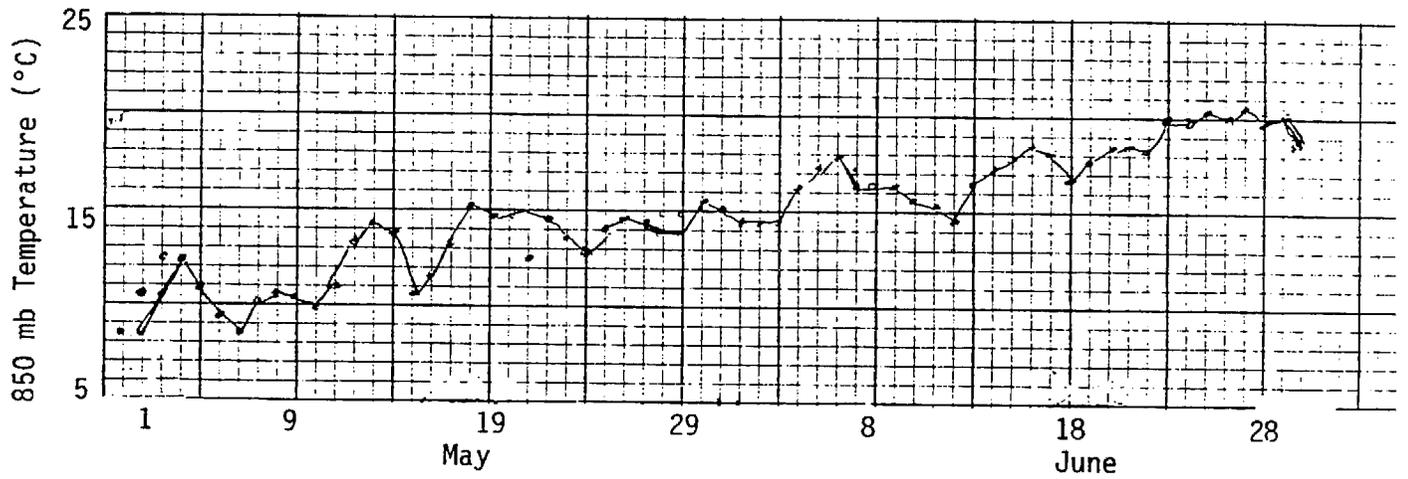


Figure 3-1. Daily Average 850 mb Temperature (Los Angeles, 1976-84).

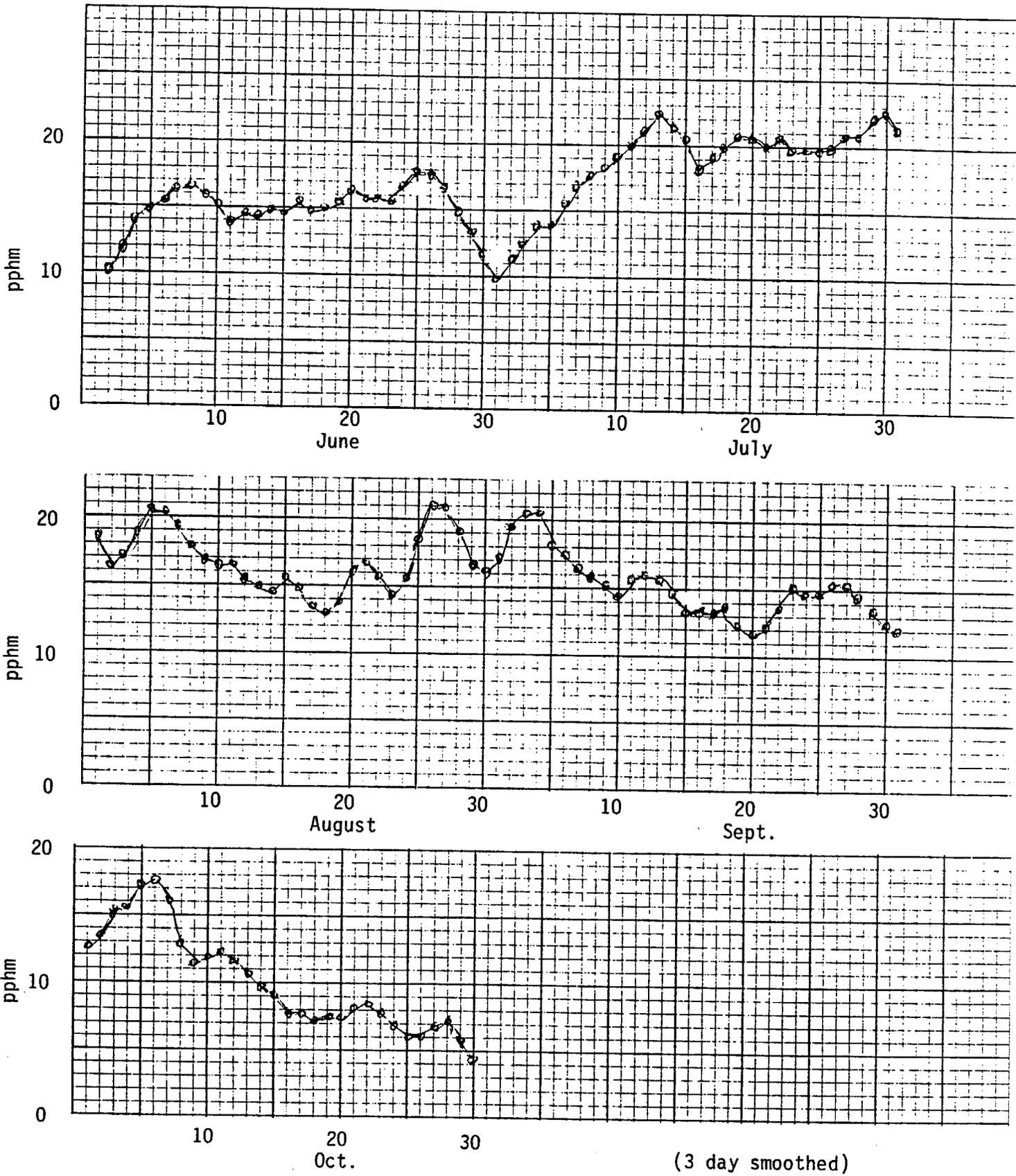


Figure 3-2. Maximum Ozone at Pomona. (Average of 1978-83.)

of primarily homogeneous chemistry as well as periods when coastal pollutants interact with water droplets which subsequently dry out as they travel inland.

The second study period suggested would be about four weeks starting in mid to late November of 1987. This period was chosen to represent winter stagnation conditions. NO₂ and CO episodes tend to occur at this time, and low inversions and cool temperatures tend to favor the accumulation of primary pollutants. This period is early enough to avoid the probability of substantial numbers of down days due to winter storms. The average daily maximum NO₂ concentrations for September-December in the SOCAB for a six-year period are plotted in Figure 3-3.

The two sampling periods were chosen to be 4-6 weeks long to minimize the probability of missing synoptic conditions of interest due to a period of unusual weather.

During each sampling period, we suggest that intensive measurements be routinely scheduled for 2-day periods starting the day before the AQMD sixth day TSP measurements. If the weather is inappropriate on that day, the start can be delayed one day. During episode conditions, an extra sampling day could be added to either the beginning or the end of the period. With this schedule, about one intensive measurement period per week would be assured, and the project would be able to make use of the regularly scheduled AQMD measurements.

3.3 SURFACE AIR QUALITY MEASUREMENT SITES

3.3.1 Measurement Site Locations and Study Region

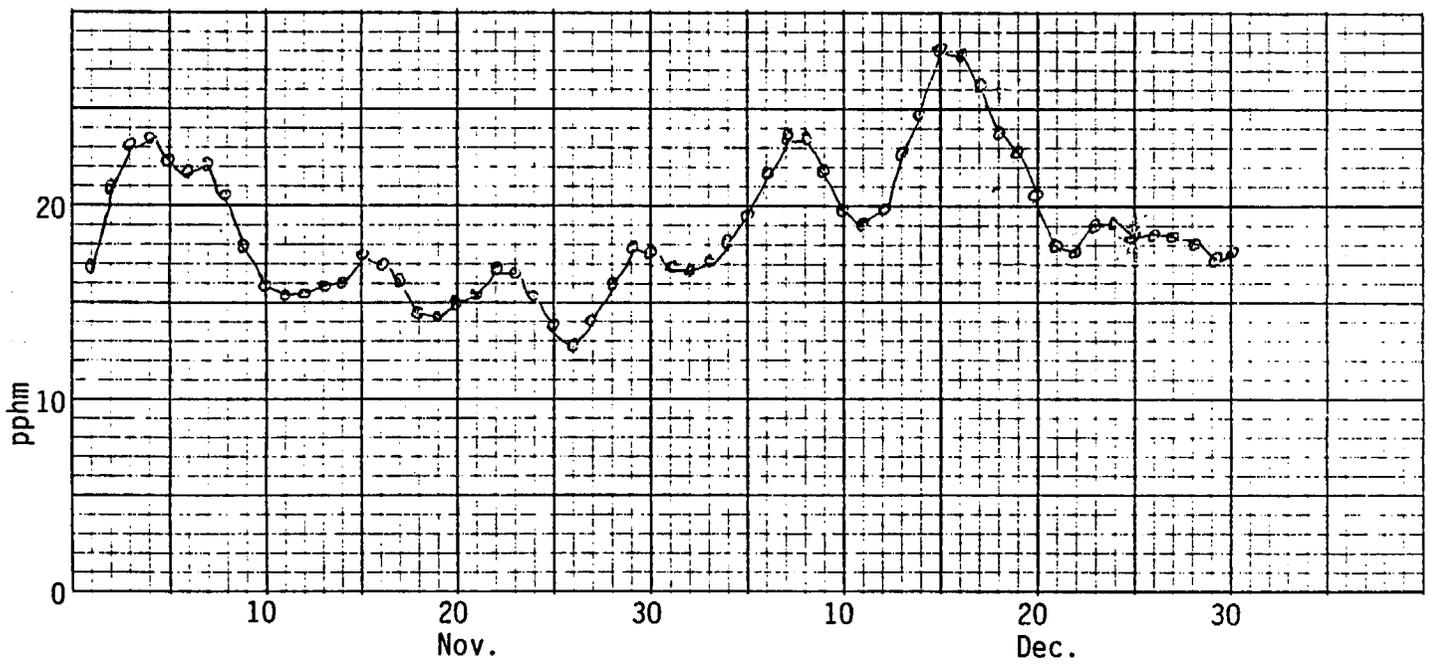
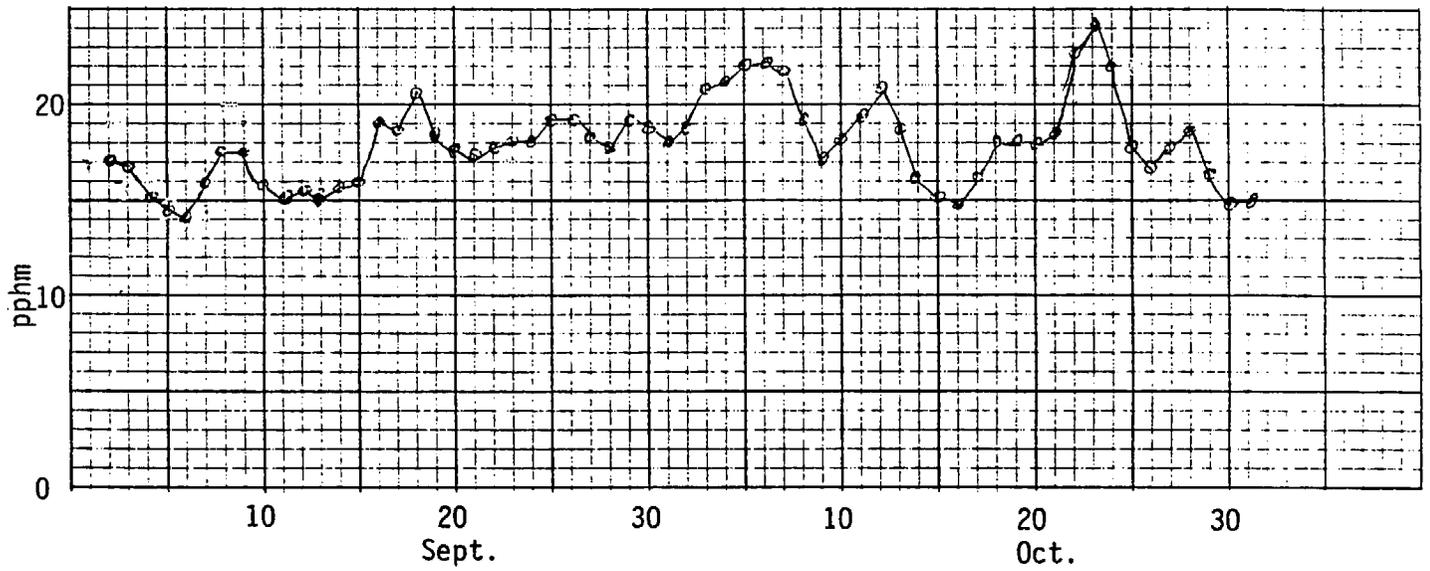
The study region includes the South Coast Air Quality Management District (SCAQMD), the upwind portions of Ventura County, and adjacent offshore regions. Three types of pollutant measurement sites are suggested in this region as indicated below.

Type "C" Sites

These sites will include the existing monitoring stations of the SCAQMD, the Ventura County Air Pollution Control District, and other stations at which air quality data are routinely collected and reported. Most of these sites are shown in Figure 2-1 and listed in Table 2-3. Data from these sites will be routinely acquired and archived by the program Data Manager. Some sites may be augmented with additional filter samplers.

Type "B" Sites

These sites will be collocated with or close to selected type "C" sites. Approximately 8 type "B" sites will be located along typical SOCAB air trajectories, and one site will be on an offshore island as a background site. Suggested onshore sites are: Anaheim, Azusa, Burbank, Hawthorne (it is planned that the SCAQMD Lennox site will be moved to Hawthorne), Long Beach, downtown Los Angeles, Riverside/Rubidoux, and Upland/Pomona. The offshore site will probably be on San Nicolas or Santa Catalina Island, depending on logistical considerations. The SCAQMD plans to implement a site on Santa Catalina Island during the approximate period of the study. Several people have suggested to us that Burbank is an anomalous site in the Basin and deserves further study. Thus, that site was chosen for the San Fernando Valley.



(smoothed 3-day mean
of daily maxima)

Figure 3-3. Maximum NO₂ - South Coast Air Basin. (Average of 1978-83.)

Type "B" sites will include the instrumentation of type "C" sites as well as substantial additional instrumentation for gas and aerosol species. The aerosol measurements at type "B" sites will have better time resolution than the type "C" sites. The instruments at type "B" sites will be operated by technicians according to specific protocols. The type "B" instruments will be operated only on "intensive" study days.

Type "A" Sites

These sites will be the base of operations for selected intensive measurements, special experiments, and individual investigators. The type "B" sites at Long Beach and at Upland/Pomona are suggested as locations for the type "A" sites. These sites represent source and receptor regions respectively. The type "A" sites will have extensive sophisticated instrumentation which will be operated by research personnel. Type "A" instruments will be operated primarily on "intensive" study days, but some researchers may operate their equipment continuously.

3.3.2 SCAQS Air Quality Measurements and Measurement Methods

The observables to be measured, their averaging times, and frequencies have been defined by the potential users of SCAQS data and are presented in the tables of Section 3.3.2. However, some of the measurement methods which are appropriate to acquire these data are still undefined. This program plan has eliminated from consideration those methods which have little or no chance of meeting the measurement requirements. For some measurements, however, several alternatives remain which are equally viable or which have not yet been characterized to an extent which will allow complete specification at this time.

Fortunately, several studies are now in progress which will result in sufficient information to select the best measurement methods prior to the SCAQS. ARB completed a nitric acid measurement intercomparison study in September of 1985, and the analysis of those results will be available by summer of 1986. These results will allow the most accurate nitric acid measurement method to be integrated into the program plan. ARB also plans an aerosol carbon intercomparison study for the summer of 1986. The results of this study must be examined prior to committing SCAQS to a method for the sampling and analysis of elemental and organic carbon. EPRI completed an extensive evaluation of visibility measurement methods in September of 1985, and these results should be reviewed prior to a detailed design of the SCAQS visibility measurements. EPA has been receiving comments on its proposed PM-10 measurement method, and it is expected that many of the controversies associated with that proposal will be resolved.

It is recommended, therefore, that the final measurement method selection be performed by the program management team prior to the final revision of this program plan. This selection should include a thorough evaluation of all relevant information which has recently been acquired. The overriding concern will be the ability to measure aerometric constituents in the ranges in which they are expected to occur with sufficient precision, accuracy, and validity to supply agreed-upon bounds around study conclusions. The next concern will be the cost of making the measurements. Tied into this will be the availability of existing measurement systems or of equipment which can be diverted to SCAQS from elsewhere.

The measurement methods specified in the following tables should be considered tentative until the final program plan is produced.

Type "C" Site Measurements

The type "C" sites are operated by the local air quality management districts and have varying levels of instrumentation. The existing sites and measurements are summarized in Table 2-3. For this study the routinely collected data from these sites will be obtained. We suggest that 8 to 10 of the type "C" sites also be equipped with samplers to measure PM-10 and fine particles (PM-2.5). In addition to the above, tracer samplers should be placed at selected "C" sites during tracer experiments. The measurements and sampling durations or averaging times typical for type "C" sites are listed in Table 3-2. The measurement methods are already in place and well-established as part of the routine monitoring network. The type "C" sites would be operated by the AQMD Staff.

Type "B" Site Measurements

The measurements recommended for the type "B" sites are summarized in Tables 3-3a through 3-3e. These measurements can be made routinely using established or semi-established methods. The measurements were selected after extensive discussions with the sponsors and the measurement and modeling communities. The methods suggested for making the measurements were generally chosen for their reliability, sensitivity, cost, availability, and compatibility with existing measurements. The reasons for including each suggested method are given in the tables. Several of these methods still require further evaluation prior to finalization. The results of recent methods evaluation studies (e.g. nitrogen and carbon) will be reviewed prior to the final choice of methods. Table 3-3a also includes estimates of the ambient concentrations, the lower quantifiable limit, and the precision for each measurement. References, notes, abbreviations, etc. are provided in Tables 3-3b through 3-3e.

The "B" site stations should be designed so that they can be easily operated by one trained technician. For intensive study days, two technicians working overtime should be able to man the stations continuously. Having the stations manned full time will enable immediate identification of problems and rapid correction. In addition, it removes the requirement for automatic sequencing of filter sample devices. We suggest that the technicians primarily perform the routine station operations and not be responsible for repairs. A separate, highly knowledgeable technician should be on call for repairs, and spares for critical components should be available at a central location.

A data acquisition system is included in Table 3-3 under the Aerosol Physical Property heading. A personal computer based system could be designed to control the aerosol equipment and to record all continuous data. The design and integration of data acquisition and aerosol measurement instruments is identified as a separate task in the cost estimates in Section 8.

For the collection of integrated or grab samples, a media management system should be designed which makes it easy for the technician to change media for sequential samples and to document all necessary parameters for each sample.

Table 3-2. Type "C" Station Measurements

	<u># days</u>	<u>Time dur./freq.</u>	<u>Analytical Method</u>
O ₃	all	hourly	UV absorption
NO	all	" "	Chemiluminescence
NO _x	all	" "	Chemiluminescence
CO	all	" "	NDIR
SO ₂	all	" "	Pulsed fluorescence
Wind speed	all	" "	Cup anemometer
Wind direction	all	" "	Wind vane
Total suspended particles	6th day	24 hrs	HiVol sampler
PM-10 (selected sites)	int. days	24 hrs	HiVol with SSI* or other size selective sampler
PM-2.5 (selected sites)	int. days	24 hrs	Size selective sampler-cyclone or dichotomous sampler
Tracer Samplers (sel. sites)	all tracer days	4 hr integration	Automated bag or syringe samplers

* Size Selective Inlet

Table 3-3a. Network Measurements at Type "B" Sites

Observable	Duration	No. per site-day	Potential meas. method	Ambient concentrations		Units*	Lower quantifiable limit	Precision**	Reason for Selection	References and notes
				typical	range					
METEOROLOGY - AQMD										
Wind speed	Cont.	24	Cup anemometer	3	0-20	m/sec	0.25	0.25	A	
Wind direction	Cont.	24	Vane	IA	0-360	degrees	IA	3	A	
Temperature	Cont.	24	Thermistor	IA	0-45	degrees C	IA	0.5	A	
Dew point	Cont.	4	Psychrometer	IA	-10-25	degrees C	IA	0.5	G	
UV radiation	Cont.	24	UV pyranometer	IA		eppleyps	IA		A	
GASES - AQMD										
O3	Cont.	24	UV absorption	30	1-400	ppb	10	15%	A	
NO	Cont.	24	Chemiluminescence	30	0-300	ppb	10	15%	A	
NOx	Cont.	24	Chemiluminescence	50	0-350	ppb	10	15%	A	
SO2	Cont.	24	Pulsed fluores.	6	0-320	ppb	10	15%	A	
CO	Cont.	24	NDIR	2	0.5-30	ppm	0.5	15%	A	
GASES - SCAOS										
SO2	4 hr.	6	Impreg. filter	6	0-320	ppb	<0.1	7%	C,E	1
NH3	4 hr.	6	Denuder tube	5	0-150	ppb	0.1	10%	D	2
HNO3	4 hr.	6	Denuder method		0-25	ppb	0.1	10%	D,K	3
Carbonyls	4 hr.	3	DNPH filter	3-7	1-30 (HCHO)	ppb	0.05	10%	C	4
C1-C10 HC	4 hr.	3	Can. or abs. & GC/F			ppbC	0.1-1ea.	10%	B	5
PAN	1 hr.	24	GC/EC	5-10	0-50	ppb	0.5	15%	C	6
H2O2	1 hr.	24	POHPAA-enzyme	5 (est)		ppb	0.5	3%	C	7
AEROSOL PHYSICAL PROPERTIES										
Size dist.	Cont.	24	OPC	IA	IA	IA	IA	IA	B	8
Size dist.	Cont.	24	EAA	IA	IA	IA	IA	Resolves diameter ratio of 1.8	E,F	9
Light scattering	Cont.	24	Integrating nephelometer	350	15-1500	Mm-1	10	10%	B	10
Data acquisition	Cont.	..	Micro computer	IA	IA	IA	IA	5mV for 10V fs.	G	
AEROSOL CHEMISTRY										
Total/fine:	4 hr.	6	Size selective sampler						J	11
Mass			Grav. or beta	40	5-220	ug/m3		7%	B	
SO4=			IC or AC	5	0.5-25	ug/m3		7%	B	
NO3-			IC or AC	8	0.5-30	ug/m3		7%	B	
NH4+			IC or AC			ug/m3		7%	B	
H+			Gran titration			ug/m3			C	
Trace elements			EDXRF or WDXRF			ng/m3	see separate table		B,G,H	
Elemental C			Ref. or therm.			ug/m3			E,G,K	
Total C			Therm.			ug/m3			C,K	
PM-10 (AQMD)	24 hr.	1	SSI-HiVol						A	12
Mass			Grav.	50	5-250	ug/m3		7%	A	
SO4=			AC	5	0.5-25	ug/m3		7%	A	
NO3-			AC	8	0.5-30	ug/m3		7%	A	
TSP (AQMD)	24 hr.	1	HiVol						A	13
Mass			Grav.	80	10-450	ug/m3		7%	A	
SO4=			IC or AC	9	0.5-30	ug/m3		7%	A	
NO3-			IC or AC	12	0.5-50	ug/m3		7%	A	
Pb			AA or EDXRF	0.2	0-2	ug/m3			A	
SIZE RESOLVED CHEMISTRY										
SO4=	4 hr.	6	UDI			ug/m3	0.4***	7%	C,D	14
NO3-	4 hr.	6	IC or AC			ug/m3	0.8***	7%	B	
NH4+	4 hr.	6	IC or AC			ug/m3	0.8***	7%	K	
Elemental carbon	4 hr.	6	Ref. or therm.			ug/m3			K	
Total carbon	4 hr.	6	Therm.			ug/m3			E,G,K	

* Units apply to both ambient concentrations and the lower quantifiable limit.

** Precision for values well above the lower quantifiable limit.

*** ug/m3 per stage

Table 3-3b. Lower quantifiable limits for X-ray fluorescence analysis of fine-particle filters.

Element symbol	Lower Quantifiable Limit (ng/m ³)	
	EDXRF*	WDXRF**
Na	80	39
Mg	12	2
Al	6	28
Si	5	4
P	4	2
S	14	5
Cl	6	2
K	2	2
Ca	2	5
Ti	0.6	2
V	0.7	4
Cr	0.7	27
Mn	1	5
Fe	1.5	12
Ni	1	6
Cu	1	12
Zn	1	5
Ga	1	--
As	1	9
Se	1	13
Br	1.5	11
Rb	2	--
Sr	2	23
Y	2	--
Zr	6	--
Pd	5	--
Ag	9	--
Cd	9	1
In	10	--
Sn	10	5
Sb	10	2
Ba	60	3
La	60	16
Hg	2	24
Pb	4	45

Assumptions: 60 lpm flow for 4 hrs. through 11.3 cm² filter area. At least 60 lpm is required to gain sufficient filter deposit in 4 hr. samples to be equivalent to a 10 lpm flow rate for a 24 hr. sample.

* Energy Dispersive X-ray Fluorescence using NEA Labs Protocol 4

** Wavelength Dispersive X-ray Fluorescence using US EPA Cr Excitation

Table 3-3c. Key to reasons for selection.

-
- A Already available at all or most of the "B" sites.
 - B Method in general use because of its sensitivity, accuracy and relative freedom from interferences. Accuracy and precision have been evaluated with field data.
 - C Only method identified with adequate sensitivity, accuracy, freedom from interferences.
 - D Interferences minimized.
 - E Accuracy of the method has been evaluated in the field.
 - F Equipment availability.
 - G Initial and operating costs.
 - H Method to be provided by a sponsor.
 - J See references and notes.
 - K Requires further evaluation.
-

Table 3-3d. References and notes.

-
- 1 Impregnated filter for sulfur dioxide. The lower quantifiable limit is small and the method has been characterized (Forrest et al. 1981) and used in the field.
 - 2 Denuder tube for ammonia (Ferm, 1979).
 - 3 Denuder method for nitric acid (Appel, Tokiwa, and Haik, 1981)
The results of the ARB intercomparison of nitrate measurement methods will provide additional information.
 - 4 2,4-dinitrophenylhydrazine (DNPH) filter method for carbonyls (Levin et al., 1985). A higher flow rate through the filter provides more sensitivity than the DNPH bubbler method.
 - 5 Cannisters-GC for hydrocarbons. There is less adsorption and desorption of hydrocarbons in electropolished stainless steel cannisters than in bags (Grosjean and Fung, 1984).
 - 6 Electron capture gas chromatography (EC-GC) for PAN (Stephens, 1969b).
 - 7 Para-hydroxy phenylacetic acid - horseradish peroxidase method for gas phase hydrogen peroxide (Lazrus et al., 1986; Kok et al., 1986; Heikes et al., 1985).
 - 8 Electrical Aerosol Analyzer (EAA). Determines aerosol size distribution data in the 0.01 to 0.3 um size range (Nominal size range is 0.003 μm to 1 μm .)
 - 9 Integrating nephelometer.
 - 10 Microcomputer data acquisition system. Flexible and cost effective. Data can be recorded in a format which can be read by most laboratories, so adding data from other experiments is possible.
 - 11 Size selective sampler. A specific sampler is not recommended at this time. Samplers may be made using design features of samplers now in use in research programs, but flow rates must be increased to obtain a sufficient filter deposit over 4 hr. sampling intervals. Size selective inlets for 10 um (Olin and Bohn, 1983) and 2.5 μm (Chan and Lippman, 1977) cutpoints at 113 l/min flow rates are available.
 - 12 PM-10 data estimated from TSP data.
 - 13 TSP data from ARB (1984).
 - 14 Uniform Deposit Impactor (UDI) (Marple and Rubow, 1984).
-

Table 3-3e. Abbreviations for analytical methods

AA	Atomic absorption spectroscopy - to determine metal concentrations.
Abs	Collection on a solid absorbing medium which is extracted in a solvent prior to presentation to an analysis method.
AC	Automated colorimetry.
Beta	Beta absorption.
Can	The determination of gas phase hydrocarbons by collection of an air sample in a stainless steel cannister which is then sent for detailed analysis by gas chromatography.
Combustion	Determination of total organic carbon by combustion of the filter deposit then determination of carbon dioxide by NDIR or by conversion to methane and flame ionization detection.
Denuder	A device which selectively removes small particles or, more commonly, gases from a sample flow by allowing them to diffuse to a surface where they are collected.
DM	Denuder method. Filter samples are collected with a denuder in the sample flow in front of the filter to remove nitric acid, and the amount of nitric acid removed by the denuder is determined.
DNPH filter	A filter impregnated with 2,4-dinitrophenylhydrazine which collects carbonyl compounds (aldehydes and ketones) for subsequent analysis by liquid chromatography.
EAA	Electrical aerosol analyzer, which obtains aerosol size distributions by electrically charging the aerosol then determining the amount of aerosol with a mobility less than each of a series of preset values.
GC/EC	Gas chromatography with electron capture detection.
GC/FID	Gas chromatography with flame ionization detector.
Gran Titr	Gran's Titration.
Grav	Gravimetric Analysis.
IA	Inapplicable.
IC	Ion chromatography to be used for inorganic anions.

Table 3-3e. (continued)

NA	Not available.
NDIR	Non-dispersive infrared absorption.
Nephelometer	Integrating nephelometer, which measures light scattering by the aerosol.
OPC	Optical particle counter - Laser based system for counting and sizing aerosol particles in the 0.1 to 2 μm size range.
PC	Computer similar to an IBM Personal Computer.
Ref	Reflectance.
Size sel. samp.	Size selective sampler which uses an inertial separation inlet to present particles within a certain size range to a filter.
SSI	Size selective inlet which removes particles larger than about 10 μm from a sample flow.
Therm	Thermometric.
UDI	Uniform deposit impactor, also called a micro-orifice impactor (MOI). A cascade impactor with very small nozzles which give 50% efficiency cut sizes in the 0.05 μm to more than 1 μm size range without the necessity of using low pressures.

To this end, we recommend that whenever possible, substrates be installed in their holders in the laboratory and that the field technicians only have to change sample cassettes.

We have recommended building, rather than buying, the grab sample system since no single system that we know of is adequate for the task. Parts of the system such as the denuder tube/filter apparatus for HNO_3 are not available commercially as pre-built systems and will have to be constructed under any circumstances. Aerosol filter sampling devices are available which will meet the needs of the study, but they are expensive and several of them will be required at each site. Caltech has designed sampling systems similar to those needed for SCAQS and will be operating them at most of the type "B" sites during the next year (Section 2-4). This sampler could be the basis for the SCAQS sampler design.

The Caltech system is set up to take samples for a single time period. For SCAQS, it will be necessary to take sequential samples and to change sampling media quickly and easily. A system similar to the Caltech system could be built with two manifolds such that the media in one could be changed while the other is sampling. Alternatively, two Caltech type devices could be used. By the time of SCAQS, the Caltech samplers will be well characterized and tested. Some modifications, however, would be needed to make the sampler easier to use and more reliable for a monitoring type environment, as well as to increase the flow rate to allow shorter sampling periods. It is possible that the existing samplers will be available for SCAQS use, thus lowering the cost of sampler acquisition.

Type "A" Site Measurements

The measurements suggested for the type "A" sites are summarized in Tables 3-4a through 3-4d. Many of the measurements suggested are quite experimental in nature and are really special studies in themselves. Some of the measurement methods indicated in the table are unique to one investigator or group. Table 3-4a is organized in the same fashion as Table 3-3a for the "B" sites. The measurements to be made at the "A" sites were suggested by the sponsors and technical reviewers and were refined to reflect the consensus of the October 1985 SCAQS workshop participants. The criteria for selection of measurement methods were similar to those for the "B" sites, even though many of the methods are quite experimental.

Most "A" site measurements will be made by individual investigators. In our cost estimates in Section 8, however, we have included an additional technician at the "A" sites to support the researchers and to perform routine sample collection and measurement tasks.

Complementary Toxics Measurements

The ARB operates a network of toxics monitoring sites. This network includes the following sites in the study area: El Monte, Long Beach, Los Angeles, Rubidoux, Simi Valley, and Upland.

The compounds currently measured at these sites are listed in Table 3-5. These measurements are made approximately three times per month for 24 hour periods. We suggest that the monitoring frequency of the Los Angeles,

Table 3-4a. Additional Measurements at Type "A" Sites

Observable	Dur- ation	No. per site-day	Potential meas. method	Ambient concentrations typical range	Units*	Lower quantifiable limit	Precision**	Reason for Selection	References and notes
ORGANIC GASES									
C1-C10 HC	1 hr.	3 more	Cannister - GC/EC		ppb			A	
C1-C6 carbonyls	1 hr.	3 more	DNPH filter	20	ppb	0.05	10%	A	
C10-Cn HC	4hr.	4	Porous plug - GC		ppb	0.1 to 1 ea.		C	
Formic, acetic acid	4hr.	6	Impreg. filter - IC		ppb				
INORGANIC GASES									
HONO	Cont.	24	DOAS (one site)		ppt	20		BF	1
HCHO	Cont.	24	DOAS (one site)		ppb	0.1		BF	
HNO3	Cont.	24	TDLAS		ppb			E	
HCl	4 hr.	6	Denuder		ppb			E	
RADICALS									
NO3	Cont.	<10	DOAS (one site)	?	ppt	1		C	2
HO	Cont.	24	FAGE					C	3
HO2	Cont.	24	FAGE					B	
RO2	Cont.	24	Chem. amplifier					F	4
ORGANIC AEROSOL									
Continuous EC, TOC	Cycle	24	Quartz filter - volatil.		ug/m3			F	
Volatility vs. temp.	4 hr.	6	Quartz filter - volatil.		ug/m3				
Carbon 14	24 hr.	1	Accelerator mass spec.						
INORGANIC AEROSOL									
Trace elements	Re-anal. selected filters from "B" sites		INA					D	
Water			Microwave? TDMA?	?	mg/m3			E	
Total acidity	4 hr.	6	Gran's titration, --					E	
AEROSOL PHYSICAL PROPERTIES									
Light absorption	Cont.	24	Spectrophone					E	
Light absorption	4 hr.	6	Filter reflectance					F,G	
Light extinction	Cont.	24	Radiance difference	350	Mm-1			C,E	
Size vs. RH	Cont.	24	TDMA; heated nephelometer		Mm-1	15-1500		F	
Volatility	Cont.	24	Heated nephelometer					F	
INDIVIDUAL PARTICLES									
Size & chem. comp.			Electron microscopy microprobe; GC/MS					C,F	
MUTAGENS									
	24 hr.	1						E	

* Units apply to both ambient concentrations and the lower quantifiable limit.

** Precision for values well above the lower quantifiable limit.

Table 3-4b. Abbreviations for analytical methods

Chem. Amplifier	A peroxy radical detector which makes use of the chain reactions with an added NO/CO mixture.
DOAS	Differential optical absorption spectroscopy.
FAGE	Fluorescence assay with gas expansion - a laser fluorescence technique for the determination of HO radical concentrations. HO ₂ can be determined by adding NO to convert it to HO.
GC/EC	Gas chromatography with electron capture detection.
GC/MS	Gas chromatography/mass spectroscopy.
IC	Ion Chromatography.
INA	Instrumental neutron activation analysis.
Spectrophone	An opto-acoustic detector which detects the absorption of light in a cell by the increase in pressure caused by heating the gas in the cell. The light is chopped at an audible frequency and the signal detected with a microphone. This device can be used to measure light absorption by aerosol suspended and dispersed as in the atmosphere.
TDMA	Tandem differential mobility analyzer - a version of the electrical aerosol analyzer in which a slot in the collector rod withdraws a sample flow containing monodisperse aerosol.

Table 3-4c. Key to reasons for selection.

A	Extension of measurements already made at "B" sites.
B	This species also measured by instrument chosen to measure another species.
C	Method has adequate sensitivity, accuracy, freedom from interferences.
D	To increase the variety of elements determined.
E	Method to be provided by a sponsor.
F	Equipment availability.
G	Initial and operating costs.

Table 3-4d. References and notes

1	Platt et al. (1980b)
2	Platt et al. (1980a, 1980b, 1984)
3	Hard et al. (1984)
4	Stedman (1983)

Table 3-5. Toxins Currently Being Measured by ARB in the Study Region.

<u>Hydrocarbons</u>	<u>Particulate Matter</u>
Benzene	Total chromium
Carbon tetrachloride	Lead
Chloroform	Manganese
Ethylene dibromide	Nickel
Ethylene dichloride	
Methyl chloroform	Arsenic*
Perchloroethylene	Beryllium*
Trichloroethylene	Cadmium*

* These compounds can be measured by ARB, but are not routinely measured.

Upland, Long Beach, and Rubidoux sites (type "B" sites) be increased during the study period to include all intensive study days, and that toxic measurements be made at all other type "B" sites during intensive study days. In this way the modeling data base could be used to assess the sources of the toxic materials measured at these sites.

3.4 AIRBORNE AIR QUALITY AND LIDAR MEASUREMENTS

Airborne measurements will be required to determine the pollutant distributions in the vertical dimension. They are especially important for documenting initial and boundary conditions, pollutant carryover, mixing layer height, representativeness of surface measurements, and nighttime chemistry aloft.

During the summer, we suggest that two aircraft be operated for three flights per day during the intensive study days. One aircraft would measure the spatial pollutant distributions in the central and inland areas, and the other would document the distributions in the coastal and upwind offshore regions. Flights would typically be in early morning (approximately 0600 PDT), in midday (approximately 1100 PDT), and in the afternoon (approximately 1600 PDT). Occasionally, the coastal aircraft would make an inland night flight at about midnight in place of an afternoon flight. The flight durations would be about 2 1/2 hours.

During the winter, one aircraft could be operated for two or three flights per day. The occurrence of fog will restrict some flights. The aircraft could measure the vertical distributions in the western source regions with one vertical spiral per flight in the eastern part of the basin. Flights would be in the morning and afternoon. Occasional night flights could be made when fog is not a problem. The flight durations would be 2 1/2 to 3 1/2 hours.

The aircraft would be equipped to make the measurements listed in Table 3-6. Each aircraft would make continuous measurements in spirals between about 5000 feet and the lowest allowable flight level (ground level at airports). Grab samples would be obtained in an orbiting pattern at a constant altitude. Approximately two sets of grab samples would be collected per flight in elevated layers or at the top of the mixed layer. Potential sampling locations would be offshore, in a source region, and in an inland area. Grab samples will take about 15 minutes to acquire. Approximately 5 spirals would be made during each flight to document the vertical pollutant distribution.

In addition to the in-situ airborne measurements, airborne lidar measurements are recommended to document the three-dimensional pollutant distribution along the slopes and offshore. In conjunction with the surface and upper air winds, the lidar could provide useful information on the fluxes into and out of the basin at the boundaries and on pollutant ventilation and carryover processes. Lidar flights should be made in early morning and in mid-afternoon. One or two flights per day could be made during intensive study days. The morning flight could document layers carried over from the previous day and could map the offshore boundary conditions. The afternoon flights could document the boundary conditions and ventilation processes. The EPA laboratory at Las Vegas has expressed interest in making these measurements.

Table 3-6. Aircraft Measurements

<u>Aircraft Measurements</u>	<u># days</u>	<u>Time dur/freq</u>	<u>Analytical Methods</u>			
O ₃	int. days 3 flts/day	Continuous over spirals and traverses.	Chemiluminescence			
NO } possibly high sensitivity	↓	↓	↓			
NO _x						
SO ₂				Spirals from surface to 5000'	Chemiluminescence	
Light Scattering (multi-wavelength)				Flame ionization		
Temperature				Integrating Nephelometer		
Dewpoint				Thermister		
Turbulence				Cooled mirror		
H ₂ O ₂				Pressure fluctuation		
PAN				POHPAA-enzyme		
Position				EC GC		
Altitude				LORAN		
Aerosol Size Distribution				Pressure Sensor		
Hydrocarbon				Laser OPC		
Filters for				2/flt in elevated layers or top of mixing layer	Canisters - GC	
SO ₄ ⁼ , NO ₃ ⁻ , NH ₄ ⁺				↓	↓	IC
trace elements						XRF
HNO ₃ ,						DDM
Carbon (elemental and organic)						Combustion
NH ₃						Denuder tube
Samplers for Carbonyls						DNPH filter

3.5 EMISSIONS

Our discussions with the modeling community have indicated that the quality of the available emissions data is one of the limiting factors in improving model accuracy. For three-dimensional grid models, an accurate, gridded, time- and species-resolved inventory will be necessary for each day to be modeled. For receptor models, detailed characterizations of the emissions from different sources will be needed for source identification (especially organics and trace metals).

To address the overall emissions issue, an Emissions Working Group (EWG) has been formed. The group consists of university, industry, and government members and will be responsible for providing the SCAQS emissions inventory. The EWG will design and execute studies to examine the accuracy of existing inventories and will coordinate special studies to improve these inventories. The EWG members are listed in Appendix A.

The EWG will be responsible for preparing an updated, quality assured, time- and species-resolved, gridded inventory for the major pollutant species including organic and inorganic gases and primary particles. The emphasis will be on those species most important for oxidant and aerosol formation. This inventory will be prepared using available inventories as a foundation and refined as necessary to include the results of special inventory characterization studies. The inventory should provide hourly-averaged emissions for each of the "intensive" study days.

The basis for the development of the inventories will be the inventory preparation process which both the SCAQMD and CARB follow in preparing their periodic inventory updates. Thus, the EWG will work closely with both agencies as they prepare their next routine inventory update scheduled for 1987. Supplementing this development process will be a series of studies aimed at quantifying the uncertainties in the inventory leading to a more accurate characterization of emission distributions in the South Coast Air Basin.

To address the problem of improving the accuracy of the inventories, a comprehensive study program will be initiated. Topics being considered for this study program include:

1. model sensitivity to emissions parameters. The EWG, in conjunction with the Model Working Group, will consider a series of model sensitivity simulations using the best available emission inventories. The intent of this effort would be to identify the sensitivity of model predictions (both ozone and PM) to uncertainties in the emissions inventory. Many emission items would be tested, including those related to numbers 2 to 10 below. Results of this sensitivity analysis would help determine priorities of these items;
2. motor vehicles exhaust emission rate and composition, including trace metals and hydrocarbon speciation. These measurements could be conducted using a tunnel field test and/or dynamometer testing;

3. aerosol size and chemical distributions from controlled and uncontrolled particle-emitting sources;
4. extension of existing inventories to include natural biogenic and geogenic emissions and ammonia. Quantify any other uninventoried emission sources;
5. fugitive hydrocarbon emissions from distributed small sources (less than 10 tons/year);
6. improving the traffic emissions estimates (the full 24 hours and the vehicle model mix as a function of location are important);
7. assessing the accuracy and consistency of the methods used for apportioning area source emissions into the grid cells;
8. developing fugitive particulate emission factors for road dust and soil dust as a function of wind speed;
9. understanding the importance of air temperature, time of day, and location on evaporative emissions;
10. improving the diurnal/seasonal and the weekday/weekend source operating profiles; and
11. compiling a comprehensive SCAQS-specific emission inventory, updated to 1987. This inventory should be completed and ready for modeling early in 1989.

3.6 METEOROLOGICAL MEASUREMENTS AND DATA ACQUISITION

A major concern of the modeling community is that adequate characterization of the three-dimensional wind field be performed. Extensive surface data exist in the study area, but upper air data are quite limited. We suggest that a contractor be selected to provide substantial additional upper air measurements and to augment the surface data in selected locations. Our discussions with modelers and meteorologists have indicated that two to four radiosondes and two to four doppler acoustic sounders should be operated in the Basin. In addition, pibal measurements could be used to fill in the network on selected days. Additional surface monitoring stations have also been suggested along the mountain slopes to document up-slope flow. Probably two or three additional slope stations would be adequate.

If possible, the meteorology of the offshore regions should also be characterized to document offshore ventilation, carryover, and re-entrainment processes. New offshore measurements would be expensive, but some of the upper air sites could be located near the shoreline, and data from existing offshore sources could be acquired and included in the data base. Some offshore meteorology measurements could also be made by the aircraft.

The routinely available surface meteorology data for the study period should be acquired by the data management contractor for all intensive study days and included in the data archives.

The meteorology contractor should be responsible for:

- Operation of 2 to 4 doppler acoustic sounders and providing hourly data for intensive study days to the data manager in an agreed upon format. The contractor may be able to obtain some data from existing sounders which he can validate and format for inclusion in the data archives.
- Operation of 2 to 4 radiosondes or airsondes each four hours on "intensive study" days. It may be possible to augment the soundings from existing sites.
- Operation of pibals at 2 to 4 selected sites each two hours on "intensive" study days.
- Operation of 2 to 3 surface wind stations along the mountain slopes for the days of the "intensive" studies.
- Operation of one or two time-lapse cameras on selected mountain locations.
- Preparation of meteorological summaries for each "intensive" study day which document: cloud locations, bases, thicknesses, and durations; mixing heights as available from temperature, wind, and acoustic sounder data; the synoptic conditions; the ARB wind field classification; and any unusual weather occurrences.
- Providing all data obtained to the data manager for inclusion in the project archives.

3.7 SPECIAL STUDIES

Some of the stated project objectives cannot be met with the monitoring data alone. Several special studies have been recommended to us to address specific questions. Some of these are outlined below. Order of magnitude cost estimates for most of these studies have been included in Section 8, but the details of their designs are not included in this plan. Each study will require a separate planning effort.

- Multiple tracer studies - Multiple tracers released from surface and elevated sources in the same vicinity will help identify effects of the height of the emissions (especially NO_x) on local and downwind pollutant concentrations. Releases should be performed near the coast and inland at varying times of the day, or possibly continuously for 24 hours, to assess differences in plume effects due to location. This study will help determine the relative contributions of sources with tall stacks (e.g. power plants) and automotive emissions on surface NO_2 concentrations and downwind ozone concentrations. The tracer data will also help document the mechanisms and amounts of day-to-day pollutant carryover, especially near the coast. (Addresses Objective 4, Issues 1, 2)

- Representativeness studies - Some monitoring stations in the SCAB have anomalous readings of certain pollutants. In addition, flow structures and localized sources can create strong gradients in pollutant concentrations in some areas. A mobile monitoring van could be used to assess the horizontal spatial scale over which selected sites are representative. The vertical scales can be assessed using the aircraft data. It will be important to determine representativeness in order to evaluate the accuracy of model predictions. The type "A" sites would be logical choices for study along with the Burbank site (an anomalous site for CO and carbon) and a coastal site. Mobile measurements of key gaseous and aerosol pollutants should be made during several meteorological conditions and during several times of the day. Measurements made in the van should be continuous measurements. (Addresses Objective 6, Issue 3)
- Aerosol, droplet, and gas chemistry in fogs and stratus - During some of the study periods, low stratus clouds and fogs will affect the resulting aerosol characteristics, but the type "A" stations may not actually be in clouds during some of the interesting time periods. In addition, no fog chemistry measurements are planned routinely for the type "A" stations. To properly model aerosol and gas processes, it will be important to understand the effects of scavenging of aerosols and gases by the droplets and the formation rates of particulate pollutants in droplets which might subsequently dry out. Thus, experiments to measure the droplet chemistry and the interstitial aerosol at the type "A" stations during fogs and at elevated locations during cloudy conditions would be useful during the study period. (Addresses Objective 3, Issue 1)
- Volatility studies - In order to compare measurements of PM-10 or fine particles to concentrations predicted by models, it is necessary to know the relationship between the aerosol concentrations in the air and the mass measured on a filter. The filter mass is obviously less representative of atmospheric concentrations if the aerosol is volatile and evaporates from the filter or if artifacts form from gases which are absorbed by a filter. Several types of measurements have been suggested to study the effects of water and organics. These measurements can be made at the type "A" sites, but they involve the performance of specific experiments rather than multiday monitoring. Experiments have been suggested to measure the effects of heating on aerosol size distribution and light scattering and the use of a beta-gauge to study changes in collected particle mass with changes in air composition. (Objective 6, Issue 2)
- Dry deposition studies - One area of uncertainty in models is the deposition rate of aerosols and gases. The relative deposition rates of acid aerosol and gases are important to

determine whether acid deposition is dominated by dry or wet deposition and by aerosols or gases. Deposition experiments have been suggested using eddy correlation techniques for gas species (and possibly for aerosols as well) and using "Acidic Dry Deposition Concentration Monitors" (EPA) (Hicks et al. 1980). Additionally, experiments have been funded by ARB to measure atmospheric concentrations of aerosol and gaseous acidic species during the SCAQS experiment period. (Objective 3, Issue 4, and Objective 5, Issue 1)

- Measurement technique intercomparison and evaluation studies - A large scale comparison of nitrogen species measurement techniques was sponsored by ARB during September, 1985. ARB will also conduct an evaluation of measurement techniques for condensable carbon species in 1986. These two studies are considered by ARB to be part of SCAQS, but they are being planned separately and are not described or costed in this project plan. These studies will allow the design of the SCAQS measurements to be modified to use the best available carbon and nitrogen measurement techniques. (Objective 6, Issues 2 and 4)
- Long term monitoring of PM-10 and fine particles - It would be useful to continue PM-10 and PM-2.5 monitoring at all of the SCAQS "B" sites after the end of SCAQS for one or more years in order to develop a long term data base adequate to test models for PM-10 annual averages. Twenty-four hour samples coincident with the SCAQMD six-day sampling cycle would be adequate. Measurement of mass alone would allow comparisons of the data with the output of the models, but continued measurement of the chemistry would allow more rigorous tests of the models. We recommend that the SCAQMD continue monitoring PM-10 and PM-2.5 mass and chemistry at the SCAQS "B" sites for at least one year on the normal 6th day schedule. We assume that sufficient equipment would be available after SCAQS to perform such monitoring and that the SCAQMD can provide the labor for operation of the samplers. The chemical analysis for this additional monitoring has been included in the special studies cost estimates in Section 8. Analyses of PM-10 and PM-2.5 filters for mass, elements (XRF), and carbon are included in the estimate. (Objective 1, Issue 1)

4. QUALITY ASSURANCE

4.1 QUALITY ASSURANCE OVERVIEW

Every measurement consists of four attributes: a value, a precision, an accuracy, and a validity (e.g. Hidy, 1985). The measurement methods described in the previous section are used to obtain the value. Quality assurance is the complementary part of the measurement process which provides the precision, accuracy, and validity estimates and guarantees that these attributes are within acceptable limits. The quality assurance component of SCAQS is essential to the attainment of Objective 1.

Quality assurance for the project will be a major responsibility of the Project Coordinator (PC). The PC must ensure that the final program design contains adequate quality control procedures and adequate external checks to assure that the data obtained will be adequate for their intended purposes. In addition, it is the responsibility of the PC to monitor the quality assurance activities during the project and to make certain that problems are rapidly identified and solved. A quality assurance program will be implemented for all repetitive measurements for which a standard operating procedure (SOP) can be developed.

The quality assurance program for SCAQS will include two types of activities: quality control (QC), and quality audits (QA). The QC activities will consist of written standard operating procedures to be followed during sample collection, sample analysis, data processing, and auditing. These procedures define schedules for periodic calibrations and performance tests. They specify pre-defined tolerances which are not to be exceeded by performance tests and the actions to be taken when they are exceeded. The QC activities are on-going activities of measurement and data processing personnel. The QC procedures will be developed, documented, and implemented by each measurement group, and reviewed for completeness by the quality auditor.

Quality auditing is an external function performed by personnel who are not involved in normal operations. The purpose of quality audits is to determine whether the QC procedures are adequate and are being followed and whether the tolerances for accuracy and precision are being achieved in practice. The quality auditing function consists of two components: systems audits and performance audits.

Systems audits will be performed for all measurements. They start with a review of the operational and QC procedures to assess whether they are adequate to assure valid data which meet the specified levels of accuracy and precision. After reviewing the procedures, the auditor examines all phases of the measurement or data processing activity to determine whether the procedures are being followed and the operational people are properly trained. The systems audit is intended to be a cooperative assessment resulting in improved data rather than a judgmental activity.

Performance audits (PA) establish whether the predetermined specifications are being achieved in practice. For measurements, the PA involves challenging the measurement/analysis system with a known standard sample which is traceable to a primary standard. PAs will be performed for those measurements for which standards are available. For data processing, the PA consists of independently processing samples of the data and comparing the results.

For this project, the position of quality audit manager (QAM) would be funded by the ARB. The QAM will be responsible for the performance of systems audits and for the coordination of performance audits. Performance audits will be funded separately and may actually be performed in part by ARB or EPA staff. The QAM will report the audit findings to the PC, and QA reports will be distributed along with the data summary reports.

Quality audit and quality control (QC) for the type "C" stations and for supplemental data will be the responsibility of the agencies operating the stations. The QAM will review and document the QA and QC procedures in use by those agencies and include such documentation with the audit reports to the PC.

For type "B" stations, the QAM will coordinate systems and performance audits for each appropriate measurement. In addition, standard QC procedures will be developed and implemented by the measurement groups. For type "A" stations, performance and systems audits will be performed for those measurement systems for which the operational procedures are standard and well documented. For more experimental measurements or those for which there is no other standard, only systems audits will be performed. It will be the responsibility of the measurement group to develop documentation and quality control procedures and to provide an assessment of the validity, accuracy, and potential sources of error in their data.

4.2 ROLE OF QUALITY AUDIT MANAGER

The Quality Audit Manager (QAM) will be responsible for the following tasks:

- work with investigators to determine the target specifications for accuracy and precision for each measurement;
- review the operational and QC procedures for each measurement and verify the assumptions on which the measurement is based;
- prepare systems audit procedures and submit to PC and measurement personnel for approval;
- perform preliminary systems audits at investigators' location with the help of the measurement groups;
- develop performance audit procedures for all core or routine measurements and submit to the PC and the investigators for approval. No performance audits will be done for experimental or special measurements since standards are not available;
- perform systems audits on field measurements and laboratory and data processing procedures during the field programs;
- coordinate performance audits on routine measurements during the field programs;
- for any problems identified in audits, inform the PC and review the issue with the investigator until auditor and

investigator agree on the existence and extent of the problem. Try to determine a course of action for remedying the problem;

- prepare short letter audit reports for the PC and investigators within 2 or 3 days of each audit; and
- prepare detailed draft reports for the PC and investigator for each audit. Revise drafts after feedback from the PC and investigator. Submit final audit reports to the PC for inclusion in the data base.

4.3 DEFINITIONS

In developing a quality assurance plan, it is important that the project participants agree on the definitions of the terms used. These definitions are continually evolving (e.g. Mueller, 1980; Mueller and Hidy et al., 1983; Watson et al., 1983; Hidy, 1985), but a suggested set is presented below for consideration. Although the definitions proposed here may change prior to beginning the SCAQS measurements, they must be fixed before that time to place all measurement processes on a common basis.

- **Measurement:** An observation at a specific time and place which possesses four attributes: (1) value--the center of the measurement interval; (2) precision--the width of the measurement interval; (3) accuracy--the difference between measured and reference values; and (4) validity--the compliance with assumptions made in the measurement method.
- **Measurement Method:** The combination of equipment, reagents, and procedures which provide the value of a measurement.
- **Quality Assurance:** A combination of procedures, reference materials, and controlled tests which assure the precision, accuracy, and validity of the measurement and minimize the exceedance of pre-set tolerances for these attributes.
- **Quality Control:** Internal procedures, documentation, and performance tests which: (1) identify deviations from measurement assumptions and (2) identify measurement values which exceed pre-set tolerances when compared to internal reference materials. Quality control identifies and corrects measurement method deficiencies and provides the information needed to assign the precision and validity attributes to the measurement.
- **Quality Audit:** External procedures, documentation and performance tests which: (1) determine the adequacy of internal procedures, documentation and performance testing, (2) ascertain the degree to which internal quality control is following the prescribed procedures, and (3) challenge the measurement methods and internal reference materials with known values derived from an external reference material. Quality auditing

identifies quality control deficiencies and provides the information needed to assign accuracy attributes to the measurement.

- Primary Standard: A known quantity of a material which is derived from fundamental physical principles, is reproducibly quantified by many different measurement methods, maintains its integrity over time, is subject to periodic and documented verification, and is accepted by all measurement methods as a standard.
- Primary Reference Material: A known quantity of a material which is reproducible within individual measurement methods, but not among methods. A primary reference material is accepted by all measurement methods as being precise, but not necessarily as being accurate.
- Transfer Standard: A physically similar quantity of material which can be directly traced to an identified primary standard or primary reference material via periodic documentation of comparisons using a prescribed measurement method. Transfer standards are used for calibration, quality control performance tests, and performance audits.
- Traceability Trail: The documentation which establishes the relationship between any measurement and all of the primary standards or primary reference materials.
- Measurement Method Validity: The identification of measurement method assumptions, the quantification of effects of deviations from those assumptions, the ascertainment that deviations are within reasonable tolerances for a specific application, and the creation of procedures to quantify and minimize those deviations during a specific application.
- Sample Validity: Procedures which identify deviations from measurement assumptions and flag individual measurements as valid, valid but suspect, or invalid based on pre-defined criteria.
- Developmental Status: Indicates the degree to which a measurement method can be expected to yield values of known precision, accuracy, and validity. Measurement status can be "established", "semi-established", or "unestablished." Established methods are those with accepted operating procedures, identified and quantified interferences, traceability to accepted primary standards, agreement with other established methods, and known levels of precision, accuracy, and validity. Semi-established methods are those with controversial operating procedures, partial characterization and quantification of interferences, traceability to one or more reference materials, disagreement with other established or semi-established methods, and known precision levels. Unestablished methods are those

with incomplete or non-existent operating procedures, no traceability to primary reference materials or standards, little or no inter-method comparison results, and unknown precision, accuracy and validity.

- Measurement Process: Established or semi-established measurement methods combined with quality control and quality auditing to provide values with known precision, accuracy, and validity.

4.4 STANDARD OPERATING PROCEDURES

Standard Operating Procedures (SOPs) codify the actions which are taken to implement a measurement process over a specified time period. These are both descriptive and prescriptive. The various SOP revisions are maintained so that subsequent users of the measurements may consult them to interpret measurements in light of new knowledge about the measurement methods being applied. Examples of this descriptive use were given in Section 2.2. The prescriptive role of SOPs is to incorporate state of the art knowledge into current measurement practice. SOPs must undergo scheduled revisions in order to fulfill this prescriptive mandate.

Standard operating procedures should be created for the routine field sampling, laboratory analysis, data processing, and quality audit activities planned for the SCAQS. These procedures will include the following elements:

- A brief summary of the measurement method, its principles of operation, its expected accuracy and precision, and the assumptions which must be met for it to be valid.
- A list of materials, equipment, reagents and suppliers. Specifications should be given for each expendible item, and its storage location should be listed.
- Designation of an individual to be responsible for each part of the procedure.
- A general traceability path, the designation of primary standards or reference materials, tolerances for transfer standards, and a schedule for transfer standard verification.
- Startup, routine, and shutdown operating procedures and an abbreviated checklist.
- Copies of all data forms with examples of filled out forms.
- Routine maintenance schedules, maintenance procedures, and troubleshooting tips.
- Internal calibration and performance testing procedures and schedules.
- External performance auditing schedules.
- References to relevant literature and related standard operating procedures.

The Project Coordinator is responsible for acquiring standard operating procedures from all measurement investigators and for scheduling procedure revisions. The Quality Audit Manager is responsible for reviewing procedures and determining their completeness and accuracy.

4.5 SAMPLE VALIDATION

The results of several measurement method validation studies have been reported in Sections 2 and 3. Other such studies are being planned prior to and as part of SCAQS as well as other studies. Section 6 specifies several projects for the interpretation of the results of these studies. These results will be needed to provide a basis for the validation of individual samples taken within the SCAQS. Three levels of validation will be applied with the result being a label of valid, valid but suspect, or invalid associated with every measurement.

Level I sample validation takes place in the field or in the laboratory and consists of: (1) flagging samples when significant deviations from measurement assumptions have occurred, (2) verifying computer file entries against data sheets, (3) eliminating values for measurements which are known to be invalid because of instrument malfunctions, (4) replacement of data from a backup data acquisition system in the event of failure of the primary system, and (5) adjustment of measurement values for quantifiable calibration or interference biases. Each measurement investigator performs Level I validation of his measurements.

Level II sample validation takes place after data from various measurement methods have been assembled in the master data base. Level II applies consistency tests based on known physical relationships between variables to the assembled data. Examples of these tests are: (1) the sum of all chemical species in a particulate matter sample should be less than or equal to the gravimetric mass of that sample, (2) size segregated particle concentrations should be less than total particle concentrations, and (3) dew point should always be less than temperature. Data adjustments for quantifiable biases are made in Level II validation if they are discovered after assembly of the master data base. The data manager, cooperating with the measurement investigators, is responsible for Level II validation.

Level III sample validation is really a part of the data interpretation process. The first assumption upon finding a measurement which is inconsistent with physical expectations is that the unusual value is due to a measurement error. If, upon tracing the path of the measurement, nothing unusual is found, the value can be assumed to be a valid result of an environmental cause. Unusual values are usually identified during the data interpretation process as: (1) extreme values, (2) values which would otherwise normally track the values of other variables in a time series, (3) values for observables which would otherwise normally follow a qualitatively predictable spatial or temporal pattern. The project coordinator, with cooperation from the data manager and data interpretation investigators, is responsible for Level III validation.

All data validation actions at each level should be recorded in a data validation summary which accompanies the data volumes. Data base records should contain flags to identify the level of validation which they have received at any point in their existence.

5. DATA MANAGEMENT

5.1 ROLE OF DATA MANAGER

The data management function will be funded by ARB. The data manager (DM) will be responsible for assembling, archiving, reviewing, and distributing the data obtained during the study. Specifically, the DM will perform the following tasks:

- With the concurrence of project participants, develop a data exchange protocol. All participants must agree to abide by the protocol in order to use project facilities and to obtain data from the data archives before publication of the final project report.
- With the help of project participants, identify all data to be considered part of the project. (Some participants or other groups may obtain data for their own use which are unrelated to the project.)
- Develop standardized data formats with the assistance and approval of the participants. All participants will submit their data to the DM in the agreed upon format and media after each study period.
- Review all data submitted to determine that formats are proper and documentation is adequate.
- Identify sources, formats, and quality of data available from existing data resources (National Weather Service, Federal Aviation Administration, AQMD, etc.) and prepare a list of data to be obtained for the study.
- For each sampling day, obtain routinely available data, convert to project format, and archive.
- For each "Intensive Study" day, obtain all project data.
- Archive all data in an easily reproducible and retrievable form. The core meteorological and surface air quality data should be archived using a disk based data base management system so that data required for specific analyses can be easily accessed.
- Perform simple consistency and validity checks on the data submitted, and flag those data points which are suspect. When possible, review suspect data with the responsible group and resolve the status of the data.
- Correct or flag data points in the master data base when errors are identified by subsequent users of the data.
- Prepare a report which inventories the data base for each study period and which documents the data formats and data access procedures. Summaries of data capture rates and data validity should be included for each intensive study period. Provide report to all participating and sponsoring organizations.

- Provide data to participants on request as required for their analyses.
- Provide a copy of the complete data archive to CARB.

The DM will design formats for the data to be submitted that are useful for the modeling community. Except for the data from the existing data resources, the DM should not have to reformat the data obtained from the participating organizations.

5.2 DATA BASE DESCRIPTION

The data base will have two components. A "core" data base will be developed for modeling and data analysis use. The "core" data will consist of the emissions data, the available routine supplementary data, the data from the types "B" and "C" stations, the aircraft data, the surface and upper air meteorology data, and data from the type "A" stations which are from regularly repeated measurements over extended time periods and which are of known accuracy and validity. The second component of the data base will be the "special studies" measurements such as the tracer studies and measurements from the type "A" station measurements which are more experimental in nature.

All data should be submitted in consistent and easily usable formats with like types of data being formatted similarly. Data formats should allow easy use of the data with graphics, statistical and modeling software. All data should be reviewed and validated by the group submitting the data, and suspect data points should be flagged in the data records.

All data submitted to and assembled by the DM should be accompanied by reports which describe the data formats, uncertainties, detection limits, and accuracy estimates for the data. Much of this information should also be included in the data records. These data reports should also provide an inventory of the data submitted and a summary of the data validity and data capture rates for each intensive study period, and describe the data collection, quality control and validation procedures used to obtain and process the data. The report should discuss potential errors, interferences, or other caveats regarding the data.

The formats of the core data should be such that they can be included in a single large data base and are easily accessible by modelers. Data records should include space for validity flags and other similar notation. Formats of the special studies data will, by necessity, be more varied and less standardized. Whenever possible, however, data records should document the position, time, and sample averaging period.

"Core" data will be reviewed by the DM and subjected to simple consistency or validity checks. Flags for suspect data points will be added to the data records by the DM.

Core data should be submitted to the DM within six months of the end of each field study and special studies data as soon as possible after that. Data should be available to participants within about 3 months after receipt by the DM. It is suggested that all core data be submitted on 1600 BPI 9-track tape in ASCII format and that a hard copy printout accompany all data tapes.

5.3 ACQUISITION OF SUPPLEMENTAL DATA

The DM will be responsible for identifying and acquiring existing supplemental data. These data include NWS, FAA, and other available meteorological data and air quality data from SCAQMD, ARB, Ventura County Air Pollution Control District (VCAPCD) and other available sources. Such data obtained by the DM will be reformatted to be consistent with the core data base formats for similar types of data. Potential sources of supplemental data are identified in Section 2.

5.4 DATA EXCHANGE PROTOCOL

A data exchange protocol will be prepared by the data manager with input from the sponsors. It will be a condition of participation in the program that sponsors and participants agree to abide by the protocol.

The purpose of the protocol is to ensure timely and complete availability of the data collected as part of SCAQS and proper attribution for data used in analyses and publications.

The protocol should embody the following principles:

1. The data collected are to be available eventually to the scientific community. Before final publication, however, the data will be made available to the SCAQS participants. It is expected that each participant will submit at least the core data from each field study to the DM within 6 months of the end of the field study. Special studies data may take a few months longer. Data should be submitted in an agreed upon format and should be reviewed and validated by the participant prior to submission.
2. All data in the SCAQS data bank should be available to any participant on request. Data in the data bank should be made available to the public after about 18 months from the end of each field study period. No participant should publish analyses or data sets which include data of other participants unless he has the permission of the other participants or the data have been formally released to the public domain. Participants may distribute or publish their own data at any time subject to the conditions in 4, below.
3. The sources of data should be cited whenever data are used in publications. If a substantial amount of data from other participants is used, that participant should be given the option of being included as a co-author on resulting publications.
4. Prior to publication or presentation, manuscripts resulting from SCAQS should be submitted to the participants and sponsors for comment. Each participant should have 30 days from receipt of the manuscript to submit his comments to the senior author. The authors should give sincere consideration to all comments. If the comments are not incorporated in the manuscript, the commenting participant may submit his comments separately to the journal to which the original manuscript was submitted.

6. DATA ANALYSIS AND INTERPRETATION

6.1 ROLE OF DATA ANALYSIS COORDINATOR

In a study of this type with many investigators and many types of data analysis and interpretation, it is necessary to have one person who can keep track of the project objectives and coordinate the diverse analysis efforts so that the objectives are met. The data analysis coordinator will have the following tasks.

- Identify a data analysis methodology to meet each of the final project objectives.
- Identify the participant who will perform each analysis task.
- Identify the information and data needs for each analysis task.
- Work with the various investigators to develop a critical path diagram and identify when the investigator will need which information or data.
- Identify milestones for review.
- Act as a facilitator to assure that the required data are made available to the investigators on schedule and that investigators are aware of complementary efforts by other investigators.
- Identify duplications of effort and work out agreements between investigators to minimize unproductive efforts and maximize the technical output from the resources available.
- Identify topics for presentation at a technical session and coordinate with the investigators to assure that papers are presented on all appropriate topics.

6.2 DATA INTERPRETATION METHODS

Measurements, by themselves, say nothing about the causes of air pollution and the likely effects of emissions reductions. It is only when these measurements are interpreted that relationships can be observed and conclusions can be drawn. The data interpretation methods which address the objectives stated in Section 1 need to be defined, at least in a general manner, before the first measurement is taken in order to assure: (1) that all information needed by the method will be available at the interpretative stage, and (2) that scarce resources will not be expended on taking measurements which do not fit within the data interpretation framework.

Section 1 stated the issues which might be resolved by the SCAQS. Section 2 specified the additional data needs which model developers and users

feel are currently lacking. Section 3 listed the feasible measurements which would fulfill those needs. The goal of this section is to identify the data interpretation methods which are expected to be used and to associate the proposed measurements with their use in these methods.

As a result of the literature survey in Section 2, it was found that data interpretation methods appropriate for attaining SCAQS objectives generally fall into one of five categories:

- Descriptive methods summarize the spatial, temporal and statistical distributions of individual observables. They include averages, standard deviations, maxima, minima, spatial isopleths and time series. A large number of measurements of each observable (typically greater than 50 to 100) is necessary to determine statistical distributions. The period between measurements needs to be smaller than that over which major changes occur, and the geographical spacing between measurements needs to be less than the spatial frequency of the observables. The results of these descriptive methods show which observables are reaching levels of concern. Descriptive methods do not yield cause and effect relationships nor do they anticipate how a change in one variable will affect the values of other variables. These descriptive methods are often useful for the display and comparison of results from other data interpretation methods.
- Co-variation methods calculate measures of association between two or more variables. These measures take on high absolute values when the variables change in the same manner over a period of time or over a geographical area; they take on low absolute values when this co-variability is lacking. Time series analysis, correlation coefficients, and principal components analysis are methods which provide these measures of association. By themselves, these co-variation methods only establish whether or not the values of a set of variables change in the same way. When these co-variational methods are combined with a physical understanding of the situation under study, cause and effect relationships among the variables may be inferred.
- Classification methods select specific periods of time, usually periods of high pollutant concentrations, and describe the physical cause and effect relationships using all data which can be acquired. Both qualitative and algorithmic classifications are possible. Regime analysis (Keith and Selik, 1977), discriminant analysis (Lin, 1982), and case studies (Blumenthal et al., 1978) have all been applied to data in the South Coast Air Basin. The case studies are particularly useful in determining the relative importance of different chemical and physical pathways. Cases are separated into dichotomous groups in which a pathway is expected to dominate or in which it is expected to have a negligible effect. If the expected consequence is observed in the first group and not observed in the second group, then the pathway

can be considered important. Most of the quantitative physical and chemical mechanisms present in current models have resulted from their identification in case studies. The importance of various reactive species, atmospheric moisture, and liquid water content of the aerosol remain to be examined by this method.

- Source oriented models contain mathematical descriptions of the interactions among variables. These models include transport and chemical mechanisms. Lloyd et al. (1979), Reynolds et al. (1976), Cass (1979), McRae et al. (1982a), and Seigneur et al. (1983b) have produced and tested such models appropriate for the SOCAB. Each of these source models requires three-dimensional wind fields (speed, direction, and dispersion characteristics at all points in the modeled area) over a period of one day or more. These wind fields can be interpolated from measurements (e.g. Goodin et al., 1980) or calculated from fundamental physical equations applied to a set of initial conditions (e.g. Pielke, 1984). Although the transport and chemical components are usually combined in the computer implementation of each model, it is possible to introduce alternative wind fields to simulate the transport mechanisms and alternative photochemical and aerosol mechanisms to simulate chemical interactions.
- Receptor models use chemical and physical measurements of sources and receptors. They require input data for the chemical compositions of the emitting sources and ambient concentrations of those same chemical species. Linear regression of species on principal components has been shown to relate sulfate concentrations to physical causes (Henry and Hidy, 1979). Chemical mass balance calculations (Gartrell and Friedlander, 1975; Miller et al., 1972; Cass and McRae, 1983; Feigley and Jeffries, 1979) can be applied in the SOCAB to determine the contributions of source emissions to receptors. Linear regressions of b_{scat} on selected chemical species or on source contributions can be applied to determine visibility extinction budgets (White and Roberts, 1977; Pratsinis et al. 1984).

Each of these data interpretation approaches has been designed around available data, with certain assumptions being made to compensate for the missing data. Most computer implementations of these models are quite flexible owing to their intended applications in many areas with varying data availability. There is no absolute list of data needs for any of these data interpretation methods. Presumably, the more data they have the better. In several cases (e.g. Seigneur et al., 1981a, 1981b), the effects of more or less data on the results of the data interpretation method have been evaluated. There is as yet, however, no objective means of defining the optimum set of data required by a data interpretation method, nor is it possible to generally determine when additional measurements would be redundant (unless those measurements are already available).

6.3 DATA USES

Data can be used for four purposes in the data interpretation process:

- Input data. Every interpretation method requires some data on which to operate for the period of time being examined. Descriptive methods require values of the variables of interest in space and time. Source models require boundary and initial conditions of precursor, intermediate, and end-product species as well as three-dimensional wind fields and atmospheric stability estimates. Receptor models require ambient concentrations and source composition. When these variables are measured for the time being simulated, they are considered input data.
- Parameters. Parameters are constants supplied to the data interpretation process by a theoretical calculation, by measurements made elsewhere and assumed to be appropriate for the place and time being studied, or by tacit assumption that the value of a variable is negligible. Reaction rates, emission rates, transformation rates, dispersion parameters, and source compositions are common parameters in source and receptor models. Values for these variables are rarely measured over the period of time being modeled. Parameters normally carry higher levels of uncertainty than input data because they are not specific to each case being studied.
- Testing data. Values yielded by the data interpretation method can be compared with measurements of the same observable to test the extent to which the interpretation represents reality. The most common test measurements are ambient concentrations of an observable which are compared with the prediction of a source model. These two values are often uncorrelated, and they often tell little about the reasons for differences between predictions and measurements. Measurements of intermediate species over the appropriate time-scales are better tests of the data interpretation method. More complete (in space and time) measurements of model input variables can also be classified as test data when they would not be available during a routine application. The difference between model calculations with and without these input data provides an estimate of the accuracy to be attached to the model results. The final use of test data is to verify that the data interpretation method is valid for a specific application. Test data can be used to quantify deviations from model assumptions. In many cases, these deviations from assumptions can be directly related to deviations of model predictions from their true values. Parameters and neglected effects are amenable to this quantitative testing of model principles and assumptions.
- Uncertainty estimation. The numerical values determined by any data interpretation process differ from reality because of both model uncertainty and measurement uncertainty. Model uncertainty results from deviations from the principles and

assumptions of the model during its application. This model uncertainty is quantified using data in its testing role, as described earlier. The measurement uncertainty of a model calculation results from the fact that each input datum and parameter does not define a single value, but an interval within which the true value of the observable should fall. The combination of all of these measurement intervals should yield an interval around the model calculation. Very few air quality models in use today provide for the estimation of this interval, and methods to calculate it are still in their developmental stages (e.g, Efron 1979; McRae et al. 1982b; Freeman et al. 1986; Watson et al. 1984). Each one of these methods requires some estimate of the statistical distribution and width of the intervals associated with the input data and parameters. This interval is typically more than the uncertainty associated with an individual measurement. Most models assume that a single point measurement represents a volume or a period of time, and an estimate of the variability of the input data or parameter over that volume or time period is required to calculate the measurement uncertainty associated with a model calculation. Measurements which are "collocated" with a resolution finer than the temporal and spatial scales of the data interpretation methods can be used to estimate the uncertainty of input data and parameters. These uncertainties can also be estimated from periodic performance tests of each measurement method (Watson et al. 1983). It is presumed that future model development will include methods to take advantage of this information and supply intervals associated with measurement uncertainty on model results.

6.4 SCAQS DATA INTERPRETATION PROJECTS

The measurements proposed in Section 3 can be used in an infinite number of combinations as input, to estimate parameters, to test the principles and assumptions of the data interpretation methods, and to estimate the uncertainty of the quantitative results of the interpretive efforts.

Data interpretation projects are described in this section which address the objectives and issues in Section 1. The projects which follow cannot identify every way in which the SCAQS data can be interpreted. The project descriptions are presented as examples to demonstrate that each piece of data collected does have a use for input, parameterization, testing, or uncertainty estimation. Although these projects are organized by the specific objectives and issues which they are intended to address, most of them are applicable to more than one objective.

Although Sections 2, 3, and 6 appear as separate entities in the program plan, they were actually formulated in an iterative fashion. Previous research in the SOGAB was studied to determine which data interpretation methods had been used in the past and the measurements they required. These were used to define an initial set of variables to be measured in SCAQS. These measurements were then incorporated into an interpretive framework which ultimately resulted in the projects described below. The measurement set was then modified to accommodate the anticipated data interpretation needs.

This iterative process is not perfect, and it may still be found that the SCAQS measurements are not totally adequate for all purposes which might be identified a posteriori. It is expected that the number of these cases will be minimized, but not eliminated, by this iterative process.

6.4.1 Objective 1: Description of SOCAB Air Quality

The data base will contain individual numbers which have been validated, corrected, and flagged. In order to be of use to researchers, this data base needs to be described statistically, graphically and phenomenologically. While most researchers will do this to a certain extent by themselves, a number of summaries have been produced in past studies which have been useful in focusing the more detailed analysis of specific situations. The data description projects are intended to provide this common denominator for subsequent projects. It is recognized that no "descriptive" study can be separated from the posing and testing of hypotheses based on previous work, and it is expected that the researchers performing projects intended to address the first objective will implicitly address other objectives as well. No attempt is made to exclude this possibility in the descriptions of the SOCAB air quality data. This speculation on cause and effect relationships is considered a "bonus" of an otherwise mundane presentation of results.

Project 1.1: Data Description Summaries of Ground-based Measurements.
Prepare statistical summaries consisting minimally of maximum, minimum, average, standard deviation, and median values for each observable at each site for the duration of both sampling periods. Express these in tabular formats and as box plots. Calculate and statistically summarize four hourly averages of one hour duration samples for comparison with the four-hour average aerosol data. Calculate correlation coefficients among each of the variables over space and time. Prepare graphical displays which include spatial isopleths of each observable for each four-hour period, time series plots of each observable, and surface wind flow patterns for each period. Produce graphs of concentrations obtained on all aircraft traverses with the flight paths clearly indicated on a map of the Basin and appropriate time-markers denoted on those paths. Plot average vertical distributions from all the spirals at each location for each measured observable. Plot temperature and wind sounding data for every sounding site and time plot. Plot gridded emission rates for each pollutant for the aggregate totals, elevated and ground level sources, and mobile and stationary sources over four hour intervals. Prepare a map of all major single point and area sources coded for source type. Prepare isopleths of the spatial distribution of the most reactive hydrocarbon emissions. To determine how random measurement errors change the data summaries, create ten or more simulated SCAQS data sets by adding and subtracting random numbers proportional to the uncertainties of each measurement and generate selected statistical and graphical summaries for comparison. Distribute these randomized outputs with the real outputs so that subsequent studies can use them to evaluate the differences in data interpretation results which might result from measurement uncertainty.

The output of this analysis project is expected to be used in subsequent analyses. In general, each investigator will produce those graphical and statistical displays which are of greatest use to him. The displays described here are the lowest common denominator for subsequent interpretive efforts, yet they will result in reams of paper.

An alternative to the generation, compilation, and distribution of hardcopies of these statistical and graphical summaries is the creation of a micro-computer based hardware/software system and appropriate documentation which would allow each investigator to classify the data base in any way he chooses, including the definition of new variables from the raw data, and to display it by any of the graphical or statistical techniques which have been designated above. Communications packages are commercially available which would allow most investigators to transfer data from their microcomputers to their larger computers for more intensive computations, should they be necessary. ARB is currently sponsoring a project which will interface its routine meteorological, emissions, and air quality data bases to IBM-XT disks. Reformatting routines and appropriate user instructions are being developed to interface these data with commercially available computer programs which perform data base management (Ashton-Tate, 1984), air quality data summaries (Odessa Engineering, 1985), spreadsheet and graphics (Lotus Development Corporation, 1983), comprehensive statistical analyses (Dixon et al., 1983), Chemical Mass Balance modeling, and elementary UNAMAP dispersion modeling (Bowman, 1985).

Another alternative to hardcopy printout is being explored by Pitchford and McGown (personal communication, 1985) in the RESOLVE program. The spatial and temporal distributions of variables have been generated on a microcomputer and recorded on video tape or a video disk. Hussey et al. (1983) applied this method to air pollution data from the SOGAB with striking results. Henry (personal communication with Ron Henry, USC, 1985) is investigating its use in visibility studies. The adaptation of such a graphics display to microcomputers and interfaces to the commercial software packages described earlier would facilitate data interpretation in the SCAQS and leave a lasting legacy for subsequent air quality measurement programs.

Project 1.2: Meteorological and Upper Air Descriptions. Describe in detail each of the episodes obtained from the SCAQS in the style of Smith et al. (1972, 1984) and Blumenthal et al. (1978). These descriptions of the meteorological evolution will provide a qualitative understanding of the transport situation, convergence zones, the potential for mixing from aloft, and carryover from previous days. This qualitative description can be used to test the assumptions of the quantitative mathematical models describing transport in the basin. Surface trajectories can be inferred from the surface wind plots. Draw cross-sections of observable values obtained from aircraft vertical soundings and estimate mixing heights. Plot isopleths of mixing height for each aircraft sampling period. Examine the synoptic weather maps and correlate with the surface and upper air observations. Examine the differences between daytime and nighttime spatial distributions and determine outflow and ventilation scenarios. Compare the SCAQS descriptions with those of earlier studies such as Blumenthal et al. (1978), Smith et al. (1972), Angell et al. (1976), and Edinger (1959, 1973).

Project 1.3: Aerosol Data Descriptions. This project consists of the examination of the chemical, spatial, temporal, and size distributions of ambient aerosols, the comparisons of ostensibly equivalent methods of aerosol measurement, and the comparison of the SCAQS aerosol distributions with those derived in previous studies of Whitby et al. (1972), Hidy and Friedlander (1972), Heisler et al. (1973, 1980), Hering and Friedlander (1982), and Stelson

and Seinfeld (1981). Calculate the material balance of the fine and coarse mass for each sample by converting elemental, ionic, and carbon measurements to probable compounds, summing, and ratioing to the gravimetrically measured mass concentration. Display these ratios as a time series and identify those which differ substantially from unity. Sum the four-hour total masses and ratio to the TSP mass concentrations for simultaneous samples. Produce pie charts which show the relative contributions of different chemical species to each fine and total mass concentration. Locate these pie charts on maps of the Basin with radii proportional to the total mass concentration at a site, similar to the display in Shah (1981). Identify the predominant size range of measured chemical species and compare with earlier findings. Plot four hour average number, surface area, and volume distributions as a function of particle size as derived from electrical mobility and optical particle counter data. Identify commonly recurring size distributions. Classify each sample according to one of the size distribution patterns. Plot the mass median diameters and standard deviations for each mode of the volume distributions on maps for each sampling period. Describe the evolution of the size distributions by location and time of day and compare to hypotheses advanced in previous studies such as Whitby et al. (1972), Hidy and Friedlander (1972), Heisler et al. (1973), and Heisler and Friedlander (1977). Examine similar size distributions and temporal/spatial plots using the chemically specific size distributions obtained from the multi-orifice impactors.

Project 1.4: Nitrogen, Sulfur, Carbon, and Oxidant Budgets.

Plot pie charts of the gaseous and particulate nitrogen (NO , NO_2 , HNO_3 , PAN, NH_3 , HONO , NH_4^+ , NO_3^-), sulfur (SO_2 , SO_4 , organic sulfur), carbon-containing (elemental and organic particles, hydrocarbons, organic sulfur), and oxidizing (O_3 , OH, H_2O_2 , PAN, HO, NO_3 , HO_2 , RO_2) species for each four hour period on a map of the Basin. The radius of each pie should be proportional to the total number of N, S, or C atoms in the budget. Also plot these totals as time series stacked bar charts for each station, with the bars divided in proportion to the species present. Compare the more completely speciated budgets at the type "A" stations with the less speciated budgets at the type "B" stations to estimate the potential magnitudes of the missing components at the more spatially representative sampling sites.

6.4.2 Objective 2: Source Characteristics for Receptor Models.

Project 2.1: Identify Chemical and Physical Properties of Sources.

Compile comprehensive primary emissions profiles for source types in the SOCAB from SCAQS source characterization tests and previous studies such as Taback et al. (1979), Mayrsohn et al. (1977), and Oliver and Peoples (1985). Classify these by source type (e.g. motor vehicle, fuel oil combustion, solvent use, natural sources, etc.), and construct comprehensive emission profiles which include gaseous as well as particulate chemical composition. Based on previous studies of chemical interactions, classify each of these species as transforming or non-transforming at distances close to and distant from an emissions source. Perform principal components analysis (e.g. Hopke, 1982 with the suggestions of Henry, 1985) on gaseous and particulate data sets at type "A" sites and determine whether or not the expected source composition patterns are reproduced. Examine the chemical species associated with each principal component and determine whether or not source categories other than those identified from the emission inventory are affecting the

receptors. Create spatial plots of selected chemical species emissions patterns and superimpose trajectories obtained from Project 1.1 to determine sampling sites and times which are most likely to be influenced by source emissions. Apply the Chemical Mass Balance receptor model using the effective variance weighting and error propagation scheme (Watson et al., 1984) to the receptor data using the profiles and chemical species for sources which are most likely to affect the receptor and which will experience minimal fractionation between source and receptor. Apply the CMB to situations when meteorological and emissions conditions mitigate against a source affecting a receptor, evaluate the consistency of the calculated source contributions with reality. Determine the variability of CMB calculations as a function of alternative, but equally valid, source profiles, the chemical species measured at the receptor and at the source, the grouping of individual sources into source types, and in response to randomized input data. Apply the singular value decomposition method of Henry (1982) to determine the multicollinearity of source profiles in different situations. Determine the minimal number of chemical species and the variability which can be tolerated in their measurement for the accurate apportionment of particulate matter, carbon monoxide, SO_2 , and hydrocarbon receptor concentrations in the absence of source profile fractionation.

Project 2.2: Source Profile Fractionation. Using simple equilibrium, reaction, decay, and deposition considerations (e.g. Stafford and Liljestrang, 1984), calculate the expected changes in source profiles as a function of meteorological variables and the presence of other species. Coordinate with source-modeling projects to obtain a better description of source profile evolution from the more comprehensive chemical transformation mechanisms included in these models, and compare the simple transformation estimates with these more complex ones. Calculate transport times below which no significant fractionation will have taken place and beyond which equilibrium will have been reached. Select those species for which fractionation estimates are reasonably robust. Select cases, using the results of Projects 1.1, 1.2, and 1.3, in which the constituents measured at one of the source-area sites follow a trajectory passing over several monitoring stations, and calculate the expected changes in the combination of source profile for the selected chemical species. Apply the CMB at each site along the trajectory. Linear combinations of fresh and aged source profiles, weighted by emission rates from the emissions inventory, should be constructed and applied to determine their value in the transport region for which equilibrium has not been reached. Determine the variability of the calculated source contributions to PM_{-10} , NO_2 , CO , hydrocarbons, and toxic substance concentrations as a function of the variables included in the CMB. Randomize the input data in proportion to their uncertainties and estimate the uncertainty which can be tolerated. Determine the multicollinearity of source profiles for various source contribution levels. Compare the effectiveness of source attribution by this method for highly reactive and non-reactive sampling periods.

Project 2.3: Attribution of PM_{-10} to Primary/Secondary and Natural/Anthropogenic Sources. Using the results of projects 2.1 and 2.2, construct source profiles for primary and secondary categories. Primary source profiles may consist of a number of individual source type profiles. Secondary source profiles may consist of those produced by several different conversion

pathways. Similarly, construct source profiles for natural and anthropogenic source types. Apply the chemical mass balance receptor models to aerosol and gas data collected at urban and non-urban sampling sites for both the winter and summer periods and for the year-long 24-hour sampling periods. Calculate the contributions of each source type to the twenty-four hour and annual average concentrations of PM-10. Examine CMB diagnostics to determine the validity of each application. To determine the uncertainty of source attribution, compare the results derived from: (1) different combinations of sources and chemical species applied to the same receptor data, (2) randomized values for the receptor and source measurements, and (3) source apportionments derived from source models applied to the same samples.

6.4.3 Objective 3. Dependence of Particle and O₃ Formation on Meteorological and Precursor Variables.

Project 3.1: Principal Components Analysis. Develop a list of phenomena which can be represented by each SCAQS variable. These phenomena may be different for the same observable measured at a different place or time in the SCAQS network (e.g. NO₂ measured at night or during the day, at ground level or above the inversion, etc.). Submit these variables, excluding particulate matter and O₃ concentrations, to principal components analysis (e.g. Henry and Hidy, 1979). Apply the PCA to various subsets of variables to (1) obtain a stable solution and (2) determine the variability within a stable solution after the fashion of Watson et al. (1985). Randomize the PCA input data in proportion to their measurement uncertainties and estimate the effects on the certainty of model results. Apply various factor rotation methods to determine the variability caused by the selection of a rotation. Associate each mathematical factor with a physical phenomenon on the basis of the variables on which it is loaded. Calculate the linear regression coefficients of fine and coarse particulate matter and ozone on the factor scores of each factor. Generate scatterplots of the values predicted by these regression equations and observations to determine how well the factors explain the observations. Recalculate these regression coefficients with a reduced data set and compare them to the coefficients obtained from the entire data set. Use the coefficients from the reduced data set to estimate particulate and ozone values which were excluded and compare the predicted and observed values. Examine the products of regression coefficients and factor scores and select very high or low values. Examine the results of projects 1.1, 1.2, and 1.3 to ascertain whether or not the principal components analysis is consistent with the qualitative meteorological and air quality features for the high and low products.

Project 3.2: Case Studies of the Aerosol Dependence on Liquid Water. Examine the temporal and spatial evolution of particle sizes and compositions yielded in Task 1.2 and explain them in terms of the variation of other atmospheric variables depicted by Task 1.1. Divide SCAQS data into periods which were preceded by or contain high and low RH, fogs and no fogs, rain and no rain. Examine the chemically speciated size distributions for these periods and determine whether or not there is a change in size or shape for ionic species. Calculate average size distributions and standard deviations for each of these dichotomous categories and determine whether or not they differ significantly to test the hypotheses of Hering and Friedlander (1982). Examine liquid water measurements to determine how the liquid water content

of the particles varies according to the ionic composition, relative humidity, and the presence of other species, and compare this to calculations using theoretical formulations (e.g. Russell et al., 1983; Stelson and Seinfeld, 1982; Bassett and Seinfeld, 1983). Calculate ion balances for cases in which liquid water is present and when it is not and infer missing species. Determine those conditions under which liquid water content can be inferred from the ionic composition measured on a filter sample which has gone through normal filter processing procedures. Identify the potential for metal catalysts which might promote liquid-phase reactions. Stratify data by cases in which photochemical and liquid phase reactions should be dominant and estimate transformation rates for SO_2 and NO_x along trajectories, then compare the results.

Project 3.3: Case Studies of Ozone Formation. Stratify episodes by high and low photochemical potential days, and compare photochemical products along trajectories identified in Project 1.1. Further stratify these episodes by ROG/ NO_x ratios in the morning at western and southern Basin sites and determine the extent to which this ratio affects the maximum ozone levels at the eastern and northern Basin sites. Recalculate ROG/ NO_x ratios for specific reactivity classes, especially aromatics, and examine receptor area ozone concentrations for cases of high and low ratios in the source areas. Examine the emissions maps to compare the quantity of fresh hydrocarbon and NO_x injected along the trajectories, and determine the degree to which this might interfere with the conclusions drawn from ROG/ NO_x ratios in the source areas. Examine aircraft traverses and compare ozone, NO_x , and hydrocarbon concentrations to simple equilibrium calculations similar to those of Calvert (1976a, 1976b). Examine nighttime concentrations of O_3 and precursors above the inversion and off the coastline to determine the degree of carryover from the previous day. Compare ROG/ NO_x ratios with those calculated from localized emissions grid squares near the western and southern sites; identify potential causes of the discrepancy. If documentable day-to-day changes in emissions patterns (temporal and spatial) occur, compare the oxidant and hydrocarbon concentrations among otherwise similar meteorological conditions (e.g. Davidson and Cassmassi, 1985). Compare oxidant values in cases with high ambient aromatic hydrocarbon concentrations to values obtained when aromatic hydrocarbon concentrations are low.

Project 3.4: Case Studies on Aerosol Sulfate, Nitrate, and Carbon Formation. Calculate equilibrium concentrations for sulfur, nitrogenous, and organic species in the gas and particle phases for each sampling site and time and compare with the aerosol measurements. Examine fine and coarse particle chemical compositions, and infer the compounds which are present. Verify these inferences via single particle analysis of selected filter samples and determine the extent to which the aerosol is internally or externally mixed. Stratify ground-based and airborne measurements by day and night and compare chemically speciated size distributions and their changes with respect to time, thereby testing the hypotheses of Richards (1983). Examine functional group analyses, selective extractions, individual particle analysis, and equilibrium estimates to estimate the fractions of organic carbon which are of primary and secondary origins. Coordinate with projects 2.1 and 2.2 to perform this primary/secondary attribution of organic carbon.

6.4.4 Objective 4. Dependence of Pollutant Spatial Distributions on Emission Height and Meteorology

Project 4.1. Case studies of natural and artificial tracer data.
Examine the results of Projects 2.1 and 2.2 to differentiate between the primary emissions from elevated and ground level source at near-source and far-source receptors. Compare these estimates with the concentrations of tracers injected at high and low elevations. Examine the vertical concentrations above ground stations to determine gradients which might be caused by elevated source emissions, and determine which sources might be the cause from the elevated emissions maps produced in Project 1.1. Examine aircraft measurements above sampling sites along well-defined trajectories between source and receptors to determine the travel time required for vertical mixing of elevated source emissions. Stratify this travel time by atmospheric stability categories, and identify significant differences. Estimate the quantity of ozone, NO_x , particulate matter and hydrocarbons which are contributed to surface concentrations by mixing as the inversion rises, and estimate the vertical distance for which vertical homogeneity is achieved as a function of time of day. Compare the results of this analysis with the assumptions of source models, and determine those cases for which the model assumptions would be valid. Examine speciated hydrocarbon and CO concentrations during high and low temperature periods to infer higher or lower evaporative fuel emissions as a function of temperature; normalizing hydrocarbon species with respect to CO may minimize the effects of different weather conditions on absolute hydrocarbon levels.

6.4.5 Objective 5. Effects of Pollutants on Visibility, Atmospheric Acidity and Mutagenicity

Project 5.1: Visibility case studies and extinction budgets.
Calculate the refractive indices for different aerosol samples and determine the effect of variations in these indices and in particle size distributions on extinction efficiencies. Include the measured fraction of liquid water in these calculations and compare the results with calculations which neglect liquid water or infer it from RH measurements. Repeat these calculations for internal and external mixtures, and compare the differences with these variabilities. Examine single particle analyses of selected samples to determine the degree of internal and external mixing in the aerosol population. Determine the extinction efficiency of each particle type, and estimate the contribution of each type to the total light extinction. Calculate extinction due to Raleigh scattering, scattering using the chemical-specific size distributions, absorption by elemental carbon, and NO_2 ; and compare the total to the scattering and absorption measurements. Identify cases of disagreement between theory and measurement which exceed estimated uncertainties and ascertain which deviations from assumptions are causing those disagreements. Calculate visibility reduction via linear regression analysis (e.g. White and Roberts, 1977) and compare the inferred scattering efficiencies with the theoretical scattering efficiencies. Calculate the relative contributions from fine and coarse particles, particles and gases, and primary and secondary species. Identify meteorological characteristics which might cause different spatial and temporal distributions of visibility impairment.

Project 5.2: Case studies of atmospheric acidity. Examine the spatial and temporal nature of atmospheric acidity and relate strong acid concentrations to sulfate, nitrate, and other ionic components in the aerosol and gas phases. Coordinate with Project 3.1 to determine differences between wet and dry oxidation mechanisms and ascertain whether or not significant differences in atmospheric acidity exist between these pathways. Compare measured acidity levels with those determined by chemical equilibrium models and determine which chemical and physical variables are required to make accurate equilibrium calculations. Apportion the acidity among the gas, particle, and droplet phases.

Project 5.3: Case studies of atmospheric mutagenicity and toxic species. Determine which organic toxic substances are present at different sites and times using the displays of Project 1.1, and compare these levels with those found in other urban areas and with levels which have been found to be harmful. Identify areas in the SOGAB where levels are consistently higher than in other areas, and examine the source emissions maps and wind flow patterns to estimate their potential origins. Identify which species are of primary or of secondary origin.

6.4.6 Objective 6. Accuracy, Precision, and Validity of Measurement Methods

Project 6.1 Evaluate Measurement Methods. As preliminary experiments to SCAQS, ARB is sponsoring intercomparisons of measurement methods for nitrogen and carbon species. These projects will provide data necessary to assess the relative concentrations determined by the different methods and to determine interferences. Duplicate samplers should also give estimates of the precision of the methods examined.

Use the data from the preliminary intercomparisons as well as SCAQS data obtained by multiple techniques and by duplicate measurements using the same techniques to assess the accuracy, precision, and validity of the SCAQS sampling methods for nitric acid, organic and inorganic carbon species, particle liquid water measurements, labile species measurements, and particle size measurements.

Project 6.2 Estimate Uncertainty of SCAQS Measurements. Combine the data from the representativeness studies, simultaneous measurements of the same observable by different methods, and the results of measurement evaluations to quantify the variability about the measurement which would be found in a representative volume around the sampling point. List all of the assumptions which must be met by each measurement method in order to yield a valid value, and identify those periods of SCAQS sampling in which those assumptions were not complied with. Quantify the effects of deviations from these assumptions wherever possible.

6.5 SYNTHESIS OF SCAQS DATA INTERPRETATION RESULTS

The projects listed in Section 6.4 represent self-contained studies, yet to fully profit from the wealth of information in the SCAQS data, the results should be synthesized and presented in a cohesive form. A separate project, headed by the data coordinator, will be needed to provide this synthesis in the following manner. Projects 1.1, 1.2, and 1.3 will be

performed first, and this descriptive information will be made available to all other researchers. Each researcher will use this information plus whatever he needs from the entire data base to perform the tasks specific to the project statement. All researchers will be known to each other, and communications among researchers will be encouraged, but not required. The data analysis coordinator will accommodate the needs of each researcher with respect to data needs and will act as a clearinghouse for information. After approximately two-thirds of the resources in each project have been expended, each researcher will write up his results and present them at a workshop. Interpretive results of one project which will enhance other projects will be identified at the workshop and collaborative agreements between researchers will be worked out. After this workshop, researchers will finish the final third of their projects with the appropriate incorporation of the work of others. The data coordinator will synthesize the papers and discussions of the workshop into a draft technical paper in the mode of Hidy et al. (1975). The paper will be reviewed by all participants and revised as appropriate. A general symposium will be established for the presentation of the final work, which will be peer-reviewed by external reviewers and published as a book or in one of the technical journals.

6.6 COMPLEMENTARY MODELING PROJECTS

Although air quality modeling is not an integral part of SCAQS, the SCAQS has been designed to meet modeling needs. Several sponsors already have planned modeling uses for the SCAQS data and have made their data needs known during the planning process. These specific needs have been accounted for in the plan. In addition, a Model Working Group (MWG) has been established to provide continuing technical input to the SCAQS design process. The MWG serves as an interface to the modeling community to assure that SCAQS data will be appropriate for modeling projects and to coordinate the modeling efforts of various participants. The MWG members are listed in Appendix A.

Some of the modeling projects currently planned by the sponsors are outlined below.

- Southern California Edison may use the meteorological measurements to evaluate a prognostic one-layer sea breeze model which was developed by the University of Washington and the Pielke (1984) primitive equations model to describe wind fields. SCE will also use SCAQS data for input to and testing of the PLMSTAR (Godden and Lurmann, 1983) photochemical model.
- The Research Division of the Air Resources Board is sponsoring the California Institute of Technology (Dr. John Seinfeld) to develop model components for the formation and dynamics of aerosols for inclusion in the Caltech urban photochemical model. In addition, Dr. Seinfeld will use the SCAQS data to evaluate the ability to simulate ozone photochemistry of a hierarchy of models and to assess the ability of his aerosol model components to predict the size, spatial and temporal distribution, and dependence on the gas phase of the SO₂ aerosol.

- The Technical Support Division (TSD) of the Air Resources Board would like to use the SCAQS data in the development of control strategies for ozone and PM-10. Over the long-term, the data will also be useful for visibility, acid deposition, and toxic substance control strategy development as well. Specifically, given adequate resources, the TSD control strategy development tasks for O₃ and PM-10 would include the following steps.
 - Identify the characteristics of ozone and PM-10 episodes, and construct annual frequency distributions of these episodes.
 - Simulate the flow fields using wind models, and compare performance against wind measurements and tracer concentrations measured in SCAQS. Evaluate the performance of wind field models and improve them.
 - Develop a grid model with improved treatments of atmospheric chemical and physical processes, dry deposition, diffusion processes, and formation of nitrate, sulfate, and organic particles.
 - Apply the wind field and chemistry model to initial and boundary conditions acquired during SCAQS, and compare calculated values with those measured at SCAQS stations throughout the SOCAB. Evaluate the need for further model development.
 - Develop lb effectiveness factors for controls on particulate matter, NO_x, SO_x, and hydrocarbons for each source type and receptor location.
 - Use cost-of-control figures, lb effectiveness factors, and PM-10 and ozone episode frequency distributions to derive cost-effective control strategies to reduce ozone levels and PM-10 levels throughout the SOCAB.
- General Motors Research Laboratories (GMR) will apply factor analysis techniques to estimate the major source contributions to PM-10 and PM-2.5 using the aerosol chemical composition data, routine gaseous pollutant data, meteorological data, emissions inventories, and emissions characterization results. GMR will also employ empirical and theoretical modeling to relate the chemical composition of the aerosol to the SCAQS visibility measurements using the chemical composition, impactor, visibility, and meteorological data. The mutagenic activity measurements will also be used in source apportionment models to identify their origins.

In addition to these projects for which commitments have been made or for which they are being actively sought, we recommend that the MWG consider projects of the following nature which are needed to attain the modeling objectives stated in Section 1:

- Although the SCAQS observables, sampling locations, and sample durations are consistent with the qualitative judgements of the modeling community, the selection presented in Section 3 may not be the optimum combination for applying and testing models. Several example model runs applied to existing data with controlled variation in the input data might be used to test alternative measurement strategies and further optimize the SCAQS measurement program. For example, the primitive equations model (Pielke, 1984) might be applied to Project BASIN (Wakimoto and Wurtele, 1984) meteorological data to determine whether or not the upper air measurement locations and periods are adequate to represent the wind field under various conditions.
- The estimation of uncertainty in model results needs to be addressed. Methods for calculating this uncertainty are not yet commonplace and need to be incorporated into the modeling process.
- Although several models will be applied to and tested against SCAQS data, there is not yet any provision for comparing the performance of the different models among themselves. A protocol for such a comparison should be formulated, and the model applications should be designed such that a common set of performance measures is produced by each model.
- Provisions for model diagnostics should be made. Intermediate and end-product species produced at various points in the model calculations should be compared with corresponding measurements at SCAQS sites to determine how well the model components are performing. The important variables need to be defined, and a method of retrieving them needs to be incorporated into each model.

7. PROGRAM MANAGEMENT PLAN AND SCHEDULE

7.1 ORGANIZATION STRUCTURE

A final organizational structure is not definable until all study participants and sponsors are determined; however, a potential management structure is outlined here. ARB has stated its tentative support for the following:

- funding of a program manager, data manager, and quality assurance activities, with assistance for the latter from EPA;
- sponsorship of a core set of measurements;
- a comprehensive program plan derived via an open planning process; and
- free data exchange among program participants and the scientific community.

ARB is required to fund self-contained projects. It is not possible to combine ARB funds with funds from other sponsors in a common contractual arrangement. The study management structure must, therefore, accommodate projects sponsored by other agencies subject to this constraint. The structure proposed in this Section is consistent with these commitments and constraints. Proposals for alternative management structures will be considered.

The proposed program management structure is outlined in Figure 7-1. The management functions will be funded by ARB, and the Project Coordinator (PC) will report to the ARB Project Officer. In a cooperative study such as this, however, the PC cannot have direct management authority over all phases of the project. In essence, his job is to manage by consensus, since direct fiscal responsibility will remain with ARB and the other sponsors for their respective contracts.

The PC will receive guidance from a Management Advisory Group (MAG) consisting of representatives of the sponsors and technical advisors selected by the sponsors. The MAG will decide the technical direction for the study. The principal role of the MAG will be to ensure that the objectives of the study coincide with the needs of the sponsors and that the project plan is technically sound and is adequate to meet the objectives. The PC will prepare a final project plan with the advice of the MAG and will submit the plan to the MAG for comment and approval. He will make changes to the plan in consideration of comments received from the MAG. The PC will then manage the project in accordance with the project plan.

The PC will have direct authority to manage the activities of the Field, Data, and Analysis Managers and to coordinate the activities of other ARB contractors. Although the PC will not have direct authority to manage the activities of participants funded by other sources, their decision to participate in the program and to follow the program plan should give the PC enough leverage to adequately manage the project.

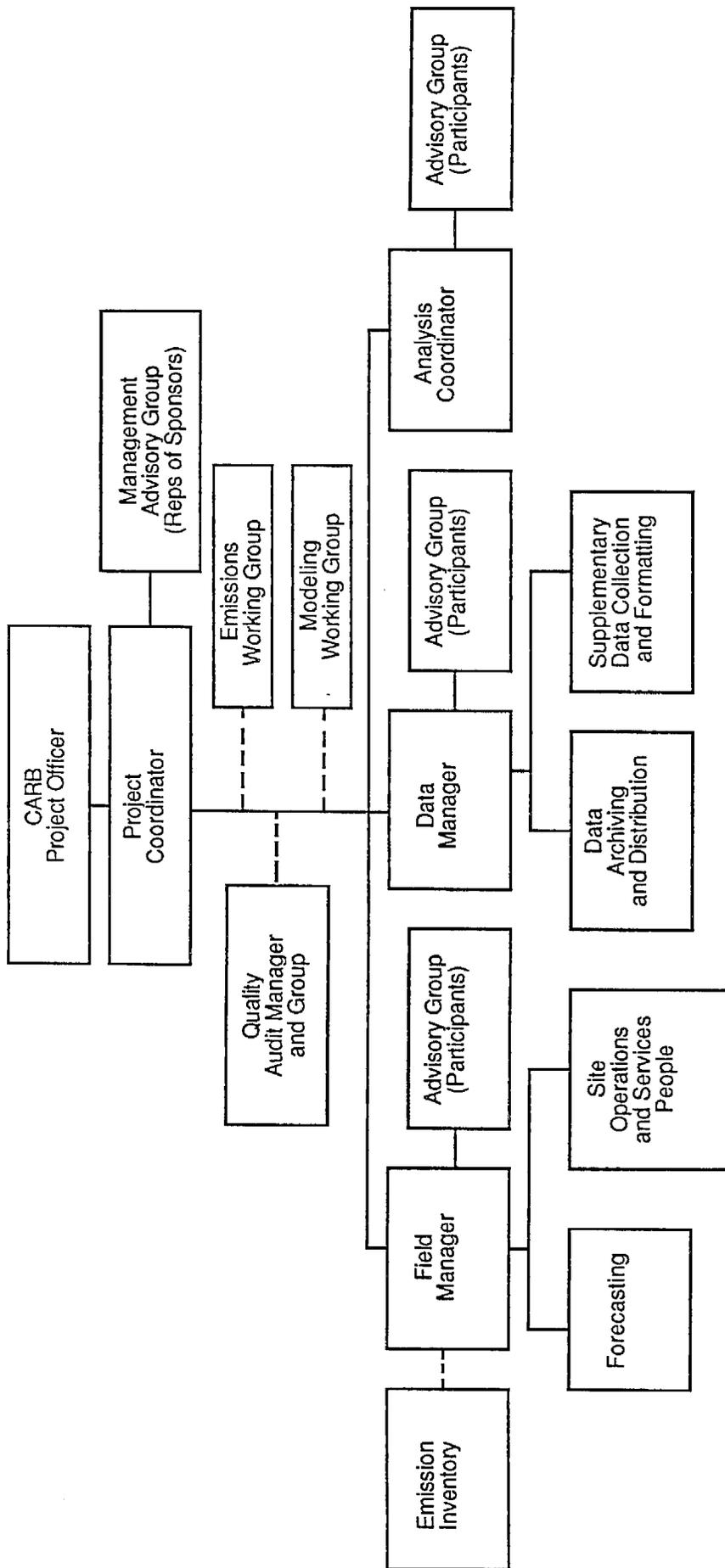


Figure 7.1. Management Functions.

The final project plan as prepared by the PC and approved by the MAG will include: a statement of the project objectives, a description of all field measurement activities, a description of the facilities and services to be provided by the Field Manager and the field measurement contractors, a data management plan including a data exchange protocol, a quality assurance plan, a data analysis plan, a management plan and schedule, and a list of milestones and reports.

During the project, the PC will be responsible for the following tasks:

- Preparation of the final project plan discussed above.
- Overall program coordination to keep the project on schedule and to resolve conflicts.
- Coordination of ARB contractor efforts.
- Coordination with the emissions contractor(s) and other complementary efforts.
- Coordination of quality assurance activities.
- Monitoring achievement of defined milestones and periodic budgetary reviews to assure that the project goals can be met with the resources available.
- Periodic revision of the project plan to take into account technical, logistical, or budgetary issues or problems which might arise.
- Preparation of short quarterly summaries of activities.
- Preparation of progress reports on a semiannual basis summarizing the progress, preliminary results, and conclusions to date of the study. This report will require technical input from all participants.
- Coordination of periodic meetings of investigators.
- Coordination of a technical session or meeting at which the final program results will be presented and coordination of the submittal of manuscripts for publication for back-to-back publication in a selected journal.
- Preparation of a final summary report which presents the results and conclusions of the study and provides a bibliography of project publications.

The roles of the Field, Data, and Analysis Managers shown in Figure 7-1 have been described in previous sections. Each of these managers will have a technical advisory group consisting of representatives of the participants. The Field Manager (FM) will prepare the measurement portion of the program plan with the input and review of his advisory group. The FM will be responsible for coordination of forecasting activities and sampling day selections and for the day-to-day interactions with the field participants. The FM will also coordinate the preparation and upkeep of the type "A" and "B" measurement sites and related facilities. The actual work, however, may be performed by another contractor.

The Data Manager (DM) will prepare the data management portion of the program plan with the input and review of the data advisory group. The DM will be responsible for the assembly, archiving, and distribution of all project data. The DM will also assemble and format data from supplementary sources.

The Analysis Coordinator (AC) will prepare the data analysis portions of the program plan, again with the input and review of the analysis advisory group. The AC will also work with the project investigators to assure that all objectives are addressed by one or more analysis efforts and to identify and eliminate redundant efforts. The AC will facilitate communications between investigators and encourage synergistic efforts.

It is possible that one person can perform more than one of the manager functions, but the roles are distinct and separate as shown on the organization chart.

Several boxes in Figure 7-1 are connected by dashed lines, indicating a consultative or coordination function. The quality audit (QA) group should be separate from the measurement groups and will report its results directly to the PC. The QA effort should be coordinated by a QA coordinator, but the actual QA work may be split among more than one contractor or sponsor. The activities of the QA group will be defined by the PC in the program plan, and their efforts will be scheduled by the PC, but their reports will be independent documents from the reports prepared by the PC. Copies of the QA reports will be provided to all participants and sponsors. It will be the responsibility of the PC to find a way to remedy any serious program deficiencies identified by the QA group.

The Model Working Group and Emissions Working Group are independent committees of participants and sponsors. Some members of both groups are planning research efforts which provide input to or make use of the SCAQS data base. Although the EWG and MWG efforts are complementary to SCAQS, their input is required for the design and operation of SCAQS. This input and interaction is accomplished directly through the Project Coordinator and as necessary through the MAG.

The emissions inventory function shown on Figure 7-1 is actually an activity which is designed and coordinated by the EWG. The inventory contractor must coordinate closely with the field manager so that he is aware of the sampling schedule and is prepared to obtain any necessary real-time emissions information on the intensive study days.

Although the management structure has been outlined above, most of the project work will be performed by contractors or participating sponsors. It is likely that the study will involve on the order of 30-50 separate contracted tasks. The division of tasks among contractors and sponsors remains to be completed. Thus, it is not possible to define the project organizational structure in more detail at this time. The tasks which should be contracted, their estimated costs, and some potential sponsors are discussed in section 8.

7.2 SCHEDULE

A preliminary schedule is outlined in Figure 7-2. We expect the dates and durations to be modified depending on climatological and fiscal considerations. The dates suggested here are to be considered only as general guidelines at this time.

7.3 REPORTS AND PRESENTATIONS

One way to keep a study on schedule and to encourage productive results is to schedule periodic reports and presentations which summarize the results and conclusions. The following reports and presentations should be prepared as part of the study.

- A Final Program Plan - to be prepared by the Project Coordinator with the help of the Field, Data, and Analysis Managers and the QA group. The field measurement portion of the plan will list the measurements to be made, the group to perform the measurements, the sponsoring agencies, the logistical requirements of the measurement groups, the services to be provided by the field manager, and a summary of the QC and QA activities. The data management portion of the plan will document the quantities and types of data to be obtained, the formats in which data should be submitted to the DM, and the formats in which data will be available from the DM. Also included will be the data exchange protocol. The analysis portion of the plan will address each objective and describe the analyses which will address the objective. The groups responsible for each analysis will also be identified. The plan will also identify technical milestones for all phases of the project and include a schedule. It is expected that the Project Coordinator will be able to expand upon the final report from the planning contract to prepare the final program plan.
- Quarterly Summary of Activities - The Project Coordinator will prepare a brief summary of the activities occurring during the quarter. In preparing the summary, the PC will review the routine monthly or quarterly progress reports of the participants and identify any instances for which the work plan or schedule are not being met.
- Six-month Progress Reports - these reports will be prepared by the Project Coordinator with input from all participants. The reports are to summarize progress to date and should include summaries of results and conclusions as they become apparent. The purpose of the progress reports is to communicate what has been learned from the project to the sponsors in an ongoing fashion. It will be expected that all participants prepare their own reports which can then be used by the Project Coordinator in the preparation of his summary report.
- Quality Audit Reports - Quality audit reports will be prepared within two months after each field program which document the QC and QA activities of the project and which describe the results of the audits and performance tests.

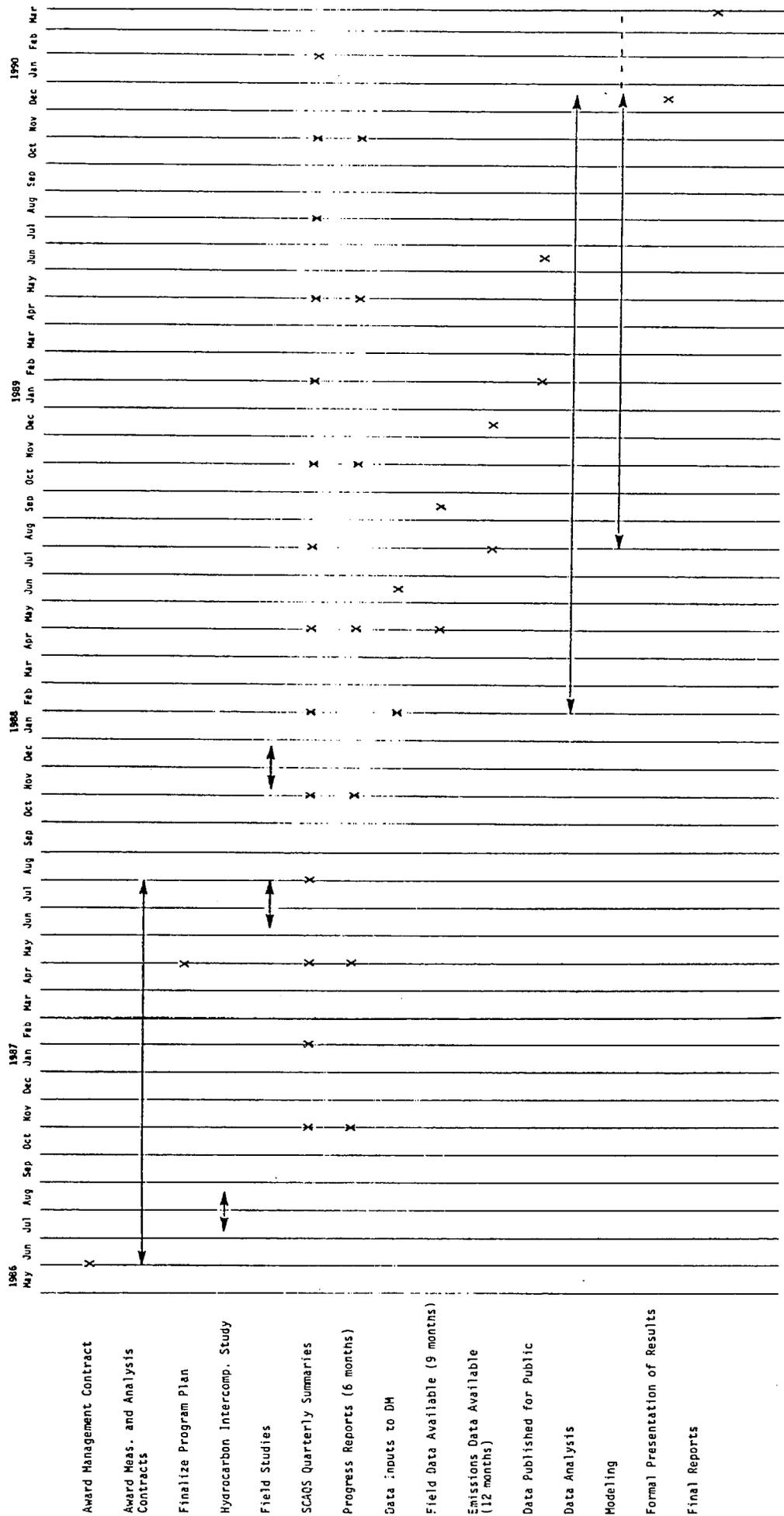


Figure 7-2. Suggested Schedule

- Data Summary Reports - reports will be prepared by the Data Manager within 9 months after each field project which inventory the data available, document the data formats, and outline the procedures for accessing the data. The reports will also document the QA procedures and assess the validity, accuracy, and potential sources of error for the various portions of the data base.
- Data Base - the Data Manager will compile all data received into an easily accessible and reproducible form and make the data available to CARB and to all participants and sponsors within 9 months after the end of each field project. This data base and the data summary report will be made available to the public approximately 18 months after completion of each field study period.
- Emissions Study Reports - within one year after each field study, the emissions contractor will report the results of his emissions inventory for the period. These reports will document the procedures used to prepare the inventory and will present graphic and tabular summaries. The report will be accompanied by a data tape which includes the gridded, time resolved emissions for the study days and by documentation of the data formats. The reports will also include the results of other analyses which are part of the emissions contract.
- Meeting Presentations - within about 18-24 months of the end of the last field study, the project coordinator will organize a session at a technical meeting for the presentation of the study results. Each study participant who is responsible for some aspect of the data analysis will be expected to present his results. The manuscripts from the session should also be submitted to a technical journal. It is expected that other presentations will be made at earlier times as results become available.
- Final Reports - each participant should prepare a final report which documents his work and summarizes his results and conclusions. The Project Coordinator will prepare a final report which describes all phases of the project and summarizes the results and conclusions. The project report will include a bibliography of all articles, reports, and presentations resulting from the study.

8. REQUIRED CONTRACTS, COST ESTIMATES, AND CANDIDATE SPONSORS

Rough costs have been estimated in 1985 dollars for the major elements of the study. Their purpose is to provide a general idea of the overall scope of the project and to allow potential sponsors an opportunity to select their most effective areas for participation. These estimates have been summarized by task, where each task represents a potential contract element. These tasks are listed in Table 8-1 along with their estimated costs. Suggested time periods by which contracts should be initiated are also listed, and potential sponsors are shown for those tasks for which a sponsor has expressed interest. Tasks which we suggest be grouped together into single contracts are grouped together in the table. If no contract start time is shown, the task is to be performed by the sponsor.

Appearance of a candidate sponsor on Table 8-1 in no way implies a commitment by the sponsor. Listing of only one sponsor for an element does not imply that that sponsor is interested in funding the whole task. Absence of a particular sponsor for an element does not necessarily imply a lack of interest. This listing is preliminary and will be subject to revision.

Estimates for the "B" site equipment and analytical costs are included in Table 8-2, and estimates for the "A" site research efforts are indicated in Table 8-3. Tables 8-2 and 8-3 were used to prepare many of the estimates in Table 8-1. Additional explanations of the Table 8-1 estimates are included in Appendix C.

Costs shown in Table 8-2 for acquisition of equipment for "borrowed" instruments are estimated costs for factory refurbishment and calibration. Costs for instruments to be "built" or purchased are rough costs per item. Estimated costs for sample analysis per site day are also indicated for grab samples. The total analysis costs shown are for all sites and all sampling days. We have assumed 12 days at 9 sites in the summer and 7 days at 5 sites in the winter for all parameters except size resolved chemistry which is estimated for 5 sites both summer and winter.

The cost estimates in Table 8-3 for chemical analyses of routine samples cover the additional sample handling and analytical costs only. The other estimates are for research contracts for which an investigator will design the experiment, perform the measurements, process the data, and provide some data interpretation. Some of the measurements for which costs are estimated will actually be performed by one of the sponsors and will not really be contracted.

An additional summary of costs by site and by major category is provided in Table 8-4. This table summarizes the information presented in Table 8-1 in a briefer form and allows comparisons of the cost estimates with previous versions of this plan.

Table 8-1. Estimated Task Costs (1985 \$) and Candidate Sponsors

<u>Tasks</u>	<u>Start Date</u>	<u>Costs</u> <u>(\$000)</u>	<u>Candidate Sponsors*</u>
<u>Management</u>			
Project Coordinator	Jun 86	154	ARB
Field Manager	Jun 86	125	ARB
Analysis Manager	Apr 87	66	ARB
	Subtotal:	345	
Q.A. Manager	Oct 86	77	ARB
Data Manager	Jan 87	175	ARB
<u>Special Equipment Acquisition and Preparation</u>			
Build H ₂ O ₂ systems	Jan 87	90	ARB
Build impactor systems	Jul 86	140	CRC, ARB
Build/test aerosol/filter sampling systems	Oct 86	234	ARB
Design, acquire parts for, and construct aerosol phys. prop. meas. and data acq. systems	Jul 86	225	ARB
<u>Site Installation and Routine Operations</u>			
Acquire/install add'l. "C" equip.	Jan 87	50	ARB
Acquire remaining "B" site equip.	Jan 87	32	ARB
Prepare "A" sites	Oct 86	200	ARB, GM
Prepare "B" sites	Jul 86	180	ARB, SCAQMD
"B" site staff training & equip. Testing	Jan 87	80	
Operate "B" sites, includ. sample handling/shipping & processing continuous data	Apr 87	244	ARB
Operate "A" sites	Apr 87	35	ARB, GM
	Subtotal:	821	
<u>Routine Sample Chemical Analyses</u>			
"B" site SO ₂ , NH ₃ , HNO ₃ gas; and aerosol organic, inorganic ion, & mass measurements, including impactor chemistry	Apr 87	467	ARB, CRC, GM
Carbonyl analyses, "A" & "B" sites	Jan 87	58	
Hydrocarbons, C ₁ -C ₁₀ , "A" & "B" sites	Jan 87	111	ARB
XRF analyses, "B" sites	-----	72	EPA
PAN analyses, "B" sites	Oct 87	29	

*See text for explanation

Table 8-1. Cont.

<u>Tasks</u>	<u>Start Date</u>	<u>Costs (\$000)</u>	<u>Candidate Sponsors</u>
<u>"A" Site Specialized Measurements</u>			
Hydrocarbons, C ₁₀ -C _n ,	Jan 87	35	SCE, CRC
Formic, acetic acid	Jan 87	20	SCE
Total acid species, gas and aerosol	Jan 87	100	ARB
HCl measurement	Jan 87	30	
HONO, HCHO, NO ₂ , NO ₃ - DOAS	Jan 87	150	ARB
Continuous HNO ₃	Oct 86	100	CRC
HO, HO ₂ , RO ₂ radicals: by FAGE	Oct 86	150	CRC
Continuous organic aerosol	Oct 86	100	
Carbon 14 measurements	Jan 87	20	CRC
Organic aerosol volatility	Oct 86	70	
Neutron activation analyses	Jul 87	85	EPA
Aerosol water analysis	Oct 86	100	EPRI
Aerosol size vs. RH	Jan 87	100	CRC
Light absorption - spectrophone	-----	160	Ford
Light absorption - filter	Jan 87	10	
Light extinction	Jan 87	50	EPA, CRC
Heated nephelometer meas.	-----	35	EPA, GM
Mutagen measurements	Oct 86	50	ARB, GM
Individual particle measurements	Oct 86	30	EPA
<u>Quality Audit Activities</u>			
All activities except QA Manager	Jan 87	423	ARB, EPA, ---

Table 8-1. Cont.

<u>Tasks</u>	<u>Start Date</u>	<u>Costs (\$000)</u>	<u>Candidate Sponsors</u>
<u>Additional Studies</u>			
Meteorology	Oct 86	350	ARB, SCE
Aircraft air qual. measurements	Jan 87	420	
Airborne lidar measurements	Apr 87	150	EPA
Tracer studies	Jan 87	500	SCE, ARB
Representativeness studies	Jan 87	150	
Dry deposition studies	Oct.86	200	ARB
Ann. ave. PM-10 monitoring	Oct 88	108	
<u>Data Interpretation</u>			
Approx. 20 analysis projects averaging \$25,000-\$75,000	Jul 87	1000	ARB, GM, SCE
<u>Model Working Group</u>			
Sensitivity studies	Jul 86	100	CRC
<u>Emissions Working Group</u>			
Emissions inventory	Jan 87	300	WOGA, MVMA, EPRI, ARB, CRC
Tunnel studies of auto emissions	Dec 87	200	CRC
	<u>Total**</u>	<u>\$8.140</u>	

**This estimate does not include carbon intercomparison studies or all of the emissions characterization measurements.

Table 8-2. Estimated Costs of "B" Site Measurements (1985 \$)

Observables	Analytical Method	Equip. Status	Equip. Cost/Site	Total Equip. Cost	Analysis Cost*** (site-day)	Total Analysis Cost	Total Measure. Cost
METEOROLOGY - AQMD							
Wind speed		avail.	--	--	--	--	--
Wind direction		avail.	--	--	--	--	--
Temperature		avail.	--	--	--	--	--
Dew point	sling psych.	purch.	250	2250	--	--	2250
UV Radiation	Radiometer	purch.	1800	16200	--	--	16200
			Subtotal:	18450			18450
GASES-AQMD							
O ₃	UV absorption	avail.	--	--	--	--	--
NO	Chemiluminescence	avail.	--	--	--	--	--
NO _x	"	avail.	--	--	--	--	--
SO ₂	Pulsed fluorescence	avail.	--	--	--	--	--
CO	NDIR	avail.	--	--	--	--	--
GASES-SCAQCS							
SO ₂	Impreg. filter	purch./build*	500	4500	150	21450	25950
NH ₃	Denuder tube	purch./build*	500	4500	150	21450	25950
HNO ₃	DDM	purch./build*	500	4500	300	42900	47400
Carbonyls	DNPH filter	purch./build*	500	4500	300	42900	47400
C ₁ -C ₁₀ HC	Cans-GC	purch.	500	4500	600	85800	90300
PAN	EC GC	rent	--	--	200	28600	28600
H ₂ O ₂	POHPAA-enzyme	purch.	10000	90000	--	--	90000
			Subtotal:	112500		243100	355600
AEROSOL PHYSICAL PROPERTY							
Size dist.	OPC	purch.	14000	126000	--	--	126000
Size dist.	EAA	borrow	2000	18000	--	--	18000
Light scat.	Nephelometer	borrow	1000	9000	--	--	9000
Data acquis.	PC	purch.	3500	31500	--	--	31500
			Subtotal:	184500			184500
AEROSOL CHEMISTRY							
Total/Fine:							
mass	size sel. samplers	build*	8000	72000	90	12870	84870
inorganics	"	"	--	--	600	85800	85800
XRF	"	build*	8000	72000	500	71500	143500
H ⁺ (fine only)	"	"	--	--	200	28600	28600
Or. & El. C	size sel. samplers	build*	8000	72000	500	71500	143500
PM-10 (AQMD):							
mass, NO ₃ ⁻	SSI-HiVol	borrow	1000	9000	--	--	9000
SO ₄ ⁼							
TSP (AQMD):							
mass, NO ₃ ⁻	HiVol.	avail.	--	--	--	--	--
SO ₄ ⁼ , Pb							
			Subtotal:	225000		270270	495270
SIZE RESOLVED CHEMISTRY**							
SO ₄ ⁼ , NH ₄ ⁺ , (NO ₃ ⁻)	2 UDI	purch.	14000	70000	960	91200	161200
Or. & El. C	2 UDI	purch.	14000	70000	960	91200	161200
			Subtotal:	140000		182400	322400
			Totals:	\$680,450		\$645770	\$1376220

* Could all be included in same sampler with manifold system.

** Only at 5 sites.

*** Assume 143 site days for all samples except Size Resolved Chemistry for which 95 site days were costed.

Table 8-3. Estimated Costs of "A" Site Measurements

Measurement	Dur- ation	# per site- day	# of sites	Method	Approximate total cost (\$000)
Organic gases					
C ₁ -C ₁₀ HC	1 hr	3 more	2	Cannister & GC	25*
C ₁ -C ₆ Car- bonyls	1 hr	3 more	2	DNPH filter	15*
C ₁₀ -C _n HC	4 hr	4	2	Porous plug & chrom.	35
Formic, acetic acid	4 hr	6	2	Impreg. filter, IC	20
Inorganic gases					
HONO, HCHO, NO ₂	cont.	24	1	DOAS (one site)	150
Total acidity **			2		40
HNO ₃	cont.	24	1	TDLAS	100
HCl	4 hr	6	2	Denuder ?	30
Radicals					
NO ₃	cont.	10	1	DOAS (see above)	--
HO, HO ₂ , RO ₂	cont.	24	1	FAGE;	150
Organic aerosol					
Continuous EC, TOC	cycle	24	2	Filter & vol anal.	100
Volatil. vs temp	4 hr	6	2	Filter & vol anal.	70
Carbon 14	24 hr	1	2	Accelerator mass spec.	20
Inorganic aerosol					
Neutron act. (INA)	add. anal. of filters from B sites				85*
Water	? 24	24	1	DMA; microwave	100
Acid species *			2		60
Mutagens			1 or 2		50
Individual particles			2		30
Aerosol Phys. Prop.					
Light absorption	Cont.	24	1	Spectrophone;	160
	4 hr	6	2	Filter	10
Light extinction	Cont.	24	2	Radiance diff.	50
Volatility	Cycle	24	2	Heated nephel.	35
Size vs. RH			1	Diff mob anal.	100
TOTAL					1,435

* Estimate for sample handling and analytical costs only

** Organic and inorganic

Table 8-4. Cost Estimates, Short Summary

<u>Program Element</u>	<u>Cost Estimate</u>
Program Management/Data Management/Analysis Coord.	\$ 520,000
Type "C" Sites - addition of PM-10, PM-2.5 to 5 selected sites	50,000
Type "B" Sites -	
Gas and Meteorological Measurements	375,000
Aerosol Physical Property Meas.	185,000
Aerosol Chemistry/Mass Meas.	818,000
Site Prep. and Personnel Training	300,000
Site Operation (2 people/site plus expenses)	244,000
Type "A" Sites -	
Organic Gases	95,000
Inorganic Gases	320,000
Radicals	150,000
Organic Aerosol including mutagens	240,000
Inorganic Aerosol	245,000
Aerosol Physical Properties	355,000
Individual Particles	30,000
Site Preparation (power, platforms, etc.)	200,000
Site Operation (1 person/site plus expenses)	35,000
Meteorological Measurements	350,000
Aircraft Measurements	420,000
Airborne Lidar	150,000
Emissions Inventory and Analysis	300,000
QA Functions	500,000
Tracer Studies	500,000
Representativeness Studies	150,000
Dry Deposition Studies	200,000
Annual Average PM-10 Monitoring	108,000
Data Interpretation to meet Specific Objectives	1,000,000
Model Sensitivity Studies	100,000
Auto Emission Tunnel Studies	200,000
TOTAL	\$8,140,000*

* This estimate does not include nitrogen or carbon methods comparison studies or emissions characterization measurements.

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Glen Cass	Caltech	Andy Ranzieri	ARB
Tai Chang	Ford	Christian Seigneur	Bechtel
Anton Chaplin	UnoCal(WOGA)	Kenneth Schere	EPA
Alan Dunker	GM	Tom Tesche	Radian
Chung Liu	SCAQMD	Gary Whitten	SAI

Other members to be determined - member from WOGA will probably be included.

APPENDIX B
SUMMARY OF AIR QUALITY STUDIES

Summary of Selected Past South Coast Air Basin Studies

<u>Study Objectives</u>	<u>Sampling Site/Location/Period</u>	<u>Observables</u>	<u>Model Used</u>	<u>Major Findings</u>
<p>Reference: Miller et al. (1972), Topic: Aerosol</p> <p>To apply the chemical mass balance model to estimate source contributions to atmospheric aerosol</p>	<p>Pasadena, CA Sept. 1969</p>	<p>11-hr TSP mass Ions (NH₄⁺, SO₄⁼, NO₃⁻)</p> <p>Carbon Elements Source sampling for soil, fuel oil, fly ash</p>	<p>Tracer solution to the chemical mass balance</p>	<p>Tracer species can be used to estimate source contributions to ambient elemental concentrations</p> <p>Major source contributions in Pasadena: Carbon (17%) Soil (9.8%) Automobile (8.2%) Sea Salt (2.5%) Fuel-Oil Combustion (0.25%)</p> <p>57% of TSP mass was unexplained</p>
<p>Reference: Friedlander (1973), Topic: Aerosol</p> <p>To state the fundamental principals of the chemical mass balance model</p> <p>To apply a carbon balance to estimate secondary conversion of organic vapors</p>	<p>Pasadena, CA Sept. 1969</p>	<p>11-hr TSP mass Carbon and carbon components Elements Source Sampling for soil</p>	<p>Least squares solution to the chemical mass balance</p>	<p>Secondary aerosol (40%) was the major contributor. Other significant contributions were 25% from primary manmade and 15% from primary natural sources</p> <p>Particle size distribution is important since the chemical composition is an average over the size spectrum</p> <p>Limitations of CMB involve chemical/physical processes, particle fractionation and variability in time and space</p>

Summary of Selected Past South Coast Air Basin Studies (cont'd)

<u>Study Objectives</u>	<u>Sampling Site/Location/Period</u>	<u>Observables</u>	<u>Model Used</u>	<u>Major Findings</u>
Reference: Hidy et al. (1975), Topics: Aerosol, Visibility				
To characterize the chemical & physical properties of urban and non-urban aerosols	12 sites for mobile labs-Berkeley, Richmond SFOAF, Fresno, Hunter-Liggett Military Reservation, Freeway Loop, Pomona, Goldstone, Pt. Arguello, W. Covina, Robidoux (Riverside), and Domingue Hills	Aerosols Total aerosol number concentrations Aerosol size distribution Size and chemically classified particles	Descriptive graphical & statistical methods Several models applied to data by other researchers	Found simplified approaches for the study of atmospheric particles Showed urban and rural aerosol mass is probably distributed bimodally in small ($dp < 3 \mu m$) and large ($3 \mu m < dp < 20 \mu m$) plus giant ($dp > 20 \mu m$) particles
To attribute ambient concentrations to primary & secondary pollutant sources		Light scattering Liquid water content		Discovered that the two mass modes have independent sources and interact minimally in the atmosphere
To identify major causes of production & visibility reduction		Particulate fallout mass and organics Gases (SO_2 , H_2S , NO , NO_2 , NH_3 , Total HC, HC, CH_4 , C_2H_4 , C_2H_2 , CO and O_3) Meteorology (WS, WD, T°, RH, radiation and rainfall)		Found that particles formed by chemical reactions in the atmosphere add to the small particle size mode Pioneered the application of receptor models
To estimate the extent of ambient air quality standards that can be achieved by existing technologies	July to Nov. 1972 July to Oct. 1973			
To evaluate the applicability of aerosol instrumentation in the study for use in monitoring networks				
To elucidate the photochemistry of aerosol formation				

Summary of Selected Past South Coast Air Basin Studies (cont'd)

<u>Study Objectives</u>	<u>Sampling Site/Location/Period</u>	<u>Observables</u>	<u>Model Used</u>	<u>Major Findings</u>
<p>Reference: White et al. (1978), Topic: Sulfate</p> <p>To examine the relationships between daily power plant SO₂ emissions and ambient sulfate concentrations in Los Angeles Basin</p>	<p>Azusa, Downtown LA, LAX, Long Beach Airport W. Covina</p> <p>May - Oct., 1975</p>	<p>Ions (24-hr SO₄²⁻)</p> <p>Gaseous (1-hr O₃)</p> <p>Meteorological parameters (RH, T850, TLA)</p> <p>Daily SO₂ emissions from power plants</p>	<p>Linear roll-back model</p>	<p>Lack of correlation between power plant SO₂ emissions and ambient SO₂ levels was found</p> <p>Power plant emissions on an average day account for 17% of the average sulfate concentrations at W. Covina (a high sulfate site)</p> <p>Factors other than sulfur emissions affect sulfate production in SOCAB</p>

10/10/75
 10/10/75
 10/10/75

Summary of Selected Past South Coast Air Basin Studies (cont'd)

<u>Study Objectives</u>	<u>Sampling Site/Location/Period</u>	<u>Observables</u>	<u>Model Used</u>	<u>Major Findings</u>
<p>Reference: Henry and Hidy (1979), Topic: Sulfate</p> <p>To empirically identify the underlying chemical and physical process for sulfate production</p> <p>To apply a principal components model which is unaffected by intercorrelations of the variables</p>	<p>Southern California sites: Anaheim, Garden Grove, Glendora, Santa Monica, Thousand Oaks, Vista, W. Covina, CA</p> <p>Jan. 1974 to Jan. 1975</p>	<p>24-hr TSP mass</p> <p>Gases (SO₂, NO_x, O₃, NMHC, total HC)</p> <p>Meteorological variables (RH, temp, WS, WD, inversion, ventilation)</p>	<p>Regression on principal components</p>	<p>Photochemical processes, SO₂ sources and atmospheric dispersion and transport are the three major causes of southern California sulfate levels</p> <p>Photochemical activity variance of (17-32%) and atmospheric moisture content variance of (9-15%) account for more than half of the sulfate variability</p>

Summary of Selected Past South Coast Air Basin Studies (cont'd)

<u>Study Objectives</u>	<u>Site/Location/Period</u>	<u>Observables</u>	<u>Model Used</u>	<u>Major Findings</u>
Reference: Tombach (1982), Topic: Hydrocarbon Sources				
<u>Receptor Model</u>	(I)	3 times/day ambient samples	Ordinary weighted least squares chemical mass balance	Receptor modeling can be used for VOC source attribution studies with good understanding of experimental method and chemical process
To apply the chemical mass balance model to volatile organic compounds (VOC)	Los Angeles Air Basin	Nonmethane hydrocarbon compounds		Relative changes in concentration between inert and reactive VOC species from the same source-type can identify sources
To determine the major contributions of ambient VOC levels in the South Coast Air Basin		Source samples included: auto exhaust gasoline, gasoline vapor, natural gas, liquified petroleum gases		The VOC source contributions varied with time of day
<u>Tracer Release</u>	(II)	Tracer release of SF ₆ gas	Dispersion Model (AQUVAL, Lissaman, 1973; Huang & Head 1978)	Auto exhaust (53%), natural gas (19%), gasoline (12%) and gasoline vapor (10%) were the major contributors of hydrocarbons to receptors
To quantify the total VOC emissions from various operations in a refinery	16 Sites at down-town and upwind			Process areas and emulsion plant (58%) and floating roof storage tanks (38%) were the major contributing operations in the refinery to the ambient NMHC levels

Summary of Selected Past South Coast Air Basin Studies (cont'd)

<u>Study Objectives</u>	<u>Site/Location/Period</u>	<u>Sampling</u>	<u>Observables</u>	<u>Model Used</u>	<u>Major Findings</u>
Reference: Cass and McRae (1983), Topic: Aerosol					
To develop better source apportionment techniques	5 SCAQMD sites: Azusa, Lynwood, Pasadena, Reseda, W. Los Angeles	24-hr TSP mass ions (SO ₄ ⁻ , NO ₃ ⁻ , NH ₄ ⁺)	24-hr TSP mass ions (SO ₄ ⁻ , NO ₃ ⁻ , NH ₄ ⁺)	Emission Inventory for fine particle trace metals can be constructed by superimposing size and chemical source compositions (resulted from source test) onto conventional TSP inventory	Emissions Inventory for fine particle trace metals can be constructed by superimposing size and chemical source compositions (resulted from source test) onto conventional TSP inventory
To assess the effects of different model structures on estimated source contributions	5 NASN sites: Anaheim, Lennox, Los Angeles, Pasadena, San Bernardino	Elements	Ordinary weighted least squares solution to the chemical mass balance receptor model	Identifying key tracer elements of emission sources is important and can be used as input to CMB Model, thereby compensating for the deficiency in HIVOL data	Identifying key tracer elements of emission sources is important and can be used as input to CMB Model, thereby compensating for the deficiency in HIVOL data
	1976 to 1977		Multiple linear regression	Consistent results were yielded by model/model comparisons	Consistent results were yielded by model/model comparisons

Summary of Selected Past South Coast Air Basin Studies (cont'd)

<u>Study Objectives</u>	<u>Site/Location/Period</u>	<u>Observables</u>	<u>Model Used</u>	<u>Major Findings</u>
Reference: Spicer et al. (1983), Topic: Photochemical Measurements	Sampling Los Angeles Air Basin	(0900 to 1700 PST)	Graphical and statistical descriptions	Average daytime distribution of NO _x at 3 sites was:
To determine the spatial and temporal distribution of oxidized nitrogen species in the Los Angeles Air Basin	3-ground sampling sites: Rubidoux, Upland, Temple City	Ions (NO ₃ ⁻ , SO ₄ ⁼ , NH ₄ ⁺)		Temple City Upland Rubidoux
To determine the extent to which measured NO _x products can account for NO _x removal from the air (i.e., nitrogen mass balance)	Oct. to Nov., 1976	Gases (SO ₂ , O ₃ , NO, NO _x , PAN, total nitrogen, NHHC, CO, CH ₄ , C ₂ H ₂ , C ₂ H ₄ , Freon-11)		NO 19% 10% -- NO ₂ 78% 66% 78% PAN 3% 22% 10% HONO-2 -- -- -- NO ₃ 1% 1% 12%
To investigate differences in the transformation processes for NO _x relative to SO _x	42 aircraft flights over 22 days	Temperature		* 11 Photochemically active days
To estimate the rate of NO _x transformation under photochemically reactive conditions				Particulate NO ₃ ⁻ exhibits a strong east-west gradient which is in contrast to SO ₄ ⁼ (relatively uniform) in the Los Angeles Air Basin
To investigate the transport of O ₃ and precursors from urban areas				70-85% of the total nitrogen can be accounted for as NO ₃ ⁻ and NH ₄ ⁺ Most of the urban NO ₃ ⁻ is present in the gas phases. Gaseous NO ₃ ⁻ /Total NO ₃ ⁻ ratio is 0.75, 0.96 and 0.45 for Temple City, Upland and Rubidoux, respectively
				NO _x transformation rate of 0.02-0.03 h ⁻¹ and removal rate of 0.16 h ⁻¹ are calculated in the study

Summary of Selected Past South Coast Air Basin Studies (cont'd)

<u>Study Objectives</u>	<u>Sampling Site/Period</u>	<u>Observables</u>	<u>Model Used</u>	<u>Major Findings</u>
Reference: Pratsinis et al. (1984), Topics: Carbon Measurements, Visibility Reduction	Duarte and Lennox July, 1980 to May, 1981	8-hr Particulate Mass HIVOL with cascade impactor (dp < 15 μm, 3.5 μm, and dp < 7.2 μm, and dp < 3.5 μm)	Thermal analysis Emission Inventory scaling Regression analysis	Major source contributions to the carbon containing component of the fine aerosol Automobile 68% Lennox 26% Duarte 12% Industrial Sources 26%
To estimate primary and secondary carbon contributions at receptors		Dichotomous sampler (3.5 μm < dp < 15 μm and dp < 3.5 μm)		A high correlation (R=0.72) was found between ozone and secondary carbon, and low correlation (R=0.65) was found between sulfate and secondary carbon
To calculate a visibility extinction budget for Los Angeles		Elements (PIXE) Ions (NH ₄ ⁺ , SO ₄ ⁼ , NO ₃ ⁻ , Cl ⁻)		The carbon containing component was responsible for 27 and 44% of the incident light extinction at Lennox and Duarte, respectively

APPENDIX C

COST ESTIMATE DETAILS

The sources or assumptions of the cost estimates from Table 8-1 are discussed in this appendix. Costs shown below were estimated in 1985 dollars and are likely to increase through inflation by the time of the 1987 measurements.

Management

Project Coordinator:

Preparation - Senior Scientist	3 mos. @ \$10,000/mo	\$ 30,000
Support	1 mo. @ \$5,000/mo	5,000
Travel, etc.		3,000
		<u>\$ 38,000</u>
Field Phase - Senior Scientist	4 mos.	\$ 40,000
Support	1 mo.	5,000
Expenses		3,000
		<u>\$ 48,000</u>
Analysis/Reports - Sr. Scientist	6 mos.	\$ 60,000
Support	1 mo.	5,000
Expenses		3,000
		<u>\$ 68,000</u>
	TOTAL	<u>\$154,000</u>

Field Manager:

Preparation - Senior Scientist	4 mos.	\$ 40,000
Support	2 mos.	10,000
Expenses		5,000
		<u>\$ 55,000</u>
Field/Report - Senior Scientist	5 mos.	\$ 50,000
Support	2 mos.	10,000
Expenses		10,000
		<u>\$ 70,000</u>
	TOTAL	<u>\$125,000</u>

Analysis Manager:

Preparation - Senior Scientist	1 mo.	\$ 10,000
Analysis/Report - Sr. Scientist	5 mos.	\$ 50,000
Support	1 mo.	5,000
Expenses		1,000
		<u>\$ 56,000</u>
	TOTAL	<u>\$ 66,000</u>

QA Manager:

Preparation - Senior Scientist	2 mos.	\$ 20,000
Support	1/2 mo.	2,500
Expenses		<u>2,500</u>
		\$ 25,000
Field - Senior Scientist	3 mos.	\$ 30,000
Support	1/2 mo.	2,500
Expenses		<u>5,000</u>
		\$ 37,500
Reports - Senior Scientist	1 mo.	\$ 10,000
Support	1/2 mo.	2,500
Expenses		<u>1,500</u>
		\$ 14,000
	TOTAL	<u>\$ 76,500</u>

Data Manager:

Preparation - Senior Person	2 mos.	\$ 20,000
Support	2 mos.	10,000
Expenses		<u>5,000</u>
		\$ 35,000
Data Collection and Archiving - Sr. Person	4 mo.	\$ 40,000
Support	10 mos.	50,000
Expenses		<u>5,000</u>
		\$ 95,000
Data Distribution and Reports - Sr. Person	2 mos.	\$ 20,000
Support	4 mos.	20,000
Expenses		<u>5,000</u>
		\$ 45,000
	TOTAL	<u>\$175,000</u>

Special Equipment Acquisition and Preparation

Build H ₂ O ₂ Systems - 9 stations @ \$10,000 each (Table 8-2)	<u>\$ 90,000</u>
Build UDI Systems - 5 stations, 4 impactors each, \$7000/impactor (per U. of Minn, Table 8-2)	<u>\$140,000</u>
Build Aerosol/Filter Systems - 9 sites each for: SO ₂ @ \$500, NH ₃ @ \$500, HNO ₃ @ \$500, Carbonyls @ \$500, Inorganics @ \$8000, XRF @ \$8000, and Organics @ \$8000. Total of \$26,000 per site (Table 8-2). Systems must include two manifolds, or two samplers for each measurement to avoid downtime while changing substrates.	<u>\$234,000</u>

Design/Construct Aerosol Phys. Prop. Meas. and Data Acquisition Systems:

Includes design of hardware/software system, preparation and testing of data acquisition software, preparation and testing of hardware, data acquisition systems will also record data from other continuous instruments.

- Aerosol phys. prop. parts (from Table 8-2)	\$185,000
- Labor to set up and test all systems	<u>40,000</u>
TOTAL	<u>\$225,000</u>

Site Installation and Routine Operations

"C" Site Installations - rough estimate \$ 50,000

Remaining "B" Site equip. acquisition -

9 sites each for dewpoint @ \$250; UV radiation @ \$1800, PM-10 @ \$1000 avg., C₁-C₁₀ H/C @ \$500 (per Table 8-2). Total of \$3550 per site. \$ 32,000

Prepare "A" Sites -

Senior Personnel	3 mos.	\$ 30,000
Support Personnel	6 mos.	30,000
Power distribution @ \$40,000/site		80,000
Platforms, facilities, other misc. expenses \$30,000/site		<u>60,000</u>
TOTAL		<u>\$200,000</u>

Prepare "B" Sites - assume \$20,000/site for 9 sites \$180,000

"B" Site Staff Training -

18 Field Staff x 2 wks @ \$25/hr.	\$ 36,000
2 Sr. Engineers x 2 wks @ \$50/hr.	8,000
Assume \$4,000/site prelim. chem. analyses for test purposes	<u>\$ 36,000</u>
TOTAL	<u>\$ 80,000</u>

Operate "B" Sites

18 Field Staff x 40/hrs wk x 7 wks @ \$25/hr. (for summer study)	\$126,000
10 people x 40 hrs/wk x 5 wks @ 25/hr. (for winter study)	50,000

Management Support - 12 wks @ \$2000/wk.	24,000
Repair Support - 10 wks @ \$1500/wk.	15,000
Expenses @ \$200/meas. day/site x 12 days x 9 sites, plus 7 days x 5 sites	<u>28,000</u>

TOTAL	<u>\$244,000</u>
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Operate "A" Sites

Assumes "A" sites are collocated with "B" sites 1 person/site x 40 hrs/wk x (2 sites x 7 wks + 1 site x 5 wks) @ \$25/hr.	\$ 19,000
Expenses \$500/meas. site day x (2 sites x 12 + 1 site x 7)	<u>15,500</u>

TOTAL	<u>\$ 34,500</u>
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Routine Sample Chemical Analyses

"B" Site SO₂, HNO₃, etc. -

SO ₂ @ \$21,450;	NH ₃ @ \$21,450;	
HNO ₃ @ \$42,900;	Aerosol organics @ \$71,500;	
Aerosol inorganic ions @ \$85,800;	Aerosol H ⁺ @ \$28,600;	
Aerosol mass @ \$12,870; and		
UDI chem. @ \$182,400 (from Table 8-2)	TOTAL	<u>\$466,970</u>

Carbonyl Analyses - "A" and "B" Sites -

"A" Sites from Table 8-3	\$ 15,000
"B" Sites from Table 8-2	42,900
TOTAL	<u>\$ 57,900</u>

Hydrocarbons, C₁-C₁₀ - "A" and "B" Sites -

"A" Sites from Table 8-3	\$ 25,000
"B" Sites from Table 8-2	85,800
TOTAL	<u>\$110,800</u>

XRF Analyses - from Table 8-2	<u>\$ 71,500</u>
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PAN Analyses - from Table 8-2	<u>\$ 28,600</u>
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"A" Site Specialized Measurements

All numbers from Table 8-3.

Annual Average PM-10 Monitoring

9 sites x 60 days x 2 samples (coarse and fine) =
1080 samples. Assume \$45/sample for carbon, \$45/sample
for XRF, \$10/sample for mass; 1080 samples @ \$100/sample

TOTAL \$108,000

Data Interpretation

Assumed at \$1,000,000; approximately \$25,000-\$75,000 per task.

Model Working Group

Sensitivity Studies

CRC budget of \$100,000 assumed for these activities.

Emissions Working Group

Emissions Inventory:

Assumed at \$300,000 after discussions with experienced
inventory contractors

Auto Emissions - Tunnel Studies

CRC budget of \$200,000 assumed for SCAQS related tunnel studies.

CARB LIBRARY



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