DEVELOPMENT OF A COMPREHENSIVE AIR POLLUTION PHOTOCHEMICAL MODELING SYSTEM FOR THE SAN FRANCISCO, CALIFORNIA REGIONAL AREA

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ABSTRACT
The goal of the project is to provide a complete photochemical modeling and analysis system for use in the development of pollution planning for ground level ozone, with future capabilities for similar support for $PM_{2.5}$ management. ENVIRON International Corporation (ENVIRON) is working with the San Francisco Bay Area Air Quality Management District (Air District) in the effort. The major components of this project are: a modeling protocol, acceptable meteorological and photochemical model simulations of three ozone episodes, performance evaluations of these simulations, acceptable estimate of future year emissions inventories, ozone simulations for future years, analysis of the sensitivity of the future year modeled ozone to changes in emissions of the oxides of nitrogen and hydrocarbons in the form of an O3 (NOx, HC) sensitivity diagram for selected sites, and a demonstration of the collective effect of alternative emissions controls upon future ambient ozone levels.

This modeling system consists of a computing system, an emissions model, a prognostic meteorological model and a grid-based photochemical model used in the work described above, including appropriate interconnections and analysis tools.

Specific project tasks include: (1) Develop Modeling Protocol; (2) Acquire Computer System; (3) Simulate Meteorological Conditions; (4) Produce Emission Inputs for Years 2000 and Future Years; (5) Simulate Ozone and Evaluate Photochemical Model Performance; (6) Simulate Future Ozone and Examine its Sensitivity to Emissions; (7) Simulate Year Future Emissions Control Strategies; and (8) Technology Transfer of the Computer and Modeling System.

INTRODUCTION

For the last thirty years the forward thinking air quality professionals of the San Francisco Bay Area have initiated sound planning principles in order to chart the best course to attain the ground level ozone air quality standards. A critical component for the attainment of the health based ambient air quality standards is the determination of the effectiveness of the emission control strategies. In order to achieve this goal the air quality agency, the Air District, engaged ENVIRON to prepare a comprehensive air pollution photochemical modeling and analysis system for the region that is being used for the development of the regulatory air quality program.

It has been the experience of the Air District that the use of a photochemical modeling system to develop an attainment strategy removes scientific uncertainty from the planning and regulatory process. By incorporating a photochemical model into the planning process the regulated and regulatory communities have been able to participate together to formulate the most expeditious and cost effective program to attain the health based air quality standards. The tools provided by a robust and properly developed photochemical modeling system have been effectively used by agency staff to determine the root causes of the problem, project the impact of future year growth scenarios, analyze the impact of the San Francisco Bay Area emissions on downwind regions, and lastly develop regulatory control programs and demonstrate their collective effect on reducing ground level ozone.

BACKGROUND

Ambient air in the San Francisco Bay Area meets the United States national 1-hour (120 pphm) and the new 8-hour (80 pphm) ground level ozone standard more than 99.9% of the time. On occasion, during hot summer afternoons, ozone concentrations may approach or even exceed the standards. These exceedances are most likely to occur in the inland valleys that are located downwind and generally to the east or to the south of San Francisco. The Air Quality District, founded in 1955, is responsible for the attainment and maintenance planning of the air quality standards. The regulatory authority to effectuate the solution to nonattainment problems is shared between the state and regional agencies in California. The California Air Resources Board has the authority to regulate motor vehicle emissions whereas the Air District regulates the industrial sources and develops transportation control measures.

The San Francisco region is noted for tourism and the lovely vistas framed by the Golden Gate Bridge. Few people realize the San Francisco Bay Area is the fourth largest metropolitan area in the United States. Over 6,760,000 persons reside in the 6,619 square miles that encompasses the region. Motor vehicles play a significant part in the cause of the ozone air pollution problem due to the 160 million vehicle miles traveled within the region every day. Mostly unnoticed is the region’s strong industrial base that contains petroleum refining, automobile manufacturing, semiconductor chip production and other general manufacturing.

Due to a concerted planning and an aggressive regulatory effort the emissions of ozone precursors (oxides of nitrogen – N0x and volatile organic compounds – VOC) have trended downward throughout the past three decades, both in the San Francisco Bay Area and nationally in the face of growing population and a growing economy. This is largely as a result of cleaner vehicles and cleaner fuels. Also, the Bay Area has made significant progress in reducing stationary source emissions.

Corresponding to the ozone precursor emissions reduction, during the last thirty years the region has made dramatic progress in meeting the health based ground level ozone ambient air quality standards. Turning back the clock, in the 1960’s the San Francisco region experienced over sixty days every year that exceeded the one-hour ozone standard (0.12 parts per million) whereas during the past three years there has been an average of less than one exceedance per year. As the result of an aggressive regulatory program, the anthropogenic emissions of ozone precursors have dropped. Since 1980 the emission of volatile organic compounds has been reduced 70 percent while the emissions of nitrogen oxides has been reduced by nearly 55 percent. Obviously the easy emission reductions strategies have been adopted and now the Air District is faced with difficult decisions on what strategies should be used to attain, and more importantly, maintain the air quality standards.

Despite the above-mentioned progress in the regulatory program, the Air District realizes it needs to continue its aggressive emission control program in order to accommodate the growing population within the region. Furthermore, the California Air Resources Board (CARB) and Air Pollution Control Districts downwind of the San Francisco Bay Area have continued interest in the role of regional transport of ozone and precursors and may consider upwind controls to help the downwind air pollution control districts meet their future air quality goals. The question remains, what emissions reduction control strategies are the most effective in meeting the health-based standards? The photochemical modeling system was developed to assist in answering this question.

DEVELOPMENT OF A PHOTOCHEMICAL MODELING SYSTEM

The photochemical modeling system developed for the San Francisco Bay Area is designed to address not only the air quality planning needs of the Bay Area, but also those contiguous areas that are affected by emissions from the Bay Area (and under some conditions, conversely, affect the air quality of the Bay Area). Thus the development of the modeling system considered several questions in its design, including:

- How do we assure that the approach being taken is acceptable to "stakeholders" (industry, public agencies, environmental organizations, public at large)?
- What pollutants are to be considered?
- What geographical area should be covered?
- How should the work being sponsored by the BAAQMD be integrated with the similar work being carried out by the State of California (Air Resources Board – CARB)
- What meteorology should be used?
- What types of emissions reduction measures will the modeling system be used to evaluate?
- What state-of-science computer modeling tools are most suited to address the complexities of the region and purpose?

To address these questions, the development of the modeling system consists of several components, both administrative and technical.

Modeling Protocol

The modeling protocol delineates the objectives, procedures, and expected results of the modeling study, and sets up a process for participation between the regulators and stakeholders to avoid potential technical conflicts. Protocol development is a dynamic process that is modified as new information is acquired. Proposed changes are to be reviewed by interested parties and incorporated if approved.

For the Bay Area, the District Board's Executive Committee serves as the policy review group, and a Modeling Advisory Committee (MAC), including stakeholders and representatives from other agencies, was assembled to review the technical aspects of the project. In any study of this type, it is important that the technical underpinnings be fully examined as they are developed. In this manner, to the extent possible, technical issues can be put aside, accepted approaches documented and followed, and the public can be better assured that the technical community has been rigorous in their review of the work.

Accordingly, a modeling protocol was developed for the photochemical modeling activities. The protocol established and described the procedures that were to be used to develop a new ozone modeling system and database for the San Francisco Bay Area, and it followed appropriate regulatory guidance.[1,2,3,4]

General Modeling Concept

Any future ozone air quality planning must include an evaluation of the effectiveness of emission control measures by simulating their effects on ambient ozone air quality during specific multi-day pollutant episodes. A three-dimensional air quality model, the Comprehensive Air Quality Model with extensions (CAMx), was used for these simulations. Air quality models require time- and space-varying inputs of emission and meteorological fields over the episodes to be considered. These fields significantly influence the results of the simulations and are the most relevant to the SIP analysis. The modeling system eventually selected for this effort consisted of the following computer modeling subcomponents:

- Emissions Processing: Emissions Modeling System, 1995 version (EMS-95)
- Meteorological Modeling: Meteorological Modeling system version 5 (MM5)
- Photochemical Modeling: Comprehensive Air quality Model with Extensions (CAMx)

The general modeling approach for evaluating control measures is to simulate one or more historic episodes (periods that violated the air quality standard) using inputs that best approximate the physical conditions that prevailed during each episode. This simulation defines a base-year reference or "base" case. If the performance of the historic base case simulation is acceptable, meaning that all evidence suggests that the model is operating correctly and appropriately reproducing the causes for high ozone where and when it was observed, then a simulation is performed using emissions that incorporate best-estimate growth projections and adopted control programs into a future year (usually the attainment year). This "future base" case is then analyzed to indicate if any additional controls are necessary to ensure attainment of the ozone standard. If necessary, then simulations are performed using emissions that introduce proposed new emission control measures ("future control" case). The differences between the "future base " and "future control" simulations represent the air quality impacts of the proposed new emission control measures.

Meteorological Episode Selection

Air quality situations, or "Episodes"' used for this analysis need to be selected carefully so that the analysis has the maximum credibility and generality. The criteria for episode selection are:

- The episode must have had an ozone measurement that exceeded the federal ambient air quality standard. The 1-hour standard for ozone is 124 ppb averaged over one hour, while the new 8-hour ozone standard is 84 ppb averaged over eight hours. Ozone observations above these standards may influence the calculation of the "ozone design value", which is the regulatory measure of ozone levels in each air basin.

- The episode must be representative of a class of episodes that occur frequently so that the simulation will presumably have greater generality to the analysis of predicted changes in the design value. Incorporating multiple episodes into the analysis will further broaden its generality. The United States EPA guidance recommends the examination of three or more episodes, unless sufficient evidence can be provided to suggest that fewer are technically acceptable.

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

Furthermore, the California Air Resources Board (CARB) and other air quality management "Districts" will be conducting regional transport assessments as a means for controlling ozone levels throughout the state. It is therefore beneficial to the BAAQMD to identify and consider the modeling episodes to be used by the CARB and other districts to specifically support the District's own evaluation of pollutant transport into and out of the Bay Area.

As a result of extensive statistical tests and meteorological analyses, two episodes were eventually selected as representing the best combination of characteristics for ambient ozone planning purposes. These two were a mid-July 1999 period, and a late July 2000 period.

Modeling Domain

The modeling domain selected for use in this study was determined by several factors. The two primary factors were: 1) consistency with work being carried out by other researchers and the State of California and, 2) adequately captured both the San Francisco Bay area air quality region and the surrounding geographically and meteorologically related regions. Figures 1a and 1b show the entire modeling domain as well as the sub-areas of special interest, including the San Francisco Bay Area.

Models Selection

An emissions, meteorological, and photochemical air quality modeling system was selected that we believed best meets the District's needs in providing high quality modeling databases that can be used for developing local San Francisco Bay Area (SFBA) and regional ozone control plans. This belief is based on the technical features of the selected modeling system and its ability to address the challenges of modeling in the SFBA, the experience and capabilities of the District staff, and the need to maximize the likelihood of a successful model application that achieves the model performance objectives. Specifically, the system we developed is comprised of the EMS-95 emissions processing model, the MM5 meteorological model, and the CAMx photochemical model.

Challenges of the Study

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

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

- Land/sea/bay breezes
- Mountain/valley wind systems in complex terrain
- Role of maritime stratus
- Mesoscale eddies
- Low-level jets
- Convergent flow regimes critical for generating high ozone in the SFBA

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

- On-road mobile sources
- Non-road sources
- Area sources
- Refinery and other industrial sources
- Electric generating sources
- Biogenic and fire emissions
- Translation from "foundation" inventories to model-ready inputs
- Quality assurance and quality control (QA/QC)

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

- Multiscale two-way nested grid resolution (e.g., 1/4/12-km)
- Sufficient vertical resolution
- Current chemical mechanisms (updated CB4, SPARC99)
- Efficient and accurate numerical solvers
- Accurate and mass consistent interface between the meteorological and photochemical grid models
- Probing tools such as Process Analysis, Decoupled Direct Method of sensitivity tracking, and Ozone Source Apportionment Technology

Regulatory Issues: The original objective of the study was to develop a photochemical modeling database that can be used for revising the SFBA 1-hour ozone SIP. Nevertheless, any air quality modeling undertaken for future regulatory analyses must be consistent with the requirements of such SIPs and must satisfy:

- EPA's SIP guideline documents and requirements including those for photochemical modeling [1,3,4]
- CARB's guidance documents including those for photochemical modeling [2]
- Continuous contact with the CARB to assure that the modeling meets CARB's approval
- Continuous contact with EPA to assure that the modeling is performed to level that leads to an approvable SIP

Strategic Issues: The modeling and computer systems set up for this project are applicable to numerous air quality issues facing the District within the next few years:

- The District will be able to use the system to develop a historical ozone modeling "climatology" and to analyze SFBA impacts on downwind areas due to transport over a wide range of episodes.
- The modeling system will be directly applicable for addressing 8-hour ozone when EPA issues the final 8-hour ozone implementation plan.
- A photochemical model that includes advanced particulate matter (PM) and toxics treatments can be readily adapted to treat many additional air quality issues
- The modeling and computer system will be powerful enough to perform real-time ozone forecasting for the Bay Area.

Selected Modeling Systems

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

Meteorological Model: Either the RAMS or MM5 prognostic meteorological models were the most logical choice for this component of the modeling system. Both models are state-of-science, have a large user community, and are available to all public agencies. Both have been used for air quality assessments for almost 20 years. Ultimately, MM5 was adopted as well for this project for consistency with modeling being undertaken by numerous groups around California (similarly to the arguments made for EMS-95).

Photochemical Grid Model: The logical candidate photochemical grid models for this study included the two leading state-of-the-science platforms currently in widespread regulatory use throughout the U.S.: Models-3/CMAQ and CAMx. Both CAMx and Models-3/CMAQ are modern codes (1995+) that incorporate state-of-the-science features for all physio-chemical processes. For this study we selected CAMx over CMAQ for several reasons, including:

1) CAMx meets or exceeds all of the process, regulatory, and strategic requirements listed above;
2) CAMx can accept meteorological input fields derived from any meteorological model, while CMAQ is limited to the use of MM5;

3) CAMx supports flexible two-way grid nesting at any nesting ratio (e.g., 2:1, 3:1, 4:1), whereas CMAQ supports only one-way nesting;
4) CAMx has demonstrated good ozone model performance in southern California [5], whereas to date only some limited CMAQ modeling for California has been undertaken;
5) Early tests with CMAQ for CCOS indicated significant performance problems, prompting the CARB to use CAMx in their Central California Ozone Study (CCOS) modeling;
6) CAMx has demonstrated successful application in several ozone SIP modeling studies nationally, whereas CMAQ has not yet been used in an ozone SIP;
7) CAMx supports a full suite of probing tools (DDM, OSAT, and Process Analysis) that may be important in ensuring that the model is working correctly, whereas the current public release version of CMAQ just supports Process Analysis;

Emissions Modeling
Effective air quality modeling requires the development of accurate temporally, spatially, and chemically resolved emission estimates suitable for input to the photochemical model. Emissions are broadly categorized into major stationary or point sources, area and non-road sources (referred to herein collectively as area sources), on-road mobile sources, and biogenics. In addition, there are many subcategories that comprise the point and area sources.

Point and Area Emissions Sources
In order to remain compatible with on-going air quality modeling and analysis activities at the CARB, we used the 1995 Emissions Modeling System, or EMS-95 [6,7,8,9,10] to prepare the spatially, temporally, and chemically resolved emissions estimates of total organic gases (TOG), oxides of nitrogen (NO_X), and carbon monoxide (CO) for the point and area sources. EMS-95 is the emissions modeling system that is currently used by the CARB in the Central California Ozone Study (CCOS). Though EMS-95 is capable of preparing biogenics and on-road mobile source emissions estimates, the CARB used separate systems to prepare these estimates.

CARB provided a copy of their version of EMS-95 for use in the current study. This ensured that emissions estimates prepared for the current study were compatible with those prepared for use in other CCOS-related studies as well as other, on-going CARB-related studies.

Biogenics
For biogenics, the CARB used the Biogenic Emission Inventory Geographic Information System, or BEIGIS [11,12] to estimate isoprene, methyl-butenol (MBO), and monoterpene emissions from the vegetation distribution over the CCOS modeling grid. Biogenic oxygenated and other volatile organic compounds (OVOCs) were estimated as thirty percent of the total isoprene, MBO, and monoterpenes [12]. Biogenic nitric oxide (BNO) was estimated using the Biogenic Model for Emissions (BIOME) [9,10], which is based on the Biogenic Emissions Inventory System version three (BEIS3) [13] and the Biogenic Emissions Landuse Database version three (BELD3) [14]. ARB [15] describes the meteorology used to estimate the biogenic emissions. EMS-95 was used to chemically speciate the biogenic emissions estimates.

Mobile Sources
For on-road mobile sources, the CARB used the Integrated Transportation Network (ITN) [16] coupled with the Direct Travel Impact Model (DTIM), and the mobile source emissions factor model (EMFAC) [17] to estimate gridded, hourly emissions. Wilkinson [16] describes how these systems and data were combined to estimate on-road mobile source emissions of CO, TOG, and NO_X (more information is provided below). Wilkinson [16] also describes the meteorology that was used to estimate on-road mobile source emissions. Again, EMS-95 was used to chemically speciate the on-road mobile source emissions estimates.

An example of the spatial distribution of emissions is shown in Figure 2.

Results to Date
Both the July 1999 and the July 2000 modeling periods are exhibiting acceptable model performance. That is, the modeled ozone concentrations for the San Francisco Bay Area are reasonably representing the ozone levels measured during each of those time periods.

In future months we will be extending the use of the modeling system by way of estimating future emissions expected in 2007 and 2013, and estimating the ozone concentrations in those years. This will represent the “future base case”. That is, the air quality in those years if no additional actions is taken by the air pollution agencies. We will then alter those future year emissions to reflect the effect of various emissions control considerations. The photochemical modeled results of those emissions changes will be used by the regulatory agencies to select the most cost effective measures to assure continued air quality improvement in the San Francisco and surrounding regions.

An example of the photochemical modeling system output of ozone concentrations is shown in Figure 3.

FUTURE PLANS
The use of the comprehensive modeling system developed by ENVIRON and the Bay Area Air Quality Management District has assisted the District in charting the best course towards the attainment of the health based ground level ozone air quality standards. The photochemical model is being used to evaluate the effectiveness of fourteen stationary source, three mobile source, nineteen transportation control measures and twenty further study measures for incorporation into the San Francisco Bay Area 2004 Ozone Attainment and Maintenance Strategy. The modeling has also been used to evaluate the transport of ozone and its precursors to the downwind regions of the Sacramento and San Joaquin Valleys.

The modeling work is not completed. The strategies for the new United States 8-hour ozone and the PM 2.5 standards need to be developed. Also, the impact of air toxics on a local neighborhood level will be challenges for the future.

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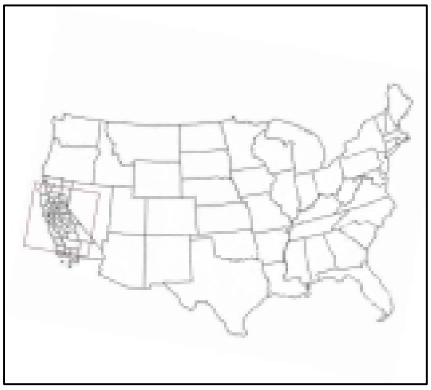

Figure 1a. Study Region (U.S. Scale)

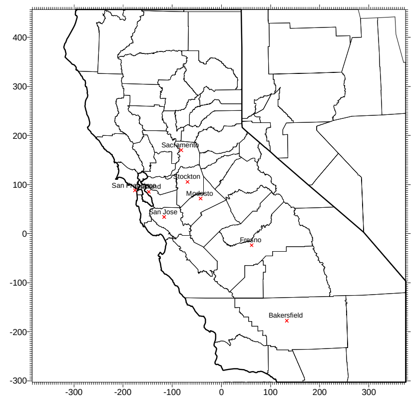

Figure 1b. Study Region (State/County Scale)

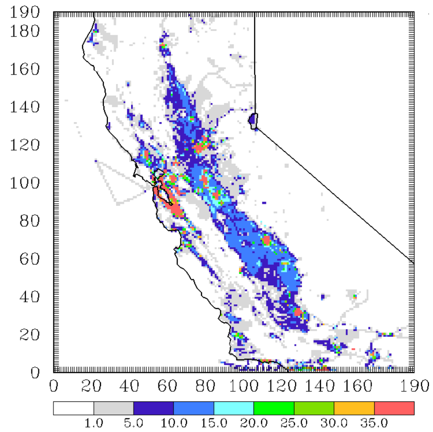

Figure 2. Example Emissions Density Plot

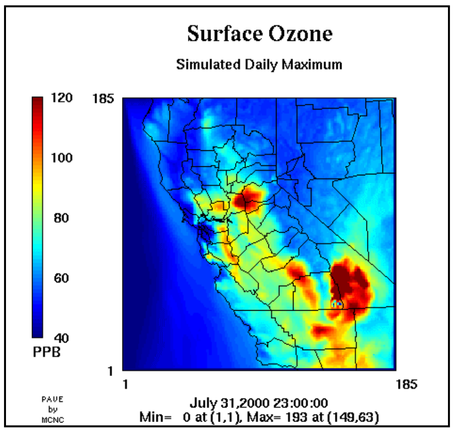

Figure 3. Example CAMx Concentration Plot