1.4 DEVELOPMENT OF A COMPREHENSIVE PHOTOCHEMICAL AIR POLLUTION MODELING SYSTEM FOR THE SAN FRANCISCO BAY AREA

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1. INTRODUCTION

The Bay Area Air Quality Management District (BAAQMD or District) is responsible for monitoring ambient air quality within the nine San Francisco Bay Area counties (Bay Area or SFBA), and for developing and enforcing emission control plans for those pollutants that have violated the National Ambient Air Quality Standards (NAAQS) and the California Ambient Air Quality Standards (CAAQS) within its jurisdiction. In 1990, the U.S. Environmental Protection Agency (EPA) designated the SFBA as being in non-attainment of the federal 1-hour ozone standard based upon historical air quality measurements within the Bay Area "airshed." Over the years, the BAAQMD has developed and submitted several State Implementation Plans (SIPs) to control ozone in the Bay Area. These plans have been effective in reducing ambient ozone levels, and since 1995 the Bay Area 1-hour ozone design value has been reduced to near the federal standard. On April 22, 2004, the EPA determined that the SFBA has attained the 1-hour ozone NAAQS. However, the original 1-hour ozone standard has now been replaced by a new and more stringent 8-hour ozone standard, and based upon air quality levels within the SFBA between 2001-2003, the area has been designated as a marginal non-attainment area of the federal 8-hour standard. Furthermore, the BAAQMD, the California Air Resources Board (CARB) and districts downwind of the SFBA have continued interest in analyzing the role of regional transport of ozone and precursors.

Given the complexities surrounding the formation and fate of ozone, the development of control strategies to mitigate precursor emissions is always a technically challenging endeavor. As a result, EPA guidance on ozone SIP development requires that non-attainment areas undertake photochemical computer modeling to understand the idiosyncrasies of their area's ozone problem, as well as to develop and evaluate ozone response to the various control scenarios under consideration. Furthermore, EPA and CARB guidance requires the development of a detailed Modeling Protocol that establishes an acceptable methodology to apply and evaluate today's state-of-the-science photochemical models and to develop various supporting datasets.

Recognizing the need to maintain a current state-of-the-science photochemical modeling capability to address the various on-going regulatory activities within the SFBA and throughout central and northern California, the BAAQMD and their contractors have been developing a new photochemical modeling system and supporting database over the past two years. The data and knowledge base gained as a key sponsor and contributor to the Central California Ozone Study (CCOS) has been essential to this effort. Integral contributions have been made by several other entities involved in CCOS, including the CARB and their associated contractors at the National Oceanic and Atmospheric Administration and the University of California at Riverside, as well as the San Joaquin Valley and Sacramento Air Districts, and their respective contractors. Given the plethora of modeling efforts conducted by each of these groups stemming from the CCOS 2000 program, the BAAQMD effort has attempted to bring together the best information and modeling approaches possible. As a result, the research, modeling, testing, and evaluation conducted in this project proved to be a rather complex and highly interactive endeavor.

This paper provides only the highlights and summary of model results fundamental to the ultimate goal of providing a working, reliable, and scientifically sound modeling system. We describe the modeling system, it's supporting databases, the methodology for its application, and results from modeling two historical multi-day ozone episodes in the summers of 1999 and 2000. Details are provided in the original project report (ENVIRON et al., 2005).

2. MODEL SELECTION

An emissions, meteorological, and photochemical air quality modeling system was selected that we

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believed best meets the District's needs in providing high quality modeling databases that can be used for developing local 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. There are numerous air quality modeling challenges in the Bay Area that must be addressed, and these are briefly described below.

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 was 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, SAPRC99)
- 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

Based upon the District's suggestions for consistency with their preexisting modeling tools and those to be evaluated by the CARB for CCOS, the following models were selected:

- Emissions Modeling System, 1995 version (EMS-95; Wilkinson et al., 1994);
- Regional Atmospheric Modeling System (RAMS; ATMET, 2004),
- Fifth Generation PSU/NCAR Mesoscale Model (MM5; Grell et al., 1994);
- Comprehensive Air quality Model with Extensions (CAMx; ENVIRON, 2004)

This modeling system contains all of the technical features necessary to simulate ozone air quality in the SFBA and throughout California. 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 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.

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. We believe that RAMS provides a better treatment of the highly non-hydrostatic processes associated with mesoscale land/sea/lake breeze and planetary boundary layer (PBL) circulations in complex terrain. The RAMS prognostic meteorological model was originally selected for the modeling system because of its demonstrated successful application in the Bay Area in the past, its inclusion of all the technical features necessary for simulating the complex Bay Area meteorology, and its familiarity to District staff. The CARB has utilized MM5 for their CCOS modeling effort and this project included an inter-comparison of RAMS and MM5 performance to select the most appropriate for use in the photochemical modeling component.

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. The CAMx photochemical grid model was selected because it is publicly available, contains all of the technical options needed to simulate ozone in the Bay Area, and contains some superior capabilities:

- CAMx meets or exceeds all of the process, regulatory, and strategic requirements listed above;
- CAMx can accept meteorological input fields derived from any meteorological model, while CMAQ was limited to the use of MM5;
- 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;
- CAMx has demonstrated good ozone model performance in southern California (Morris et al., 2002), whereas to date only some limited CMAQ modeling for California has been undertaken;
- Early tests with CMAQ for CCOS indicated significant performance problems, prompting the CARB to use CAMx in their CCOS modeling;
- CAMx has demonstrated a successful track record in several ozone SIP modeling studies nationally, whereas CMAQ has not yet been used in an ozone SIP;
- CAMx supports a full suite of probing tools (DDM, OSAT, and Process Analysis);
- The District had a greater familiarity with CAMx and had used it before.

3. EPISODE SELECTION

Modeling episodes needed to be selected carefully so that the analysis possessed the maximum credibility and generality. Several criteria for episode selection are provided in EPA modeling guidance (EPA, 1991; 1999), and these address such considerations as peak concentrations, number of exceedances, number of valid measurements, and episode representativeness. Furthermore, the CARB and other Districts are conducting regional transport assessments as a means for controlling ozone levels throughout the state. It was 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.

BAAQMD staff investigated the categorization of 1-hour ozone exceedances in the Bay Area for the period 1995 through September 2002 in order to find representative exceedance days to be used for SIP modeling. Two main categories of exceedance patterns were found: (1) when high values occurred at several sites and in many areas throughout the SFBA; and (2) when high ozone values occurred at an isolated individual site within the SFBA. Based upon frequencies of exceedance events by day of week and month of year, year-to-year trends, and a statistical cluster analyses, four periods were selected as candidate episodes for modeling (2 in each cluster). Meteorological and trajectory analyses were conducted on each of these periods to compare and contrast them. Based upon the extensive review, and the criteria for data availability, we elected three exceedance days for the SIP modeling: July 31, 2000; and July 11/12, 1999. The July 2000 episode included August 1 and 2 as well, to pick up exceedance days in the Sacramento and San Joaquin Valleys. The July/August 2000 period occurred during the CCOS, and July 31 fell into the “Type 2” pattern (1 site exceedance per day). The 1999 days represented the “Type 1” pattern and indicated many more measured exceedances. July 11 was a Sunday and July 12 was a Monday, which satisfied the need to evaluate weekend-weekday issues. Data for these periods were quality assured and archived by various agencies. Based on preliminary back-trajectory analyses, all episode days indicated potential transport paths from the Bay Area into the downwind areas of Sacramento and the San Joaquin Valleys.

As observed over the past decade or so, the 1-hour SFBA ozone exceedances in both episodes were measured in the eastern inland valleys , most commonly in the Livermore Valley, and secondarily in the Concord area. Table 1 summarizes the three SFBA episode days described above.

4. SUMMARY OF MODELING APPROACH AND RESULTS

4.1 *RAMS Meteorological Modeling*

ATMET (2004) presents a brief analysis of the meteorology for the July 2000 and the July 1999 ozone exceedances episodes in and near the Bay Area. The observations in these cases, as with numerous other ozone episodes in other locations, indicate that convergence zones are important in focusing ozone and the precursors. The convergence zones in these cases were caused by the interaction of the on-shore seabreeze flow within the marine layer with the easterly large-scale flow forced by Eastern Pacific subtropical high pressure. When the winds and temperature allow, the easterly flow can erode the marine layer over the Central Valley and Coastal Range, causing near-surface convergence zones to occur. An important finding in the analysis shows that the convergence zone frequently does not extend to the ground. This finding has significant implications for verification and four-dimensional data assimilation applications.

Table 1. Summary of episode characteristics for SFBA photochemical modeling.

Episode Dates	Days of Week	Peak ozone (ppb)	# Exceedances	Category
July 11-12, 1999	Sun, Mon	156 Concord	6	1
July 31, 2000	Mon	126 Livermore	1	2

RAMS was configured with four 2-way nested domains with 48/12/4/1 km grid spacing, with the finest resolution placed over the immediate Bay Area. The model employed 41 vertical levels up to ~20 km. Overall, the RAMS simulations performed for the July/August 2000 and the July 1999 episodes show verifications that are consistent with past simulations of this type, with errors of especially wind speed and temperature within the range expected. When temperatures were adequately simulated, RAMS tended to over predict wind speeds in the coastal sea breeze zones. While the error statistics were acceptable for the most part, there were various aspects of the simulations of this region that need to be addressed to make significant improvements in the results:

- Even with 1 km grid spacing, higher resolution may be needed to resolve the important topographical features and land use features such as coastlines, wetlands, urban areas, etc.;
- There was no information on which areas were in active irrigation during these episodes, which may be critical to accurately determine sea breeze and other mesoscale circulations. There was circumstantial evidence in the observational temperature and dewpoint data that various areas were actively irrigated.

The complexity of the central California meteorology, with complex terrain and land use features, along with the interactions of marine and mountain flows, poses a difficult situation to simulate with current models. This puts a reliance on the FDDA to introduce large scale changes into the mesoscale domains. But too often, the FDDA also serves the purpose of attempting to correct model errors, sometimes with undesirable results. The situations in these cases point this out very clearly; the vast majority of the observed data used in the FDDA are taken at or very near the surface. However, the primary forcing mechanisms for the important flows may not ever become apparent at the surface. And there were far too few observations taken above the surface, even during CCOS with the profilers and RASS, to adequately resolve the horizontal structure of the meteorology above the marine layer.

We also found that it is imperative in these complex layers of stability that the subgrid turbulence scheme employed in the meteorological model be able to correctly treat elevated well-mixed, neutral layers. Simple, surface-based PBL schemes either: 1) produce a single PBL from the surface to some defined PBL height, usually resulting in a too deep boundary layer that mixes out the shallow surface stable layer, or 2) overemphasize the effect of the surface stable layer and shut down vertical mixing throughout the PBL. It is necessary to employ a TKE-based scheme that has all of the necessary physical terms (advection, production, diffusion, dissipation) to correctly handle elevated mixed layers and these types of elevated convergence zones.

4.2 *MM5 Meteorological Modeling*

Initial MM5 simulations were performed for the CCOS July 2000 episode by the CARB and their meteorological modeling contractor at NOAA/ARL, concurrent with the RAMS simulations undertaken for the District. Subsequent MM5 modeling of the July 2000 and July 1999 episodes was undertaken by both the CARB and BAAQMD. The meteorological model was run with 3 one-way nested domains with 36/12/4 km grid spacing and 50 vertical levels; the finest grid encompassed the CCOS 2000 field study area (Figure 1). Among various MM5 simulations with different combinations of surface and boundary layer parameterizations, we found that overall the most accurate simulation was produced when using the Eta planetary boundary layer scheme (a reduced-form TKE algorithm), the NOAH land surface model (LSM), and FDDA.

Direct meteorological comparison between the model simulation and the observations from the CCOS 2000 field experiment (Emery and Tai, 2004a) indicated that the errors in the simulated low-level winds and surface temperature varied from one area to another, although the model simulated large-scale pattern was in fairly good agreement with analyses. In terms of time series, the simulated low-level winds were generally in better agreement with the observations in SFBA than in the central valley areas. The opposite was generally true for temperature, where the time traces followed observations better in the central valley areas. However, according to daily-average bias and error statistics, performance was superior in the SFBA for all three meteorological parameters – consistent performance issues were noted for winds, temperature, and humidity throughout the central valley. The use of the NOAH LSM led to more accurate simulations of surface temperature and moisture in the central valley areas. FDDA of the observed winds significantly improved the simulated wind field, and reduced the cold bias in the simulated temperature field. Good agreement was found between the area average observed and simulated boundary layer heights except for the area immediately inland of the SFBA.

The CARB and BAAQMD conducted MM5 modeling of the July 9-12, 1999 period using the MRF PBL algorithm, the simple 5-layer soil scheme, and various incarnations of FDDA. Horizontally, MM5 was applied on the CCOS modeling domain, but only ~30 vertical layers were specified in the July 1999 simulations. The CARB simulation included observational FDDA to an original unscreened meteorological dataset that they compiled in early 2003. The BAAQMD applications tested the model with no FDDA whatsoever, analysis nudging toward EDAS, observational nudging toward a screened/improved observation dataset, and runs testing the impacts from using the Eta PBL scheme and the NOAH LSM. Graphical and statistical results showed that the original CARB run consistently performed better than any

BAAQMD FDDA sensitivity test. Analysis nudging improved wind speed performance in the SFBA, but it was clearly the worst run in all other respects. An MRF "phase-lag" problem for wind speed was clearly evident for areas in the central valley. Wind direction performance especially was unacceptable on July 11-12 in the central valley. The SFBA was too warm and the central valley (particularly the southern SJV) was too cool in all runs. Humidity was not evaluated due to lack of data, but a cool bias in the central valley was likely associated with a positive moisture bias as seen in the CCOS 2000 modeling results.

BAAQMD tests using the Eta PBL fixed the wind speed phase-lag problem associated with the MRF PBL scheme. However, no significant impacts were seen for direction, and a slight degradation of temperature performance was seen in the central valley. The "best" MM5 simulations for this episode were only moderately acceptable relative to performance benchmarks established from a vast array of meteorological modeling conducted across the country. This may be as much related to the complex terrain over such a vast area as to the quality of the data used in the performance evaluation. The best MM5 simulation does not always lead to the best CAMx performance. Remaining issues include:

- Proper temperature performance leads to overly high SFBA winds, and vice-versa;
- There may be a need for more terrain-induced "drag" on the winds, including proper resolution of terrain elevation in the modeling grid, valley channeling, and effects of unresolved terrain features that add to surface roughness;
- The default MM5 surface roughness values as a function of land cover category are now known to be too low; tests in other studies outside of California have shown improved results when higher values for roughness are employed.

4.3 *Emissions Modeling*

In order to remain compatible with emissions preparation activities at the CARB for CCOS, we used EMS-95. Specifically, the CARB provided a copy of their version of EMS-95 for use in the current study. This ensured that the District's emissions estimates were compatible with those prepared for use in other CCOS-related studies as well as other on-going CARB-related studies. EMS-95 was used 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, mobile, and area sources. EMS-95 was used to prepare model-ready emissions estimates for CB-IV and SAPRC99 speciation for both the July 1999 and July/August 2000 episodes.

CARB (2004a) describes the methods used to prepare stationary and area source emissions estimates for use in CCOS, including the methods to prepare certain day-specific emissions estimates for the July/August 2000 episode. Note that day-specific point and area emission estimates were not included in the July 1999 episode due to the lack of data; however, as with the July/August 2000 episode, day-specific emissions were estimated for the biogenics and on-road mobile sources using methods described by Wilkinson (2004) and CARB (2004a,b,c). Although EMS-95 is capable of preparing biogenic emission estimates, the CARB used the Biogenic Emission Inventory Geographic Information System (BEIGIS) to estimate biogenic VOC emissions from the vegetation distribution over the CCOS modeling grid. Biogenic nitric oxide (BNO) was estimated using the Biogenic Model for Emissions (BIOME), which is based on the Biogenic Emissions Inventory System version three (BEIS3) and the Biogenic Emissions Landuse Database version three (BELD3). EMS-95 was used to chemically speciate the biogenic emissions estimates.

The July 2000 CCOS episode was characterized by a heavy contribution from forest fire smoke, particularly from fires in the southern Sierra Nevada mountain range. The smoke plumes from this and other large regional fires in Oregon and Nevada were detected aloft on several days by multiple aircraft and ozonesonde samples taken throughout central California. Therefore, day-specific wildfire emissions were estimated for the July 2000 episode by the CARB. This issue has affected every major area in California conducting air quality modeling for this CCOS episode, and arguments have been made concerning the representativeness of fire-dominated episodes for use in ozone SIPs in California. A special set of "fire-augmented" boundary conditions were developed for the July 2000 episode to account for the influences of regional fires. The July 1999 episode was not nearly affected by forest fire smoke, as fire activity levels were more representative of a "typical" ozone day (i.e., no single fire impacted ozone air quality in any California ozone nonattainment areas). Therefore, the emission inventory for July 1999 contained standard season day fire estimates.

The BAAQMD project team undertook additional analyses to improve emission estimates for marine shipping in the San Francisco Bay and at the ports. Specifically, we estimated day-specific NO_X and VOC emissions for oceangoing and San Francisco Bay commercial marine traffic. The original CCOS inventory for this category contained estimates for monthly ship emission values. The work conducted in this study acquired data on day to day variations in SFBA ship movement and used this information to scale the monthly emission estimates to daily levels.

4.4 *CAMx Applications*

CAMx was run for the two historical episodes of July 31–August 2, 2000 and July 11–12, 1999 on a single large modeling domain that covers most of California with 4-km grid spacing (Figure 1). The performance of the model was evaluated against available air quality data; the purpose of the evaluation was to build confidence in the model's reliability as an ozone prediction tool. The proposed evaluation plan followed the procedures recommended in the EPA and CARB guidance documents for 1-hour ozone (EPA, 1991; CARB, 1992), and draft guidance for 8-hour ozone (EPA, 1999). The philosophical approach to the model performance evaluation for this project is provided in the project Modeling Protocol (ENVIRON et al., 2002).

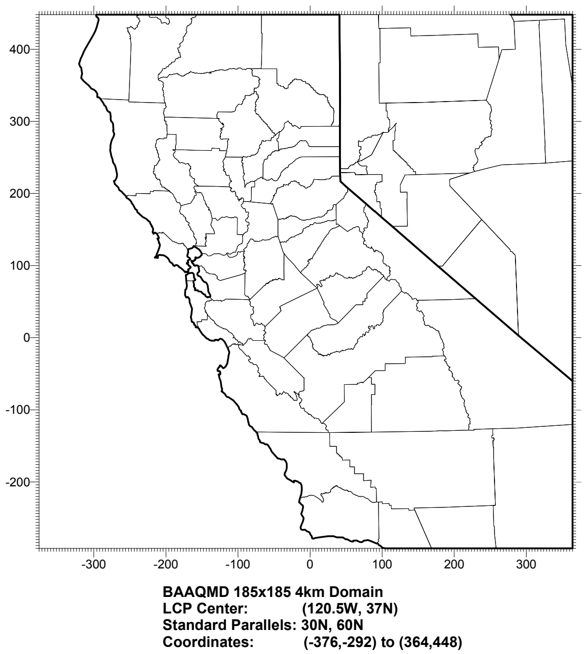

Figure 1. The coverage of the CARB/CCOS air quality modeling domain. Grid spacing over the entire region is 4 km. Map projection is MM5-based Lambert Conformal.

4.4.1 *Developmental Simulations*

Since the fall of 2002, when the initial emission inventory and preliminary meteorological simulations first became available, ENVIRON and the BAAQMD conducted on the order of 50+ CAMx simulations. Considered to be "developmental" model applications, most of these runs were made for the July 2000 episode each time the emission and/or meteorological inputs were incrementally updated; later, developmental CAMx runs were also made for the July 1999 episode as inputs became available. A portion of these runs were made with the interim versions of the emission and meteorological inputs to test photochemical model sensitivity to various options, treatments, and ancillary inputs. All developmental simulations were run using CAMx v3.10 with the Carbon Bond IV (CB-IV) chemistry mechanism. A mixture of RAMS and MM5 meteorology were used to drive the photochemical model.

The specific sensitivity tests conducted as part of the developmental process included: numerous increased/descreased emission scenarios for both NOx and VOC applied to various source categories; use of alternative CB-IV speciation profiles; modifications to key input meteorological fields; horizontal grid resolution over the SFBA and vertical depth/resolution over the entire domain; influences from initial and boundary conditions; role of fire emissions; meteorological impacts on certain emission components; and impacts of various CAMx model options. Results from these tests are summarized by ENVIRON et al. (2005).

Throughout the course of these developmental CAMx applications, two key performance issues constantly emerged in both episodes: (1) the emissions inventory (using CB-IV speciation of VOC) did not appear to be sufficiently reactive in producing ozone, suggesting that major proportions of emissions were either lacking or incorrectly speciated; and (2) flow fields in the Bay Area meteorology were either too fast and/or insufficiently convergent in the east bay, leading to over-ventilation of both precursors and ozone. Initially, these problems led to under predictions of peak observed ozone in the Bay Area by ~40 ppb, yet this deficit was incrementally improved to a shortfall of ~15-20 ppb after numerous updates to the emission and meteorological inputs. Furthermore, significant under predictions were seen throughout central California, particularly in the central and southern San Joaquin Valley (SJV), where even larger ozone shortfalls were simulated.

4.4.2 *VOC and Process Analyses for July 2000*

A large body of evidence was compiled from the developmental simulations conducted in this project, as well as from modeling undertaken by the CARB and Alpine Geophysics for the San Joaquin Valley (Tesche et al., 2004), which strongly suggested that CAMx ozone under predictions were chiefly a result of insufficient VOC emissions and/or incorrectly speciated CB-IV compounds. An analysis was undertaken by ENVIRON that compared VOC measurements and CAMx predictions for the July 2000 episode in the Bay Area, Sacramento Valley, and San Joaquin Valley (Emery and Tai, 2004b).

There exists a large level of uncertainty concerning overall data quality in the CCOS VOC dataset, both for 3-hour canister and 1-hour GC-MS samples. While certain findings from the analysis are significant, they may be overly influenced by the inclusion of poor quality samples that appear to be reasonable from casual inspection without further supporting evidence to suggest otherwise. Generally, there are consistent model performance issues that we have identified in the three basins and among most sites with useable measurements. First, there is a general under prediction of total VOC and this is mainly attributable to insufficient PAR (since this contributes the bulk of VOC mass). VOC performance in the SFBA showed consistent under predictions of total VOC, with some sites indicating under predictions for reactive species (OLE, TOL, XYL). There is evidence from "background" sites that PAR is too low, although this could be caused by old smoke plumes originating well to the north of the CCOS domain. Limited VOC:NOx ratio data and model predictions both indicate that the eastern areas of the SFBA are NOx-rich and VOC-limited.

VOC performance in the Sacramento region indicated mixed performance for total VOC. Some sites indicated reasonable model performance across the CB-IV species, while others showed significant under predictions of PAR, OLE, and carbonyls. Observations and predictions of VOC:NOx ratios agree that conditions east of Sacramento are NOx-rich. VOC performance in the SJV region showed consistent under predictions of total VOC, and CB-IV species were under predicted across the board. VOC:NOx analyses also suggest a problem with disproportionate VOC and NOx emissions in the SJV.

Vizuete et al. (2004) detailed the application of the Process Analysis (PA) Tool in CAMx to study modeling phenomena in the San Francisco Bay Area during the CCOS episode of July 30 – August 2, 2000. This evaluation employed CAMx with some code modifications to the PA Tool applied by the University of Texas. CAMx was configured to run two process analysis domains over the eastern San Francisco Bay Area (Figure 2). Evaluation of the Integrated Process Rate (IPR) and Integrated Reaction Rate (IRR) output generated for the Bay Area PA domain was then performed. The focus of the analysis was on the key episode day of interest, July 31, 2000.

Vertical advection was found to play an important role in the transport of pollutants across the boundaries of the process analysis box. This can be attributed to the heterogeneity of the terrain under analysis. These differences in terrain account for a wide range of mixing and vertical advection. The process analysis tool determined that the modeled atmosphere is NOx-rich and VOC-limited. The composition of the VOC that was available in the atmosphere was predominantly low-reactive paraffins. Since the analysis area incorporated natural terrain a significant amount of biogenic isoprene was emitted during the day into both process analysis boxes. Nevertheless, there were still inadequate amounts of reactive VOC available to generate large amounts of ozone chemically. The chemical NOx cycles, radical cycles, chemical production of ozone, and percentage of OH reacting with VOC were all at insufficient levels to simulate ozone production at observed levels.

The low concentrations of highly reactive VOCs (toluene, olefins, xylene, and aldehydes) in the atmosphere were not consistent with observed VOCs, and were under predicted by as much as a factor of 5. The model's inability to generate the observed concentrations of aldehydes could be evidence that the model is not fully capturing all the atmospheric VOC chemistry. However, some reactive olefins (OLE) are also classified as ALD2 which points to an underrepresented emission inventory. Observed ethylene concentrations were consistent with model values. This suggests that the meteorology of the model has been properly simulated and is not the cause of the OLE/ALD2 discrepancies. Further investigation is needed to explore the discrepancies found in the OLE emission inventory. The strongest possibility for the low reactivity could be the lack of total VOC and/or the improper speciation of the general anthropogenic emission inventory.

4.4.3 *Use of Decoupled Direct Method for July 1999*

ENVIRON used the Decoupled Direct Method (DDM) Probing Tool in CAMx to investigate the sensitivity of ozone to boundary conditions of ozone and VOC during the July 1999 episode. Further, the DDM was used to assess ozone sensitivity to emission categories and emission source regions as a first glimpse into potential transport impacts. Figure 3 shows the source regions that were individually tracked with DDM sensitivity coefficients.

The maximum Bay Area ozone sensitivity to boundary conditions relative to total peak ozone in the eastern SFBA was ~35% in these tests (mainly from north boundary ozone and VOC). However, the key result of the boundary condition analysis was that the low model top (~5 km) and fairly large ozone top boundary conditions specified by the CARB (70 ppb) did not significantly impact model performance in areas of central California where high ozone was simulated.

Appropriately, ozone sensitivity to emissions was found to be much larger than to boundary conditions. Ozone is nearly as sensitive to biogenic VOC as anthropogenic VOC in all regions. The Bay Area shows the most sensitivity to NOx and VOC emissions. Less anthropogenic and/or biogenic VOC will reduce ozone in the eastern SFBA, while less anthropogenic NOx will increase ozone. Ozone in the southern Sacramento and northern SJV regions is only modestly sensitive to Bay Area NOx and VOC emissions. In the central valley, ozone in the major urban areas is insensitive to NOx, but very sensitive to VOC; rural areas are equally or more sensitive to NOx than VOC (Figures 4 and 5).

4.4.4 *Summary of BAAQMD CAMx Simulations for CCOS 2000*

The MM5-CAMx couple using the SAPRC99 chemical mechanism produced reasonable predictions

Figure 2. The locations of the two 640 km^2 PA sub-domains, outlined in black.

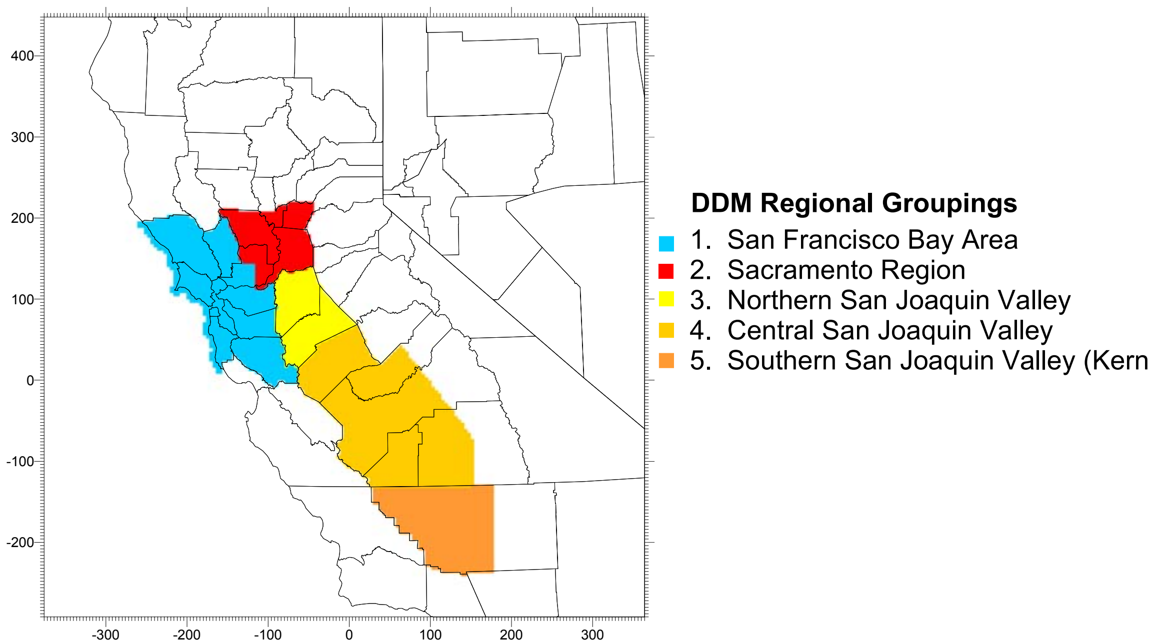

Figure 3. Definition of source regions for the CAMx DDM application.

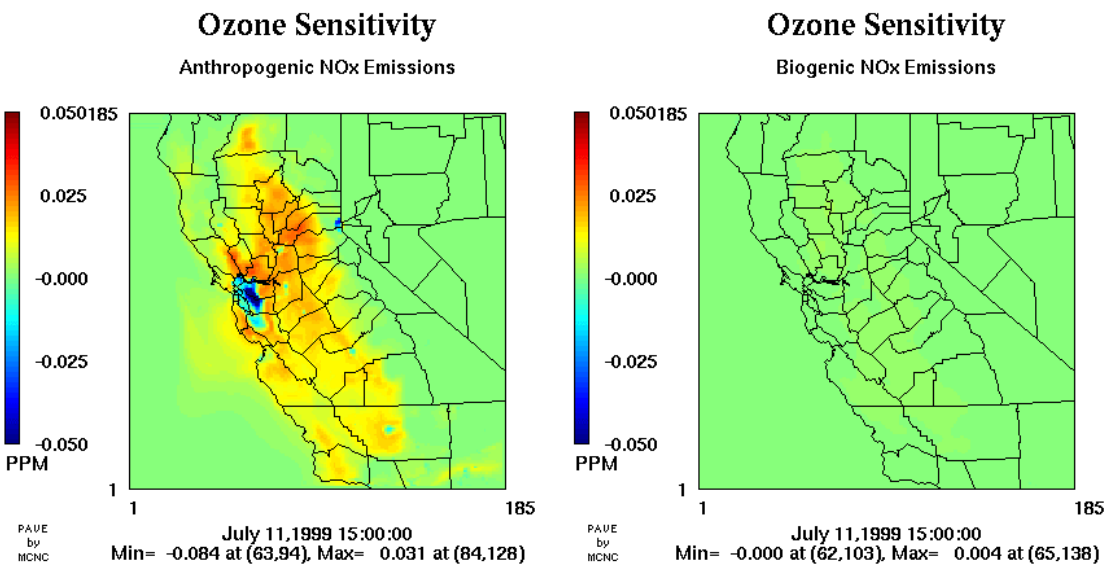

Figure 4. DDM ozone sensitivity coefficient field for total anthropogenic and biogenic NOx emissions at 3 PM local time on July 11, 1999.

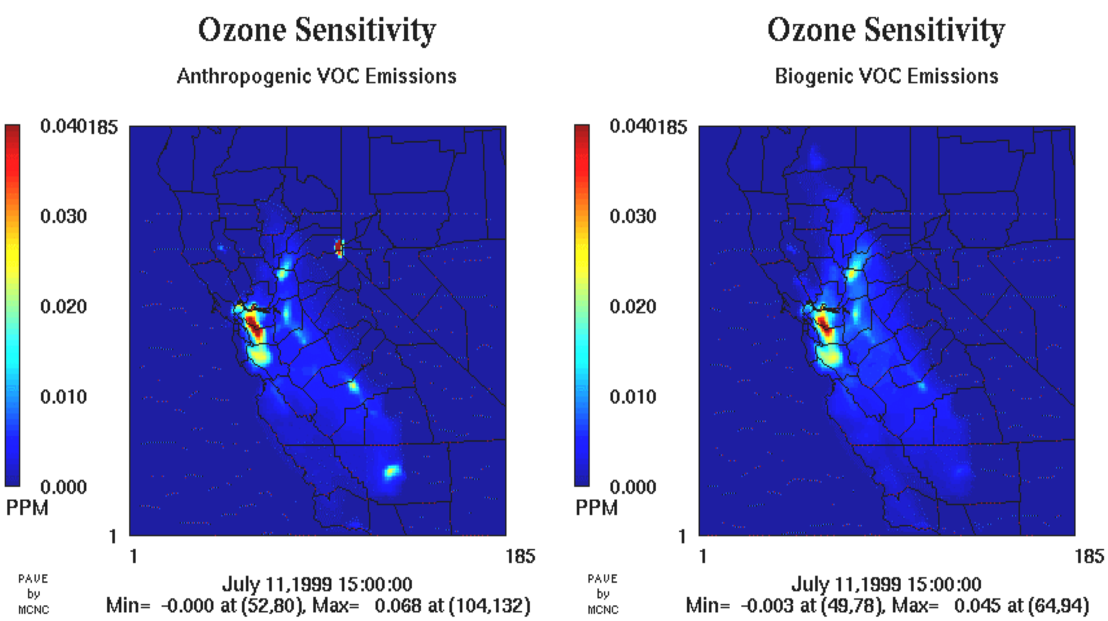

Figure 5. DDM ozone sensitivity coefficient field for total anthropogenic and biogenic VOC emissions at 3 PM local time on July 11, 1999.

of ozone in central California during the July 31-August 2, 2000, period. It also produced reasonable predictions of the locations and timing of peak ozone in the SFBA on July 31, 2000 (Figure 6). The prediction skill varied from region to region and from time to time. Under predictions continue to be a problem for the modeling in Sacramento and the southern SJV on their specific days of interest (August 1 and 2, 2000, respectively).

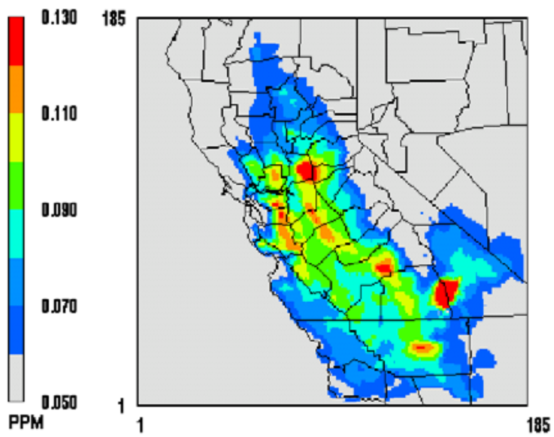

Figure 6. Simulated ozone distribution over the CCOS domain at 1600 PST, July 31, 2000.

Locations of the wind convergence zone and the locations of simulated high ozone were found to be closely related (Figure 7). The overall surface-wind patterns in the SFBA are similar in the three MM5 realizations used to drive CAMx, but there were subtle differences in the wind patterns among the runs in and near the Livermore Valley. The MM5 runs with the 5-layer soil model under predicted Central Valley temperatures and therefore produced a weaker sea breeze. This weaker sea breeze created a convergence line close to Livermore and produced an ozone pattern that, among the three simulations, compared best with observations. The MM5 runs using the Noah LSM, while producing a reasonable Central Valley temperature, created a much stronger sea breeze. This stronger sea breeze moved the convergence zone about 20 km east of Livermore.

This trade-off between accurate inland temperature and accurate sea-breeze predictions may indicate a deficiency in the current MM5 model. There are several possible explanations for this problem. The first is that the second-order advection scheme used in MM5 requires such large diffusion values that the mountain-blocking effect is reduced and the sea breeze front is propagated too far inland. Another possible explanation is the lack of a mountain drag parameterization that would tend to reduce the speed of the sea breeze in the Tri-Valley and more accurately channel the flow. A third possible explanation is the lack of vertical resolution in the original data input to MM5 to define the inversion layer during this high ozone period. A comparison between the MM5 output and the observed vertical profiles of temperature did show that the strength of the

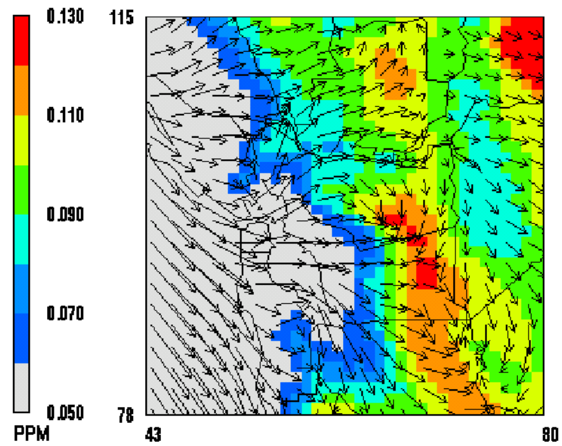

Figure 7. The simulated ozone distribution over the SFBA at 1600 PST, July 31, 2000, with wind vectors overlaid.

inversion is under predicted. An important conclusion, then, is that some relatively subtle flow features, which may not be fully appreciated in meteorological model performance evaluations, can have a significant influence on the performance of a photochemical model.

4.4.5 *Summary of BAAQMD CAMx Simulations for July 1999*

The BAAQMD undertook photochemical modeling of the July 9-12, 1999 period using two different sets of meteorological input fields (CARB's MM5/MRF run and BAAQMD's MM5/Eta run) and two different chemical mechanisms (CB-IV and SAPRC99). Besides meteorology, the only other significant difference in model configuration between the CCOS2000 and July 1999 simulations was the lower model top (set at 5 km in the July 1999 applications).

CAMx tests conducted with different meteorological inputs used the SAPRC99 chemistry. Both sets of meteorological inputs resulted in much higher ozone concentrations over the entire urbanized portions of the modeling domain than achieved in the July/August 2000 episode, with simulated ozone reaching near 150 ppb in several areas each day. Given that the input emissions for this episode are not dramatically different from the July/August 2000 episode, the higher and more widespread ozone patterns generated by CAMx in this simulation suggests a more extreme meteorological condition conducive to poor ozone air quality was successfully modeled with MM5 and translated to CAMx. This is particularly evident from the fact that high ozone concentration patterns were pushed to the coast and even offshore along the central California coastline, suggesting proper replication of the offshore wind system that set up between July 11 and 12.

In the SFBA, the MM5/MRF meteorology generally leads to less of an under prediction of the highest observed ozone levels, but very little difference (statistically) resulted from the two meteorological realizations. The daily unpaired peak and bias metrics are quite good on both days and for both sets of meteorological inputs. However, the gross error is rather high in all cases (but still within EPA acceptance). There is no obvious best case for the SFBA. In Sacramento, differences are more obvious among the two simulations both visually and statistically; however, the mix of improvements and degradations result in no clear winner in this region as well. The unpaired peak accuracy shows extreme under predictions on July 12 for both sets of meteorology, but gross error is not impacted by the different cases. In the SJV, both simulations are very similar and show the consistent under predictions of high ozone and over predictions of low ozone. Model performance shows very little skill in this region. Peak ozone performance is not sensitive to meteorology, but bias and gross error are worse in the BAAQMD MM5/Eta run. We conclude that CAMx performance is slightly degraded in the central valley with the use of the BAAQMD MM5/Eta meteorology.

Example CAMx ozone results using SAPRC99 with the MM5/MRF meteorology are shown in Figures 8 and 9. For the July 1999 episode, SAPRC99 has a tendency to over predict the low to moderate observed ozone concentrations throughout the SFBA. In Sacramento, CAMx performs well over the entire range of concentrations, but the single peak observation on July 12 is under predicted by a large margin. Over the entire SJV, the model performance is quite promising for July 11 and 12, with the metrics at or well within the EPA acceptance criteria.

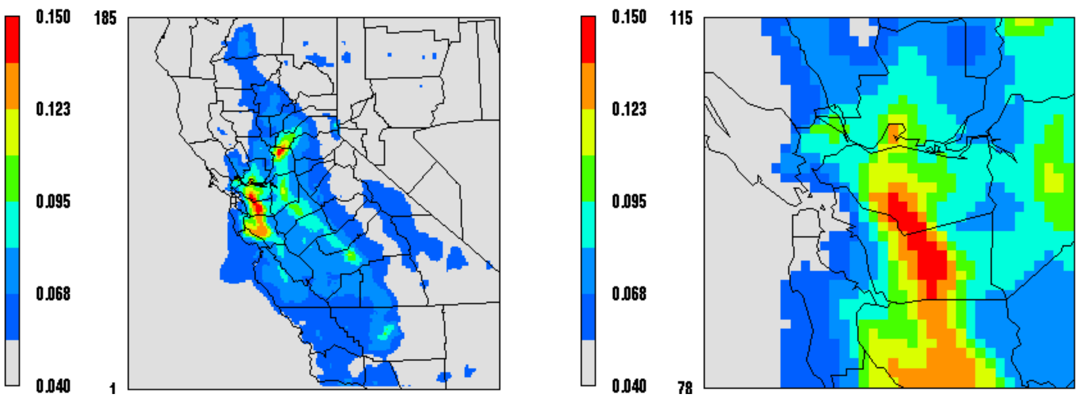

Figure 8. CAMx/SAPRC99 simulated ozone on July 11, 1999 at 1400 PST (a) over the entire domain and (b) over the SFBA region.

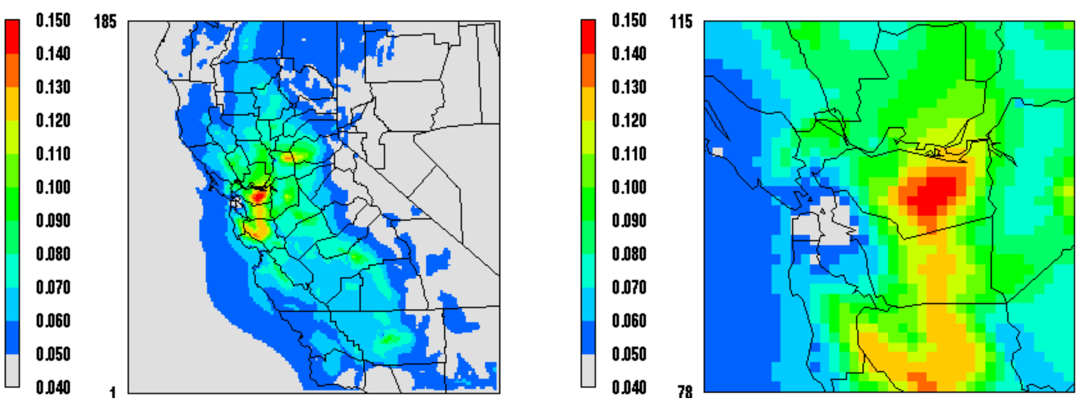

Figure 9. CAMx/SAPRC99 simulated ozone on July 12, 1999 at 1400 PST (a) over the entire domain and (b) over the SFBA region.

5. FUTURE WORK

The objective of this effort has been the development of a technical platform for photochemical modeling that is comparable to that which exists at the Air Resources Board and is state of the science. The District has made remarkable progress in the development of a highly respected technical capability in photochemical modeling. Such complex modeling capabilities are absolutely necessary tools for use by the District in assessing a range of issues, both present and future, and will allow the District to make policy decisions based upon sound atmospheric science. The issue of attainment and maintenance of the NAAQS in the Bay Area is closely related to the relationship of the Bay Area "air basin" to that of the Sacramento and the San Joaquin Valley regions. Therefore, the current modeling system has been designed to be able to examine the inter-basin effects of emissions controls in one region on the air quality in another. While the system has been designed to encompass the entire area here described, further work must be done to fully qualify its performance as acceptable in such complex, far reaching modeling. As the District moves forward with air quality planning in the Bay Area, it will need to continue to develop the following:

- Improve Meteorological Modeling
- Improve Precursor Emissions for Future Years
- Enhance Modeling System Utility and Sensitivity Assessments
- Assess Impacts of Future Ozone Strategies
- Assess Alternative Episodes

REFERENCES

ATMET, 2004: RAMS Simulation for San Francisco Bay Area Air Quality Episodes. Prepared for the Bay Area Air Quality Management District, San Francisco, CA, by ATMET LLC, Boulder CO, June 2004.

CARB, 1992: "Technical Guidance Document: Photochemical Modeling," California Environmental Protection Agency, Air Resources Board, April 1992.

CARB, 2004a: "Preparation of Emissions." http://eos.arb.ca.gov/eos/ARB_Modeling/JulyAug2000_SIP_Modeling_Doc_Ch4_11-26-03.pdf.

CARB, 2004b: "Biogenic Emissions." http://eos.arb.ca.gov/eos/ARB_Modeling/JulyAug2000_SIP_Modeling_Doc_AppB_11-26-03.pdf.

CARB, 2004c: "Treatment of OVOCs." http://eos.arb.ca.gov/eos/ARB_Modeling/Addition_of_OVOCs.doc.

Emery, C.A. and E. Tai, 2004a: "Standardization of MM5 statistical performance evaluation for CCOS applications." Memorandum to the Bay Area Air Quality Management District and the Modeling Advisory Committee, prepared by ENVIRON International Corporation, Novato, CA, March 12, 2004.

Emery, C.A. and E. Tai, 2004b: "CAMx model performance for speciated and total VOC for July/August 2000." Memorandum to the Bay Area Air Quality Management District and the Modeling Advisory Committee, prepared by ENVIRON International Corporation, Novato, CA, April 13, 2004.

ENVIRON, ATMET, Alpine Geophysics, and BAAQMD, 2002: "Modeling Protocol (Fourth Draft): Development of a Photochemical Modeling System to Support the Bay Area Air Quality Management District's 2004 State Implementation Plan." Prepared for the Bay Area Air Quality Management District, San Francisco, CA., December 2002.

ENVIRON, 2004: User's Guide, The Comprehensive Air quality Model with extensions (CAMx). Prepared by ENVIRON International Corporation, Novato, CA (www.camx.com).

ENVIRON, Alpine Geophysics, ATMET, San Jose State University, BAAQMD, 2005: "Development of a Photochemical Modeling System for the Bay Area Air Quality Management District to Support Ongoing Ozone Air Quality Analyses." Final Report prepared for the Bay Area Air Quality Management District, San Francisco, CA, January 2005.

EPA, 1991: "Guideline for Regulatory Application of the Urban Airshed Model," U.S. Environmental Protection Agency, Office of Air Quality Planning and Standards, Research Triangle Park, NC 27711, July 1991 (EPA-450/4-91-013).

EPA, 1999: "Draft Guidance on the Use of Models and Other Analyses in Attainment Demonstrations for the 8-Hour Ozone NAAQS." U.S. Environmental Protection Agency, Office of Air Quality Planning and Standards, Research Triangle Park, NC 27711, May 1999 (EPA-454/R-99-004).

Grell, G.A., J. Dudhia, and D.R. Stauffer, 1994: "A Description of the Fifth Generation Penn State/NCAR Mesoscale Model (MM5)." NCAR Tech. Note, NCAR TN-398-STR, 138 pp.

Morris, R.E., G.M. Wilson, G. Yarwood. T.Darlington, J. Heiken, J.Heuss, G. Wolff, A. Dunker, S. Yamazaki and S. Chatani, 2002: "Evaluation of the Air Quality Impacts of Zero Emission Vehicles (ZEVs) and a No ZEV Alternative in the South Coast Air Basin of CA". Presented at the 95th Annual Air and Waste

Management Association Meeting and Exhibition, Baltimore, MD, June 24-26.

Tesche T. W., D. E. McNally, J. G. Wilkinson, H. E. Jeffries, Y. Kimura, C. Emery, G. Yarwood, and D. R. Souten, 2004: "Evaluation of the 16-20 September 2000 Ozone Episode for use in 1_hr SIP Development in the California Central Valley." Prepared for the California Air Resources Board, by Alpine Geophysics, LLC, Ft. Wright, KY, O3 Chemistry, NC, University of Texas, Austin, TX, and ENVIRON International Corporation, Novato, CA (AG-90/TS201).

Vizuete, W., D.T. Allen, C.A. Emery, G. Yarwood, H. Jefferies, 2004: "Evaluation of the July 31, 2000 Ozone Episode in the San Francisco Bay Area with the Process Analysis Tool." Prepared for the Bay Area Air Quality Management District, San Francisco, CA, by the University of Texas, Austin, TX, ENVIRON International Corporation, Novato, CA, and the University of North Carolina at Chapel Hill, NC.

Wilkinson, J. G., C. F. Loomis, R. A. Emigh, D. E. McNally, T. W. Tesche, 1994: "Technical Formulation Document: SARMAP/LMOS Emissions Modeling System (EMS-95)." Final report prepared for the Lake Michigan Air Directors Consortium, Des Plaines, IL, and the Valley Air Pollution Study Agency, Sacramento, CA, by Alpine Geophysics, Fort Wright, KY, (http://www.ladco.org/emis/guide/ems95.html).

Wilkinson, J. G., 2004: "Development of the California Integrated Transportation Network (ITN)." Final report prepared for the California Air Resources Board, Sacramento, CA, by Alpine Geophysics, LLC, La Honda, CA (AG-TS-90/155).