# EXECUTIVE SUMMARY

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. Based upon historical air quality measurements within the Bay Area "airshed", the U.S. Environmental Protection Agency (EPA) has designated the SFBA as being in non-attainment of the federal 1-hour ozone standard. Over the years, the BAAQMD has developed and submitted several implementation plans 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. The original 1-hour ozone standard has now been effectively 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 nonattainment 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 described in this report was a rather complex and highly interactive endeavor; it would be nearly impossible (and not particularly useful) to document every detail associated with the modeling and analyses undertaken in this study. Thus, only the highlights and model results fundamental to the ultimate goal of providing a working, reliable, and scientifically sound modeling system are presented herein.

This report provides an updated photochemical modeling protocol that describes 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. The report also includes a conceptual model review for ozone events in the SFBA and an episode typing analysis as part of the modeling episode selection process. The original protocol (ENVIRON et al., 2002) was developed at the beginning of the project to establish model selection and application/ evaluation methodologies, and to provide peer and stakeholder review and acceptance of the proposed approach.

## PURPOSE AND GOALS

The original purpose of the current study was to modernize the District's modeling capabilities to align with the modeling systems to be evaluated by the CARB under the CCOS program, and to use those systems to develop a new photochemical modeling database to support the 2004 Bay Area SIP revision. With the recent elimination of the need to submit a 2004 SIP revision for 1-hour ozone, the objectives of the study have shifted slightly, but the overall focus remains the same.

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

> Immediate and foremost goal:
> Provide the District with a photochemical modeling system and technical analyses consistent with CARB to support future Bay Area SIP submittals, including assessment of projected future year ozone levels in the SFBA, examination of local and regional control strategy effectiveness, and analyses of the impact of those strategies on regional ozone throughout central California.
>
> Longer-range goal:
> Provide the District with a modern tool base that they can use to build a modeling "climatology", consisting of many additional historical episodes with which to evaluate local/regional ozone patterns and issues surrounding inter-basin transport.

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

Both of these phenomena can be addressed from the photochemical modeling system developed in this study. Pollutant mass transport can be explicitly addressed because the modeling domain used in this study extends well beyond the SFBA, thus accounting for such air mass movement within the modeling system. The movement of vehicles can be addressed through the use of complex transportation model output results being used in estimating mobile source emissions. Such transportation models are used by Metropolitan Transportation Commission (MTC) in the San Francisco area, and Sacramento Association of Governments (SACOG) in the Sacramento area. As described earlier, Alpine Geophysics developed a California-wide Integrated Transportation Network that should facilitate such analyses in the future.

## MODEL SELECTION

Based upon the District's suggestions for consistency with their preexisting modeling tools and those to be evaluated by the CARB for CCOS, the original scope specified the use of the following models:

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|---|---|
| Emissions Processing: | Emissions Modeling System, 1995 version (EMS-95) |
| Meteorological Modeling: | Regional Atmospheric Modeling System (RAMS) |
| Photochemical Modeling: | Comprehensive Air quality Model with Extensions (CAMx) |

This modeling system was originally selected for this study because it contains all of the technical features necessary to simulate ozone air quality in the SFBA and throughout California. The same EMS-95 emissions processor and input databases used by the CARB were used in this project to assure CARB compatibility and acceptability. 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. Meanwhile, the CARB has utilized the Fifth Generation PSU/NCAR Mesoscale Model (MM5) for their CCOS modeling effort. The original protocol was therefore revised to include an inter-comparison of RAMS and MM5 performance and to select the most appropriate for use in the photochemical modeling component. Ultimately, the District also undertook MM5 simulations on their own and we evaluated both CARB and District MM5 applications in this project. The CAMx photochemical grid model was selected for the modeling system as it is publicly available, contains all of the technical options needed to simulate ozone in the Bay Area, and contains some superior capabilities to the other state-of-science models.

## EPISODE SELECTION

Episodes used for this analysis needed 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. 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 CARB and other 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.

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 regions; 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): July 11-12, 1999; June 15, 2000; July 31, 2000; and July 9-10, 2002. 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 initially elected four exceedance days for the SIP modeling, in the following order:

1) July 31, 2000
2) June 15, 2000
3) July 11 and 12, 1999.

The June and July 2000 days occurred during the CCOS, and both of the 2000 days fell into the "Type 2" episode category. The 1999 days represent the other frequently occurring ozone pattern category. July 11 was a Sunday and July 12 was a Monday, which satisfied the need to evaluate weekend-weekday issues. Data for this period was quality assured and archived by various agencies. Also, the July 1999 episode experienced more widespread Bay Area exceedances than other periods (3 per day). 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 Valley. Ultimately the June 2000 episode was dropped from consideration since it was a redundant "Type 2" category and was not considered by CARB in their statewide modeling analyses.

## SUMMARY OF MODELING APPROACH AND RESULTS

### 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 sea breeze flow within the marine layer with the easterly large-scale flow forced by the subtropical high. 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.

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. We have pointed out various issues with the input datasets that have been used for the verifications and the four-dimensional data assimilation schemes.

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 a 1 km resolution grid, it is our opinion that even higher resolution may be needed to resolve the important topographical features and land use features such as coastlines, wetlands, urban areas, etc.
- With the higher resolution also comes the need for higher resolution datasets of topography and land use, since the datasets used by atmospheric models are usually 30 second (about 1 km) resolution. Much higher resolution datasets do exist, especially for topography.
- There was no information on which areas were in active irrigation during these episodes. There was circumstantial evidence that various areas were active, since stations located very close together in the Central Valley sometimes had very different temperatures and dewpoints.

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.

There is one other important meteorological modeling implication of the elevated convergence zone. It is imperative in these complex layers of stability that the subgrid scheme employed in the meteorological model be able to correctly treat elevated well-mixed, neutral layers. Models such as MM5 use simple, surface-based PBL schemes that 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) overemphasizes the effect of the surface stable layer and shuts 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.

**MM5 Meteorological Modeling**

Initial MM5 simulations were performed for the CCOS July/August 2000 episode by the CARB and their meteorological modeling contractor at NOAA/ARL, concurrent with the initial ATMET RAMS simulations undertaken for the District. Later, the BAAQMD instituted their own internal MM5 modeling effort for the July/August 2000 episode. Subsequent MM5 modeling of the ancillary July 1999 episode was undertaken by both the CARB and BAAQMD.

A case study was carried out for the July/August 2000 CCOS period in which the output from various CARB and BAAQMD MM5 simulations was compared with the wind profiler/RASS and surface observations of wind, temperature, and humidity. The meteorological model was run on a 36-12-4 km one-way nested model domain of 50 vertical levels, with the 4 km domain encompassing the CCOS 2000 field study area. 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, the NOAH land surface model (LSM), and FDDA.

The direct meteorological comparison between the model simulation and the observations from the CCOS 2000 field experiment indicates 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. Overall, the MM5 configuration using the Eta PBL with NOAH LSM and FDDA was the best performer for all parameters and in all areas. Good agreement was found between the area average observed and simulated boundary layer heights except for the area immediately inland such as the San Francisco Bay Area.

The CARB and BAAQMD conducted MM5 modeling of the July 9-12, 1999 period using the MRF PBL scheme, the 5-layer soil model, 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 the 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 the screened/improved observation dataset, and runs testing the impacts from using the Eta PBL scheme and the NOAH LSM.

Graphical and statistical results show that the original CARB run consistently performed better than any BAAQMD FDDA sensitivity test. Analysis nudging improves wind speed performance in the SFBA, but it is clearly the worst run in all other respects. The 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 the 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. Results from tests using the NOAH LSM were not available in time for this report.

The "best" MM5 simulations for this episode are 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.

## 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 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, 2004d, 2004e).

Although EMS-95 is capable of preparing biogenic emission estimates, the CARB used the Biogenic Emission Inventory Geographic Information System, or 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/August 2000 CCOS episode was characterized by a heavy contribution from forest fire smoke, particularly from fires in the southern Sierra Nevada. 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-August 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 1-hour ozone SIPs in California. A special set of "fire-augmented" boundary conditions were developed for the July/August 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.

## CAMx Applications

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

### Developmental Simulations

Since the fall of 2002, when the initial emission inventory and preliminary meteorological simulations first became available, ENVIRON and the BAAQMD have conducted on the order of 50+ CAMx simulations. Considered to be "developmental" model applications, most of these runs were made for the July/August 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 CB-IV chemistry mechanism. A mixture of RAMS and MM5 meteorology were used to drive the photochemical model.

Developmental CAMx simulations were discussed at the Model Advisory Committee meetings, and the results have also been documented on the project web site (www.environ.org/basip2004/results.html, user=basip2004, password=goldengate) through early spring of 2004, when the CAMx modeling effort shifted primarily from ENVIRON to the Bay Area District. Throughout the course of these CAMx applications, two key performance issues constantly emerged in both modeling 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 the 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.

It should be noted that the CB-IV chemistry mechanism was used in the developmental simulations because of it's speed and the preponderance of evidence (by many groups involved in CCOS) that the common signal from SAPRC99 is a <10 ppb increase in peak simulated ozone levels formed from NOx-rich urban environments. That is, the SAPRC99 chemical mechanism was not seen as the key solution for the various California-wide under prediction problems, but was rather reserved as a final "polish" once an acceptable BAAQMD simulation was achieved and all major inventory and meteorological improvements were stabilized.

The specific sensitivity tests conducted as part of the developmental process (excluding the numerous major meteorological and emission updates) included the following:

- Impacts from reducing area + mobile NOx by 30%
- Impacts from increasing area + mobile VOC emissions by 50%
- Impacts from increasing biogenic VOC emissions by 50%
- Impacts from NOx+VOC mobile emission scaling to reflect Harley (2003) emission estimates based on basin-specific fuel consumption
- Impacts from using EPA CB-IV speciation profiles in place of CARB profiles
- Impacts from reducing winds speeds 50%
- Impacts from reducing PBL depths by 50%
- MM5 vs. RAMS meteorology
- Use of high-resolution meteorological fields (~1 km grid spacing)
- Influences from initial and boundary conditions
- Role of fire emissions
- Role of temperature on biogenic emission rates and ozone predictions
- Role of temperature on motor vehicle emission rates and ozone predictions
- Impacts from invoking the Plume-in-Grid option
- Impacts from invoking drought stress (affects deposition rates)
- Impacts from reducing horizontal diffusion by a factor of 3

Results from these tests are summarized in Section 7 of this report. Additional information for each run is provided on the project web site at the "CAMx Results" link (www.environ.org/basip2004) and in the MAC presentation documents provided at the "Documents" link.

Performance Evaluation for VOC

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/August 2000 episode in the Bay Area, Sacramento Valley, and San Joaquin Valley (Emery and Tai, 2004b). Our conclusions from this analysis are as follows:

- The 3-hour canister data from most CCOS sites exhibited very few hydrocarbon species samples relative to the 1-hour GC-MS sites. Because of this, the 3-hour dataset did not provide sufficient information over CB-IV species and/or time period to allow inclusion into our analysis. We therefore believe the 1-hour data to be more robust.

- In spite of the assertion above, there still exists large uncertainty concerning overall data quality in the CCOS VOC dataset, both for canister and GC-MS samples. While certain findings from the analysis reported here 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.

- We wish to stress that the performance results reported here should not be taken as an implication of the emissions inventory only. If we are to believe the measurement data, then certainly some aspects of the results (e.g., significant differences for certain species, disagreement among observed/predicted VOC:NOx ratios) are likely associated with deficiencies in emissions, either in total mass, speciation profiles, temporal profiles, spatial allocation, etc. However, there exists a large range of plausible explanations that involve meteorological performance (inaccurate mixing heights, wind field errors that cause the modeled urban plumes to miss the monitors, etc.), and at this point none of these should be ruled out.

- 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). Second, the model lacks sufficient levels of higher aldehydes (ALD2), usually by large factors of 2 or more. This is a surprising result and possible explanations are made difficult by the fact that model-to-sample comparisons are largely an "apples-oranges" dilemma. Most ALD2 in the model is secondarily formed with some contributions from emissions (e.g., biogenics). ALD2 in the measurements is primarily from direct emissions, pieces of which are allocated to the CB-IV ALD2 bin for reactivity purposes (i.e., they are not necessarily carbonyl type compounds).

- VOC performance in the SFBA showed consistent under predictions of total VOC. A large discrepancy between 1-hour and 3-hour samples at Sunol (mainly PAR) remains unexplained. The Sunol site indicates under predictions for reactive species (OLE, TOL, XYL) in both 1-hour and 3-hour samples. There is evidence from Bodega Bay that background levels of PAR are too low, although this could be caused by old smoke plumes originating well to the north of the CCOS domain. Generally, performance for individual CB-IV species other than PAR was acceptable (with a few exceptions). Limited VOC:NOx ratio data and predictions indicate that the east bay is NOx-rich.

- VOC performance in the Sacramento region indicates mixed performance for total VOC on August 1. Granite Bay indicates just a slight over prediction of 1-hour data, with generally good performance across CB-IV species, while San Andreas shows significant under predictions of 3-hour PAR, OLE, and carbonyls. There were insufficient data to compare 1-hour and 3-hour data at Granite Bay. Observations and predictions of VOC:NOx ratios at Granite Bay agree that conditions east of Sacramento are NOx-rich.

- VOC performance in the SJV region showed consistent under predictions of total VOC, with especially poor performance at the Parlier GC-MS site. CB-IV species were under predicted across the board at that site. Results in Turlock were better, with a slight under prediction of total VOC from low PAR, OLE, and ALD2. There were insufficient data to compare 1-hour and 3-hour data at Parlier. VOC:NOx analyses also suggest a problem with disproportionate VOC and NOx emissions in the SJV.

Application of the Process Analysis Tool

Vizuete et al. (2004) detail the application of the Process Analysis 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 v4.03, with process analysis code modifications applied by the University of Texas (UT). Other code differences between v4.03 and v3.10 (used in developmental simulations) are minor and do not lead to significant differences in air quality predictions. ENVIRON configured version 4.03 of the model to run a process analysis domain over the eastern San Francisco Bay Area and ran the model for the episode. Evaluation of the Integrated Process Rate (IPR) and Integrated Reaction Rate (IRR) output generated for the Bay Area PA domain was then performed by UT. 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.

The low concentrations of reactive VOCs in the atmosphere were not consistent with observed VOCs. The model under predicts the amount of highly reactive VOCs (toluene, olefins, xylene, and aldehydes) 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.

Use of the Decoupled Direct Method for July 1999

ENVIRON invoked the Decoupled Direct Method (DDM) probing tool in CAMx v4.03 to investigate the sensitivity of ozone to boundary conditions of ozone, VOC, and CO. Further, the DDM was used to assess ozone sensitivity to emission categories and source regions as a first glimpse into potential transport impacts. The maximum Bay Area ozone sensitivity to boundary conditions relative to total peak ozone in the east bay was ~35% in these tests (mainly from north boundary ozone and VOC). However, the key result of the boundary condition analysis is that the low model top (~5 km) and fairly large ozone top boundary conditions specified by the CARB (70 ppb) do not significantly impact model performance in areas of central California where high ozone is simulated.

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, VOC, and CO emissions (as opposed to boundary conditions). More anthropogenic and/or biogenic VOC will increase ozone in the east bay, while less anthropogenic NOx will also increase ozone. Ozone in the southern Sacramento and northern SJV regions is modestly sensitive to Bay Area NOx and VOC emissions (sensitivity coefficients are ~10 ppb). 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.

Summary of BAAQMD CAMx Simulations for CCOS 2000

We have shown that the MM5-CAMx couple using the SAPRC99 chemical mechanism produced reasonable predictions 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. 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, respectively).

Locations of the wind convergence zone and the locations of simulated high ozone were found to be closely related. The overall surface-wind patterns in the SFBA are similar in the 3 MM5 runs used to drive CAMx, but there are 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 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.

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 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 this area.

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.

CAMx tests conducted with different chemical mechanisms used the CARB MM5/MRF meteorological inputs. Ozone performance differences between the two mechanisms were minor on all days and for all three analysis regions; this result is much more in line with expectations as opposed to the surprisingly higher peak ozone achieved in the July/August 2000 episode using SAPRC99 over CB-IV. This difference in sensitivity among the episodes apparently is related to the different local meteorology (which differs substantially from the CCOS episode) than any differences in emissions (which are very similar among the episodes). However, it is difficult to explain how the meteorological differences play into the CB-IV/SAPRC chemistry differences. Tools such as Process Analysis are needed to further understand the source of the CB-IV/SAPRC signal among these two episode.

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.

## 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. For approximately the last 24 months, 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. In fact, that objective is already achieved, in large measure through the very effective technical oversight and guidance provided by the District's Modeling Advisory Committee.

The main impetus for this developmental effort had been the historical exceedance of the National and California 1-hour ambient air quality standards for ozone. With the newly affirmed National Ambient Air Quality Standards for 8-hour ozone and PM2.5, the scope and purpose of the photochemical modeling in the Bay Area must also be expanded to maintain technical credibility with the U.S. EPA, CARB, other Districts, and other agencies such as MTC and ABAG. The current photochemical modeling system is able to address issues of 1- and 8-hour ozone as well as PM2.5.

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 region 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.

Many key achievements have occurred during this developmental effort.

- The District has developed an air quality modeling capability for two meteorological episodes, one (July 1999) that is fully characteristic of a multi-region buildup/transport case, and one that fulfills CARB's recommendations for modeling an intensive monitoring event (July/August, 2000).

- The District has contributed significantly to the CARB's compilation of the CCOS air quality and meteorological database, particularly in the area of quality assurance and control.

- The District has contributed significant and substantial improvements to the CARB's ozone precursor emission inventories (NOx, VOC, and CO) to provide the most accurate and comprehensive modeling inventory for the Bay Area and Northern/Central California.

- The District has fully engaged the CARB, other districts, other state agencies, environmental groups, industry, and EPA and MTC, among others, through the Modeling Advisory Committee;

- The framework has been set for a continuation of state-of-the-science photochemical (including 8-hour ozone, PM2.5 and air toxics) modeling in the San Francisco Bay Area.

As the District moves forward with air quality planning in the Bay Area, it will need to continue to develop this expertise.

**Improve Meteorological Modeling**

As described in this report, meteorological modeling has been conducted by several groups involved in CCOS. All models employed to date exhibit key performance problems, mostly related to the complex geography of the central/northern California modeling domain. Work must continue in this area to:

- Continue to improve meteorological modeling for both 1999 and 2000 episodes, based on Bay Area specifics such as climatology, topography, land-sea interactions;
- Refine existing modeling (meteorological and photochemical) capabilities to 1 km cell size (or smaller) to allow for better capture of terrain influences on flow and dispersion characteristics;
- Consider examining the utility of using RAMS simulations completed to date as a guide for further improvements in MM5 simulations;

- Explore the utility and possible improvements related to use of WRF;
- Evaluate 2002 episodic modeling being carried out by DRI;

**Improve Precursor Emissions for Future Years**

A very large effort has been put forth to develop episodic base-year emissions (July 1999 and July/August 2000). Work must continue to finalize future year base case emission forecasts of NOx, VOC and CO and to address alternative future emissions for assessing possible control strategy impacts on future year ozone:

- Refine existing emissions modeling capabilities to 1 km cell size (or smaller) to allow for better sub-regional impact assessments for planning decisions;
- Provide both tabular and graphical representation of emissions and emissions changes from 2000 and 1999 base years, both spatially and temporally as appropriate (by source category, etc.), for future years;
- Quality-assure all emission estimates received from CARB and correct identified errors;
- Prepare future year model-ready emissions files.

While the U.S. EPA 8-hour ozone implementation rule does NOT require ozone modeling for an area designated as "marginal", such as the Bay Area, being able to quantify the effect of emissions changes upon future 8-hour ozone levels is important in answering two logical questions: 1) What is our future air quality expected to be, and how much within the standard are we estimated to be (i.e., what is our expected "headroom" for growth)? 2) How do our emissions relate to attainment of the 8-hour standard in those areas that MUST (according to the same U.S. EPA rule) carry out photochemical modeling of attainment of that standard, such as Sacramento and San Joaquin Valley? Work must continue in this area to:

- Develop emissions for additional future year base case episodes similar to that already done for the current BAAQMD 1-hour study, but for additional 8-hour attainment years. At this time, two future years will need to be examined: 2007 (Bay Area attainment year) and 2013 (San Joaquin Valley and Sacrament attainment year);

**Enhance Modeling System Utility and Sensitivity Assessments**

While we have many fine technical assessment tools available through our work to date, the complexities of meteorological and photochemical modeling are well addressed through the use of visualization techniques and so-called "probing tools." The visualization techniques serve a diagnostic use to the technical person, but equally important, allow a better communication of results to decision makers and the public.

The cause-effect relationship between pollutant emissions and air quality are at the heart of the purpose of the photochemical modeling system. Once the system is believed to be offering acceptably accurate performance, it is critical to begin to examine the relationship between various emission sources or other assumptions and the resulting air quality predicted by the modeling system. Such sensitivities include: altering the emissions from certain major point sources, area sources, or categories of such sources; altering assumptions on growth rates and patterns (future vehicle counts and emission factors by type mix; population density, urban growth boundaries and land use changes, etc.); altering transportation assumptions (VMT and travel demand from various alternative transportation plans, mass transit vs. private auto, etc.); altering assumed technical assumptions in the models themselves that may affect the response of the model to emissions changes (vegetative distribution and emission rates for biogenics, assumed fire emissions, certain meteorological parameters, deposition algorithms, etc.).

The following should be carried out for both the 1-hour and 8-hour ozone standard as appropriate:

- Conduct extensive "Probing Tool" applications to fully describe likely cause-effect relationship between emissions (growth, distribution, source types, controls) and air quality changes (both temporally and spatially). Special attention should be focused upon effects of Bay Area control on downwind regions of SJV and Sacramento; transport and valley growth impacts on Bay Area air quality; transportation improvement impacts; port activity emissions control impacts; etc.;
- Given input from various local agencies, examine longer term effects of alternative assumptions on growth (population, VMT, vehicle mix), land use changes, and alternative economic assumptions;
- Design and develop “EKMA-like” NOx/VOC/ozone isopleths resulting from a series of CAMx simulations at key sites throughout the Bay Area where air quality assessments are most critical for attaining and maintaining the air quality standards.

**Assess Impacts of Future Ozone Strategies**

As just described, the cause-effect relationship between emissions changes and ozone air quality changes, both within the Bay Area modeling domain and within the much larger CCOS domain (thus including the San Joaquin Valley and Sacramento regions) will be characterized in terms of sensitivities. As a result, initial insight will be available as to which emissions reductions would be most effective (on a ton for ton basis) in reducing ambient ozone in various areas of the study domain. That information will be extended to characterize the specific air quality changes that are likely to result in various emissions reduction measures and groups of measures (strategies), as appropriate for 1-hour and 8-hour ozone standards:

- Review current proposed control measures, and identify additional “most probable” measures that are identified for further study;
- Estimate emissions reductions (or changes) resulting from the implementation of such measures to all applicable sources of such emissions;
- Develop combinations of proposed control measures, thus composing one or more emissions control strategies;
- Execute the emissions preprocessor system to estimate the emissions reductions associated with the selected sets of control strategies;
- Using “EKMA-like” ozone response curves, identify the control strategies that are likely to provide acceptable future ozone levels;
- Refine and expand on likely candidate control strategies through detailed and specific CAMx modeling results of ozone concentrations in the modeling domain.

**Assess Alternative Episodes**

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. Episodes need to be selected carefully so that the analysis has the maximum credibility and broad applicability. Furthermore, the CARB and other 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 modeling episodes to be used by the CARB and other districts.

At the time of episode selection for the work done thus far, the District was tasked with developing a revised SIP to attain the 1-hour ozone standard. While we believe that the episodes ultimately chosen for the current effort would provide an adequate base for initial 8-hour ozone assessments as well, the BAAQMD will be cognizant of more recent ozone episodes that have occurred in the 2001-2003 8-hour designation period (or new summer episodes in 2004 and later) to update their modeling library. The following should be carried out:

- Revisit methods used in the previous 1-hour ozone episode selection and determine the degree to which these methods should also be used in the evaluation of an 8-hour episode. Recommend alternative evaluation techniques as appropriate;
- Examine episodes that have occurred in the 2001-2003 time period (and later) and characterize them in a manner similar to that used in characterizing 1-hour episodes for July 2000 and July 1999;
- Rank both the 2000 and the 1999 episodes, along with episodes in the 2001-2003 time period for potential value for additional air quality modeling.