

ENVIRON

MEMORANDUM

To: Bay Area 2004 SIP Modeling Advisory Committee (MAC) Participants

From: Chris Emery,
BAAQMD Staff and Management

Date: September 6, 2002

Subject: Response to comments received on the draft Modeling Protocol.

By August 1, 2002 the Bay Area Air Quality Management District (BAAQMD or District) and ENVIRON received comments on the subject protocol from the following MAC members:

- Carol Bohnenkamp, U.S Environmental Protection Agency, Region IX (EPA IX);
- John DaMassa, California Air Resources Board (CARB);
- Bob Nunes, Monterey Bay Unified Air Pollution Control District (MBUAPCD);
- Steve Ziman, Western States Petroleum Association (WSPA);
- Rob Harley, University of California at Berkeley.

We have placed these comments on the project web site (www.environ.org/basip2004). To a large extent the comments received expressed similar concerns among the reviewers. In fact, the bulk of comments could be easily grouped into the following broad categories:

- 1) Episode Selection
- 2) Domain/Grid Extent and Regional Transport
- 3) Model Evaluation Methodology
- 4) Emissions Processing

Other comments received concerned various miscellaneous issues, and minor edits to the text.

ENVIRON and the BAAQMD management and staff appreciate the MAC members' time and effort to review the draft Modeling Protocol and to forward their thoughtful comments, questions, and issues to our attention. This memorandum attempts to address the concerns raised from this review in a succinct manner. Since so many of the comments could be grouped under the four topics listed above, and were quite similar in nature, we provide a general response under each topic area. This alleviates the need for repetitive responses for each individual reviewer comment. Other miscellaneous comments are addressed individually. The minor text edits were all applied directly to the revised protocol.

EPISODE SELECTION

Comments on this subject primarily focused on the need to provide a representativeness analysis in the protocol for the two CCOS episodes to be modeled. The revised protocol will include the results of such an analyses for exceedance events from 1995 to 2001. As the study progresses and additional results from CCOS are made available, the final project report will include additional references and discussions of episode characterization.

Upon further inspection of ambient ozone data from the CCOS period, it became quite evident that these episodes either lack sufficiently high ozone (as in the July-August case with a peak of 126 ppb), or will be quite difficult to model given the extreme localization of exceedance-level ozone in Livermore. Furthermore, both of these episodes are quite similar in nature and fall into just one of the two major categories identified from cluster analyses (discussed in the revised protocol). Two monitors were in operation in Livermore during the summer of 2000, Rincon Avenue and First Street, separated by only ~1.5 km. During the June 15 episode the highest 1-hour ozone was 152 ppb at Rincon and 137 ppb at First Street. The 15 ppb difference could be explained by the effects of local sources, probably higher NO_x at the First Street site, but the time averaging of the data may also have contributed to the difference (caused by differences in when the peak ozone arrived at a given site). The next highest ozone reading in the Bay Area on June 15 was only 86 ppb at Concord (a difference from the peak of 66 ppb). Our experience with photochemical models warns us that replicating the conditions in Livermore on June 15 will be incredibly difficult, even with a 1-km grid spacing.

Therefore, we have decided to include a third episode to (1) augment the chosen CCOS periods for wider representation of episode types (including ability to evaluate weekday/weekend effects), and (2) provide a backup episode to the CCOS periods in case acceptable model performance is not achieved. Given the limited ozone exceedances in the Bay Area during the summer of 2000, we decided to choose an episode among several that occurred in 1998 and 1999. Review of ozone measurements from these two summers reveals a good set of widespread multiple-day ozone events. The event in July 1999 is especially attractive as it includes high ozone over a weekday/weekend period; this would directly address concerns raised by the MAC regarding the effects of ozone control strategies on day type. This approach has been discussed with John DaMassa at CARB, and he concurs with the approach for a third episode. The protocol has been updated to include a description of the chosen episode, and procedures for additional emissions processing outside the CCOS period.

DOMAIN/GRID EXTENT AND REGIONAL TRANSPORT

Comments on this subject concerned the size/extent of the 4-km nested grids in the meteorological and air quality models, the effects of nesting on the proper simulation of regional transport, the vertical depth of the air quality modeling domain, and the ambiguous language in the protocol suggesting less emphasis on the analysis of regional transport.

We recognize that the evaluation of control strategy impacts on regional transport is an



important aspect in the development of a SIP plan. This is in fact mentioned in the draft protocol. However, we agree with reviewer comments that the language concerning transport was rather ambiguous in several areas of the protocol, further suggesting that this was not to be addressed in the study. We have revised the protocol to remove this ambiguity; indeed the impacts of Bay Area controls on ozone transport to neighboring basins and districts will be addressed in the simulations, both explicitly and implicitly given that the entire modeling domain encompasses all of the central California non-attainment areas. In other words, every control strategy/sensitivity simulation run will show the ozone impacts throughout the domain, and any downwind dis-benefits predicted by the model will be seriously considered by the District.

We now turn to the specific grid configuration. First, it should be noted that both RAMS and CAMx utilize two-way grid nesting. This means that the grids are run simultaneously, whereby information is allowed to pass up-scale and down-scale between the grids interactively. Models that can only run in one-way nested mode require that each nest be run separately, and that information is only transferred in the down-scale direction from coarse resolution grids (run first) to higher resolution grids via boundary conditions. This can certainly have a dire impact on accurately resolving transported mass across grid boundaries. Depending upon how the meteorological data are developed, one-way nesting can also lead to inconsistent realizations of mass fluxes (e.g., different directions) on the grid boundaries. Two-way nesting, as will be used in this study, avoids both of these problems.

Concern was raised as to whether an adequate meteorological simulation could be realized in the central valley if the 4-km RAMS grid does not include the northern and southern boundaries of the valley. Since the 4-km RAMS grid is two-way nested within a 12-km grid, the effects of the northern and southern boundaries are directly included in the simulation, albeit at a coarser resolution. This would not be expected to result in an unacceptable simulation of mesoscale meteorology in the central valley. However, the District has requested that the 4-km RAMS grid be expanded to cover the same area as the CCOS 4-km modeling grid as a way to maximize flexibility in running various 4-km nests in CAMx. This allows the RAMS 4-km grid to cover the entirety of the central valley. The revised protocol reflects this change.

Another concern raised the possibility of mass reflections in the air quality model at a fine-coarse boundary interface and its effects on properly treating regional transport from the Bay Area to downwind areas in the 12-km domain. Reflective properties at grid boundaries are generally associated with wave energies within meteorological models; air dispersion models (at least CAMx) are simply large mass accounting programs that determine fluxes cell-to-cell and so should not cause mass reflections on grid boundaries (we certainly have never experienced this with any photochemical model).

A more legitimate concern is the proper resolution of urban plumes exiting the Bay Area and moving out to the 12-km domain. Several reviewers expressed concerns that sudden dilution effects crossing from 4 to 12 km grids would tend to artificially diffuse the plumes thereby possibly under predicting Bay Area contributions to ozone downwind. This can present a

problem if the grid structure is not carefully designed (i.e., the fine grid boundary is moved too close to the key source area). In the draft protocol, the 4-km grid was set to cover the Bay Area and major urban areas directly downwind, to include Stockton, Modesto, Sacramento, and Monterey. This establishes a consistent grid structure for medium-range transport to and from these areas. As urban plumes move downwind, they will become more widespread and diffuse, and at some point are resolved just as well with the coarser 12-km grid spacing. The distance from the southern Santa Clara Valley and Livermore to Fresno is nearly 200 km. It is felt that the Bay Area ozone (and NO_x) plume, as diffuse as it may already be in exiting the Bay Area, will be sufficiently resolved with 12-km grid spacing out to Fresno and Bakersfield. This issue could be evaluated by additional simulations.

Bob Nunes made a strong case to extend the 4-km nest further southward as the current edge was placed at just about the location of Pinnacles National Monument, where an important monitoring site is located. We have made this modification in the revised protocol. No other changes were made to the extent of the 4-km grid.

Several reviewers were concerned about the depth of the air quality modeling domain. A depth of 3-4 km was described in the draft protocol. Several salient points were raised concerning this height relative to the topography in the domain, and possible impacts on vertical circulation systems. We have therefore increased the depth of the domain in the revised protocol to 7-8 km. We have also added detailed layer structure definitions in the text to provide readers with more information concerning vertical resolution in both RAMS and CAMx.

MODEL AND CONTROL EVALUATION METHODOLOGY

Comments were received concerning the evaluations to be employed for both RAMS and CAMx. Both are addressed below.

For RAMS, comments centered on a lack of any discussion on “mechanistic” or “phenomenological” analyses, as opposed to relying on statistical comparisons between predictions and observations over the entire domain. First, we agree that statistics calculated over the entire domain are not particularly revealing. The RAMS tool called REVU-GS does allow sub-regional statistical performance measures to be calculated, and the protocol section on statistical analyses has been revised accordingly. Second, a discussion on mechanistic evaluations of RAMS performance has been added, including possible data sources (satellite, etc.) to facilitate such analyses. The evaluation of slope-flows, location and formation of maritime stratus, boundary layer depths and wind flows, and three-dimensional trajectories, are all discussed.

Understandably, a wide range of comments were received concerning the evaluation of CAMx base case performance and the effects of emissions reductions. Issues included comparing CAMx simulations to CARB’s modeling results, using probing tools to bolster the analyses, uncertainty, probabilistic, and significance evaluations, and performance on sub-domains. All



of these comments were quite helpful. The protocol text has been revised in an attempt to clarify that the evaluation of CAMx for the base case and for the emission reduction tests will rely on a flexible evaluation approach, using the data and tools available to the project study team as schedule and resources permit. Many of the comments are directly addressed in the revised text.

Sub-regional performance in replicating base year ozone will certainly be a key to the performance evaluation. The focus will be on the quality of the Bay Area ozone simulation, but certainly if performance in other sub-regions is far outside that which is typically achieved, then an investigation into possible compensating errors will need to be undertaken. However, marginal performance in southern San Joaquin Valley, for example, will have less bearing on accepting a base case simulation than will marginal performance in areas much closer to the Bay Area, such as Stockton or Sacramento. The approach should not force acceptable performance by choosing from available meteorological simulations, or setting initial/boundary conditions, that serendipitously result in the best CAMx performance. Instead, the approach should evaluate the reasons for good and/or poor performance. If, after a good-faith effort, an acceptable simulation is not possible for a given episode, then it should be rejected from consideration in the analysis of SIP controls. See a discussion to this effect in the draft and revised protocol document, under Section 7: Approach to Model Performance Evaluation.

Comments associated with uncertainties in addressing weekend/weekday effects should be satisfied by the addition of a third episode as described above.

EMISSIONS PROCESSING

The following issues were raised concerning emissions development for base and future years:

- The specific data files provided by CARB to the study team;
- The loose usage of “VOC” (volatile organic compounds) in the draft protocol versus “TOG” (total organic gasses), which of these will be provided by CARB, and which of these will be used by the air quality modeling;
- The need to include soil/biogenic NO_x;
- The need to examine/improve NO_x from marine vessels;
- The use of 2000 census data in surrogate development;

The draft protocol has been revised accordingly to include new sections for the development of biogenic NO_x and marine emissions. The specific emission data files and formats to be acquired from CARB have been updated. A new section was added detailing how emissions for a third non-CCOS episode will be processed for modeling. Other portions of the emissions processing approach have been expanded to provide more detail. As described in the revised protocol, CARB’s current 4-km and 1-km spatial surrogate files to be used in this study are based on pre-2000 conditions; developing new activity and surrogate data using 2000 census data is beyond the scope of this study, and would depart from CARB’s emissions database.



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MISCELLANEOUS ISSUES

John DaMassa and Steve Ziman commented on the specification of initial and boundary conditions. The draft protocol has been revised to expand on that topic, to include the use of aircraft data if and where available, and to test the influence and sensitivity of initial/boundary conditions on the model simulation.

Rob Harley's comment regarding the Carbon Bond IV chemical mechanism:

“...I am concerned by the inclusion of the Carbon Bond-IV mechanism as part of a “current” and “state-of-the-science” modeling effort. The Carbon Bond IV or “CB4” mechanism provides a description of the relevant atmospheric chemical reactions that form ozone, as summarized by Gery et al. in the late 1980s. Although an up-to-date chemical mechanism (SAPRC99) is mentioned, it is made clear elsewhere in the protocol document (see p. 6-6) that CB4 is the “default” mechanism that will be used in this study, and that SAPRC99 may not be used at all.”

CAMx includes a newer CB4 mechanism (circa 1995) with updated radical termination reactions and isoprene chemistry as used for the EPA OTAG modeling of the eastern U.S. Alternatively, CAMx may also be run with the SAPRC99 mechanism. While SAPRC99 is newer, provides up-to-date reaction rates, and the hydrocarbon lumping scheme resolves VOC more precisely, to our knowledge it has not definitively performed any better than CB4 in terms of ozone air quality model predictions. As an example, in one test that we have conducted in Los Angeles using CAMx, SAPRC99 led to degraded performance relative to CB4 (obviously, conclusions relating the performance of the two mechanisms cannot be drawn based on this single test). SAPRC99 also contains many more reactions and species than CB4, and this leads to model run times are nearly twice that of CB4. Our approach is to use CB4 as the default mechanism in developing the base cases for each episode, and to compare results with SAPRC99 in sensitivity tests. If a clear case can be made for improved model performance in simulating both ozone and precursors over all episodes, then we would use SAPRC99.

Steve Ziman's comment regarding uncertainty and probabilistic evaluation:

“...Under Strategic Issues, I have two which should also be discussed in more detail in later chapters. The first is whether the predictions for attainment can be placed in a probabilistic framework, per some of the work that S. T. Rao has published. The second is whether the changes in ozone with respect to changes in emissions are significant, or within the noise of the system. This has been a real issue in previous regulatory actions, as for instance with respect to the Bay Area refinery NOx rule. Certain agencies considered changes in ozone as real and significant even though the response to emissions reductions was 1 ppb or less. One may think of this as uncertainty analysis, and it needs to be addressed. A reference to recent work by



Moore and Lodergan , under API support, speaks to one approach, and can be found in Atmos. Envir. 35, 4863-4876 (2001).”

We appreciate the potential benefits that are derived from expressing the results of air quality modeling into probabilistic terms, and one cannot argue against the merits of such analyses, especially, as Steve points out, in allowing for a “significance” determination of an ozone response. We are familiar with the work undertaken by Rao and others whereby they systematically altered almost every model input variable and internal parameter in order to develop an output probability envelope. Our understanding is that this approach required a good deal of time to develop, undertake, and evaluate. Unfortunately, the project schedule constraints, and the limited resources available with which to undertake this SIP modeling project, preclude modeling analyses of that order. We will attempt to qualify model uncertainty from the sensitivity and diagnostic analyses discussed in the revised protocol.

Steve Ziman’s comment regarding ozone response surfaces:

“While it is mentioned in the next chapter, I would encourage generation of ozone response surfaces (see page 8-2, Matrix) be done on the base case simulation rather than on the future case simulation. While I recognize that estimates of growth could shift the sensitivity of precursor, a matrix analysis done on the future base case incorporates all of the uncertainties associated with growth projections, and adds uncertainty to the resultant ozone response surface. This is minimized in the base case. Moreover, application to the base case, with generation of response surfaces for many sites allows comparison of these results to those generated through observational modeling. It also allows one to look at reductions and use process analysis to understand how the underlying chemistry responds to reductions.”

We certainly agree with the point that that the process of projecting future year emission estimates leads to a large component of uncertainty that is additive to the uncertainties associated with ozone response surface derived from systematic NOx and VOC reductions. It would be interesting to generate and analyze both base year and future base response surfaces. However, the District needs to develop the response surface for the future year base case so that effects of emission reductions can be directly ascertained, and given the very tight budget and schedule for this study, that will be our intent. If time and budget allow, we will consider comparing the future year base matrix response to a base year response, with the understanding that there will be many competing demands for additional topics to investigate.

Steve Ziman’s comment regarding the development of a plausible “set” of future year base case emission inventories:

“With respect to the future year emissions inventory, the protocol lays out the normal approach to projection to 2006. However, there are few instances in which these projections have really come close to reality on a retrospective review. It is clear that in 1999 no one would have predicted the “dot com” crash, and the impacts that economic event had on area and mobile source emissions. Recognizing that there is

probably little flexibility in the regulatory guidance with regard to use of more than one projected future inventory, there is still need to project a few alternatives so that for some major source categories we have upper and lower bounds estimates. We need to at least make a set of future base case simulations with these alternative projections to see if there are significant differences in ozone reduction. This is particularly important given that most of the stationary sources are already controlled to the point that very little additional reductions will occur within that category regardless of projections. But with mobile and area sources probably responding to different economic projections more than all other sources, and also being the largest categories, alternative future base year emissions inventories should be estimated and simulated.”

At this point, it is our understanding that the CARB will provide only one set of future year base case emissions data for use in the air quality modeling efforts. The emissions control scenarios that will be developed during the study will be applied to the single future year base case. Development and use of alternative future year base case emissions scenarios in an air quality modeling study enhances the study results. However, the process of developing such alternative future year emissions scenarios can be resource intensive. Should additional resources be provided to this study, we would be pleased to examine alternative future socio-economic-land use-transportation network alternatives.