PEER REVIEW OF ARB OZONE MODELING FOR SOUTHERN CALIFORNIA

Report to the
California Air Resources Board
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Summary

The California Air Resources Board (CARB)'s air quality modeling procedures that are underway or being proposed for the 2003 ozone SIP are critically reviewed, and areas of concern and recommendations are summarized. This review is based on a reading of the September 18, 2000 draft of the CARB's ozone SIP modeling protocol document, discussions and meetings with the CARB staff in June 2001, and the reviewer's experience in chemical mechanism development and VOC reactivity modeling. This document gives a summary of what this reviewer sees as an ideal ozone SIP modeling procedure given the current state of knowledge and data availability, and discusses general and specific aspects of the current CARB modeling plan in light of these considerations. It is concluded that for the most part the models and modeling procedures being proposed for use represent the state of the art and incorporate significant improvements over past SIP modeling, but there are potentially significant concerns and recommendations. The major recommendations concern using more episodes in the control strategy modeling to represent the distribution of relevant conditions, discontinuing use of model components, such as the Carbon Bond mechanism, that are out-of-date and have known errors and biases, more comprehensive analysis of uncertainty and bias, and improved documentation of the process and results, especially to policymakers. Recommendations are also made concerning the process for review and external input.

Background

In 2003 California is required to submit a State Implementation Plan (SIP) indicating how it intends to meet ambient air quality standards for ozone in Southern California. Air quality modeling, which is used to estimate the extent to which planned emissions changes will result in air quality improvements, is an important component of this SIP. Ozone is not emitted directly, but is formed from a complex series of reactions of oxides of nitrogen (NO_x) in the presence volatile organic compound (VOC) and sunlight. Because of the complexity and nonlinearity of these processes, modeling provides the only reasonably credible means to estimate the effects of proposed emissions changes on ozone, and thus is the only available means estimate the likelihood that planned controls will achieve the ambient ozone standard in the required time period. However, air quality modeling is an evolving science, and current models have many uncertainties that affect the credibility of their predictions. For this reason, it is essential that the modeling procedures used to support the SIP and other regulatory planning ensure not only that the modeling reflects the best available knowledge and science, but also that the results, and their limitations, are appropriately understood when they are used in formulating public policy.

The California Air Resources Board (CARB), which is primarily responsible for technical support for the modeling needed for the ozone SIP, recognizes the importance of their modeling efforts reflecting the best available science. The CARB has been in the forefront of supporting applied and even some basic research needed to improve its ozone modeling. The CARB was a major sponsor of the 1997 Southern California Ozone Study (SCOS97) to collect data needed to support and evaluate ozone modeling in Southern California. The CARB staff has been working with regional stakeholder agencies in developing a modeling program to support their planning needs. Industry groups such as the Coordinating Research Council and the Electric Power Research Institute provided support to SCOS97 and hopefully will be providing input into the modeling process as it proceeds. This input from stakeholder groups is important to the credibility of the regulatory modeling process but by itself is not sufficient because by definition stakeholder groups have an interest in the results that may affect perceptions of objectivity.

External peer review by appropriate experts provides another means of enhancing quality and credibility of the process. Ideally, the reviewer should not be represent a stakeholder in the process and be able to provide input from an objective perspective. As such, this provides the best complement to stakeholder input. In practice, however, most qualified experts would have some stake in the process as well, particularly with regard to research on modeling analyses or developing model components or inputs. This can be addressed in part by using reviewers with differing areas of expertise and by taking the reviewers interests into account when assessing his or her input. In any case, the CARB requested that the University of California (UC) conduct a scientific peer review of their air quality modeling work in support of 2003 clean air planning requirements. The three reviewers chosen were Dr. Richard Turco of UCLA Dr. Robert Harley of UC Berkley, and Dr. William Carter of UC Riverside, the author of this report. Although Dr. Turco was unable to conduct the review because of contracting problems, both Dr. Harley and this reviewer were able to participate. This report gives the results of the review by the author. His background and experience, and potential areas of conflict of interest that must be borne in mind when assessing this review, are discussed in the following section. This is followed by a brief summary of the review process and then the review itself.

Reviewer Background

Qualifications and Experience

My research concerns the gas-phase atmospheric reactions of volatile organic compounds and the assessment of reactivities of VOCs in the atmosphere. This includes developing chemical mechanisms for airshed models, testing and refining these mechanisms using environmental chamber data, utilizing these mechanisms in airshed models to develop ozone reactivity scales for VOCs, and directing environmental chamber programs to provide data to test the mechanisms and evaluate VOC reactivities. Current projects include developing a new environmental chamber facility for more comprehensive evaluation of mechanisms for gas-phase and particle formation reactions, and developing improved experimental methods for VOC reactivity assessment that can be applied to compounds where environmental chamber methods are not suitable. I am the developer of the SAPRC-99 gas-phase chemical mechanism that is considered by some to represent the current state of the art in this area, and developed the Maximum Incremental Reactivity (MIR) ozone reactivity scale that is incorporated in several VOC regulations adopted by the CARB. More information about my research, list of publications and downloadable versions of most of his recent reports and presentations is available at http://www.cert.ucr.edu/~carter.

I am a past member of the CARB's Modeling Advisory Committee and the South Coast Air Quality Management District's Science Advisory Council and is a current member of the Texas Air Research Center Advisory Board. I am also a past peer reviewer of the EPA's RADM2 model development effort, and in that capacity assisted in the evaluation of the RADM2 chemical mechanism. I am a currently an active participant in the Reactivity Research Advisory Group (RRWG), where I served as the leader of the team developing the Reactivity Science Assessment document and research plan. The RRWG is a partnership of industry and regulatory groups formed to coordinate VOC-reactivity relevant research to inform the development of the EPA's VOC regulation policies.

Potential Conflicts of Interest

Most qualified reviewers in areas of air quality modeling derive some benefit from work related to modeling or model development that may be relevant to the modeling efforts being reviewed. As discussed below, this reviewer is no exception in this regard. This needs to be borne in mind when assessing the comments and recommendations made in this review.

A non-negligible portion of my research has been funded by the CARB, and the CARB has been or is planning to use the results of some of this research in its modeling and regulations. Most relevant to this review is the fact that my SAPRC-99 chemical mechanism is one of the two proposed for use in the 2003 SIP ozone modeling. This mechanism was developed under CARB funding, and a solicited proposal I submitted to evaluate and update it for low NO_x conditions is now being considered by the CARB Research Screening Committee. Past CARB projects supported the development and recent updates to the MIR scale for VOC reactivity, the CARB is currently supporting my project to develop new procedures to evaluate VOC reactivity, and CARB support for additional research concerning architectural coatings reactivity is pending. The CARB, along with various private sector groups, has supported a number of environmental chamber projects in my laboratory, though most of my current funding for environmental chamber studies is from the EPA project to develop the new environmental chamber facility for improved mechanism evaluation. However, a limited amount of support for experiments in this facility is included in the pending CARB project to evaluate architectural coatings reactivity, and additional proposals to the CARB for research using this facility are anticipated. Assessments of uncertainties in the ozone SIP modeling that is discussed in this review may well affect the priorities set by the CARB concerning funding this mechanism development, VOC reactivity, and environmental chamber work.

One of the recommendations in this review is to use consistent speciation assignments in model simulations using different chemical mechanisms. I have submitted pre-proposals to the RRWG and the American Chemistry Council to carry out work to address this need, and if this is funded I plan to ask the CARB to collaborate and provide in-kind support for this effort. This was brought up in the peer review meeting discussed in the following section and in follow-up communications with the Planning and Technical Support and Research Division staff.

Another recommendation in this review is to use the RACM chemical mechanism be used at least for diagnostic purposes in its SIP modeling. If this is adopted, the CARB may ask me to evaluate this mechanism against chamber data or to assist in making emissions assignments utilizing existing procedures and databases developed for SAPRC-99.

Review Process

John DaMassa of the CARB staff provided me with the September 18, 2000 draft of the document entitled "Modeling Protocol for Regional 1-Hour and 8-Hour Ozone Modeling in Southern California for the 2003 State Implementation Plans (Draft #3)". I read the document and provided a series of written questions and possible areas of concerns that can serve as a basis for subsequent discussions to Don McNerny and John DaMassa by email. Brief discussions were held with Arthur Winer of UCLA about the biogenic emissions work and somewhat more extensive discussions were held with Joe Norbeck of UCR about his concerns with the mobile source emissions inventory. I then traveled to Sacramento and spent most of a day in meetings primarily with John DaMassa, Don McNerny, Bruce Jackson, Luis Woodhouse, Paul Allen of the Planning and Technical Support Division, and Dongmin Luo of the Research Division. Eileen McCauley of the Research Division, Ed Yotter from our Mobile Source Analysis Branch, Michael Benjamin from the Emissions Inventory Branch and Jinyou Liang of my staff was also present. Of the Planning and Technical Support Division also attended for part of the time. The matters discussed included the details on the work on the biogenic and mobile source emissions inventory, other inventory issues, the choice of modeling episodes and the factors that need to be considered, meteorological models (primarily to educate the reviewer in this area), the various models proposed to be used (with emphasis on the chemical mechanism), and current problems of model evaluations. This review document was prepared the week following the meeting.

Recommended SIP Modeling Procedure

A summary of what I see as an ideal ozone SIP modeling procedure given the current state of knowledge and data availability is given in this section, along with my overall recommendations both for the current 2003 SIP effort and for longer term goals for future SIPs. My assessments and recommendations for the individual components of the current SIP are summarized in the section following this.

Choice of Modeling Episodes

Ideally, episodes being modeled for SIP and most other planning applications should represent the full distribution of meteorological conditions that are relevant to the problem being assessed. In the case of the ozone SIP these are not only conditions where the highest ozone occurs, but also other conditions, which may have quite different transport patterns, and thus possibly different dependences of emissions on air quality in different areas. The distribution of meteorological conditions is particularly important when considering transport from one region to the other, which is an important part of the overall SIP development process. The episode selection process should be made based on an assessment by meteorologists of the different types of relevant meteorological conditions that occur in Southern California, their frequencies of occurrence, and the types of ozone exceedences that occur in each. This information can then be used to assess an appropriate distribution of modeling episodes that adequately represents this distribution.

The use of an appropriate distribution of modeling episodes is important because air quality in different episodes may respond differently to proposed emissions changes. For example, one of the important factors that needs to be assessed in developing an ozone SIP concerns the relative benefits or dis-benefits of NO_x controls. It is known that different regions in the same episode respond quite differently to NO_x controls, and by the same reasoning it is quite possible that the same region in different episodes may also respond differently. Use of varying episodes is also necessary to test the extent to which the “relative reduction factor” (RRF) varies with conditions, which policy makers need to know if they are relying on this approximation in their planning. Use of different episodes is also necessary for determining the extent to which sensitivities to uncertainties vary with conditions, and for other diagnostic purposes.

The current procedure for choosing modeling episodes for SIP planning is based primarily on considerations of data availability and the magnitude of the peak ozone concentration. With regard to the latter, if only one episode can be modeled, as has been the case in the past, modeling the “worst case” scenario is probably the best compromise. However, a control strategy that meets the standard in the worst-case episode may not necessarily meet the standard in other episodes where present ozone may not be so high. For example, NO_x controls may reduce ozone more in high photochemical reactivity scenarios, where O_3 tends to be NO_x limited, while it may reduce it less or even make it worse in lower photochemical reactivity scenarios where the fact that NO_x slows down the rate of ozone formation may be relatively more important. Only by modeling episodes that represent different current (and potential future) non-attainment conditions can one assess the effectiveness of controlling for the worst-case conditions in improving air quality under more moderate conditions that may occur more frequently.

Data availability is currently the most important factor governing episode selection in the current modeling approach. Episodes with good data availability and quality obviously are the best for model performance evaluation, but they may not be the best or sufficient in number to represent all conditions that should be considered for control strategy modeling. Just because a certain type of condition is not well characterized for model performance evaluation does not mean that it should be ignored in planning applications. Representing such conditions approximately is better than ignoring them entirely.

One way to address this problem is to use the episodes with good data availability for model evaluation, but supplement them with other episodes developed using generally available meteorological information and expertise to represent the other meteorological conditions that need to be included in a comprehensive planning analysis. The episodes with good input and evaluation data can be used to develop and test the model inputs and components that are common to all episodes, which would include the emissions inputs and the ability to predict their chemical transformations. These are probably the most important uncertainties in predicting relative reduction factors caused by emissions changes. The main model components that change when modeling different episodes are meteorology and to a lesser extent boundary conditions. Uncertainties in boundary conditions can be minimized by appropriately expanding the domain, the approach adopted by the ARB in the present modeling plan. Although uncertainties in meteorological representation are critically important in model evaluations involving comparing predictions to ambient measurement data, they are less important in planning modeling where the main objective is to predict how emissions changes will affect future air quality in general *types* of episodes. Modeling past episodes for evaluation is the means to that end, but not the end in itself.

Use of a distribution of variety of approximately represented conditions has to be used for predicting long term averages, which though not applicable to the present ozone SIP is applicable to other planning applications. It is also the approach used when developing the MIR and my other VOC reactivity scales that are intended for application under a range of environmental conditions. Research may be needed to improve our confidence in developing reasonable, consistent, and credible meteorological inputs representing conditions with only routine supporting data, and without excessive cost in terms of person-hours and computer time. I am not sufficiently knowledgeable in meteorology to assess this, but prognostic modeling appears to me to be the appropriate approach. If this is not currently feasible, research in this area needs to be a priority for future ozone SIPs, as well as for the other planning modeling applications as indicated above.

The draft modeling protocol lists six episodes being considered, with all but one being based on data obtained in the SCOS97 campaign. The CARB staff believes that this represents a good distribution of “episode types” based on their classifications of episodes in terms of transport between the various urban areas in Southern California. This is a significant improvement over most previous SIP modeling in that at least more than one episode is being used, and that an attempt is being made to represent different episode. However, the document does not contain a discussion or a reference to previous work for an analysis of episode types, and whether other considerations besides inter-urban transport might affect how air quality depends on emissions. Certain episodes such as September 26-29 and October 30-November 1, 1997 appear to be de-emphasized because their ozone concentrations are not as high in the SCAB, but they appear to me to be sufficiently different from the others that they should be in a comprehensive analysis. These episodes will be modeled as part of other projects being undertaken by the CARB in conjunction with the regional agencies, so they might as well be included in the ozone SIP modeling. At a minimum they should be used to evaluate the applicability of RRF assumptions.

Treatment of Uncertainty

Uncertainty is unavoidable in model applications, but if their effects on model predictions can be quantified, then planners can take them appropriately into account when using the model results when recommending public policy. It is critical that the modeling plan include an attempt to assess the effects of the magnitudes of the important known uncertainties, and that the documentation on the results of the modeling analysis explain these uncertainties in a manner that is understandable and useable to the policymakers and their advisors that will be using the results. The CARB clearly understands the importance of this, as evidenced by the fact that the modeling plan includes an extensive set of diagnostic simulations and that the CARB has funded work on quantifying uncertainties. However, additional work and better documentation in this area may be appropriate as part of the SIP modeling process.

Quantifying uncertainty is difficult, but it is not infeasible for at least some of the major model inputs and components that may be important in affecting policy-relevant results, particularly those, such as mass emissions, based on scalar values. At least subjective but expert numerical estimates of uncertainty can and should be made for important inputs such as emissions, boundary conditions, light intensity, the more important uncertain parameters used in the chemical mechanism and probably other types of parameters or inputs in the model. This will allow for systematic assessments of the effects of these uncertainties on model predictions. Because of their potential importance, such estimates should be ideally included in the modeling input databases. Contractors developing emissions databases should be required to provide uncertainty ranges as part of the overall projects, and results of mechanism uncertainty studies such as by Milford and co-workers could be used to determine the most important *known* quantifiable mechanism uncertainties could be used. Box models or other types of appropriate simplified models or analysis methods could be used to assess relative importances of the various types of uncertainties to determine which subset or combination of parameter values would be the most useful to examine in diagnostic calculations using the comprehensive models.

This type of systematic analysis is probably not feasible for meteorological inputs or other model components that are multi-dimensional, or for model components where it is uncertain whether the parameterization is appropriate, such as aspects of the chemical mechanism or some of the numerical algorithms. In this case diagnostic simulations using a reasonably varied set of inputs, assumptions, or methods are needed. Ideally, this should be done with only one type of uncertainty varied at a time. This way one gets a more unambiguous assessment of which type of uncertainty is most important and the contribution of that type of uncertainty to the overall result, and there is less chance of errors of one type compensating for errors in another. This will also give a better idea of priorities for future model improvements. For example, comparing simulations with entirely different models, with different chemical mechanisms, resolutions, solvers and emissions processing assignments is much less useful than using simulations where, for example, only the mechanism or only the resolutions or only the solvers are changed. Considerations with regard to particular types of uncertainty are discussed where appropriate in the following section. In many cases limitation of current model software inhibits systematic assessments of different types of uncertainties, and software improvements to make such assessments more feasible are needed. This is also discussed later.

Treatment of meteorological uncertainty is a special case because considerations of this type of uncertainty are quite different in policy-relevant calculations than in simulations of past episodes carried out for model evaluation. In the latter case meteorological uncertainties are extremely important because they have large effects on predicted concentrations at specific times and locations, and must be properly taken into account when evaluating model performance. A decision on whether non-meteorological model components such as the treatment of emissions or chemistry are or are not consistent with the data must be made based on an assessment of meteorological uncertainty and how it affects the predictions of the observations. It is my understanding that major efforts are made in the current and planned model evaluation process to properly consider the effects of meteorological uncertainty on evaluation results, but I am not fully qualified to evaluate their adequacy. However, specific concerns in this regard are discussed later in this report.

As discussed above, meteorological uncertainty concerning exact representations of specific past episodes are much less important in planning modeling, except to the extent that the evaluation results affects conclusions concerning the uncertainties of the non-meteorological model inputs and components. For planning modeling, the most relevant meteorological uncertainties concern how well the selected episode(s) reflect the distribution of conditions of relevance to the planning assessment, and the variability of policy-relevant results with respect to meteorological conditions. Simulations of episodes representing differing meteorological conditions provide the means for assessing this, as discussed in the previous section. This is an important part of the planning modeling procedure that has not been adequately utilized in the past. As indicated above, the current SIP modeling plan represents a significant improvement in this regard, but its practice of only using the most data-intensive episodes for planning modeling means that the representativeness of the episodes used is more a matter of serendipity than planning.

Treatment of Biases

Bias refers to a type of uncertainty where the input or component is considered to be significantly more likely to err in one direction than the other. The now-classic example concerns past vehicle emissions inventories, which many if not most experts thought were low, and few if any thought were high. This may not be the case for vehicle emissions inventories now (some think the bias may be in the other direction), but may be the case in other aspects of the model inputs or components. Examples include treatment of unknowns in biogenic and anthropogenic inventories, known or probable biases in the Carbon Bond mechanism proposed for use in some of the modeling, possible inventory biases that might be suggested by comparing model calculations with measurements of emitted species, and probably others that I am not currently aware of. These specific concerns are discussed where appropriate below. In this section, I give comments that I think should be applicable to all types of biases.

Ideally, known biases in the emissions inventories and where feasible other areas should be eliminated from the models before they are used for planning. This can be done by adjusting the biased inputs until approximately an equal number of experts think they are too high as too low. Procedures for doing this, probably by using advisory panels, should be included in the modeling protocol. Diagnostic calculations and uncertainty analyses could then be done to assess the magnitudes of the corrections and uncertainties. Removing biases in this way may increase the overall modeling uncertainty, but uncertain models without known biases are better for policy analyses than biased ones. The documentation of the results should include a discussion of the adjustments that had to be made, and the how the adjustments and uncertainties affect the policy-relevant results. If the biases are large and the adjustments to remove them affect policy-relevant conclusions, this is something that the policy makers definitely need to understand.

The contractors responsible for developing components of the emissions inventories should obviously be among the experts used when assessing inventory biases, though they probably should not be the only ones. As indicated above, such contractors should be required to include estimates of uncertainties in their data. As part of that, they should also be required to indicate where they think biases may exist and to provide estimates as to the likely magnitudes of the biases. Furthermore, as discussed below, they should not be allowed to treat unknowns considered to be non-negligible as if they do not exist. They should provide their best estimates as to the amount of unknowns present and their uncertainty range, and make recommendations on how they should be represented in the model (i.e., what types of chemical species might be appropriate surrogates for them). Lack of knowledge should not be accepted as an excuse for not providing such recommendations. Proper modeling procedure requires that unknowns that may have non-negligible effects be represented somehow, and the contractors familiar with how the data are obtained usually can make more educated (or less uneducated) guesses about the data than the modeler.

Some types of known or potential biases may not be possible to assess using the types of procedures discussed above. Model components with known biases should not be used in planning calculations if better alternatives are available, though in some cases simulations with the biased component may be useful for diagnostic purposes. (An example is the chemical mechanism, which is discussed below.) Whenever possible, effects of biases that cannot be readily removed should be examined with appropriate diagnostic calculations to determine the types of effects they may have on results of planning calculations. Based on this, the likely biases in terms of policy-relevant predictions should be explained in the documentation so they are understood by those using the results. If it is not possible to assess the biases in this way, the documentation should still indicate the existence of the biases, and the direction and reasonable upper limit magnitude for the resulting bias in the policy-relevant result. Known biases should never be treated as if they do not exist.

State of Science of Model Components

The CARB recognizes the importance of its planning models representing the state of the science, as indicated by past research projects and its planned use of the most advanced models, so this need not be discussed in detail here. Whenever feasible it is best to use more than one approach and representation for an uncertain model components such as the chemical mechanism, treatment of the meteorology, and numerical approximations used in the model software, so effects of uncertainties that are otherwise difficult to quantify can be examined. Ideally, the alternative approaches should be as different as possible yet equally represent the state of the art, though this ideal is difficult to achieve in most cases. However, the more common approach is to compare a state-of-the-art model or component with one that is known to be outdated. This is better than no comparison at all, but does not necessarily indicate the uncertainty of current model, only the extent to which advances in our knowledge since the latter was developed have changed model predictions. Such comparisons may give misleading uncertainty assessments without a detailed consideration of the nature of the updates and the remaining uncertainties. Discussions of specific components that I am aware of are given below.

The CARB's modeling plans include use of different models and in some cases different model components in their performance evaluation studies. Some of the models and components discussed in the modeling protocol document reflect more of the state of the art than the others. The less advanced models should probably not be used for planning purposes, though will probably be useful for diagnostic purposes. Although as discussed above it is better that errors in model components be assessed systematically by comparing state-of-the-art alternatives and by varying one component at a time, the CARB's planned comparisons are better than nothing when such a systematic evaluation is not feasible, and may provide the most straightforward way to test for gross problems and errors.

An important model component that may not be receiving adequate attention is the model software. The internal software design and code documentation should be such that programming improvements can be carried out relatively easily by programmers who did not work on the original code.

Just as the CARB should not use proprietary models for regulatory applications, so should it not use models whose code cannot be understood or appropriately by qualified CARB staff or independent reviewers and contractors. All contractors doing software development work for the CARB should be required to produce well documented and publicly available source-code, and software developed internally by CARB staff should be held to the same standards.

Software limitations that prevent useful diagnostic simulations from being carried out or that introduce known errors into the model should be removed to the extent feasible. For example, most models and emissions processing software systems do not readily permit use of different chemical mechanisms in a consistent manner, and errors are introduced into model simulations because the software does not permit input of aircraft emissions into elevated layers. The chemical mechanism implementation modules should be such that new chemical mechanisms, including those using variable parameters that depend on the compounds being represented, can be readily implemented and the implementation readily verified. The emissions processing software and database design must allow efficient processing of emissions for different mechanisms in a consistent manner. This will not only aid in the implementation of updated mechanisms in those models where this is needed, it will also improved capabilities for diagnostic calculations to evaluate chemical mechanism uncertainty.

Model Performance Evaluation

Because of the many uncertainties involved in the model application, model performance evaluation is necessary, though not sufficient, to provide some degree of credibility to its predictions. The theory is that if a state-of-the-science model with credible inputs can correctly simulate observations in a past episode, then it *may* be able to simulate what happens if emissions change in some future episode. The CARB recognizes the critical importance of model evaluation, so this need not be discussed in further detail here. The CARB also recognizes that there is always concern for compensating errors or “giving the right answer for the wrong reasons”, and that this is why the model must utilize the best science and inputs available. This is also why any adjustments or modifications made to the model specifically to improve its performance must be made with great care, and with an appreciation that the adjustments may be covering up an error of a totally different type than the parameter being adjusted,

Model performance evaluation should be carried out with a proper appreciation of the critical role of meteorological uncertainty in the model evaluation process. This is because predictions of observations at specific sites are highly sensitive to meteorological inputs, but meteorological inputs are held constant when carrying out control strategy predictions. Indeed, meteorological uncertainties are actually of secondary importance in control strategy modeling, since the objective is just to represent a *type* of episode, not an actual past event. Because of this, inappropriate adjustment of meteorological parameters to compensate for errors in the emissions or chemistry may result in a model that is actually *less* accurate in control strategy predictions than might otherwise be the case.

The modeling protocol document does not include adequate discussion of the steps being taken to assure that assure that meteorological input adjustments are not being made to compensate for non-meteorological errors. Adjustments to fit purely meteorological observations such as wind or temperature fields are clearly appropriate if done in a physically reasonable manner, but adjustments to fit observations of pollutants must be done with greater care and always be clearly documented. Adjustments to fit slowly reacting primary species such as CO or morning NO_x might be appropriate if their emissions are reasonably well established and if there is independent evidence supporting the adjustment. Adjustments to fit secondary species such as O_3 should be done with much greater care, and probably should be avoided unless it can clearly justified and supported by other observations.

Diagnostic simulations to determine effects of the adjustments on control strategy predictions should be conducted if meteorological adjustments that may compensate for errors in emissions inventories or chemical mechanisms have to be made to obtain satisfactory model performance.

There is always the possibility that the model performance will be unsatisfactory in some respect, unless adjustments that are otherwise difficult to justify are made. Ideally all the different types of uncertainties that may cause the bias should be examined, to determine the effects of the different types of errors on control strategy predictions. For example, if the model does not correctly predict the morning concentrations of NO_x, the error could be in the emissions or the emissions or in the mixing heights. Control strategy predictions using models with the meteorological or with emissions adjustments can be compared to assess the uncertainty in the policy-relevant result indicated by this model performance problem. If the model predicts that the ozone is too low in mid-basin regions, the error could be in the emissions, the chemical transformation rates (i.e. the mechanism or the light model), or the winds. Each of these kinds of adjustments should be assessed to see if they improve model performance, and if so what differences they cause in policy-relevant predictions. Although the appropriate adjustment may be uncertain, at least policy makers would get some idea of the uncertainty in the model predictions that may be indicated by the poor model performance.

Since the actual objective of the SIP modeling process is to predict effects of emissions changes on air quality, the most directly relevant model performance test wold be to see if the model actually predicts the results of past and ongoing emissions changes. Emissions changes occur every weekend, and it is now recognized that weekends have statistically different air quality than weekdays. Indeed, weekend/weekday ozone ratios have been used as an indicator of the relative sensitive of ozone to NO_x and VOC controls. Therefore, a very useful performance evaluation test would be to see if the model could predict these weekend/weekday differences. This is can be done by modeling weekday episodes using weekend emissions, and vise-versa. Such an assessment is feasible now because the CARB now has separate weekend inventories, and certainly should be carried out for all the episodes being considered. However, at present but the applicability of the results may be too uncertain to draw definitive model performance conclusions because of the uncertainty in the weekend inventories, and because the limited number of model scenarios does not allow for an adequate comparison with statistical air quality data. Reducing the uncertainty of this very useful type of model performance evaluation is one reason that improving the quality of weekend inventories should be a high priority. This is also another reason why a more comprehensive set of model scenarios needs to be developed, as discussed above.

Documentation

Proper documentation is a critical component of the modeling process. It serves two important functions. The first is to convey to the policymakers the policy-relevant results of the analysis and the assumptions, caveats and uncertainties involved. The second is to document the process for technical experts in the stakeholder and research community, and for the public record. These are essentially separate documents, though they should be consistent and lead to the same conclusions.

The executive summary and recommendations for the policymakers is probably the most important output of this process, because it determines what the public gets for all this effort that it paid for. This is also probably the most difficult to produce properly. Not only must the general methods and the results be given in an understandable and meaningful way to a largely non-technical audience, it must make this audience appreciate and as much as possible understand the uncertainties and potential biases involved. If insufficient information or caveats are provided than the results may be misused and inappropriate decisions may be made. If too much detail is given then the information will probably not be read or assimilated and the result would be the same if it had not been provided in the first place.

This reviewer is not an expert in preparing executive summaries for policymakers, and therefore cannot provide specific recommendations other than that a significant effort be expended to see that this is done as well as possible. One suggestion is to use members of the CARB or stakeholder legal staffs as test subjects to serve as surrogates for the intelligent but not necessarily technically trained audience that the summary is designed to reach. The subjects would then be given a limited amount of time to read the summary and then asked to present their assessments of the results and their uncertainties. If the subjects misinterpret or cannot properly assimilate the information in the amount of time that one might reasonably expect a policymaker to spend on it, then the summary would need to be revised and re-evaluated using another set of test subjects. The cost and effort of this procedure may well be worth it in terms of how well the overall modeling process ultimately benefits the public.

The technical documentation and to some extent the policymaker summary should include a discussion of the episode types used in the modeling evaluation in terms of all relevant meteorological variables, and a discussion of the extent to which the episodes used for modeling represents this distribution of episode types. This needs to know this when assessing the implications of the modeling results. All adjustments made to the model to improve model performance, other than error fixes or corrections to input data, need to be listed and clearly documented. There exists (fairly or unfairly) a perception that the models contain so many ad-hoc adjustments to give desired evaluation results that the evaluation is not a real indicator of model validity. One way to combat this is to make the adjustment process completely transparent. Various other items that are recommended for the technical documentation and/or executive summary are indicated where relevant elsewhere in this review. The other components of an appropriate technical documentation are probably adequately known to the CARB staff, and need not be listed here.

Discussion of Specific Components

This section gives my comments and recommendations about specific components of the modeling plan as described in the protocol document and as discussed with the CARB staff, in light of the more general comments given in the previous section. The extent of discussion of the various components reflects primarily my level of familiarity with the components, and not necessarily their relative importances.

Modeling Episodes and Domain

The expansion of the modeling domain to cover the major Southern California source areas represents a major improvement over previous modeling procedures. The domain appears to appropriately minimize problems with boundary conditions, since the most of the boundary areas have relatively low emissions. Inclusion of the urban areas in Northern Mexico is appropriate, although the greater uncertainty of Mexican emissions is uncertain, this approach is treating Mexican pollution as a boundary condition. The inclusion of the other Southern California Air Basins besides the SCAB permits improved planning for the other basins and better assessment of transport issues, as the protocol document indicates.

Southern California appears to be fortunate compared to the East Coast in that it is less important to model half the continent to adequately deal with the major transport and boundary issues. However, the documentation should include some discussion of the extent to which Southern California gets pollution from very long-range transport outside this domain. For example, I understand that PM pollution from Asia can occasionally be significant. Although this may not be an ozone issue, it suggests that very long-range transport may be non-negligible, especially in future episodes if U.S. pollution decreases faster than in other countries.

As discussed above, the choice of episodes for modeling appears to be based more on evaluation issues than on planning considerations. However, the 1997-1998 episodes listed in the protocol document at least represent different transport conditions, and as such provide some ability to test how control strategy effectiveness may vary with meteorological conditions. It may not be feasible to develop entirely new episodes for the current SIP, even if they are used only for planning and rely on modeling of the other episodes for evaluation of the non-meteorological components. However, it may be feasible to us episodes set up previously for modeling to represent other meteorological conditions in the planning modeling for the current SIP. The main difficulty may be expanding the domain to the extent used in the SCOS97 episodes. If it is feasible to obtain credible meteorological inputs (at least in terms of representativeness of a *type* of meteorology) for these past episodes, the SCOS97-evaluated emissions, chemistry, and models can be used to represent these conditions in planning modeling. The feasibility of this should be explored for the current modeling plan. Obviously, this is only worth considering if the meteorological conditions they represent are sufficiently different to complement those in the current episodes.

In any case, as discussed above the SCOS97 episodes considered of secondary importance for SCAB SIP modeling in the discussion in the protocol document should be included as part of the SCAB SIP modeling, if only to provide a more comprehensive test of the RRF approach. Because of the nonlinearity of the processes, the RRF may be quite different in different episodes.

Chemical Mechanism

In terms of predictions of effects of future emissions changes on ozone, the chemical mechanism is probably the second most important model component after the emissions. (Meteorology is probably more important than the mechanism in the performance evaluation modeling, but as indicated above that is a separate process than control strategy modeling.) The CARB recognizes the importance of the chemical mechanism (at least for VOC reactivity modeling) and has been the only significant supporter of chemical mechanism development in the United States in the last decade.

The current modeling plans include use of models with both the Carbon Bond IV (CB4) and the SAPRC-99 mechanisms. Use of SAPRC-99 is appropriate since the CARB supported its development and peer review for VOC reactivity modeling, and has incorporated or is considering incorporating a VOC reactivity scale based on it some of its stationary source regulations. The CARB's Reactivity Science Advisory Panel supported the conclusions of the peer reviewer that it represented the state of the art for reactivity modeling, and also recommended it be used in the CARB's regional modeling. The main problems with this mechanism are its relatively large computational demands and more its complex emissions processing requirements compared to mechanisms used previously in such models. However, advances in computer technology has made the computational demands relatively less important than in the past, and the CARB staff has already implemented its special emissions processing procedures at least for some models.

Use of the CB4 mechanism is included in the plans because it is by far the most widely used in regulatory modeling in the United States, because it has been optimized for computational efficiency, and because emissions processing procedures and databases have been well established for it for many years. For this reason, modelers have a large body of experience and degree of comfort with this mechanism. However, it was developed in the late 80's and there have been numerous advances in our knowledge of atmospheric chemistry and in modeling reactions of VOCs since that time. Although it was evaluated against chamber data, the data used were relatively poorly characterized outdoor chamber experiments, and the treatment of photolysis reactions in the model is inadequately documented and probably not consistent with their treatment during the evaluation. Despite that, the mechanism has undergone essentially no updates since that time, other than updating PAN rate constants in the mid 80's, fixing a numerical instability problem due to an omission in the peroxy + peroxy chemistry in '93, and most recently updating the representation of isoprene. In addition, the mechanism has known errors and biases that could affect control strategy model predictions. Its treatment of reactions of internal olefins (including terpenes that are important in biogenic inventories) ignores their important reactions with ozone, which Paulson and co-workers propose may be an important source of OH radicals at nighttime and other conditions. Its treatment of large molecules is not consistent with the fact that they usually become stronger radical sinks as they become larger, and is not conducive to appropriately modeling secondary organic aerosol formation. Perhaps more significantly in terms of ozone SIP modeling, the limited number of systematic studies carried out thus far suggest that this mechanism predicts ozone formation occurs significantly slower under relatively high NO_x conditions than is the case for more up-to-date mechanisms that have been more comprehensively evaluated against chamber data. This represents a known bias in planning modeling.

For this reason, and the fact that there are alternatives available that are more up-to-date and have fewer known errors and biases, the CB4 should no longer be used in modeling for policy development. However, diagnostic modeling using CB4 is still appropriate and is probably necessary. Implementing a new mechanism into an airshed model is a complex process that is subject to errors, and comparisons against the well-established and (probably) already debugged CB4-based models provide a useful debugging tool. Care must be taken to assure that causes of any differences between models with updated mechanisms can be understood in terms of differences in the mechanisms themselves, and not to implementation or emissions processing errors. The CB4 mechanism also provides a useful method to test the implementation of “flexible mechanism” software into airshed models where CB4 is “hard-wired”. Furthermore, since CB4-based modeling has been used for almost all U.S. regulatory modeling in the past, comparisons of planning predictions of the newer models with CB4-based models provides a link to the past that will probably be useful for some purposes.

Note that when comparing CB4 with other mechanisms care must be taken to be sure that the comparisons are done on an equal light intensity basis. Failure to do this is apparently a problem with some of the CARB’s mechanism comparison and UAM/CB4 vs. UAM-FCM/CB4 tests.

Because of its known biases and errors, comparisons of diagnostic calculations using CB4 with updated mechanisms do not provide an appropriate indication of the effect of chemical mechanism uncertainty. If the differences observed are primarily due to mechanism updates and improvements, then the comparison may over-estimate the effects of mechanism uncertainty. On the other hand, if some highly uncertain process is represented based on the same assumptions in both mechanisms, then the comparison may under-estimate the effect of mechanism uncertainty. This means that such comparisons are not particularly useful for either upper or lower limit uncertainty determination. Although comparing equally state-of-the-art mechanisms also suffers from the problem that both may make similar assumptions about some uncertain processes, at least the results would be useful for lower limit uncertainty determination.

One of the arguments for using CB4 is its computational efficiency, which makes it greatly preferred by many modelers for routine use, especially for applications where a detailed representation of the chemistry is not considered to be needed. If this is important, then the approach should be develop a condensed version of a current mechanism rather than continue to use an out-of-date one with known errors and biases. The position of the CARB staff appears to be that the advantages of improved computational efficiency is not sufficient to justify the cost of work needed to condense an existing mechanism, especially since existing mechanisms tend to be updated from time to time, making condensed versions of them out-of-date. However, it would not be as out-of-date as CB4. Furthermore, an appropriately designed research program examining effects of various condensation and implementation efficiency improvement approaches for molecularly-based mechanisms could probably provide relatively straightforward and inexpensive procedures for updating condensed in the future. I suspect that developing a new condensed current mechanism is given low priority because use of CB4 is available as an option when computational efficiency is important. The priority may be different if the option of using a mechanism with known biases and errors is removed.

If my recommendation to de-emphasize use of the CB4 is adopted, then as presently proposed the CARB's regulatory modeling will be left with only one mechanism. The complexity and uncertainties in the chemical mechanism, and its importance to ozone modeling, makes reliance on only a single mechanism a source of concern. Fortunately, SAPRC-99 is not the only state-of-the-art mechanism that is currently available for use in regional models. The RACM mechanism of Stockwell and co-workers was developed around the same time frame as SAPRC-99, and is widely used in Europe. Because it does not represent the hundreds of types of VOCs that are represented in SAPRC-99 it is not as well suited for VOC reactivity assessment, but it is sufficiently detailed for regional modeling, being comparable to the fixed parameter version of SAPRC-99 in this regard. In addition, it may have a more accurate representation of the peroxy + peroxy reactions that are important under low NO_x conditions, so it would be particularly useful for comparison with SAPRC-99 under low NO_x conditions. Although it has not been as extensively evaluated against chamber data as SAPRC-99, its evaluation is probably sufficient to establish that it does not have major biases. Most of the emissions processing used for SAPRC-99 could be used to derive emissions assignments for RACM with relatively little effort[1].

Because of this, I recommend that the CARB consider implementing the RACM chemical mechanism in at least one of the state-of-the-art models it is proposing to use, and at a minimum conduct mechanism comparison simulations using it for diagnostic purposes. Because of its use in existing models in Europe and its similarity to the fixed parameter version of SAPRC-99 in terms of structure and emissions assignments, I believe that this should feasible for the 2003 SIP. This should be a priority if significant differences between SAPRC-99 and CB4 are found in the model performance that cannot be attributed to the known deficiencies of CB4. However, even if this is not the case, the different way RACM treats low NO_x chemistry compared to SAPRC-99 and CB4 makes it possible that RACM may give different low NO_x predictions than both these mechanisms. Results of past mechanism intercomparisons with RADM2, which has a similar treatment of low NO_x chemistry as RACM, may provide useful guidance in this regard, if any such intercomparisons exist.

Note that any mechanism comparisons, whether with CB4 or state-of-the-art mechanisms, need to be done on a consistent basis in terms of representing different VOCs species in emissions profiles. This is particularly a problem with CB4 where many profiles are assigned directly to model species without specifying the individual contains.

It should be noted that some of the models simulate quite high altitudes that are beyond the likely range of validity of the current mechanisms, particularly for the reactions of the higher VOCs. This may

[1] The reviewer has a conflict of interest in making these recommendations. See "Reviewer Background" section, above.

not be a concern if the chemistry of higher VOCs is not important at higher altitudes and if the most important reactions at higher altitudes are the simpler ones where the temperature and pressure dependences are known and adequately represented. However, it may be appropriate to consider if there may be cases where this could be a concern.

Air Quality Model Selection Process

The CARB is evaluating use of a number of state-of-the-art airshed models for its 2003 ozone SIP modeling. It has not made the final determination on the ones that will primarily be used, except that the out-of-date CB4 will be de-emphasized and non-public domain models will not be used. This is the appropriate procedure. The CARB recognizes that the version selected should represent the state of the science, including use of a current chemical mechanism. Intercomparison of different models is important, though as discussed above it most useful when the different components can be varied independently. Although the modeling protocol document is somewhat vague on the criteria that will be used to select among the recently developed models, the reviewer is reasonably confident that the CARB staff will probably make the appropriate choices.

Since as discussed above out-of-date mechanisms should only be used when appropriate for diagnostic purposes, If SAPRC-99 or an alternative state-of-the-art mechanism cannot be implemented into the model with the funding and time available for this SIP, then that model should not be used. Mechanism implementation is discussed in more detail below.

Mechanism Implementation in Models

The mechanism implementation capability of some of the models being considered for use have been or are being improved as part of the CARB's modeling efforts. The problems with the chemical solver in the original version of the CALGRID model have apparently been fixed, and updated flexible mechanism implementation software is being developed for it. The CARB is funding the implementation of a fixed-parameter version of the SAPRC-99 mechanism into CAMx, to be compatible with the version that is implemented into Models-3. However, if these implementations lack the capability to readily modify the variable product yield parameters in the SAPRC-99 mechanism, it will not permit use of the full capability of this mechanism to represent effects of changes in current or future emissions inventories.

The CARB spent considerable resources to develop the SAPRC-99 mechanism and support the experiments necessary so it could predict ozone and other impacts of the many types of VOCs that are emitted. The variable parameter features of this mechanism permit this chemical detail to be incorporated into airshed models. This is an important feature for assessing the effects of VOC composition changes in emissions, particularly in future year scenarios where emissions compositions may be quite different. Software implementations that do not permit use of this feature means that a less accurate mechanism has to be used in future year simulations than would otherwise be the case. As indicated elsewhere, every effort should be made to remove from the models software limitations that artificially limit the model's accuracy whenever this is feasible. Certainly development of new mechanism implementation systems that lack this capability should not be supported.

The mechanism implementation system used in the UAM-FCM is optimum for use with the SAPRC mechanisms because it fully supports the use of the variable parameter of the mechanism and because it uses the same mechanism compiler as used when the mechanism was developed and evaluated. This means that updated versions of the mechanism can be implemented readily and with significantly reduced likelihood of errors. Unfortunately, the UAM-FCM is being phased out because of limitations of the UAM as a whole, and the CARB apparently has no plans to implement it into more state-of-the-art models. The original version of CALGRID had an earlier version of the SAPRC implementation software that was used as the starting point in the UAM-FCM development, and it could be updated for use with SAPRC-99 with probably relatively modest effort. However, but the CARB staff is apparently developing an entirely new mechanism implementation system for it that uses a different input format and that may lack variable parameter capability. It seems to me that updating the CALGRID mechanism implementation software to the level of UAM-FCM would have been more cost-effective and more beneficial to the CARB in the long run.

The Models-3 software has a flexible mechanism compiler that allows implementation of fixed parameter mechanisms, and files implementing SAPRC-99 into that system are available. Although it lacks variable parameter capability, the model can be run with variable parameter capability by re-compiling the mechanism whenever the parameters are varied. However, my understanding is that some programming is needed so that it can be used in this way without a large level of effort. This capability may be developed for the EPA under separate funding from the American Chemistry Council, but if this does not occur then the development may need to be carried out by the CARB if it wishes to use the full capabilities of SAPRC-99 with Models-3[2].

I understand that the CARB is funding Environ to implement a fixed parameter version of SAPRC-99 into the CAMx model. The implementation should be such that the mechanism can be readily recompiled with different parameter values without having to have a separate contract with Environ. The CARB should be aware that Yosuke Kimura at the Center for Energy and Environmental Resources at the Univ. of Texas at Austin is working on a adapting the UAM-FCM software into CAMx so it can be used with SAPRC-99 in the full parameter mode, though he is apparently doing this with limited resources had is currently experiencing problems. I recommend that the CARB staff most familiar with the UAM-FCM determine the status of Mr. Kimura's efforts, assess its probability of success, and provide whatever assistance may be useful. A subcontract to Environ to provide technical assistance would probably be the most effective approach, and in the long run would probably be the most cost-effective if the CARB plans to extensively use this model[3]. Alternatively, the necessary funding to complete the FCM implementation in CAMx may be obtained from the State of Texas, in which case the CARB should take advantage of the results[4].

I am not familiar with the mechanism implementation system in SARMAP and the amount of work required to implement SAPRC-99 in that model. I am told that it has a flexible mechanism input capability, but I am unsure of the extent to which it supports use of variable parameter mechanisms.

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[2] The reviewer has a conflict of interest in making this recommendation since he is participating as a subcontractor in a proposal by MCNC to the ACC to do this implementation. See "Reviewer Background" section, above.

[3] The reviewer has a conflict of interest in making this recommendation because CAMx is implemented at CE-CERT and has collaborative programs with Environ using CAMx, and if CAMx had the FCM capability it would significantly enhance our ability to conduct reactivity-relevant research using a state-of-the art model.

[4] The reviewer is engaged in discussions with Dr. Dave Allen of the University of Texas regarding model development work related to this.

Diffusion and Transport Solvers

No discussion is given as to mathematical problems some models have in representing diffusion and transport. I am not an expert in this area, but I understand from discussions with Akula Venkatram that this may be a serious problem. The CARB staff appears to acknowledge that this may be a problem, but apparently does not feel that this is equally a problem with all current models and that much can be done about it at the current time. However, some considerations of the types and magnitudes of any biases this may introduce in model applications or evaluations need to be carried out and discussed in the modeling support documentation. If it is concluded that this is probably a minor problem then documentation or references supporting this conclusion should be given. If it may significantly affect evaluation or application modeling, then appropriate caveats must be given in the documentation, and appropriate priority should be given for research in this area. Known problems should not be ignored even if they cannot be readily solved.

Horizontal and Vertical Grid Resolution

Although I am not an expert in this area, the horizontal and vertical grid resolution used for the more state-of-the-art models being considered appear to represent an improvement over modeling for past SIPs, and probably represent the state of the art. The resolution is less for the UAM models, but its use is being de-emphasized. However, the need to use finite grid resolution may introduce biases in the evaluation or planning modeling, and either previous studies giving information in this regard should be included in the modeling documentation, or diagnostic calculations where resolution is varied should be included as part of the modeling process. Ideally, simulations of selected evaluation and future-case should be carried out with enhanced resolution to determine if the improvements result in significant differences, and if so in what direction. If this isn’t feasible (and I understand that enhancing vertical resolution is difficult) then diagnostic calculations can be carried out with the resolution degraded to obtain information on possible biases by extrapolation.

Meteorological Models and Inputs

I am not an expert in meteorology and am not really able to adequately peer review the CARB’s performance and plans in this regard. It is unfortunate that none of the current peer reviewers are experts in meteorology, and a meteorologist should be among the reviewers of the evaluation results (see discussion of Technical Oversight and Review, above.) However, the CARB modeling process has extensive input from meteorologists in stakeholder agencies. My general impression based on previous experience, the modeling protocol document, and discussions with the CARB staff has led me to believe that CARB’s current meteorological modeling and input preparation efforts represent the state of the art.

The use of both prognostic and diagnostic models as alternative approaches for preparation of meteorological inputs appears to be an appropriate and prudent procedure for model evaluation, since they are entirely different approaches with presumably different strengths and weaknesses. I get the impression that prognostic models are considered to be more state-of-the art, but may not always be as successful as diagnostic models in reproducing observations. Although data assimilation is used with the prognostic models, apparently it is not always sufficient to make the model adequately agree with the data. It is not clear to me what procedures will be used if the two procedures give significantly different model performance evaluation results, and what procedures will be used if the temperature fields and other meteorological observations are not well predicted by the models.

It seems to me that prognostic models would be most useful for developing inputs for episodes to represent meteorological conditions for which data are insufficient for evaluation modeling. In this case, it would be useful to evaluate whether models using meteorological inputs derived from prognostic models tend to give different control strategy predictions than those with inputs derived using diagnostic models that give better fits to the meteorological observations. My suspicion is that although the predictions of observed pollutant concentrations at fixed locations may be different, the RRF predictions would probably be similar. If they are not, it would suggest that control strategy effectiveness may be highly dependent on scenario conditions, making it all the more important that an adequate distribution of conditions be represented in multiple scenarios. The prognostic model inputs may not be properly representing the historical episode being modeled for evaluation purposes, but it may well be that a some episode in 2010 may be better represented than those inputs than inputs that exactly duplicate a 1997 SCOS episode.

One type of meteorological input that in the past has not received adequate attention is the characterization of the solar light intensity and spectral distribution, and how it varies with time. These are critically important inputs that affect model predictions of how rapidly the overall photooxidation processes occur. Improper treatment of this is exacerbated by use of older models, such as the UAM, which treats photolysis rates as if they only depend on the chemical mechanism and the solar zenith angle. State-of-the-art models (and the UAM-FCM) do not have this problem, and require separate input of the actinic fluxes as part of the scenario conditions.

The CARB has come to recognize the importance of light characterization as a model input, and included a number of light characterization studies as part of SCOS97. An analysis by Vuilleumier and co-workers suggest that there are problems with the NO_2 actinometry measurements made during this study, and work carried out at our laboratories indicate that standard “UV radiometers” do not give consistent measurements and should not be used for model input. However, the other light measurements provide useful model input that should be incorporated in the SCOS modeling. Note that Vuilleumier and co-workers and others find that aerosol pollution probably has a non-negligible effect on photolysis rates and that this should be taken into account for comprehensive modeling. At a minimum, diagnostic calculations should be conducted to determine if this might be a significant factor. In addition to potentially affecting evaluation results, future reductions in haze may cause non-negligible changes in photolysis rates that may affect ozone formation. This may not be a large effect but until it is assessed it will be an uncertainty.

Day-Specific Emissions

The CARB is making a major effort to improve day-specific models, and it appears that good progress has been made. Weekend emissions are still more uncertain than weekday, but I get the impression that this is improving. Reducing uncertainty in weekend emissions is important not only for model evaluation of episodes that occur over weekends, but for evaluating the models’ ability to predict weekend/weekday effects, as discussed above. Estimates of the level of uncertainty in the weekend inventory and diagnostic simulations to determine the effects of these uncertainties may be useful.

I understand that an important uncertainty in this regard is weekend emissions on surface streets (freeways seem to be much better characterized in this regard). Because of the utility in testing model predictions of weekend/weekday effects, I recommend that priority be given to reducing this uncertainty. Although I am not an expert in this area, it seems to me that conducting traffic counts on appropriately selected surface streets would provide the type of data needed. I have not been informed of ongoing research in this area, if any.

Chlorine Emissions and Model Representation

If sufficient chlorine or other chlorine containing species that rapidly photolyze to form chlorine are emitted into an air basin, the chlorine atoms they form can contribute significantly to the rate of ozone formation. Chlorine emissions from industrial sources have been shown to be important in affecting ozone formation in Houston, and it has been proposed that non-negligible amounts of photoreactive chlorine-containing species may be formed in heterogeneous reactions of sea-salt aerosol in Los Angeles. If this is so, its emissions and chemistry must be accounted for in the model. The CARB staff informs me that research is underway to assess chlorine emissions in the SCAB, and that steps will be taken to represent it in the models. Note that if it is important in the coastal areas of the SCAB, it may also be important in other coastal areas such as Santa Barbara or San Diego.

Note that incorporating chlorine chemistry into the model require a major expansion of the chemical mechanism and a significant increase in its size. Researchers in Texas are working on adding a chlorine module to the SAPRC-99 mechanism, and also conducting experiments concerning the effects of chlorine on ozone and other measures of air quality. If the CARB decides it needs to incorporate chlorine in its models it should coordinate with and take advantage of the Texas work to avoid duplication of effort and obtain maximum benefit for the available research funding. Work conducted at our laboratories with several chlorine and bromine-containing compounds suggest that we cannot successfully model all the significant atmospheric reactions of halogen-containing species. Therefore, the ability of mechanisms to accurately represent the effects emissions of chlorine or chlorine-containing species will be highly uncertain.

HONO Emissions

HONO may be either emitted or heterogeneously formed from primary emissions, since it has been observed in the atmosphere. Like chlorine, if it is emitted in sufficient quantities it can significantly enhance the photochemical reaction rates, though in this case no changes need to be made to the mechanisms to represent this. Currently NO_x emissions are assumed to include 2% of HONO, and CARB staff informs me that diagnostic calculations indicate that the model is not highly sensitive to HONO at this level. This may need to be verified with the updated models and emissions, particularly for low VOC/NO_x scenarios that will be most sensitive to radical initiators. HONO emissions from diesel vehicles may be much greater than that. This is indicated by environmental chamber studies with diesel exhaust in the Euphore chamber by Wiesen and co-workers, and also by chamber experiments in our laboratory. In particular, under CARB funding we did experiments with exhausts with a number of types of vehicles and fuels, and could get fair to good fits of model simulations to the experimental data for all except for the one experiment with diesel exhaust. Subsequent to writing the report I found that adding 5% HONO to the NO_x in the experiment. Work needs to be carried out to evaluate HONO emissions from diesel vehicles in California, and the sensitivity of the model to higher HONO from diesel emissions may need to be investigated.

Testing the VOC Inventory with Measurements

The model performance evaluation plan includes testing VOC emissions inventories by comparing speciated VOC emissions measurements with model predictions. This is done by converting the speciated VOC measurements to the corresponding lumped species that are represented in the model. The CARB staff recognizes the problems involved with spatial variations of primary pollutants, and presumably will adopt procedures to take this into account in the data analysis. But measurement biases are also important, as discussed below.

The main problem with speciated VOC measurements by GC is that they tend to be biased low, for several reasons. First, VOC emissions and oxidation products include polar and low volatility compounds that either can't be sampled quantitatively or don't make it through a GC column, or (usually) both. Appropriate sampling methods such as Tenax cartridges permit better sampling of such compounds, but this is not sufficient if the compounds can't make it through the GC column. Furthermore, almost all analyses include non-negligible amounts of unidentified GC peaks, and these are often not included or quantified in the analyses. Contractors conducting VOC measurement campaigns should always be required to report unknowns and provide estimates as to their quantities, but this practice has not always been followed in the past. Finally, multitudes of small peaks that are not resolved in the GC analysis can be treated as baseline using conventional analysis procedures. The significance of the latter is suggested by done with "2-D" GC analysis, where greatly enhanced resolution indicated that a substantial amount of the carbon is in small peaks that contribute to higher baselines and thus escape detection. The significance of undetected VOCs in general is supported by results of Paulson's work where a total carbon analyzer is found to detect more carbon than speciated GC analysis. Although this carbon is undetected, it may be represented in the emissions inventory and converted to model species in the simulations.

There are apparently no plans to test the VOC inventory using ambient total hydrocarbon measurements. Commercial FID total carbon analyzers are probably not useful because of the size of the methane interference in total carbon analyzers, because of the unreliability and problems with backflush models, and because of FID carbon response differences. However research into alternative total carbon analysis methods, such as that developed by Paulson, should be supported. Use of 2-D GC studies of air samples in the SCAB should also be investigated, if feasible. For SCOS evaluation, comparisons of total VOC measurements or 2-D GC analyses with speciated GC analyses using the methods employed during SCOS might provide a means to correct the data for inventory evaluation purposes. However, I suspect that current data are inadequate to assess whether the VOC inventory is high, but it may provide an indication whether it is low.

Evaluation Using NO_x and CO Data

Although CO is a non-negligible O_3 precursor, the primary importance of the CO inventory is that it provides a means to test meteorological and transport inputs to the model, because of its low consumption rate due to chemical reactions or deposition. Therefore, the accuracy of the CO inventory is important for that reason. Accuracy of the NO_x inventory is critical to O_3 modeling for reasons that are obvious to the CARB. Although NO_x species react rapidly, the consumption of total NO_x is slower, and comparison of modeled vs. measured NO_x in the morning in source areas also provides a test to the inventory or the relevant meteorological inputs. Because of the importance of NO_x emissions, any discrepancy between measured and modeled morning NO_x in the source areas would be a major concern. Comparisons of CO data with observations should be used to assess whether problem is due to meteorological or mixing model. If CO model agrees with data, possible biases in the NO_x inventory needs to be considered. NO_x and CO measurements on non-photochemical days could also be used to assess the inventory for these species, if relevant meteorological parameters are sufficiently well characterized.

Use of "NO_x" or "NO_y" data in non-source areas is *not* recommended for model performance evaluation except in the most qualitative sense. Fitz and co-workers in monitored a simplified irradiated VOC surrogate + NO_x air mass with multiple instruments used in the SCOS field study and found that different instruments of the same model give different readings. Data from the NO_x channel of converterbased analyzers should only be used for model performance evaluation if there is good reason to believe that the NO_x species present are primarily NO or NO_2.

Vehicle Emissions

The CARB recognizes the critical importance of having accurate vehicle emissions inputs in the models, and has undertaken major efforts to improve these inventories and remove the biases that have existed previously. This includes work in both traffic models and in vehicle emissions models. Some biases may remain, and because of the importance of vehicle emissions and the known biases in previous inventories, all known or suspected biases should be dealt with as discussed above in the "Treatment of Bias" section.

Some are concerned about whether the CARB's vehicle models adequately predict in-use emissions, and about possible biases that may result if deterioration factors are not correctly predicted. However, the CARB has an ongoing random in-use vehicle testing program that appears to go a long way towards providing the type of data needed. Reactivity of in-use emissions is also a concern, both evaporative and exhaust. The in-use vehicle testing program conducts speciation measurements on 10% of the in-use vehicles tested, both of the exhaust and the gasoline in the tank (the latter being useful not only for assessing evaporative speciation but also for the reactivity of gasoline in the marketplace). Presumably the results from this program are being incorporated into improving the vehicle emissions model and also the vehicle emissions speciation profiles.

Variability information (in speciation as well as mass) obtained in the vehicle emissions testing programs should also be used for uncertainty analysis. Because of its importance, systematic uncertainty analyses of vehicle emissions models should be carried out to assess the importance of this variability to model predictions, or at least to the total inventory.

There seems to be considerable ongoing work in improving vehicle activity estimates. The data for modeling freeway traffic activity appear to be adequate, but surface street activity is more uncertain, particularly for weekend differences as indicated above. The assumption that surface activity is proportional to freeway activity may be reasonable in the aggregate, though one would expect great variations in the weekday/weekend ratios relative to the freeway for surface streets in weekday-only business areas compared to residential neighborhoods or weekend-intensive retail areas such as by malls. Hopefully, weekend/weekday traffic differences are treated differently in these types of cases.

The reactivities of gasolines and exhausts appropriate for use in future-year scenarios are highly uncertain, but I am told they may be important in affecting attainment modeling. I am concerned about "reactivity neutral" assumptions that are apparently being made when deriving future vehicle emissions profiles. Gasoline formulators may well achieve future emissions standards using gasolines with varying reactivity, regardless of whether the standards are reactivity-based. If the reactivity of future exhaust is highly uncertain, it may need to be examined in diagnostic simulations. But artificial assumptions should not be made to make the uncertainty look like it is less than it really is, as it may introduce biases in the control strategy modeling. As discussed below, biases that are more important in the future-year scenarios than in the base case or evaluation simulations are of particular concern in this regard.

Biogenic inventory

The expanded domain used in the current modeling program may reduce the importance of background pollutants, but it makes biogenic emissions, and their corresponding uncertainties, relatively more important. Biases are also a particular concern in the biogenic inventory, because biogenics are expected to be much more important in the future year simulations than in the current episodes.

Diagnostic modeling already carried out has indicated that this is the case. This means that errors in the biogenic inventory may not have large effects on the performance evaluation or base case model results, but may significantly affect attainment demonstration or carrying capacity simulations. This would lead to biases in control strategy predictions.

The CARB recognizes the importance of reducing uncertainties in the biogenic inventories, and is supporting considerable research in this area. The various areas of research in this area were discussed in detail in the peer review meeting, and to a lesser extent in the modeling protocol document. The "GAP" database is used to estimate plant species distributions, work is ongoing to improve this, and the CARB Research Division has a project to look at these databases. The species estimates they incorporate are highly approximate but are better than nothing, and do not appear to be a source of known bias. The CARB participates in biogenic working group with EPA and others, but much of the work applicable to the East Coast not applicable to California, and vise-versa.

The one major concern I have with the current biogenic inventory concerns treatments of unknowns. Unidentified or unknown species constitute a non-negligible portion of the biogenic mass (one estimate I was given was ~30%), and yet they are not included in the biogenic databases. In other words, they are treated as if they are not there, even though they are really present and, like most biogenic VOCs, are probably quite reactive. This is a totally unacceptable and avoidable source of bias. Until data are concerning these unknowns are available, the modelers will need to contact appropriate estimates as to the amount of unknown mass that would remove this bias (see discussion of biases, above), and guidance as how best to represent them in the model. In the future, as indicated above, contractors need to be required to report the unknowns and provide estimates on their quantities and likely identities, because they are in a much better position to make more educated estimates than the modelers.

The BEGIS biogenic emissions database needs to be expanded to incorporate these "unknown" measurements or estimates and their recommended speciations. Note that consideration of most likely speciation of unknowns may vary with type of plant species, so the database should have the flexibility to add other types of chemicals.

In this regard, the speciation assignments for biogenic species should *always* be in terms of actual chemicals and *never* have direct assignments to lumped species used by the model. My understanding is that the biogenic speciation databases used by the CARB only allow for classification as isoprene, "terpene" or m-butenol. Note that different terpene isomers can have quite different reactivities and the SAPRC-99 is capable of representing these differences at least for the major isomers that have been studied. Therefore, the databases should allow for the ability to assign individual terpene isomers when such information is available. In addition, the databases should permit the assignments of unknowns to the most appropriate types of chemical species without constraint. The determination of how to represent these in the model is a chemical mechanism implementation issue that should not be mixed in with the inventory databases and assignments. This is discussed further below.

Speciation Databases and Emissions Speciation Processing

The CARB is making a significant effort to improve the quality of the speciation databases, though improvements are needed to the biogenic speciation database as indicated above. The most important are probably the vehicle emissions speciation databases, and work in this area is discussed above. The previously all-too-neglected stationary source inventory speciation profiles are also undergoing improvement, though this probably driven more by the CARB's implementation or considerations of reactivity-based stationary source controls than any perceived importance of such profiles to SIP modeling.

Work is needed, however, to improve the organization of the speciation databases, and in particular the methods used to classify the various types of VOCs in the profiles. The categorization used by the CARB is no longer consistent with that used by the EPA, even though they were apparently the same at one time. The present categorization used by both includes complex mixtures and ambiguous classifications that are not real compounds, and assigns lumped model species directly to them. Directly assigning model species to mixtures is an amalgamation of chemistry and emissions that makes consistent treatment of the emissions by different mechanisms difficult, and complicates both new mechanism implementation and emissions speciation improvement. Mixtures should always be defined by specifying (or guessing) either the actual chemical compounds they are thought to contain, or by making a best estimate of a surrogate mixture of actual chemicals that might be an appropriate basis for representing them in a model. Model species should only be assigned to actual chemicals and never to mixtures. This allows mechanisms to be compared on the basis of the same emissions inventory assignments, frees the mechanism developer from having to make guesses about emissions, and frees emissions database developers from having to make judgements about particular mechanisms used in models.

The CARB is working on improving the speciation databases by gradually removing mixtures from its profiles as data become available. However, the EPA is probably not progressing as rapidly on this front, and neither the EPA nor the CARB are making any apparent attempt to make their categorization consistent. This inconsistency makes the problem of implementing new mechanisms into new databases almost twice as difficult. It is recommended that the CARB collaboratively support the development of a new speciation classification and mechanism assignment system that allows for consistent species classification and mechanism assignments in all regulatory models used throughout the United States. The system should be structured so that direct assignments of lumped model species to mixtures or profiles is no longer an option, but otherwise implemented so they can be interfaced to emissions processing systems[5].

Finally, it should be noted that my experience indicates that emissions processing procedures and databases provide the major obstacle to implementing new mechanisms in models or conducting systematic investigations of effects of mechanisms on model predictions. Since as discussed above comparing mechanisms should be an important part of the model evaluation process, work is needed to improve emissions processing procedures and databases to permit such evaluations to be readily conducted. For example, such improvements would make my recommendation to conduct diagnostic simulations using the RACM mechanism much more likely to be implemented.

Mexican Emissions

Uncertainties in emissions from Mexico can affect evaluation and control strategy simulations in San Diego and might also affect SCAB simulations as well, under certain transport conditions. The CARB recognizes the importance of this and is funding a contractor to conduct an independent review and update of a previous inventory developed by another contractor. However, future-year Mexican

[5] The reviewer has a conflict of interest in making this recommendation because he has distributed pre-proposals to do this work, as discussed in the “Reviewer Background” section above. Even if another contractor carried out this task, it would benefit the reviewer by making the job of implementing new mechanisms for the CARB and the EPA significantly easier.

emissions are particularly uncertain, and the problem of how to deal with this was not discussed in the protocol document or during the review meeting. Diagnostic simulations should be included to assess the effects of current Mexican emissions uncertainties on both the evaluation and the control strategy predictions, and of future Mexican emissions on the control strategy results.

I understand that the CARB is involved in a separate process involving border modeling issues, so these types of simulations may be planned as part of that process. However, some of the modeling for this process may be relevant to the ozone SIP, if only to show that Mexican emissions uncertainty is not a major issue in this regard.

Initial and Boundary Conditions

My impression is that for the most part there seem to be an adequate assessment of boundary condition uncertainties in the diagnostic simulations, with the possible exception of Mexico. No mention is made of transport from the east over the deserts or from Kern County. I assume this is because they have already been shown to be relatively unimportant or that they will be adequately evaluated in the diagnostic simulations. The possibility of very long range transport being influential in future year scenarios also needs to be assessed, as indicated above.

Model Evaluation Using Radical Measurements

I understand from Gail Tonnesen that models perform poorly in simulating radical levels measured in special studies. I understand that Bob O'Brien made some radical measurements in conjunction with SCOS97 but has no funding for data analysis. The CARB should consider including in the model evaluation process an analysis of this potentially valuable and unique dataset whose collection has already been paid for.

Technical Oversight and Review

The ozone SIP modeling is being carried out in coordination with a number of Southern California Stakeholder groups consisting of the affected regulatory or government agencies. They hold 3-4 meetings a year with these groups, and also have a separate meteorological working group including meteorologists from those agencies that meet periodically. Meetings of transport working groups, presumably also with various regulatory or government agencies, have begun, though the major effort in this regard is not yet underway.

This participation by stakeholder regulatory or government agencies is obviously necessary and important, and it appears that the CARB is doing what needs to be done in this regard. The UC Peer review provides a useful supplement to this, though the absence of an expert meteorologist among the reviewers is unfortunate, given the importance of meteorological issues in both the evaluation and policy planning process. Although the most technical reviewers will have some conflicts of interest and biases if they have sufficient expertise and experience to conduct a meaningful review, in general these will be different than those for most of the other stakeholders, and thus provides a useful supplement to the stakeholder input.

Another set of stakeholders that may not be adequately represented at this point are the various industry groups. Some of these significantly co-funded SCOS97, have considerable modeling and other relevant technical expertise, and presumably at are carrying out an independent analysis of the results. They will obviously provide input at the end of the process if the regulations affect their companies' bottom line. The CARB would be better off to have their input earlier in the process, when it is time to deal with it effectively.

The stakeholders should participate in the performance evaluation process and the considerations of the appropriate steps to take should performance be less than satisfactory. However, the CARB and the other regulatory stakeholder agencies are also under considerable pressure to have a satisfactory evaluation so they can go ahead with policy-relevant modeling that their leaders are really interested in. Therefore, the perception exists, however unfairly, that they may be tempted to gloss over or under-represent important problems revealed in the evaluation. For this reason, external objective peer review may be particularly useful during the period when the initial performance evaluation and associated diagnostic calculations are completed, but there is still time to do additional analysis before the policy recommendations have to be made. This is the time that decisions are made on what additional adjustments or diagnostics are needed, and how to appropriately proceed with the policy relevant analysis. External input at this point would probably be more helpful than at the end of the process, when the same criticisms would inevitably be raised, but when it will be too late to deal with them.

Summary Of Recommendations

I think the models and modeling procedures being proposed for use by the CARB for the 2003 ozone SIP for the most part represent the state of the art, and has significant improvements over past SIP modeling. I believe that the CARB staff understands the major issues and concerns involved, and are committed to conducting the most technically defensible modeling process possible for the resources available. However, the modeling process has many difficulties and uncertainties, and there will always be concerns about whatever process is employed and recommendations on how to do it differently. These concerns are listed below. Note that some if not most of these are probably being addressed at least to some extent in the present SIP or are priorities for future research, but are included in the list below either to emphasize their importance, or because I am uncertain of the CARB's priorities concerning them.

It is probably not feasible to carry out all of these recommendations for the 2003 ozone SIP, and some of the concerns and recommendations may already be adequately addressed. However, I believe that the CARB should consider the feasibility of carrying out at least some of these recommendations in the near term if they are not already being addressed, and in the other cases consider them as recommendations for future research.

- The portion of the documentation containing executive summary and recommendations for the policymakers is probably the most important output of this process. A major effort should be made to assure that it conveys all the caveats and uncertainties in a manner they can assimilate and properly interpret. The ability of the documentation to communicate the needed information to non-technical audiences should be evaluated using appropriate personnel as test subjects.
- Episodes modeled for control strategy assessment should represent the full distribution of meteorological conditions that are relevant to the problem being assessed, and not just those with sufficient data available for full model performance evaluation. Model performance evaluation should not be necessary for all episodes used for control strategy predictions, if the major components affecting such predictions are adequately tested in other representative episodes.
- Known biases should be removed from model inputs whenever possible. In some cases this can be done by adjustments so equal numbers of experts think they are high as low. Diagnostic calculations should be used to estimate effects on control strategy predictions of more complex biases that cannot be removed, such as grid resolution effects.
- Model components that are significantly out of date or have known biases or errors should not be

used except perhaps for diagnostic purposes if better alternatives are available. This is the case for the Carbon Bond mechanism, whose use in control strategy modeling should finally be discontinued. Condensed versions of up-to-date mechanisms should be developed if computational efficiency is the main reason that CB4 continues to be widely used.

- Models should never ignore unknowns that may have make non-negligible contributions, and must incorporate best estimates as to the amounts and nature, even if subjective guesses. Emissions databases need to include unknowns. This is particularly critical in biogenic emissions databases because ignoring biogenic unknowns can bias control strategy predictions.
- In this regard, contractors developing emissions inputs should be required to provide uncertainty and (if applicable) bias estimates for all the data they provide. They should also be required to report and estimate amounts of unknowns, and provide recommendations as to what types of compounds might be the least inappropriate to serve as the basis for representing them in models.
- Any adjustments or modifications made to the model specifically to improve its performance in simulating observed pollutant concentrations must be made with an appreciation that they may be covering up an error of a totally different type than the parameter being adjusted. All such adjustments should be clearly documented and diagnostic calculations should be used to evaluate the effects of alternative adjustments on control strategy predictions. Of particular concern is meteorological adjustments compensating for emissions or chemistry errors, or vise-versa.
- A second external peer review should be carried out after the results of the initial model performance calculations have been analyzed, but before final decisions have been made on how the control strategy modeling will be carried out. At least one of the reviewers should be an expert in meteorology who has not previously been part of this modeling process.
- Attempts should be made to obtain input from industry groups in the modeling process before it is too late to incorporate their input or effectively respond to their concerns.
- A priority should be given to determining whether the model can simulate observed weekend vs. weekday effects. This may require research into improving weekend inventories, particularly models for weekend traffic activity on surface streets.
- It should be feasible to systematically quantify effects on control strategy predictions for the major model components, such as emissions, that are based on scalar values. Subjective expert judgment can be used to obtain uncertainty ranges where needed. Diagnostic calculations should be used to estimate effects on control strategy predictions of more complex types of uncertainties, such as chemical mechanisms effects. Ideally, only one type of uncertainty should be varied at a time in such assessments.
- Because of mechanism uncertainties and possible errors in implementation, the CARB should not rely on only one mechanism for modeling. The RACM mechanism is about as up-to-date as SAPRC-99, is widely used in Europe, and may have a more accurate representation of some low NO_x reactions. It should be implemented in the CARB models to provide an up-to-date alternative to SAPRC-99 for evaluation.
- Software limitations that prevent useful diagnostic simulations from being carried out or that introduce known errors or otherwise unnecessary approximations into the model should be removed to the extent feasible. Chemical mechanism implementation and emissions processing software should be improved so that diagnostic simulations varying the chemical mechanism or lumping assignments can be more routinely carried out, and so that all the capabilities of SAPRC-99 for representing chemical detail can be incorporated. The quality, documentation,

flexibility, and ease of modification of model software should be among the criteria used in model selection.

- The effects of uncertainty in light intensity on evaluation and control strategy predictions need to be investigated. Some (but not all) of the light characterization data obtained during SCOS97 may be useful in assessing and reducing this uncertainty.
- The possibility that mathematical problems some models have in representing diffusion and transport may cause biases in model evaluations and control strategy predictions may need to be assessed, or at least ruled out.
- "Reactivity neutral" assumptions should not be made when estimating speciation profiles for future vehicle emissions, as they may introduce biases in control strategy modeling.
- The effects of uncertainties in Mexican emissions, particularly in future year scenarios, need to be evaluated.
- If ongoing research suggests that the role of chlorine needs to be investigated, then the CARB should take advantage of the major efforts underway in Texas concerning modeling chlorine chemistry.
- The possibility that HONO emissions from diesel may be significantly greater than from gasoline vehicles should be investigated.
- Evaluations of VOC emissions with ambient speciated measurements needs to appropriately take into the fact that such measurements are probably biased low. Research with improved total carbon analysis methods and very-high-resolution gas chromatography should be supported. Contractors conducting VOC measurement campaigns should always be required to report unknowns and provide estimates as to their quantities.
- Any discrepancies between observed and modeled NO_x and CO data in source areas should be analyzed to determine the extent to which they may indicate a problem with the NO_x emissions inventory, as opposed to uncertainties in meteorological inputs.
- The CARB should consider supporting analysis of radical measurements made during SCOS97 as part of the model evaluation process.
- Speciation assignments for complex mixtures in the anthropogenic inventory should always be in terms of actual chemical species and never as lumped species associated with particular chemical mechanisms. Contractors developing speciation profiles should be required to estimate what chemicals are most appropriate to represent unknowns or to serve as surrogates to represent complex or uncharacterized mixtures. The speciation databases and software used by the CARB and the EPA need to use consistent chemical classifications and not permit direct assignments of lumped model species to mixtures.
- "NO_x" or "NO_y" measurements made using commercial chemiluminescent analyzers should not be used for quantitative model evaluation. Eppley UV radiometer measurements should not be used for light model evaluation or input.