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The Importance of Using Alternative Base Cases in Photochemical Modeling



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The Importance of Using Alternative Base Cases in Photochemical Modeling

Health and Environmental Sciences Department

API PUBLICATION NUMBER 4616

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ABSTRACT

Satisfactory photochemical model performance is apparently possible despite evidence suggesting significant biases in emissions estimates. This study assessed the influence of compensating modeling input errors on estimates of the effects of emission control scenarios. Specifically, a series of Urban Airshed Model (UAM) sensitivity studies have been carried out using simulations of two summer ozone episodes from the Southern California Air Quality Study (SCAQS) of 1987. These episodes were chosen because they provided the most comprehensive databases available at the inception of this study for supporting photochemical grid modeling. Existing simulations yielded inadequate performance, so it was necessary to identify UAM performance problems, implement appropriate modifications to model inputs, and assess the model's suitability for use in subsequent analyses. Plausible alternative conditions were established to define acceptable base cases; some alternative base cases were identified that provided a level of UAM performance comparable to the best achieved for the episodes. Several UAM sensitivity runs were made to determine whether the choice of base case had a significant influence on simulation results for hypothetical emission reduction strategies. The alternative base cases used in this study produced significant differences in estimates of the air quality benefits associated with hypothetical emission control scenarios. For example, one set of base cases indicated NO_x controls would be counterproductive in reducing the estimated peak O₃ concentration in part of the modeling domain; another base case suggested that such controls would yield almost no change in the peak value. These analyses provide a lower bound estimate of the uncertainty attending modeling results of the air quality benefits associated with emission control plans. It is strongly recommended that current photochemical modeling practice be extended to include such analyses. These efforts will help reduce the risk of focusing emission control efforts on the wrong precursors, underestimating control requirements needed to meet air quality goals, or incurring costs to implement unnecessary controls.

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EXECUTIVE SUMMARY

The 1990 Clean Air Act Amendments require states to demonstrate attainment of the ozone (O_3) National Ambient Air Quality Standard through use of grid-based photochemical models. In developing inputs to such models for the simulation of historical O_3 episodes (also termed base case simulations), "best estimates" are normally used for each category of input variables. Examples include the magnitudes of aggregated emissions and the fluxes along the upwind boundary of the region. While these estimates are judged "best," inputs of somewhat lesser or greater magnitudes - but within the range of uncertainty - may be equally acceptable, given our knowledge. It is quite possible that different combinations of model inputs, selected within the ranges of uncertainties, will yield acceptable performance levels of comparable quality. For example, one combination of inputs might produce a gross bias of 10 percent and an aggregate average discrepancy between model estimates and observations of 30 percent. A second combination, constructed by increasing emissions, decreasing boundary concentrations, and maintaining other variables constant, might produce a gross bias of 7 percent and an average aggregate discrepancy of 33 percent. In terms of overall quality of performance, these two cases might be judged approximately equivalent.

If the predictive performance of the model using various combinations of inputs is indeed approximately equivalent, there is no way to discriminate among the alternatives in selecting a base case for further use. Each is equally plausible. However, when emissions are reduced in the evaluation of a candidate control strategy, each alternative base case may produce different levels of improvement in O_3 concentrations. Since the base cases are equally acceptable, each estimated improvement should also be equally acceptable. This range of improvements provides a lower bound estimate of the uncertainty of the benefits associated with instituting the candidate strategy. Particular attention will need to be given to the interpretation of modeling results in situations where the choice of alternative base case has a significant influence on either the magnitude or important spatial and/or temporal aspects of estimated future year concentrations. Furthermore, the utility of modeling results may be quite limited in situations where the choice of precursor to

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control (i.e., volatile organic compounds [VOCs] and/or NO_x) is not consistent among the alternative base cases

The objective of this investigation is to demonstrate how to identify alternative base cases and to assess their influence on estimates of air quality benefits associated with future year emission control scenarios. To achieve this objective, a series of Urban Airshed Model (UAM) sensitivity studies was performed based on existing model applications for the South Coast Air Basin (SoCAB). The SoCAB was selected because, at the inception of this study, this area had the best available emissions, meteorological, and air quality data base with which to support such a photochemical modeling activity.

Upon initiating this investigation, a review of existing UAM simulation results for O₃ episodes occurring in June and August of 1987 indicated that the model was not replicating important features of the O₃ concentration field. Thus, it was necessary to diagnose the possible causes of these problems, to implement appropriate modifications to model inputs, to reevaluate the model's performance, and to assess its suitability for use in subsequent analyses. Although improvements in model performance were realized, the model was still not correctly simulating all important atmospheric phenomena. Nevertheless, model performance was deemed acceptable for the purposes of this demonstration study. At this point, plausible alternative conditions that might define acceptable base cases were established, and UAM simulations were conducted to identify alternative base cases that provided a level of model performance comparable to the best achieved for both the June and August 1987 episodes. Then several UAM sensitivity runs were made to ascertain whether the choice of base case had a significant influence on simulation results for hypothetical emission reduction strategies.

Note: Only hypothetical emission reduction scenarios were examined in this study. It was not the intent of this investigation to assess the impacts of proposed emission control plans or to even suggest suitable directions for control in the South Coast Air Basin.

The key findings of this investigation, their implications for regulatory modeling practice, and the applicability of the results to other studies follow.

FINDINGS

It is feasible, for a given air quality episode, to develop two or more alternative base cases that display equivalent performance.

Alternative base cases for both the 23-25 June and 26-28 August 1988 SCAQS episodes were identified, differing primarily in the treatment of VOC emissions, boundary values, mixing heights, and wind fields. Equivalence of the alternative base cases was established based on model performance measures for O₃ and NO₂. Specifically, five of seven candidate base cases for the June episode were judged equivalent. Two candidate base cases for the August episode, similar in many respects to two base cases studied using the June episode, were examined and also found to be equivalent.

Equal emissions reductions can produce different responses in O₃ fields, i.e., the decreases in estimated O₃ concentrations and their patterns can differ among alternative base cases.

The alternative base cases employed in this study produced the following range of percent reductions in the peak estimated O₃ concentration in the eastern portion of the modeling domain for various hypothetical emission control scenarios:

Percent Emission Reduction ¹		Range of Percent Reductions in Peak O ₃ Concentration			
VOC	NO _x	24 June	25 June	27 August	28 August
50	0	31-42	28-31		
50	25	21-30	23-31	5-38	18-40
0	25	2-14	(-3)-13		
0	50 ²	0-1	0-1		

¹ Only anthropogenic emissions were reduced in this sensitivity study.

² Only NO_x emissions from large point sources were reduced (i.e., sources that emit pollutants aloft in the UAM)

Three of the June base cases were used to assess the effects of a 50 percent reduction in anthropogenic VOC emissions. All base cases yielded lower estimated peak O₃ concentrations. For 24 June, the estimated reductions in peak O₃ ranged from 31 to 42 percent; on 25 June, the

percentage reductions in peak values were more closely grouped, ranging from 28 to 31 percent. For the scenario in which anthropogenic VOC and NO_x emissions were reduced by 50 and 25 percent, respectively, two of the three alternative June base cases indicated that the additional NO_x control would be counterproductive (i.e., would yield a smaller reduction in the peak O₃ concentration than was estimated for the case where VOC emissions alone were reduced). The third June base case yielded peak O₃ concentrations that were essentially the same as those resulting from the scenario in which only VOC emissions were reduced. Simulations were also performed for this emission reduction scenario employing the two August alternative base cases; the percentage reductions in peak O₃ were quite different for 27 and 28 August. When a 25 percent reduction in anthropogenic NO_x emissions was studied (with no change in VOC emissions), one June base case indicated a modest reduction in peak O₃ (i.e., a 13 to 14 percent reduction), whereas a second alternative base case yielded very little change in the peak concentration (i.e., a 2 percent decrease to a 3 percent increase). For a scenario involving a 50 percent reduction in NO_x emissions from large point sources, the two alternative June base cases employed here indicated little effect on the peak O₃ in the eastern portion of the domain. In the area northeast of Long Beach and portions of the San Fernando and San Gabriel Valleys, differences in the estimated percentage reduction in the gridded peak O₃ values ranged from 9 to 16 percent.

The range of outcomes, both among alternative base cases and alternative emission reduction outcomes, are indicative of a lower bound on the range of uncertainty for the specific case.

Alternative base case analyses are carried out by varying model inputs within their range of uncertainty. The range of estimated concentrations is indicative of the uncertainty in model results. Since such analyses are conducted for a limited set of alternative input conditions, the results represent a lower bound on the range of uncertainty; the use of additional alternative base cases can only broaden the bound.

The UAM did not provide an accurate simulation of some features the O₃ and precursor concentration fields observed during the June and August 1987 SCAQS episodes.

Upon initiating this investigation, a review of existing UAM simulation results for O₃ episodes occurring in June and August of 1987 indicated that the model was not replicating important features of the O₃ concentration field, including the relatively high peak concentrations reported at inland monitoring stations and the formation of an extensive layer of high O₃ concentrations aloft. Attempts to diagnose and to rectify these problems were only partially successful. Although improvements in model performance were realized, the model was still not simulating O₃ formation aloft to the extent indicated by available measurements. Moreover, the model generated O₃ concentrations in an area north of the San Fernando Valley that were much higher than the observations. The accuracy of VOC and NO₂ estimates was poorer than that for O₃, indicating that the model was not adequately simulating these species.

IMPLICATIONS

There is a need to recognize the presence of uncertainty in modeling results, to determine the extent to which it can be quantified, and to prescribe and implement methods for doing so.

The uncertainty in modeling results stems from (1) biases in procedures employed to develop model inputs and in the conceptual representation of atmospheric processes within the model, (2) the imprecision in data employed to develop inputs, and (3) the natural variability or stochastic character of the atmosphere and the ability of a deterministic model (such as UAM) to provide only a single realization of such phenomena. It is essential that the presence of uncertainty in modeling results be recognized and considered as part of the decision-making process. Of particular concern is that biased or inaccurate modeling results may cause decision makers to make inaccurate judgements concerning the most appropriate means for achieving a future air quality goal. In this case, efforts must be made to reduce bias in modeling results to an acceptable level. Once this has been accomplished, procedures should be implemented to quantify the remaining modeling uncertainties.

A process for quantifying uncertainties might include the following steps:

- assess overall model performance and perform basic sensitivity runs to insure that the model provides a reasonable simulation of key atmospheric phenomena;

- summarize the uncertainties in model inputs as well as the uncertainties inherent in the model formulation itself,
- use the uncertainty estimates to identify possible alternative base cases and then conduct model simulations to ascertain which base cases provide a level of performance comparable to the best achieved for each episode;
- develop a lower bound estimate of the range of uncertainty in modeling results for proposed emission control scenarios by assessing the air quality benefits of each scenario using the alternative base cases. The range of O₃ concentration reductions or increases represents the range of uncertainty in the modeling results.¹
- conduct corroborative and other supplemental analyses to support the findings of modeling studies.

To implement this process, it will be necessary for regulatory agencies with modeling expertise to develop pertinent information concerning the uncertainties in the model's formulation and its inputs. Model application programs will need to include time and budgetary provisions for evaluating model performance and conducting sensitivity, alternative base case, and corroborative analyses. We strongly recommend that existing regulatory modeling guidance be extended to encourage and require the estimation of uncertainties in modeling results and to indicate how such information should be employed by decision makers.

In cases for which approximately equivalent alternative base cases can be developed, their study and analysis should prove useful to policy makers in their deliberations.

Since equivalent base cases yield results that are equally plausible, the findings of emissions reduction simulations using alternative base cases are also equally plausible. Thus, using a suite of "equally plausible" cases (perhaps three to six in number) to examine the consequences of emissions reduction options provides an attractive and effective means for characterizing a lower

¹For example, suppose that three alternative base cases are used to provide a lower bound estimate of the range of uncertainty of the air quality benefits associated with a particular emission control scenario. Further suppose that, upon conducting the three alternative base case simulations, peak O₃ levels are reduced by 10, 12, and 15 percent. From these results, we estimate that the control scenario will produce a 10 to 15 percent reduction in the peak O₃ concentration. The range of outcomes (i.e., a 10 to 15 percent reduction) represents a lower bound estimate of the uncertainty in the modeling results since additional alternative base case simulations might produce percentage changes in peak O₃ that are somewhat smaller than 10 percent or greater than 15 percent.

bound on the range of uncertainties that attends the estimation of control outcomes. Information of this type should prove valuable to the decision maker confronting the classical dilemma: minimizing the chances of not meeting defined air quality goals versus minimizing the chances of incurring unnecessary control costs.

Whereas it is recognized that routine data bases are deficient, the experience of this study suggests that "richer" data bases, such as SCAQS, may also be deficient for supporting adequate performance evaluation. That is, the existence of a "rich" data base does not insure adequacy.

The SoCAB was selected because the SCAQS data base represented the best available at the outset of this study to support photochemical modeling. In the course of working with these data, we encountered difficulties in fully understanding important phenomena that were taking place during the episodes of interest. In particular, it was not possible to accurately describe how an extensive layer of high O₃ concentrations formed during the June SCAQS episode. This may be attributed in part to the lack of sufficient wind observations aloft with which to characterize O₃ and precursor transport. Additional aircraft data would have helped us to understand how far offshore pollutants were transported during the episode and to establish boundary concentration inputs.

The difficulties in achieving adequate model performance given this relatively "rich" data base demonstrates that the availability of special field measurements that does not assure a successful performance evaluation outcome, or more fundamentally, that the existing data base is sufficient in variety, quantity, and/or quality to support the modeling needs. Moreover, the uncertainties associated with current emissions estimates are a key limitation even in a region with "rich" meteorological and air quality data bases. Particular attention must be given to designing and implementing field programs that adequately characterize all important atmospheric phenomena. Moreover, efforts must be undertaken to provide more accurate emissions estimates. In many areas of the country, photochemical modeling is being conducted using much more limited data bases than that employed in this study. Given the large uncertainties in model inputs in these situations, the possibility for introducing compensating errors is quite significant. Even in the

absence of compensating errors, there appears to be incentive for defining alternative base cases due simply to the significant uncertainties associated with model inputs.

APPLICABILITY OF STUDY

Since the model was not simulating important phenomena observed during the June and August 1987 SCAQS episodes, a decision was made to proceed, assuming that the model provided a true simulation of a hypothetical set of conditions in the SoCAB (i.e., the set of conditions represented by the meteorological, emissions, air quality, and other inputs).

In its current state, the model cannot be viewed as providing an accurate, reliable simulation of O₃ formation during either the June or August 1987 SCAQS episodes. For a regulatory application of the model, there is no question that further efforts should be devoted to diagnosing and rectifying the remaining performance shortfalls. However, a key issue faced by the study team was whether or not to devote additional project resources to deal with the remaining problems, especially since the intent of the investigation was to examine the potential importance of compensating errors, not to develop emission control policies or regulations for the SoCAB.

Of particular importance is whether the model is functioning adequately for the intended purposes of this study. For example, the ability to simulate the formation of high O₃ concentrations aloft is of particular concern if the aloft air mass mixes to the surface. Underestimation of O₃ levels aloft that are entrained into the mixed layer as the mixing height increases during the morning hours can lead to the underestimation of O₃ concentrations at the surface. This problem may be contributing to some of the underestimation bias in the June results. Another key problem is that reasonable estimation of peak O₃ levels could only be achieved through use of increased VOC emissions. Although the overall scaling factor of 2.2 for VOC emissions was based on comparisons of early morning emissions estimates and ambient observations of VOC/NO_x data, the simple scaling factors employed in this study provide only an interim "fix" to the emissions inputs. More accurate corrections to emissions inputs must await the availability of pertinent source test results

The achievement of better model performance was expected to be a costly and time consuming endeavor. For example, one possible further study might have involved the development of revised wind fields using a prognostic meteorological model. There are currently no good means for improving emissions estimates.

In assessing the modeling situation, a judgment was made to proceed with the proposed study. Basically, we attempted to achieve the best performance possible within the constraints of schedule and budget. In using the model for subsequent studies, we assume that it is being applied to a hypothetical situation as represented by the most acceptable (yet still inadequate) model inputs. Under these circumstances, it is possible to examine the potential influence of alternative base cases for this set of hypothetical conditions. We strongly recommend that caution be exercised in any attempt to extend the model application results cited herein to emission control policies in the SoCAB.

This study demonstrates the potential importance of alternative base case analyses and illustrates how to conduct such assessments. The methodology must be applied to individual urban areas to ascertain the importance and implications of such results.

The most relevant findings of this work concern the potential need to examine the influence of alternative base cases on the air quality benefits of future year emission control plans. The methodology for such assessments involves (1) identifying candidate alternative base cases, (2) conducting model sensitivity runs and evaluating the equivalence of the candidate cases, (3) performing simulations for key sensitivity and emission control scenarios using the alternative base cases, (4) estimating the uncertainties associated with model application results, and (5) assessing the implications of the alternative base case analyses as they pertain to emission control policies and other issues. Since the present study considered only a single area, namely the SoCAB, it is not possible to stipulate the conditions for which such analyses may or may not be important for other urban areas. We recommend that alternative base case analyses be conducted in other areas to provide specific information concerning the importance and implications of such results.

Section 1

INTRODUCTION

BACKGROUND

The 1990 Clean Air Act Amendments require states to demonstrate attainment of the O₃ National Ambient Air Quality Standard (NAAQS) with grid-based photochemical models for all designated nonattainment areas classified as serious and above. Interstate moderate areas are subject to similar requirements. Furthermore, intrastate moderate areas must demonstrate attainment through modeling, but the use of grid models is optional. The Urban Airshed Model (UAM) is the EPA-recommended grid-based model for use in O₃ NAAQS attainment demonstrations.

In developing inputs for a grid model simulation of an historical O₃ episode (also termed a base case simulation), "best estimates" are normally used for each category of input variables. Examples include the magnitudes of aggregated emissions and the fluxes along the upwind boundary of the region. While these estimates are judged "best", inputs of somewhat lesser or greater magnitudes - but within the range of uncertainty - may be equally acceptable, given our knowledge. It is quite possible that different combinations of model inputs, selected within the ranges of uncertainties, will yield acceptable performance levels of comparable quality. For example, one combination of inputs might produce a gross bias of 10 percent and an aggregate average discrepancy between model estimates and observations of 30 percent. A second combination, constructed by increasing emissions, decreasing boundary concentrations, and maintaining other variables constant, might produce a gross bias of 7 percent and an average aggregate discrepancy of 33 percent. In terms of overall quality of performance, these two cases might be judged approximately equivalent.

If the predictive performance of the model using various combinations of inputs is indeed approximately equivalent, there is no way to discriminate among the alternatives in selecting a base case for further use. Each is equally plausible. However, when emissions are reduced in the evaluation of a candidate control strategy, each alternative base case may produce different levels of improvement in O₃ concentrations. Since the base cases are equally acceptable, each estimated

improvement should also be equally acceptable. This range of improvements provides an indication of the range in uncertainty of the benefits associated with instituting the candidate strategy. Particular attention will need to be given to the interpretation of modeling results in situations where the choice of alternative base case has a significant influence on either the magnitude or important spatial and/or temporal aspects of the estimated concentrations. The utility of modeling results may be quite limited in situations where the choice of precursor to control (i.e., VOCs or NO_x) is not consistent among the alternative base cases.

STUDY OBJECTIVE

The objective of this investigation is to demonstrate how to identify alternative base cases and to assess their influence on estimates of air quality benefits associated with future year emission control scenarios. To achieve this objective, a series of Urban Airshed Model (UAM) sensitivity studies was performed based on existing model applications for the South Coast Air Basin (SoCAB). The SoCAB was selected because, at the inception of this study, this area had the best available emissions, meteorological, and air quality data base with which to support photochemical modeling. In particular, during the summer of 1987, supplemental meteorological and air quality monitoring activities were carried out as part of the Southern California Air Quality Study (SCAQS). The background and study design for SCAQS are described by Lawson (1990). Elements of the SCAQS data base of particular interest were the upper air meteorological soundings, air quality data collected by aircraft, and VOC speciation measurements. Such observations are not typically collected in routine monitoring networks. Two SCAQS O₃ episodes have been the subject of considerable study, namely those that occurred during 23-25 June 1987 and 26-28 August 1987.

We would have preferred to select a study area that was somewhat more representative of those regions in which photochemical modeling is currently being performed. However, there was no other region with as good a data base to support this demonstration study. While the specific SoCAB simulation results presented in this report may have limited applicability to other areas, the procedures used to identify alternative base cases and to assess their effects on the estimated

air quality benefits of emission control scenarios should be applicable to other contemporary modeling studies.

At the outset of this investigation, a review of UAM performance for the June and August SCAQS episodes indicated that some improvement to the representation of atmospheric processes was needed prior to undertaking subsequent modeling work. Discussions involving members of API's Air Modeling Task Force and the California Air Resources Board (CARB) early in the study indicated a common interest in diagnosing and rectifying UAM performance problems and in examining issues associated with the possible existence of multiple base cases. Thus, it was agreed that the study team and CARB personnel would collaborate in trying to resolve UAM performance problems and in studying model sensitivity issues of common interest. In rectifying these problems, particular emphasis was given to assuring that any changes to model inputs were soundly based and were not merely attempts to "tune" the model. (Tuning a model refers to a process wherein modifications are made to model inputs for the sole purpose of achieving better agreement between estimated and measured concentrations). A protocol was developed for this study describing key technical and administrative issues and the activities to be carried out by the participants. The protocol is included as Appendix A. Note that the present report documents the activities carried out by the API-SCE study team.

STRUCTURE OF THE STUDY

This investigation was carried out in three phases. Phase 1 involved efforts to improve model performance. The study team obtained UAM input and output files for the 23-25 June 1987 episode and was able to adequately replicate simulation results provided by the South Coast Air Quality Management District (SCAQMD). Diagnostic analyses were conducted to identify shortcomings in existing simulations for the June episode

Phase 2 of the study involved the identification of alternative base cases for the June episode. In addition, a limited effort was carried out to ascertain whether the findings derived from use of the June episode were also valid for the August conditions. In conducting the Phase 2 activities, the

study team carried out an assessment of the base cases developed in Phase 1. In light of these analyses, plausible alternative conditions that might define an acceptable base case were defined. Analyses of the SCAQS data reported by Lurmann and Main (1992) indicated that VOC and CO emissions may be underestimated and that NO_x emissions may be relatively unbiased. On this basis, modifications were made to precursor emission and boundary condition inputs, as well as wind and mixing height inputs in an attempt to identify conditions that provided comparable model performance.

Phase 3 is concerned with ascertaining whether the choice of base case has a significant influence on UAM simulation results for hypothetical emission reduction strategies. If the model exhibits significant sensitivity to the choice of base case, particular attention would need to be given to any interpretation of results concerned with emission control strategy assessment. Emission scenarios included various combinations of across-the-board reductions in VOC and NO_x emissions from all anthropogenic sources in the study area, as well as an assessment of the effects resulting from reductions in precursor emissions from elevated point sources. Again, most UAM sensitivity runs were carried out using the June episode, with the conduct of a few confirmatory simulations using the August conditions.

STRUCTURE OF THIS REPORT

Section 2 discusses the efforts in Phase 1 to improve model performance for the June SCAQS episode. Section 3 documents the Phase 2 activities concerned with the identification of alternative base cases. Section 4 presents the UAM sensitivity studies conducted in Phase 3 to assess the influence of the choice of alternative base cases on estimates of the effectiveness of hypothetical future year emission control scenarios in reducing O₃ concentrations. Finally, Section 5 summarizes the implications of this work for regulatory modeling activities.

Section 2

PHASE 1--IMPROVING MODEL PERFORMANCE

OBJECTIVES OF PHASE 1

At the inception of the study, a review of Urban Airshed Model (UAM) simulation results for both the 23-25 June and 26-28 August 1987 Southern California Air Quality Study (SCAQS) episodes indicated a need to improve the representation of model inputs prior to conducting the investigation to assess the possible importance of alternative base cases. For example, an inability of the model to adequately simulate the formation of O₃ aloft was noted by Roberts and Main (1992a,b) based on analyses of UAM results using the SCAQS data base. The specific objectives of Phase 1 activities were:

- to identify UAM performance problems in existing simulations for the June 1987 SCAQS episode;
- to diagnose the possible causes of UAM performance problems;
- to identify and implement appropriate modifications to model inputs; and
- to evaluate the model's performance and assess its suitability for use in subsequent activities in Phases 2 and 3.

GENERAL RULES FOR ALLOWABLE CHANGES TO THE MODEL AND ITS INPUTS

Efforts to improve model performance were designed to reduce the discrepancies between model estimates and observed air quality levels where these could be logically defended based on sound scientific principles through (preferably) analyses of relevant, site-specific data. Three principles governed the model improvement activities:

- any changes to the model or its inputs were to be documented;
- any changes to the model or its inputs were to be supported by scientific evidence, analysis of new data collected for the purpose, or by reanalysis of the existing data where errors or misjudgments may have occurred; and

- all proposed changes to the model or its inputs were to be subject to review by all project participants.

To help assure that the proposed diagnostic and model improvement activities would not be viewed as a "tuning" exercise, the study team discussed the proposed modifications to existing inputs for the June episode with project oversight personnel prior to exercising the model and evaluating its performance.

PROCEDURES AND CRITERIA FOR JUDGING MODEL PERFORMANCE

To assess the adequacy of the model's concentration estimates, we compared the calculated surface O_3 concentrations with the available measurements using performance measures identified in the study protocol (see Appendix A). Since such comparisons do not constitute a stressful test of the model, we also examined other aspects of model performance, including its ability to accurately estimate precursor concentrations and to simulate important characteristics of the concentration fields aloft. Figure 2-1 shows the locations of air monitoring stations in the SoCAB. We refer the reader to Appendix G for a more detailed discussion of the procedures and criteria used in this study for judging performance.

DIAGNOSIS OF MODEL PERFORMANCE PROBLEMS

For the UAM simulation of the 23-25 June 1987 episode using inputs developed by the South Coast Air Quality Management District (SCAQMD), the model exhibited little overall bias, but the average normalized error was 39 percent on both 24 and 25 June. A particular concern was that peak O_3 concentrations were underestimated at several monitoring stations where relatively high concentrations were reported (e.g., Azusa, Banning, Burbank, Glendora, Pasadena, Reseda, and Upland). Hourly-averaged NO_2 concentrations tended to be underestimated by 24 to 32 percent, and the normalized error ranged from 45 to 52 percent.

For comparison purposes, UAM simulation results for the 26-28 August 1987 episode using inputs prepared by the SCAQMD exhibited little overall bias, and the normalized error ranged

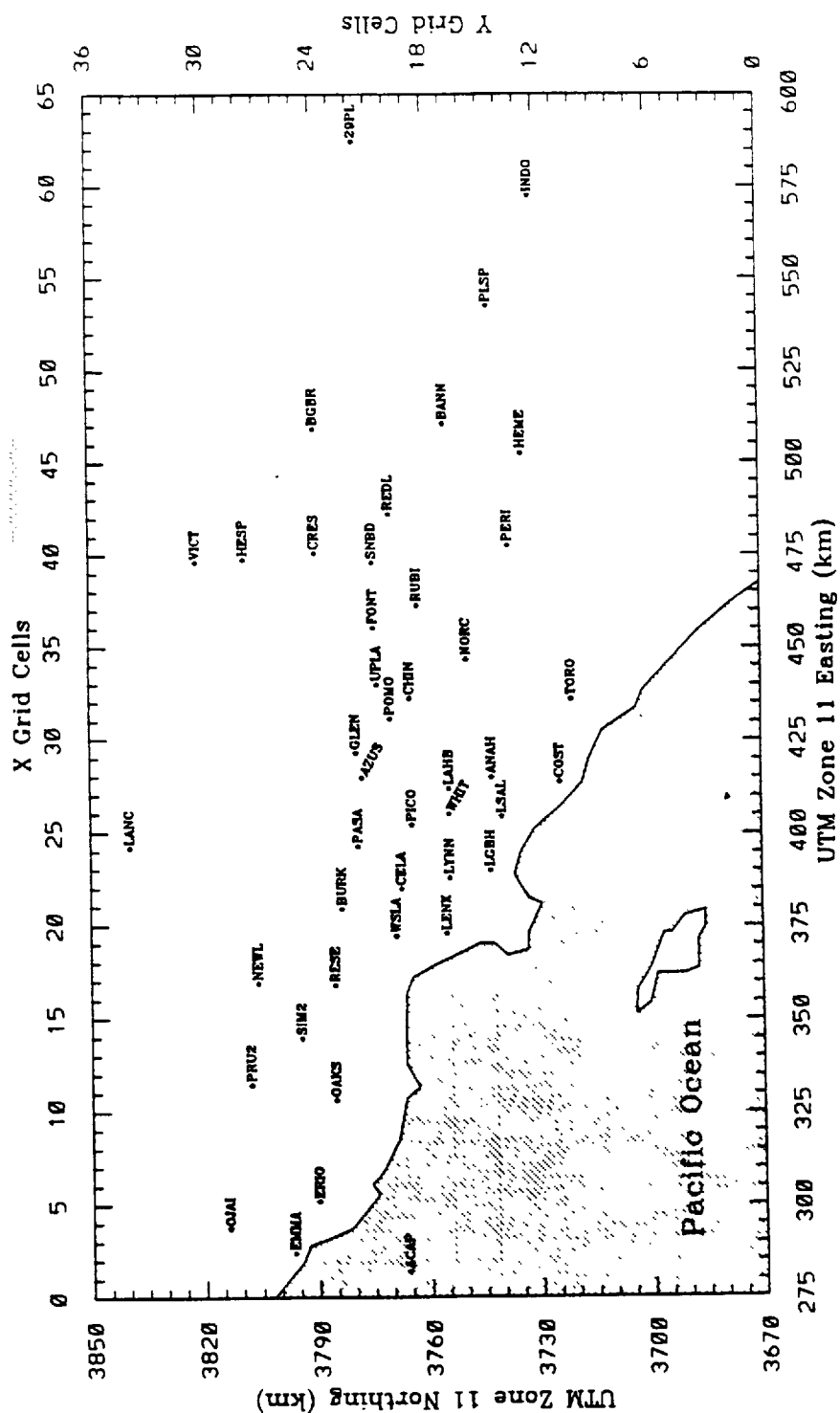


Figure 2-1. The UAM modeling domain and locations of air monitoring stations

from 24 to 32 percent. The small bias figures can be attributed to fortuitous cancelling of larger over- and underestimation biases, as indicated by the normalized error results. In addition, significant discrepancies existed between estimated and measured peak O₃ concentrations at several stations (e.g., Crestline, Glendora, Hesperia, Pomona, Rubidoux, and Victorville). The normalized error for hourly-averaged NO₂ concentrations was 58 percent for both 27 and 28 August.

Roberts and Main (1992a,b) examined UAM simulation results for the June episode in light of the SCAQS aircraft observations. As shown in Figure 2-2, the observations point to the existence of a layer of high O₃ concentrations aloft. However, when they examined available UAM results, they found that the model was significantly underestimating O₃ aloft, as illustrated in Figure 2-3.

An inability both to accurately replicate the peak O₃ measurements at several important air monitoring locations and to simulate the formation of high O₃ levels aloft indicated a need to develop improved representations of model inputs in the hope that this would lead to better model performance.

Analyses of existing model inputs using the SCAQS data and discussions with CARB personnel concerning their work with the August episode indicated a need to implement changes to several model inputs, including

- the simulation starting time
- the height and vertical resolution the modeling grid
- wind fields and mixing heights
- initial and boundary concentrations
- photolysis rates
- emissions

These revisions to model inputs are discussed in Appendix B.

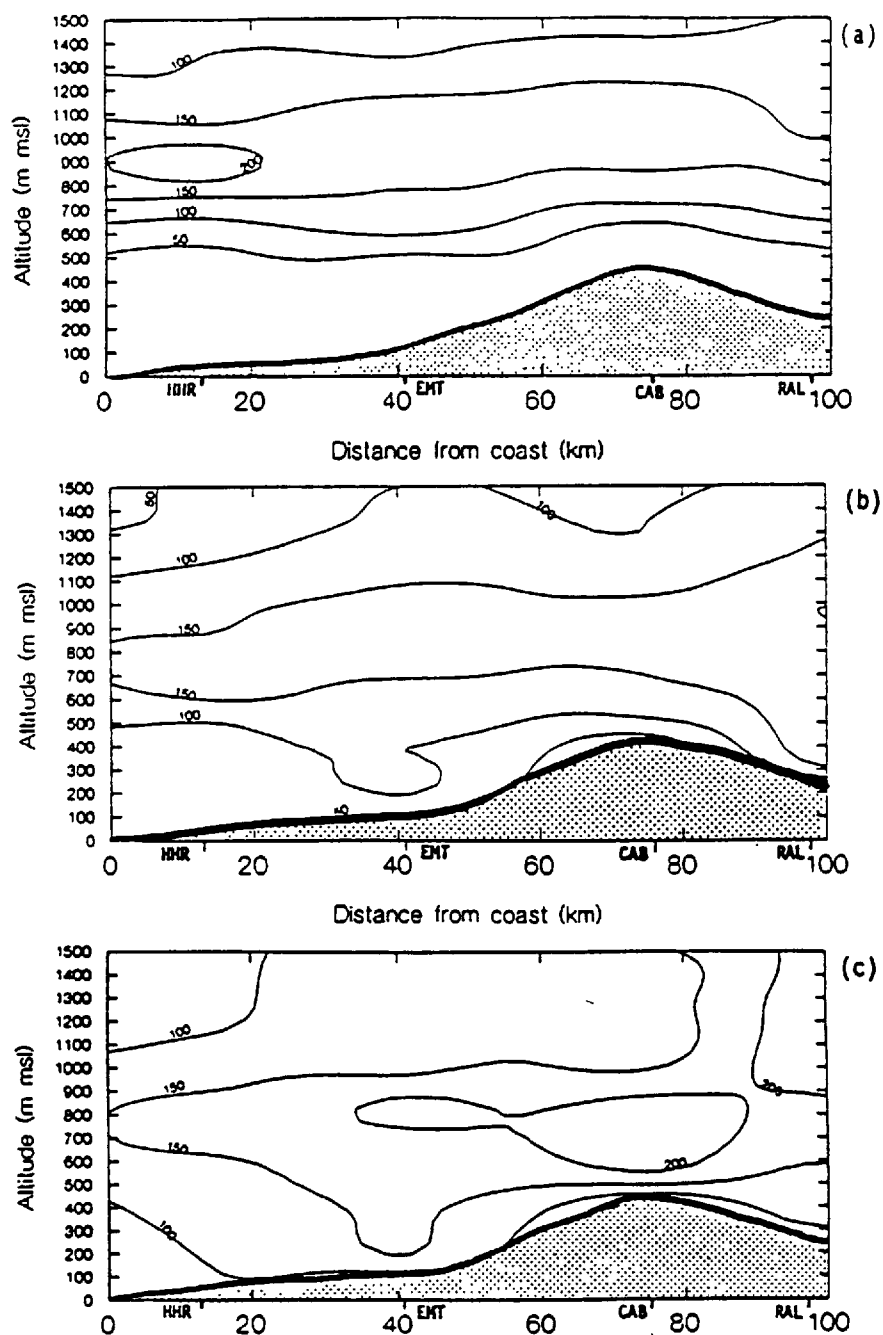
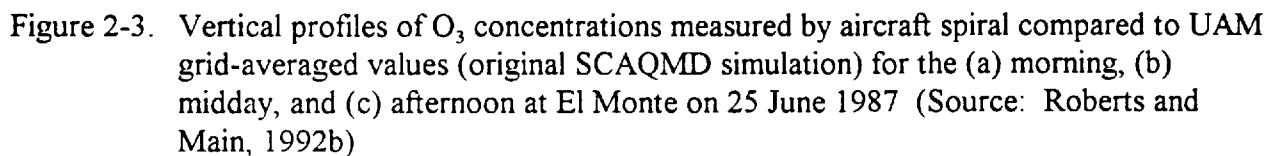


Figure 2-2. O₃ concentrations aloft during the (a) morning, (b) midday, and (c) afternoon of 25 June 1987. O₃ contours, in ppb, generated along a west-to-east plane from the coast near Hawthorn to Riverside using data from aircraft spirals. The shaded area approximately represents the ground. (Source: Roberts and Main, 1992b)



DISCUSSION OF RESULTS

This section focuses on results of UAM simulations developed using the inputs described in the previous section. In addition, we summarize model performance for the original UAM simulation of the June episode provided by the SCAQMD. These simulations are designated as follows:

- Run J1--the simulation of the 23-25 June 1987 episode using revised model inputs as described in the previous section (including use of nominal VOC emissions estimates increased by a factor of 2.2); and
- Run J2--the simulation of the 23-25 June 1987 episode using inputs prepared by the SCAQMD.

The assessment of model performance is presented in two parts. First, we examine the overall results, considering the spatial distribution of peak concentrations over the modeling domain, as well as the calculated performance measures determined using the complete set of available pairs of estimated and measured concentrations. In the second part of this presentation, we discuss model performance on a subregional basis.

Note that all figures referenced in this discussion of results will be found at the end of Section 2.

Overall Model Results

The highest estimated one-hour averaged ground-level concentrations for O₃ for 24 and 25 June based on the inputs developed in this study (Run J1) are illustrated in Figure 2-4 and 2-5, respectively. The small numbers printed on these figures represent the corresponding measured values. Values enclosed in a rectangle and preceded by an "H" or "L" designate maxima and minima, respectively, in the spatial field of estimated concentrations. Of particular note are the high estimated concentrations in the northwestern portion of the domain in the vicinity of Newhall. Peak O₃ levels in this area are overestimated by almost a factor of two. The location of the highest concentrations in the eastern portion of the domain are within about 10 to 20 percent of the observed values on 24 June. The highest estimated values in the eastern area on 25 June may be situated approximately 20 km too far south, although available measured values at sites

surrounding the location of the highest peak value seem in reasonable agreement with the estimates. Unfortunately, there were no measurements in closer proximity to the location of the highest value with which to assess the accuracy of this estimated concentration.

Figures 2-6 and 2-7 depict the peak estimated O_3 concentrations on 24 and 25 June, respectively, from the simulation using inputs originally developed by the SCAQMD (i.e., Run J2). Note that the SCAQMD simulation does not produce exceptionally high estimates of O_3 concentrations in the northwest portion of the domain. Peak estimated O_3 levels in the eastern portion of the domain for the two simulations are within about 1 pphm. CARB staff have noted a tendency for the model to produce very high O_3 concentrations to the north of the San Fernando Valley in various sensitivity runs carried out for both the June and August SCAQS episodes. This problem may be caused by an inaccurate specification of wind velocities and/or mixing heights in this area of significant terrain features. In addition, an examination of ambient VOC measurements at Burbank (upwind of the high O_3 area) indicated that several organic species were significantly overestimated during the morning prior to the time when the high O_3 levels were calculated (as discussed in the next subsection).

Peak NO_2 concentrations for 24 June for both Runs J1 and J2 are shown in Figures 2-8 and 2-9, respectively. Note that the highest NO_2 concentrations are estimated in the San Fernando Valley in Run J1 and to the north of stations in the San Gabriel Valley in Run J2. Although the peak estimated values differ by only about 1 pphm, the differences in locations are most likely indicative of the differences in wind inputs employed in these two simulations. For Run J1, peak estimated concentrations in the San Gabriel Valley underestimate the observed values, while in the San Fernando Valley, peak NO_2 levels are overestimated. For Run J2, the model tends to overestimate the peak values in the San Gabriel Valley. In general, observed peak levels range from 5 to 9 pphm over much of the central basin, San Gabriel Valley, and San Bernardino areas. Model estimates in these areas for both simulations are also generally in this range.

Exhibits 2-1 through 2-3 summarize the calculated values for the various performance measures identified in Appendix G for Run J1 for O_3 , NO_2 , and NO_x . Similar results for Run J2 are given in Exhibits 2-4 through 2-6, respectively. Since results for 23 June may be significantly influenced by uncertainties in initial concentration inputs, we focus this discussion on the results for the last two days of the simulation, namely 24 and 25 June. Model results for Runs J1 and J2 are summarized in Table 2-1.

Note that performance for NO_2 and NO_x is not as good as that for O_3 . Model peak and bias performance metrics for O_3 exceed the thresholds triggering concern cited in Appendix G. In general, the overall bias and error metrics for Runs J1 and J2 are quite similar in magnitude. This is an interesting finding considering that these two simulations employ different model inputs--especially VOC emissions that differ by a factor of 2.2. A review of the estimated O_3 spatial concentration fields indicates that both runs fail to replicate the formation of the significant layer of O_3 aloft, as shown in Figure 2-2.

Subregional Model Results

Figures 2-10(a) through 2-10(i) provide time series displays of estimated and measured concentrations on 23-25 June for O_3 , NO_2 , and NO_x at representative stations within each of the nine subregions described in a previous subsection. These displays show results for Runs J1 and J2, as well as one of the alternative base case simulations (Run J7), which is discussed in Section 3. A complete set of time series displays for all monitoring stations is provided in Appendix C.

Figures 2-11(a) through 2-11(h) provide time series displays for various organic species collected at the Claremont College, Long Beach City College, and Burbank monitoring sites. VOC sampling was carried out a few times per day at eight locations in the basin during the June episode. VOC speciation results for individual compounds were combined in accordance with the definitions of Carbon-Bond species to facilitate comparison with the model estimates. A complete set of VOC time series plots are included in Appendix D.

Table 2-1. Summary of model performance measures for Runs J1 and J2

	Run J1	Run J2
peak estimation accuracy (location of highest observation)		
O ₃	underestimates by 25 - 28%	underestimates by 6 - 48%
NO ₂	underestimates by 14 - 40%	underestimates by 20 - 39%
NO _x	underestimates by 80%	underestimates by 59 - 67%
average peak estimation accuracy (all locations)		
O ₃	21 - 23%	24 - 26%
NO ₂	36 - 45%	38 - 47%
NO _x	41 - 51%	50%
normalized bias		
O ₃	underestimates by 21 - 23%	underestimates by 7 - 20%
NO ₂	underestimates by 33 - 38%	underestimates by 24 - 32%
NO _x	underestimates by 27 - 35%	underestimates by 13 - 26%
mean bias		
O ₃	underestimates by 1 - 3 pphm	underestimates by 1 - 3 pphm
NO ₂	underestimates by 2 pphm	underestimates by 1 - 2 pphm
NO _x	underestimates by 2 pphm	underestimates by 1 - 2 pphm
normalized error		
O ₃	30%	32%
NO ₂	50%	45 - 52%
NO _x	50%	51 - 56%
mean error		
O ₃	3 - 4 pphm	4 pphm
NO ₂	2 pphm	2 pphm
NO _x	3 pphm	2 - 3 pphm

The time series plots provide an indication of how well model estimates conform with the observations at particular locations. Note that some caution must be exercised in the interpretation of such results since model estimates represent concentration values that are spatially-averaged over several square kilometers, while the measurements are taken at a point. This can be a problem when an air monitoring station is situated near a heavily-travelled roadway or other large sources. In such situations, we would expect the model to underestimate precursor concentrations.

Exhibits 2-7 and 2-8 provide summaries of performance metrics for peak accuracy, bias, and error for each subregion for Runs J1 and J2, respectively. Results are provided for O₃, NO₂, NO_x, and various Carbon-Bond species.

Key findings concerning O₃ and NO_x subregional model performance are as follows:

- estimated O₃ and NO_x concentrations at stations within the coastal and Ventura County subregions are generally in good agreement with the observations.
- O₃ concentrations are underestimated during the late morning and afternoon at several sites in the Central Basin and Eastern subregions (e.g., Los Angeles, Pico Rivera, Whittier, Pasadena, Glendora, and Upland).
- the relatively high O₃ concentrations reported at stations in the Far Eastern area are not accurately estimated; this problem appears to be caused by inaccurate estimates of wind directions in areas to the east of San Bernardino, which significantly influence when the polluted air mass that has been transported across the basin reaches these stations; the Diagnostic Wind Model has difficulty in estimating the easterly movement of the convergence zone that forms in the Far Eastern subregion.
- significant O₃ underestimation problems in the SCAQMD simulation for 24 June (Run J2) occurring during midday hours when relatively high O₃ concentrations were reported at Reseda, Burbank, Pasadena, Glendora, Azusa, and Fontana were much reduced using the revised inputs of this study (Run J1);
- a tendency to overestimate NO_x concentrations in Run J2 at some stations in the Coastal and Central Basin subregions was mitigated in Run J1.

- high NO_x concentrations reported at San Bernardino, Upland, Fontana, and Pomona were underestimated in both Runs J1 and J2.

In their assessment of the composition of ambient and emissions data, Lurmann and Main (1992) found that olefin emissions were overestimated and aromatics and carbonyls were underestimated. Considering data collected in the summer, the reactivity of the mix of organic species included in the emissions inventory appeared to be about 10 percent greater than the mix of pollutants in the ambient air samples. These speciated VOC measurements were available at a few times a day on 24 and 25 June at eight sites in the modeling domain and provide a limited basis for evaluating the model's VOC performance. Key findings from an examination of model VOC results follow:

- RHC (the sum of all Carbon-Bond species) estimates for Run J1 are generally in reasonable agreement or modestly underestimate the observed values; RHC values from Run J2 generally exhibit a greater underestimation tendency than those from Run J1 (perhaps not surprising since Run J1 uses emissions that are 2.2 times those employed in Run J2) and significantly underestimate reported values at Los Angeles and Burbank.
- ALD2 (high molecular weight aldehydes) are systematically underestimated in both Runs J1 and J2 in all subregions by from 65 to 82 percent; FORM (formaldehyde) levels are overestimated on the average in Run J1 by about 20 percent and in Run J2 by from 12 to 44 percent.
- ETH (ethene) and OLE (olefinic carbon bonds) tend to be overestimated on the average in Run J1 by 13 to 30 percent, with results in the coastal and San Fernando Valley subregions being overestimated by as much as a factor of two; ETH and OLE tend to be underestimated in Run J2 by 5 to 42 percent.
- TOL (toluene) tends to be overestimated in Run J1 in the Coastal, Central Basin, and San Fernando Valley subregions by from 29 to 80 percent; in contrast, TOL tends to be underestimated by from 11 to 53 percent in the Central Basin, San Fernando Valley and Eastern subregions and overestimated in the Coastal subregion by about 27 percent. For Run J1, XYL (xylene) tends to be overestimated in the Coastal and San Fernando Valley subregions and underestimated in the Central Basin and Eastern subregions. For Run J2, XYL is underestimated in all subregions by from 28 to 65 percent.
- PAR (paraffinic carbon bonds) tend to be underestimated in all subregions for both Runs J1 (on the average by 1 to 17 percent) and J2 (on the average by 9 to 26 percent).

Overall, the subregional results indicate that the model is not accurately simulating all relevant phenomena. VOC and NO_x results exhibit a level of performance that is poorer than that for O₃. Model performance in the Coastal and Ventura County subregions was good, indicating that boundary concentration inputs may be specified reasonable well. Discrepancies between estimated and measured VOC and NO_x concentrations suggest that further attention must be given to developing more accurate specifications of emissions inputs. Problems in estimating O₃ concentrations in the northeastern and far eastern portions of the modeling domain point to a need for further work to develop better estimates of wind inputs in these areas.

IMPLICATIONS OF PHASE 1 RESULTS

Several modifications to existing model inputs were implemented in efforts to improve performance for the June 1987 SCAQS episode. These modifications included revisions to the wind fields, simulation of an additional "ramp-up" day, calculation of episode-specific photolysis rate constants, extension of the top of the modeling domain from 1000 to 1500 m, use of an increased number of vertical grid cells, revision of boundary concentration inputs, and increase of VOC emission inputs. All of these modifications were implemented in an effort to get model inputs to conform more closely with available aerometric data collected during the SCAQS episode.

An assessment of model results for the June episode indicated that some performance improvements had been achieved, especially with regard to the estimation of peak O₃ levels at inland locations where relatively high concentrations were reported. However, a number of shortfalls in performance remain. In particular, the model does not adequately simulate the formation of a layer of high O₃ concentrations aloft that extends over a large portion of the central basin, and estimates of bias and error for O₃ and especially NO_x and VOCs indicate that the model is not providing an adequate simulation of all important physical and chemical phenomena that influence air quality during the June episode.

The SoCAB was selected for this study because the SCAQS data base represented one of the best available to support photochemical modeling. The difficulties in achieving adequate model performance given this relatively good data base cast concerns regarding the utility of modeling, especially regulatory applications. In many areas of the country, photochemical modeling is being conducted using much more limited data bases. Given the large potential for uncertainties in model inputs, the potential for introducing compensating errors is real. Even in the absence of compensating errors, there appears to be good potential to define alternative base cases due simply to the significant uncertainties associated with model inputs.

In its current state, the model cannot be viewed as providing an accurate, reliable simulation of O_3 formation during the June 1987 SCAQS episode. For a regulatory application of the model, there is no question that further efforts should be devoted to diagnosing and rectifying the remaining performance shortfalls. However, a key issue faced by the study team was whether or not to devote additional project resources to deal with the remaining problems, especially in a situation where the intent of the investigation was concerned with examining the potential importance of compensating errors, not the development of emission control policies or regulations for the SoCAB.

Of particular importance is whether the model is functioning adequately for the intended purposes of this study. For example, the ability to simulate the formation of high O_3 concentrations aloft is of particular concern if the aloft air mass mixes to the surface. Underestimation of O_3 levels aloft that are entrained into the mixed layer as the mixing height increases during the morning hours can lead to the underestimation of O_3 concentrations at the surface. This problem may be contributing to some of the underestimation bias in the June results. Another key problem is that reasonable estimation of peak O_3 levels could only be achieved through use of increased VOC emissions. Although the overall scaling factor of 2.2 for VOC emissions was based on comparisons of early morning emissions estimates and ambient observations of VOC/ NO_x data, the simple scaling factors employed in this study provide only an interim "fix" to the emissions

inputs. More accurate corrections to emissions inputs must await the availability of pertinent source test results.

The achievement of better model performance was expected to be a costly and time consuming endeavor. For example, one possible further study might have involved the development of revised wind fields using a prognostic meteorological model. There are currently no good means for improving emissions estimates.

In assessing the modeling situation, a judgment was made to proceed with subsequent phases of the proposed study. Basically, we attempted to achieve the best performance possible within the constraints of schedule and budget. In using the model for subsequent studies, we assume that it is being applied to a hypothetical situation as represented by the existing model inputs. Under these circumstances, it is possible to examine the potential influence of alternative base cases for this set of hypothetical conditions. We strongly recommend that the reader exercise caution in any attempt to extend subsequent model application results to emission control policies in the SoCAB. The most relevant findings of this work concern the potential need to examine the influence of alternative base cases on the air quality benefits of future year emission control plans.

Run J1 Maximum Estimated and Observed Concentrations of O₃ (pphm) on 24 June 1987

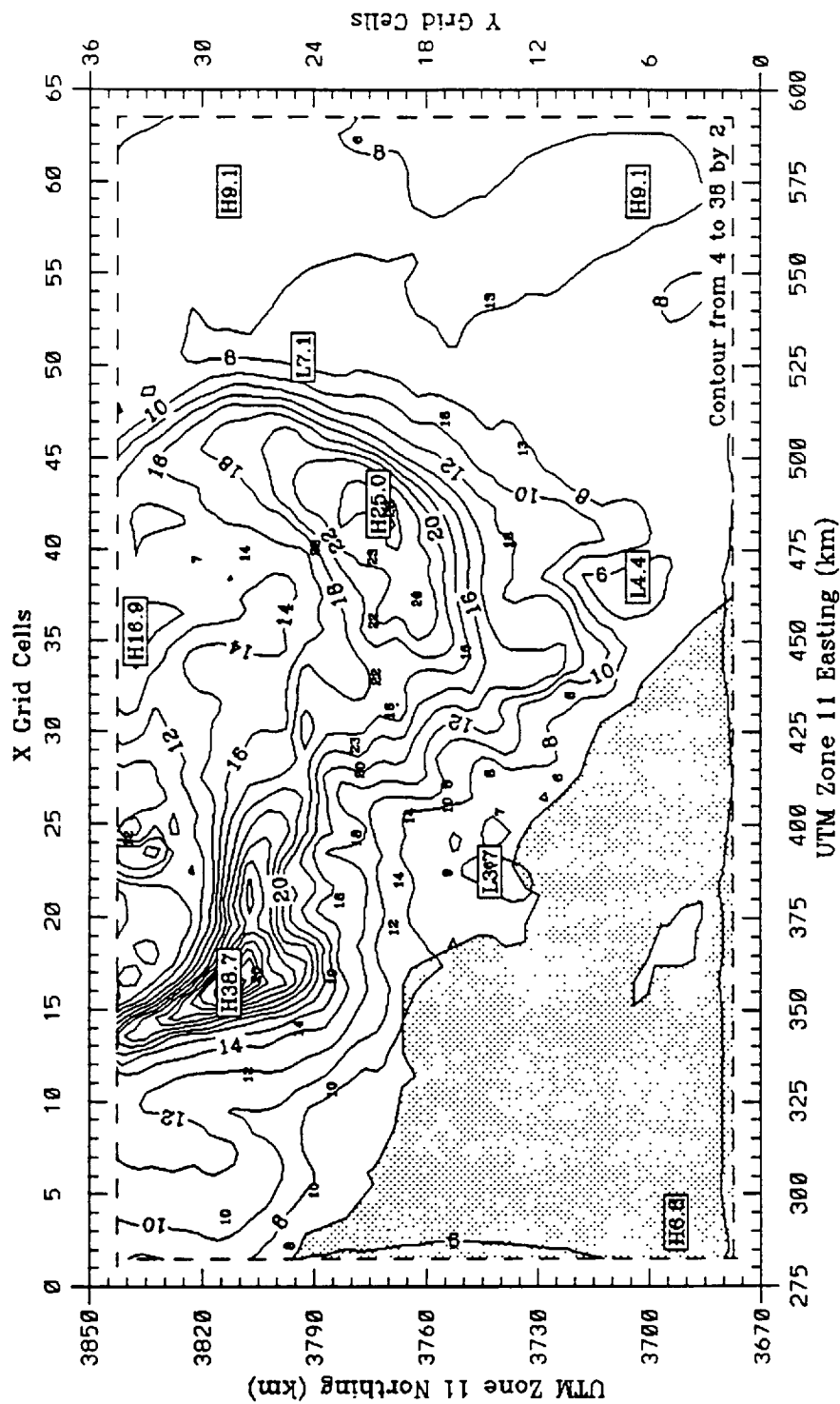


Figure 2-4. Run J1 maximum estimated and observed concentrations of O₃ (pphm) on 24 June 1987

Run J1 Maximum Estimated and Observed Concentrations of O₃ (pphm) on 25 June 1987

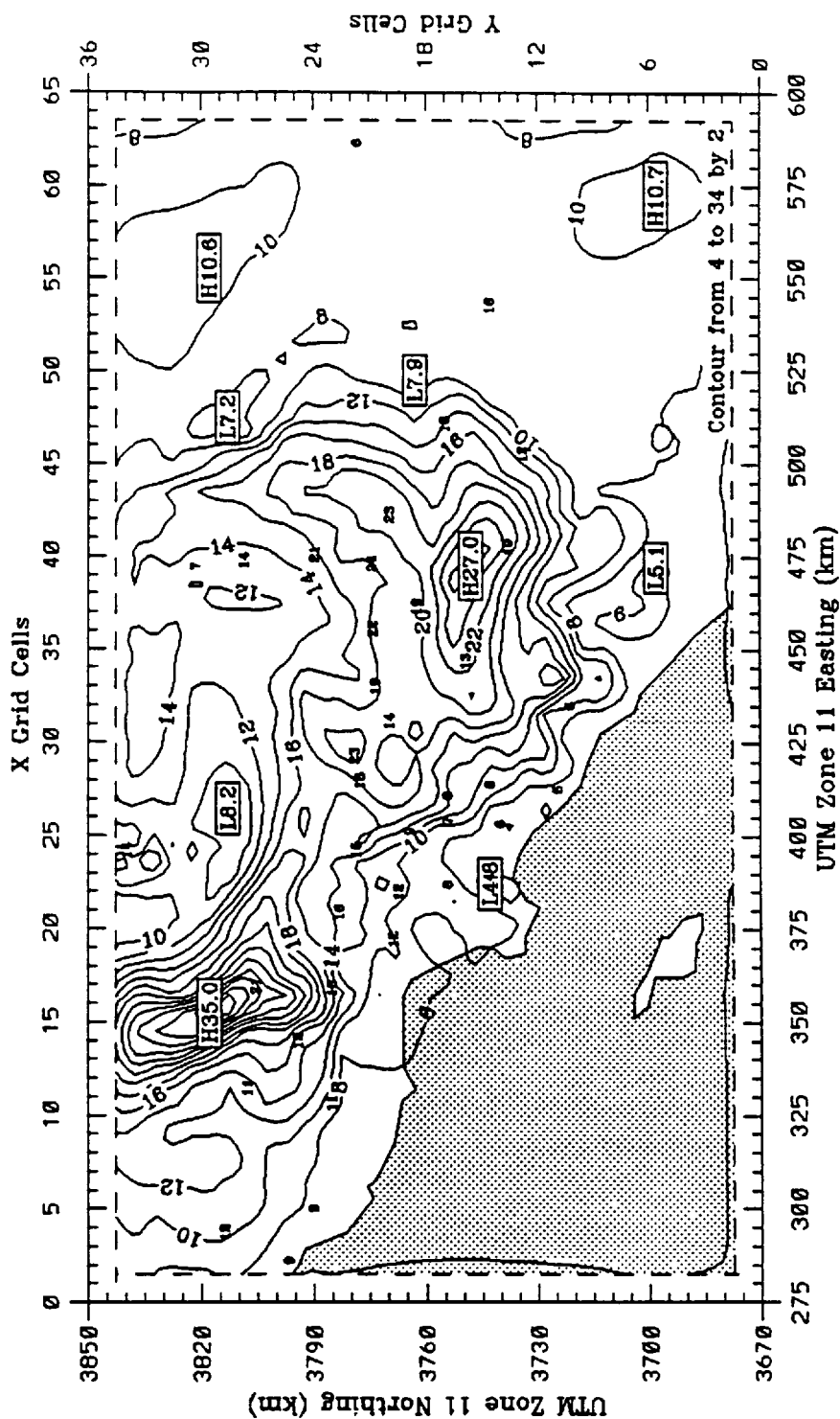


Figure 2-5. Run J1 maximum estimated and observed concentrations of O₃ (pphm) on 25 June 1987

Run J2 Maximum Estimated and Observed Concentrations of O₃ (pphm) on 24 June 1987

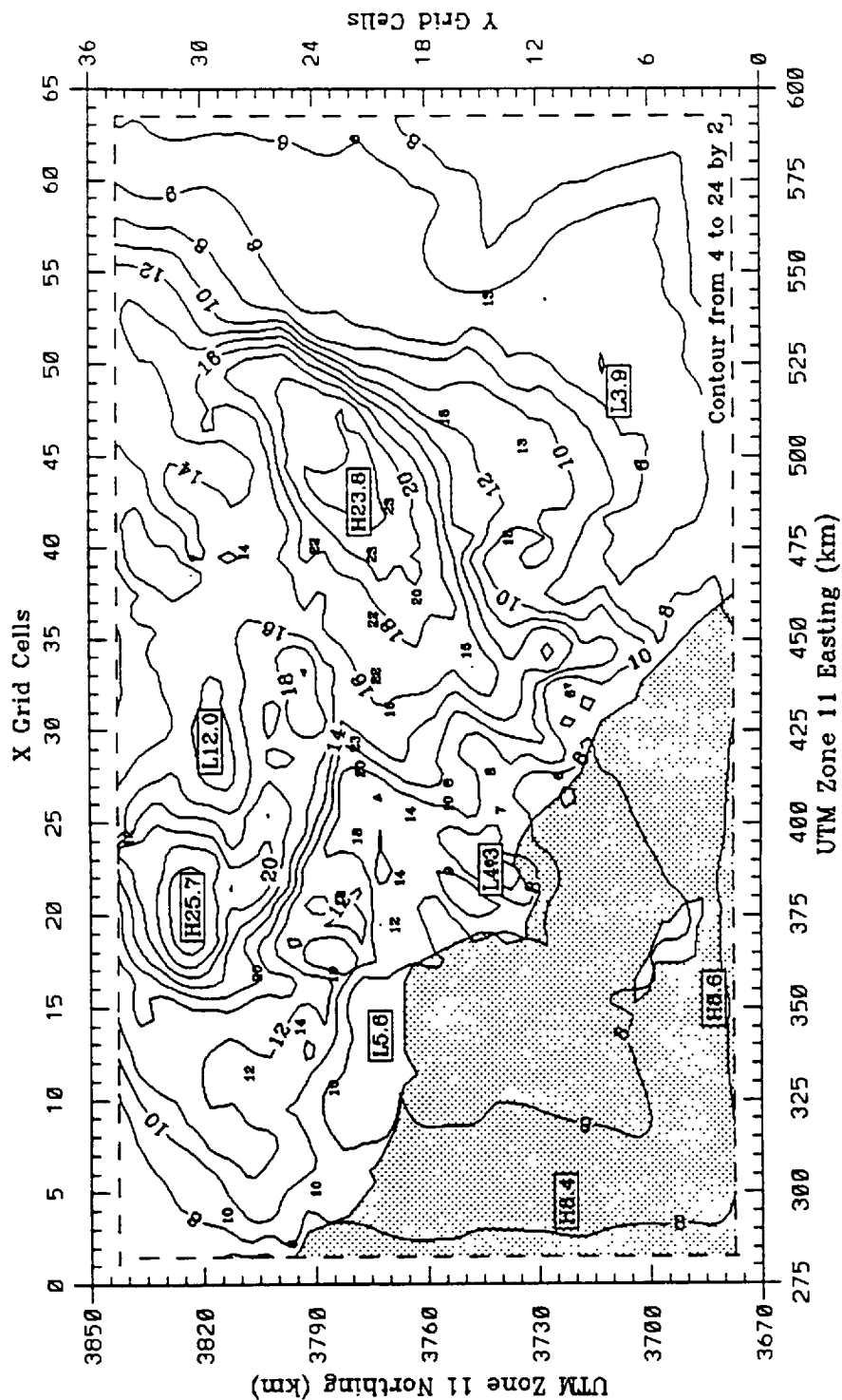


Figure 2-6. Run J2 maximum estimated and observed concentrations of O₃ (pphm) on 24 June 1987

Run J2 Maximum Estimated and Observed Concentrations of O₃ (pphm) on 25 June 1987

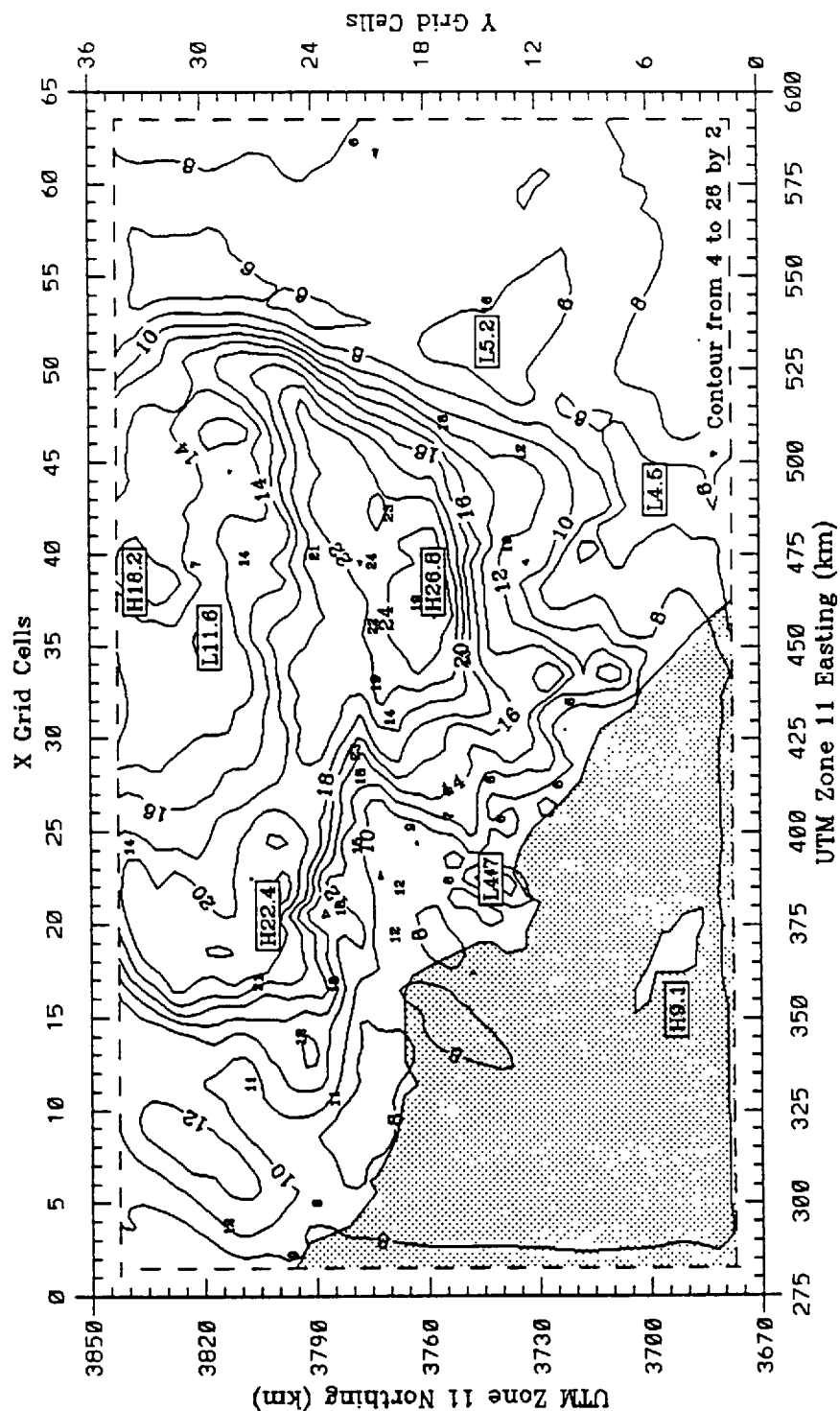


Figure 2-7. Run J2 maximum estimated and observed concentrations of O₃ (pphm) on 25 June 1987

Run J1 Maximum Estimated and Observed Concentrations of NO₂ (pphm) on 24 June 1987

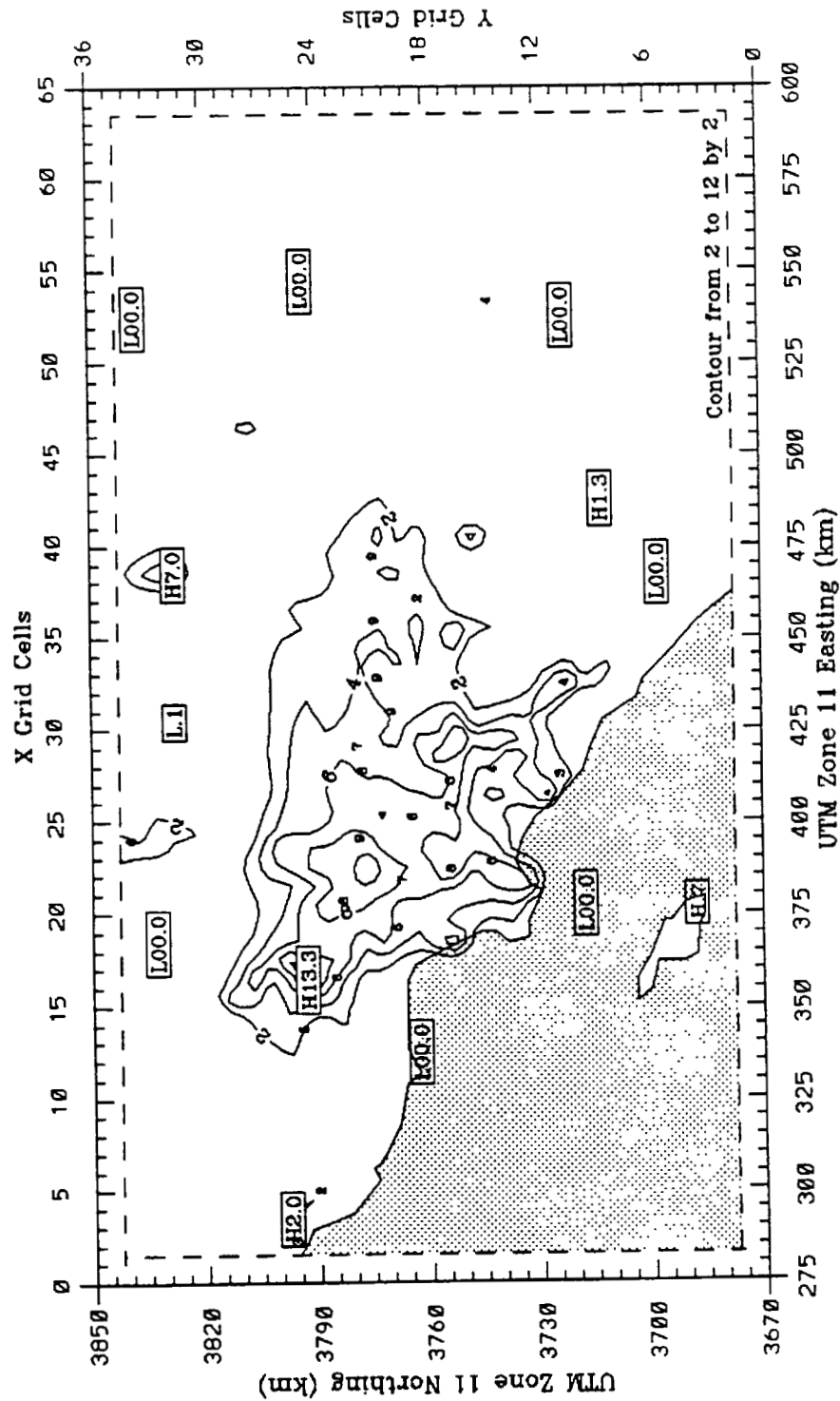


Figure 2-8. Run J1 maximum estimated and observed concentrations of NO₂ (pphm) on 24 June 1987

Run J2 Maximum Estimated and Observed Concentrations of NO₂ (pphm) on 24 June 1987

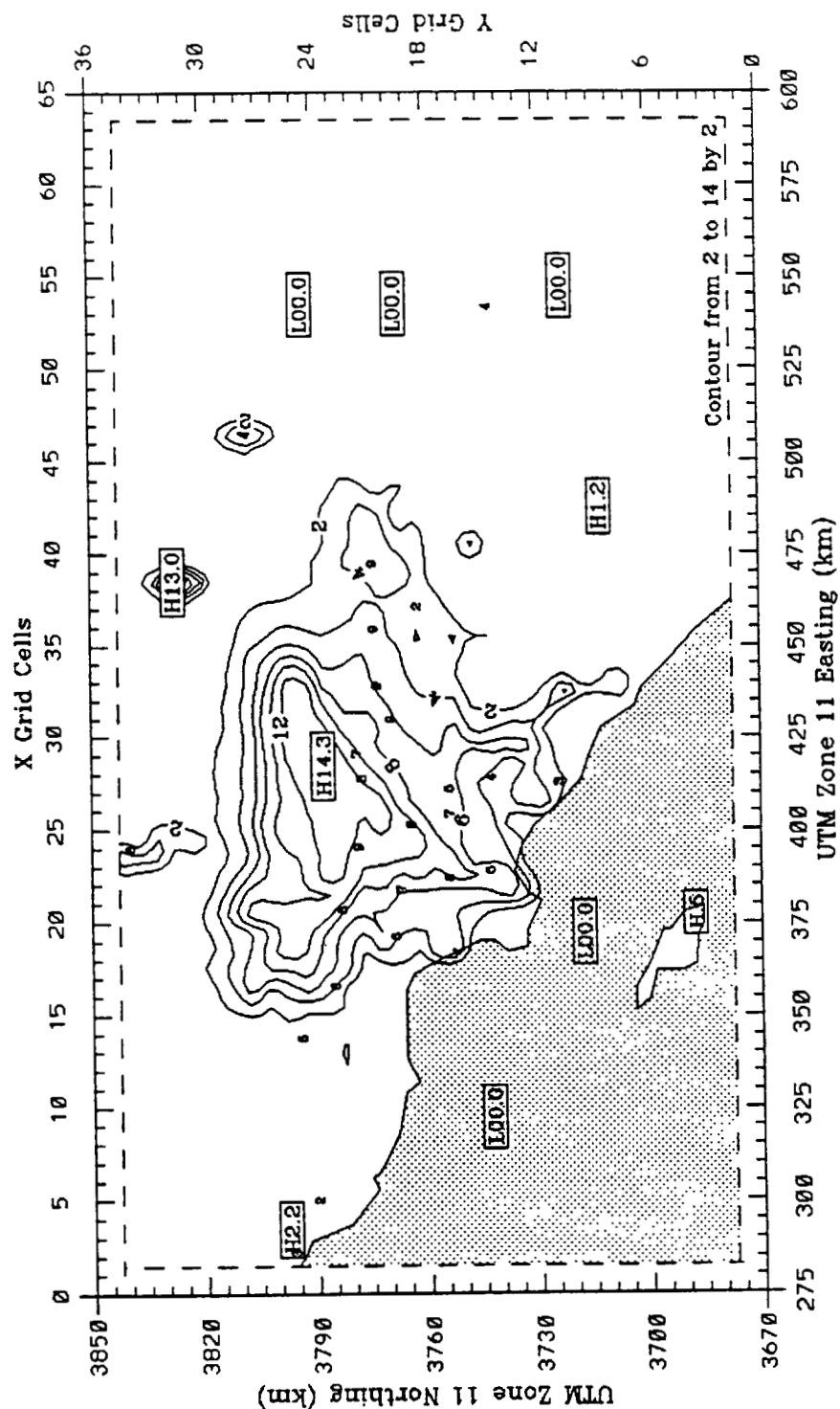


Figure 2-9. Run J2 maximum estimated and observed concentrations of NO₂ (pphm) on 24 June 1987

UAM Simulation Results for 23-25 June 1987

Location: LGBH Runs: J1, J2, and J7

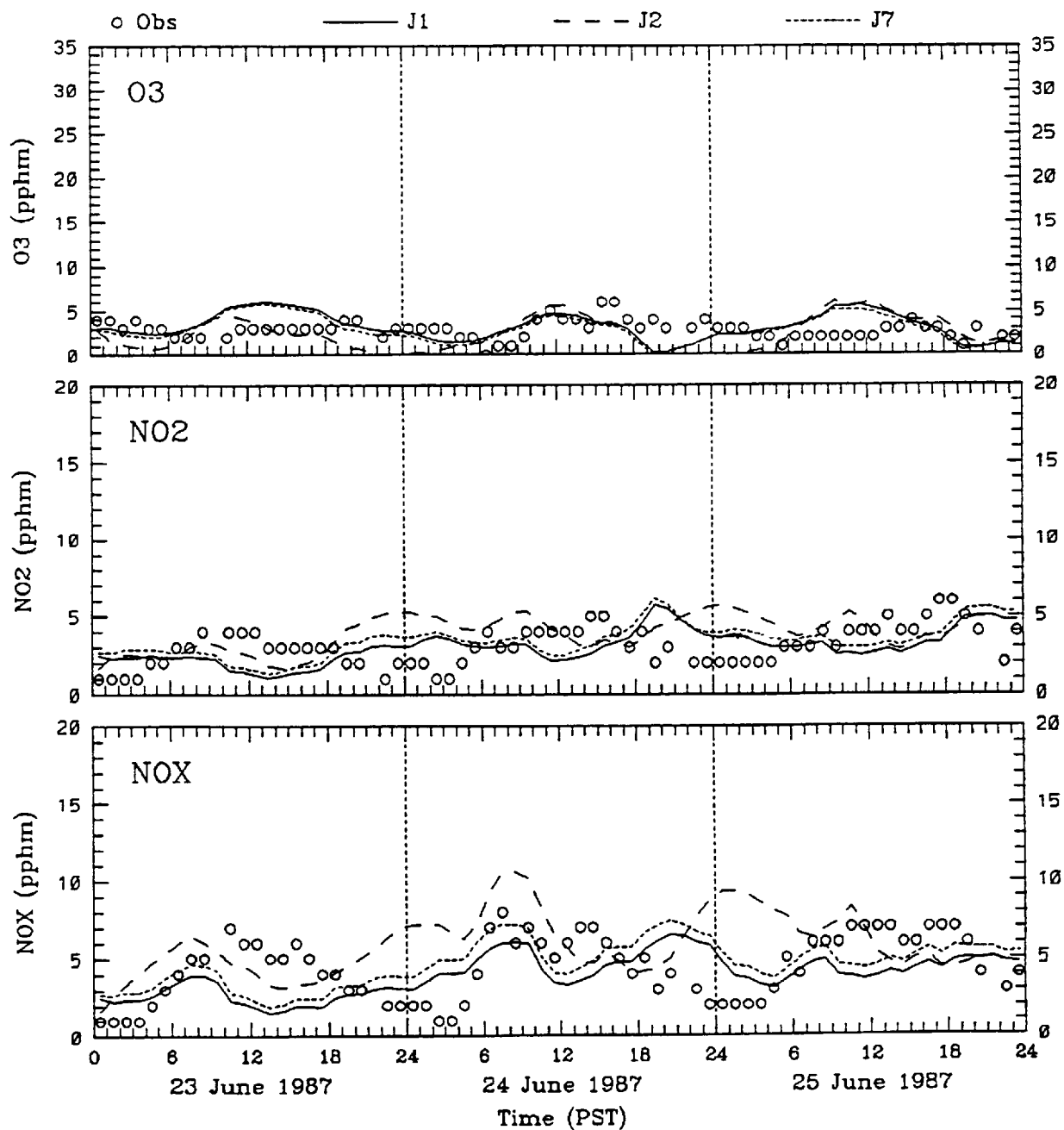


Figure 2-10(a). UAM simulation results at Long Beach

UAM Simulation Results for 23-25 June 1987

Location: CELA Runs: J1, J2, and J7

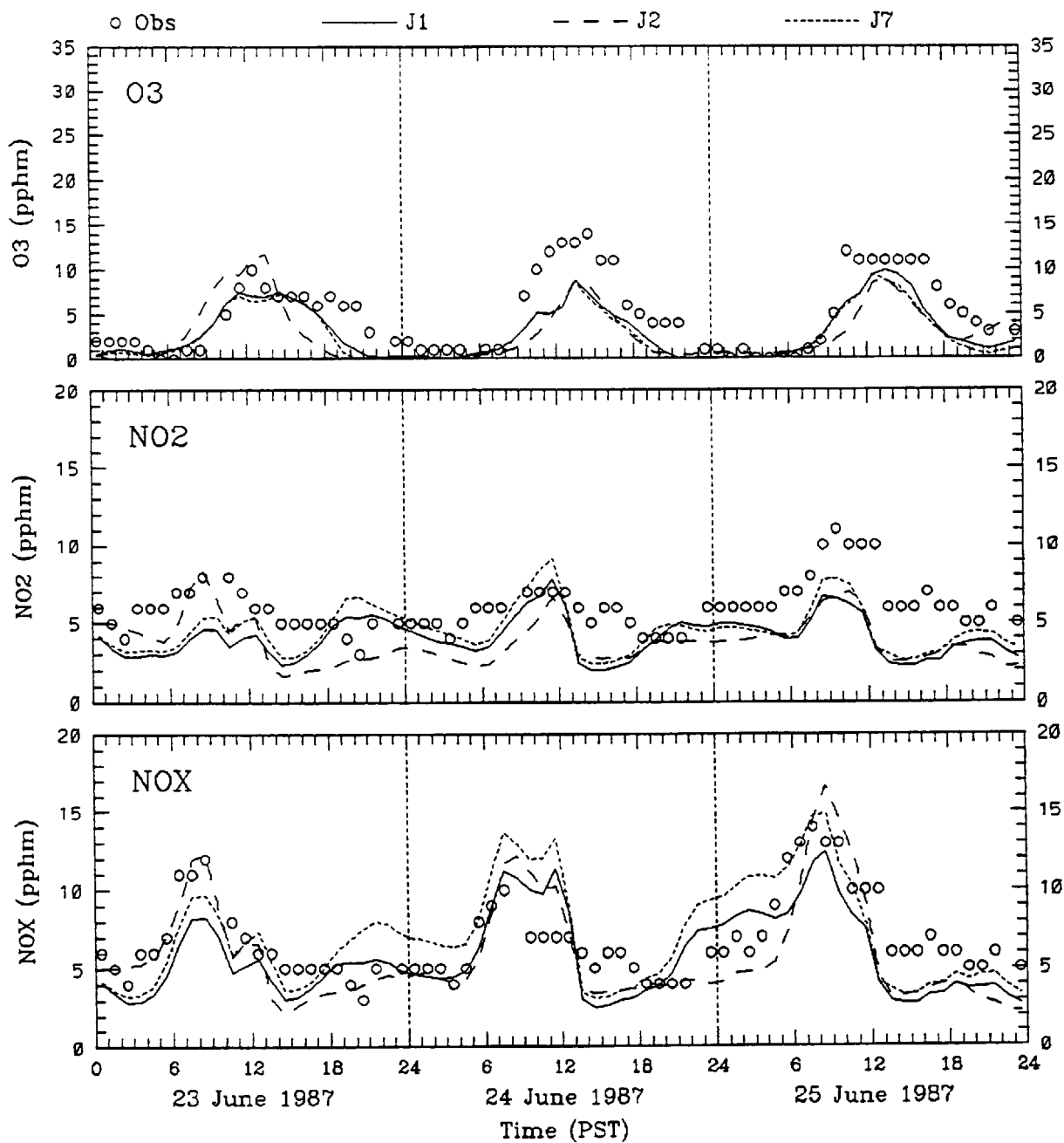


Figure 2-10(b). UAM simulation results at Los Angeles