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The Importance of Using Alternative Base Cases in Photochemical Modeling

STEP
Strategies for Today's Environmental Partnership

American Petroleum Institute
1220 L Street, Northwest
Washington, D.C. 20005

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Strategies for Today's Environmental Partnership

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The Importance of Using Alternative Base Cases in Photochemical Modeling

Health and Environmental Sciences Department

API PUBLICATION NUMBER 4616

PREPARED UNDER CONTRACT BY:

STEVEN REYNOLDS, HARVEY MICHAELS, AND PHILIP ROTH
ENVAIR
12 PALM AVENUE
SAN RAFAEL, CA 94901

T.W. TESCHE AND DENNIS MCNALLY
ALPINE GEOPHYSICS
P.O. BOX 2059
CRESTED BUTTE, CO 81224

LUANN GARDNER AND GREG YARWOOD
SYSTEMS APPLICATIONS INTERNATIONAL
101 LUCAS VALLEY ROAD
SAN RAFAEL, CA 94903

JULY 1994

American
Petroleum
Institute

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API STAFF CONTACT

Howard Feldman, Health and Environmental Sciences Department

MEMBERS OF THE API AIR MODELING TASK FORCE

Kenneth W. Steinberg, *Chairman*, Exxon Research & Engineering
Charles H. Schleyer, *Vice-Chairman*, Mobil Research & Development

Doug N. Blewitt, Amoco Corporation
Lee K. Gilmer, Texaco Research
Allan A. Hirata, Unocal Corporation
John A. King, Shell Development Company
George A. Lauer, ARCO
Rory S. MacArthur, Chevron Research & Technology
Robert L. Peace, Jr., Unocal Corporation
Chris Rabideau, Texaco Inc.
Stephen D. Ziman, Chevron Research & Technology

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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 O_3 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

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 O_3 episodes occurring in June and August of 1987 indicated that the model was not replicating important features of the O_3 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 O_3 and NO_2. 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 O_3 fields, i.e., the decreases in estimated O_3 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 O_3 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 O_3 concentrations. For 24 June, the estimated reductions in peak O_3 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 O_3 concentration than was estimated for the case where VOC emissions alone were reduced). The third June base case yielded peak O_3 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 O_3 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 O_3 (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 O_3 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 O_3 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 O_3 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 O_3 episodes occurring in June and August of 1987 indicated that the model was not replicating important features of the O_3 concentration field, including the relatively high peak concentrations reported at inland monitoring stations and the formation of an extensive layer of high O_3 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 O_3 formation aloft to the extent indicated by available measurements. Moreover, the model generated O_3 concentrations in an area north of the San Fernando Valley that were much higher than the observations. The accuracy of VOC and NO_2 estimates was poorer than that for O_3, 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 O_3 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

[1]For 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 O_3 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 O_3 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 O_3 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 O_3 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 O_3 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 O_3 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 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 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 O_3 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 O_3 NAAQS attainment demonstrations.

In developing inputs for a grid model simulation of an historical O_3 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 O_3 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 O_3 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 O_3 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 O_3 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

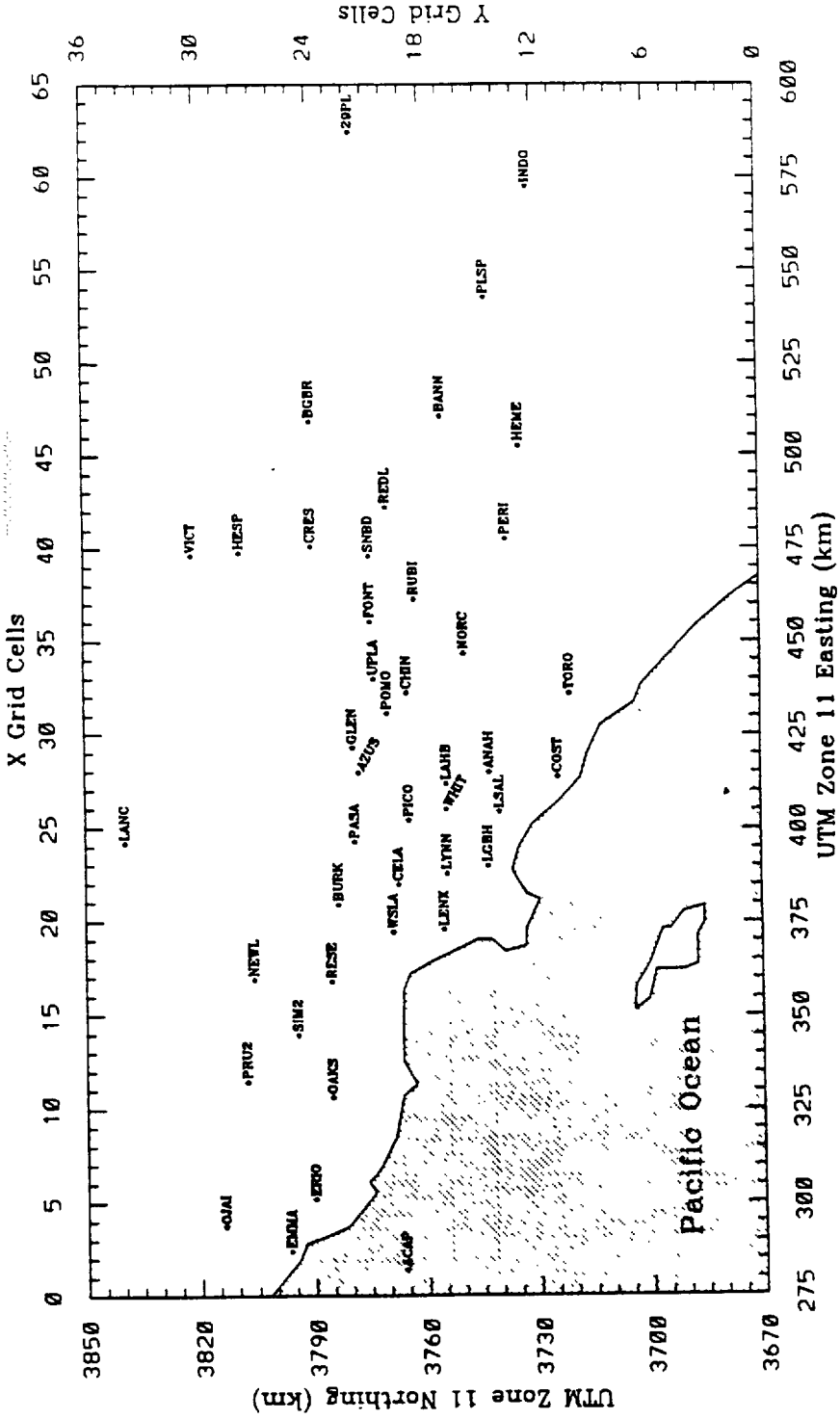


Figure 2-1. The UAM modeling domain and locations of air monitoring stations

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 O_3 concentrations at several stations (e.g., Crestline, Glendora, Hesperia, Pomona, Rubidoux, and Victorville). The normalized error for hourly-averaged NO_2 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 O_3 concentrations aloft. However, when they examined available UAM results, they found that the model was significantly underestimating O_3 aloft, as illustrated in Figure 2-3.

An inability both to accurately replicate the peak O_3 measurements at several important air monitoring locations and to simulate the formation of high O_3 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.

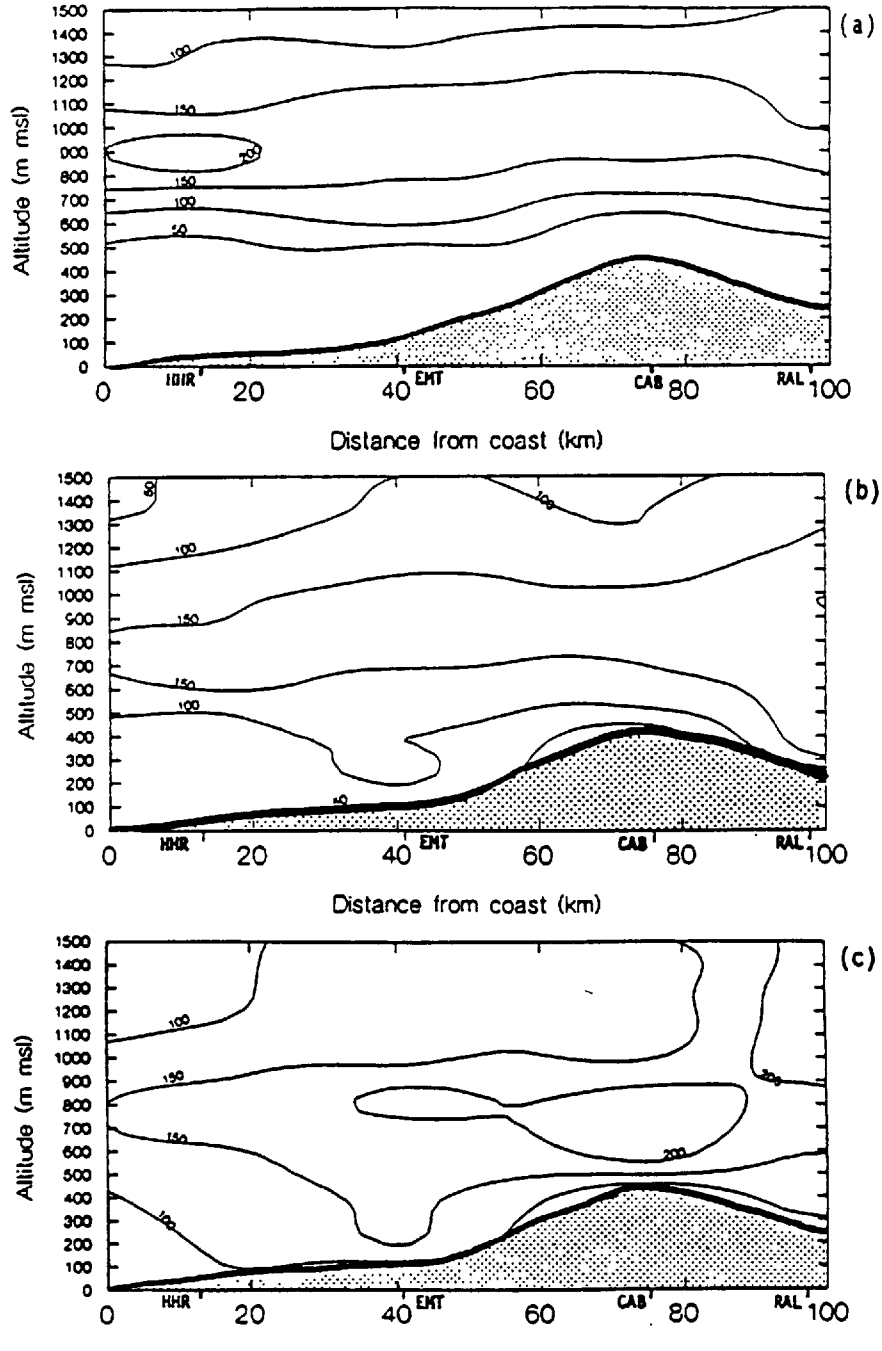


Figure 2-2. O_3 concentrations aloft during the (a) morning, (b) midday, and (c) afternoon of 25 June 1987. O_3 contours, in ppb, generated along a west-to-east plane from the coast near Hawthorn to Riverside using data from aircraft spirals. The shaded area approximately represents the ground. (Source: Roberts and Main, 1992b)

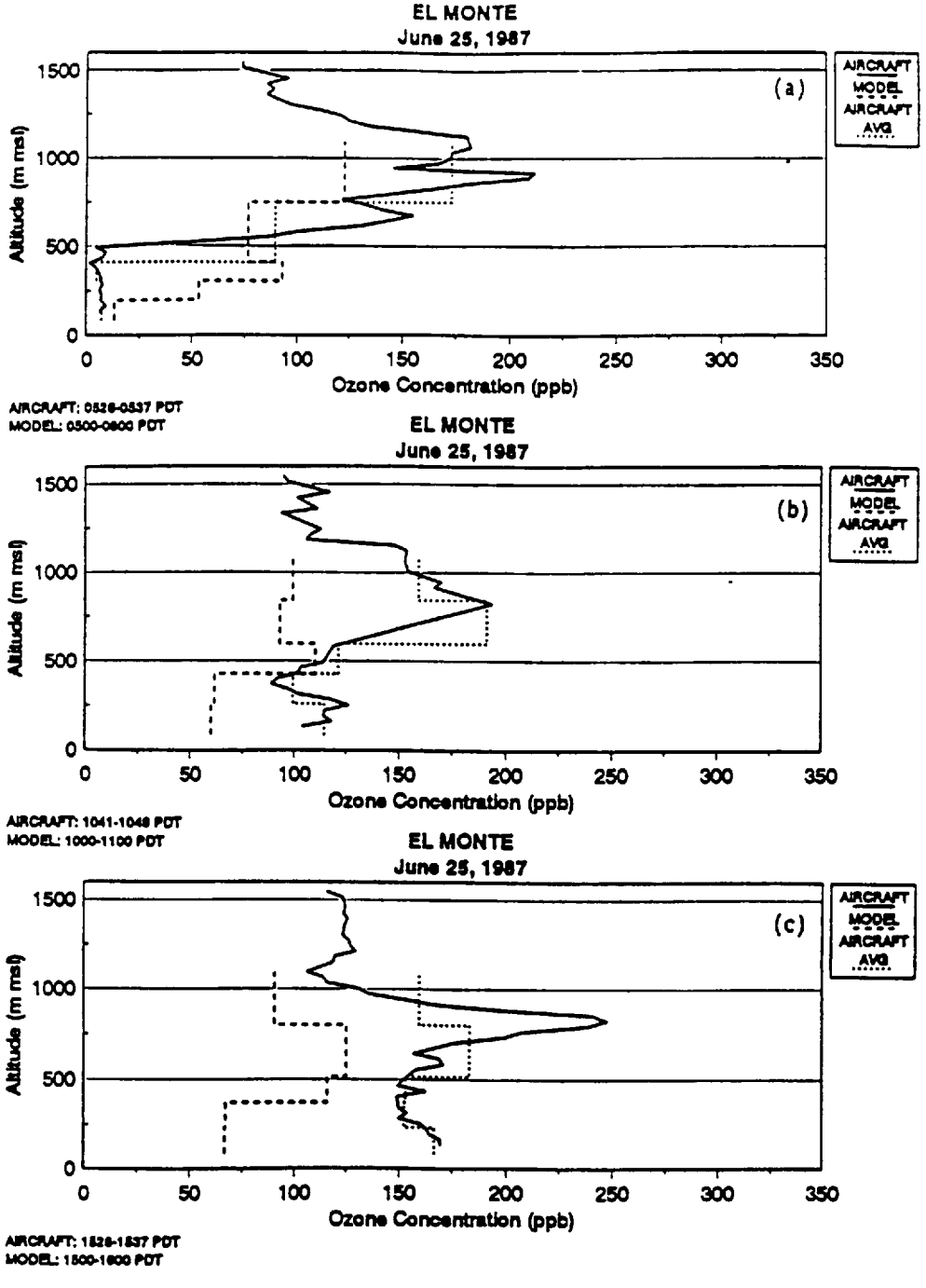


Figure 2-3. Vertical profiles of O_3 concentrations measured by aircraft spiral compared to UAM grid-averaged values (original SCAQMD simulation) for the (a) morning, (b) midday, and (c) afternoon at El Monte on 25 June 1987 (Source: Roberts and Main, 1992b)

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 O_3 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 O_3 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 O_3, NO_2, NO_x, and various Carbon-Bond species.

Key findings concerning O_3 and NO_x subregional model performance are as follows:

- estimated O_3 and NO_x concentrations at stations within the coastal and Ventura County subregions are generally in good agreement with the observations.
- O_3 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 O_3 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 O_3 underestimation problems in the SCAQMD simulation for 24 June (Run J2) occurring during midday hours when relatively high O_3 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 O_3. 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 O_3 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 O_3 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 O_3 concentrations aloft that extends over a large portion of the central basin, and estimates of bias and error for O_3 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.

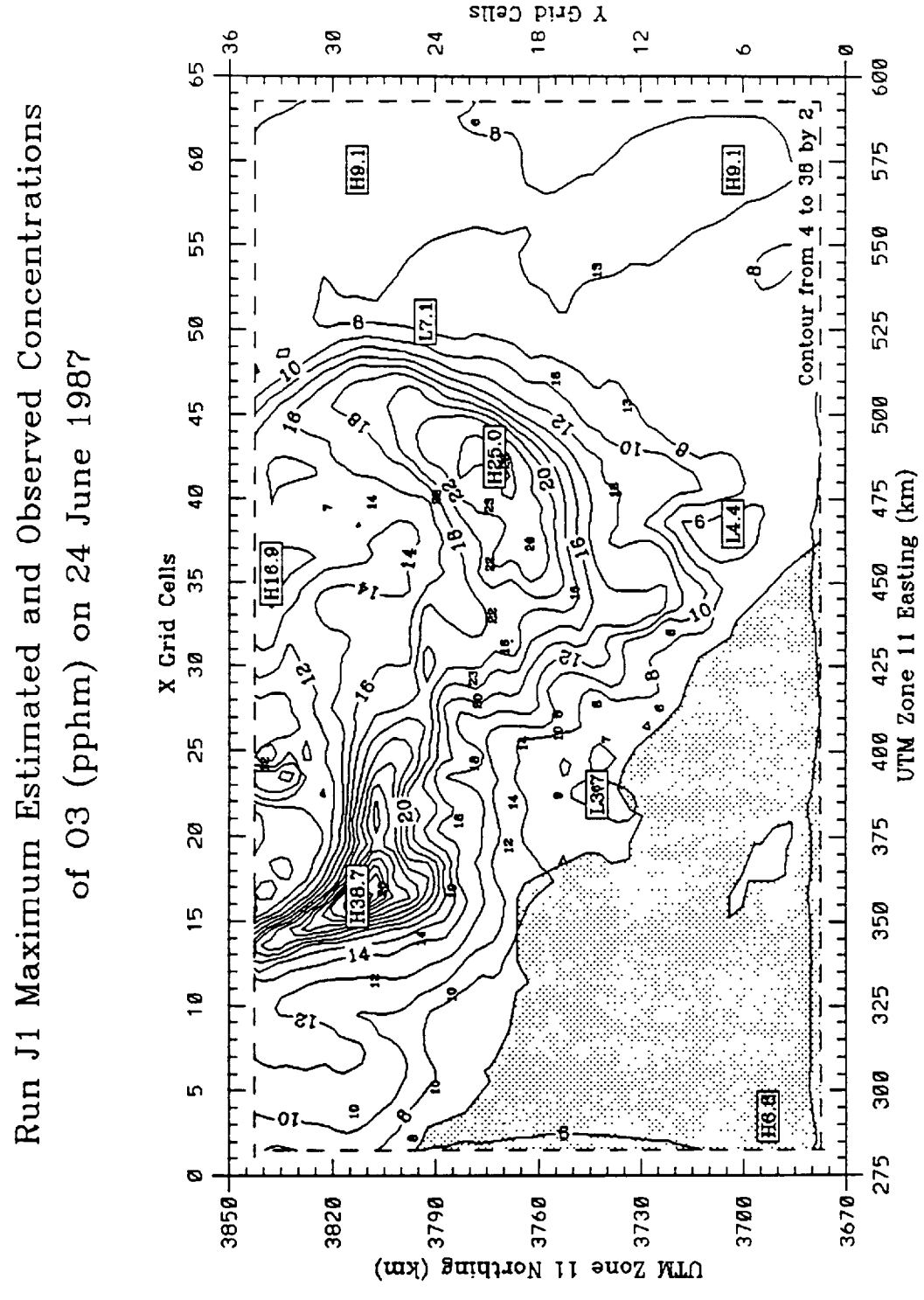


Figure 2-4. Run J1 maximum estimated and observed concentrations of O_3 (pphm) on 24 June 1987

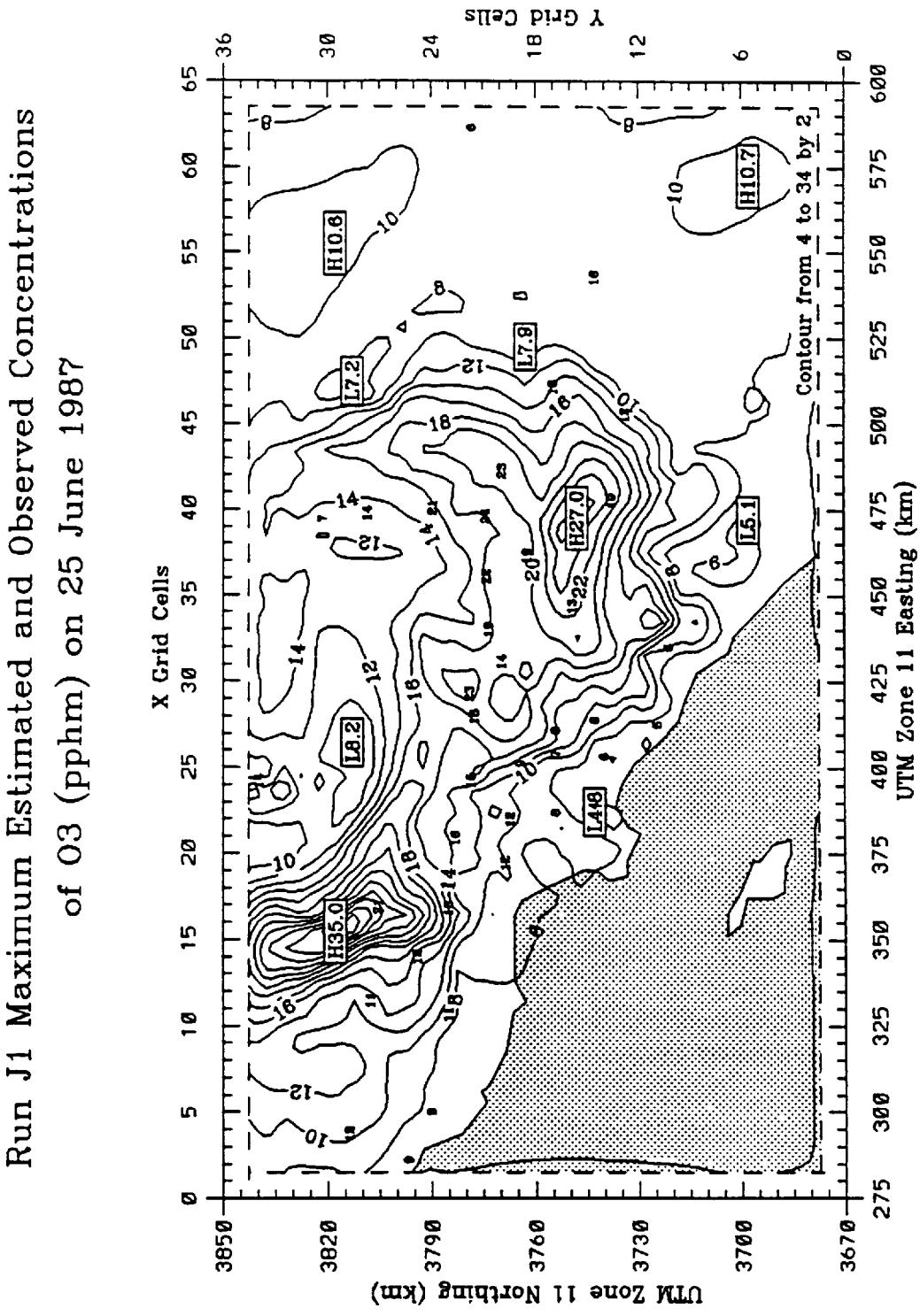


Figure 2-5. Run J1 maximum estimated and observed concentrations of O_3 (pphm) on 25 June 1987

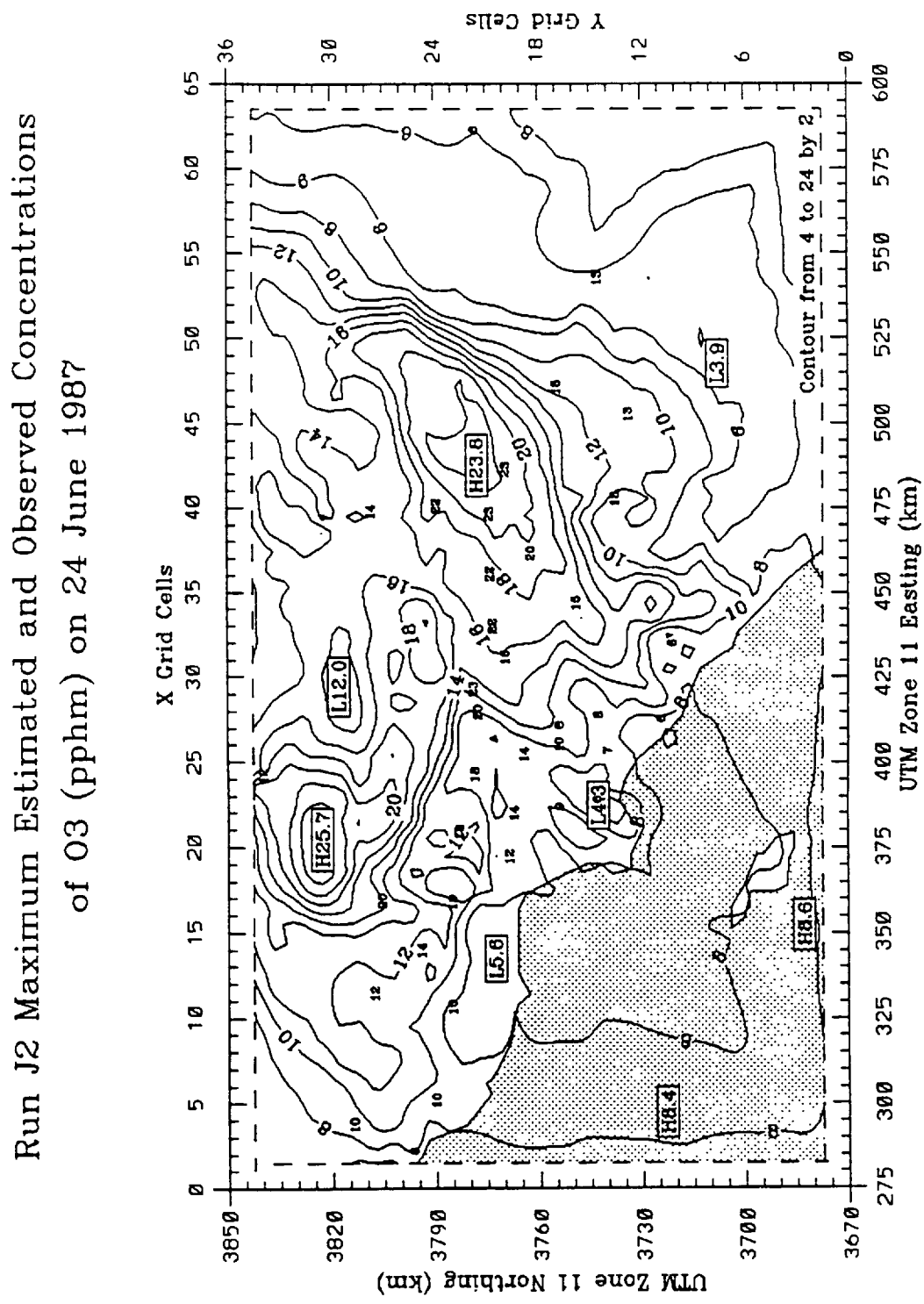


Figure 2-6. Run J2 maximum estimated and observed concentrations of O_3 (pphm) on 24 June 1987

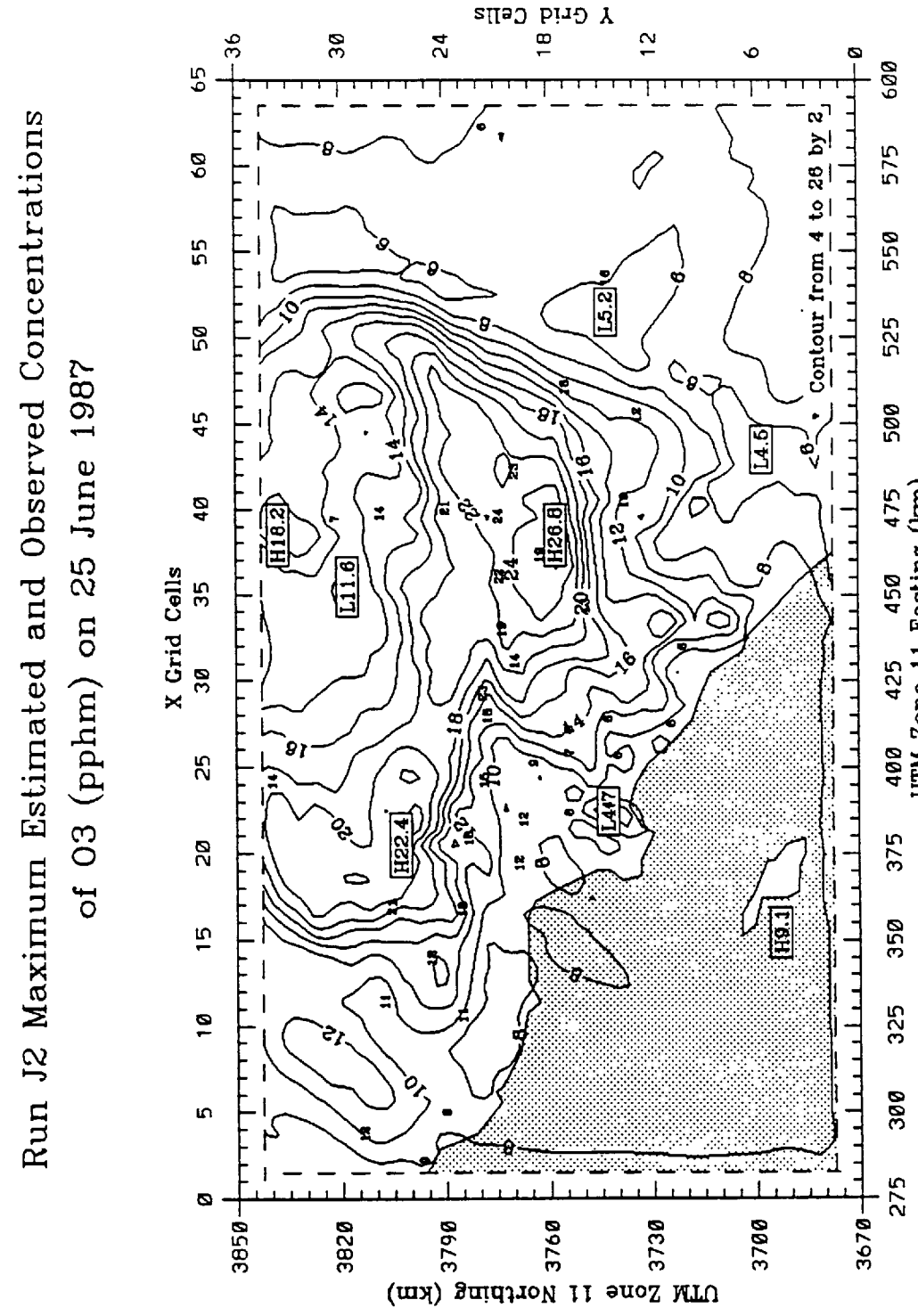


Figure 2-7. Run J2 maximum estimated and observed concentrations of O_3 (pphm) on 25 June 1987

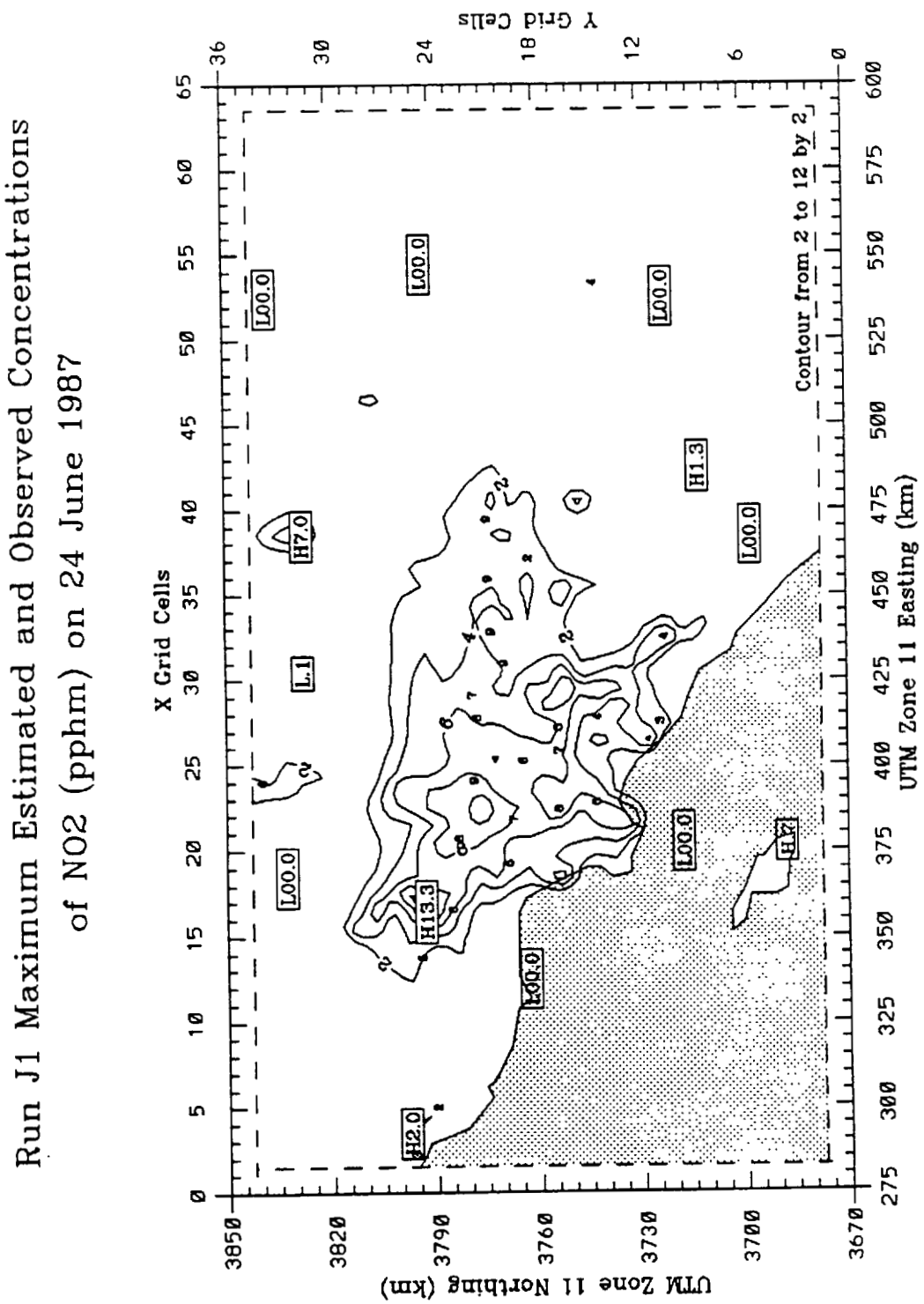


Figure 2-8. Run J1 maximum estimated and observed concentrations of NO_2 (pphm) on 24 June 1987

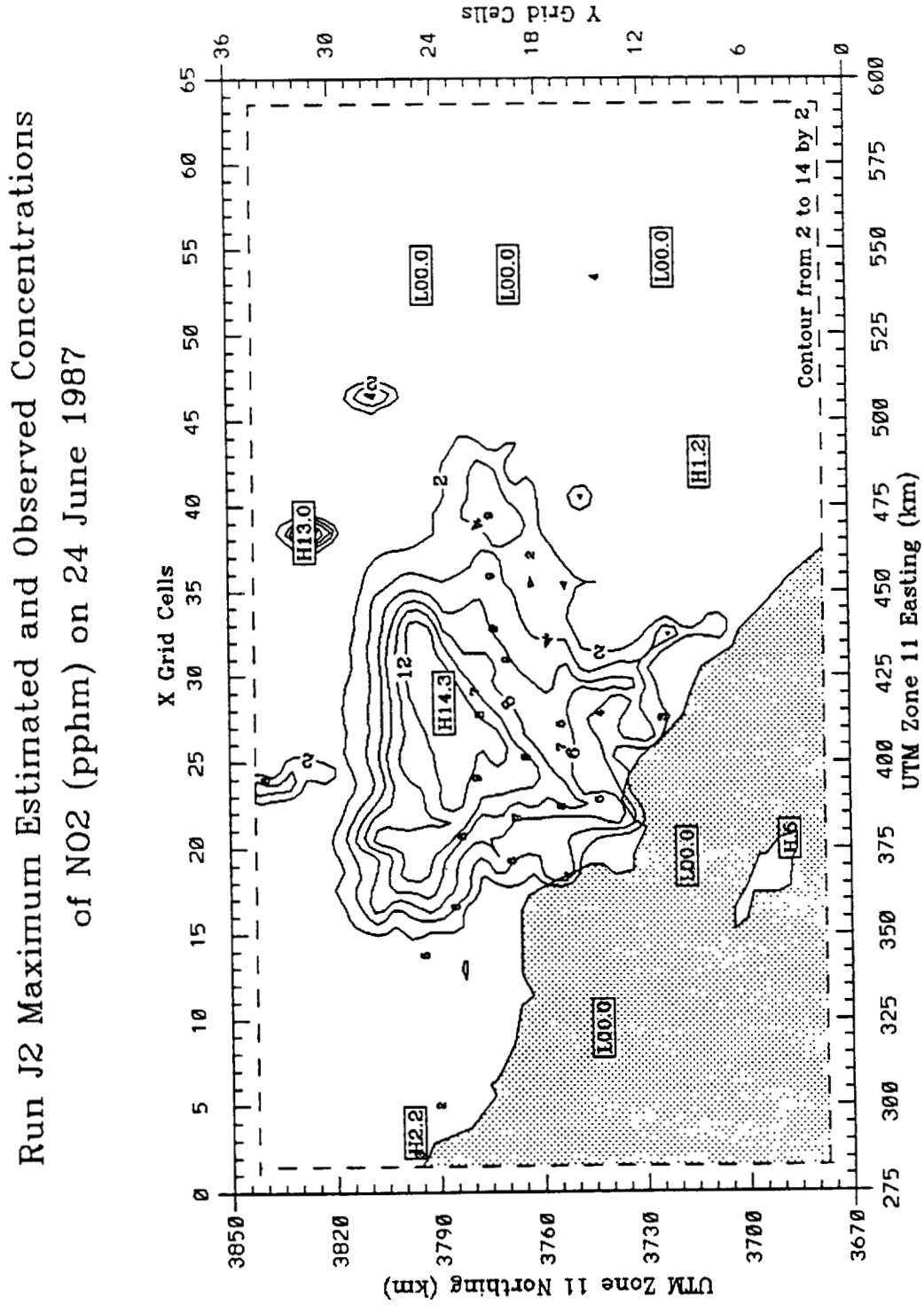


Figure 2-9. Run J2 maximum estimated and observed concentrations of NO_2 (pphm) on 24 June 1987

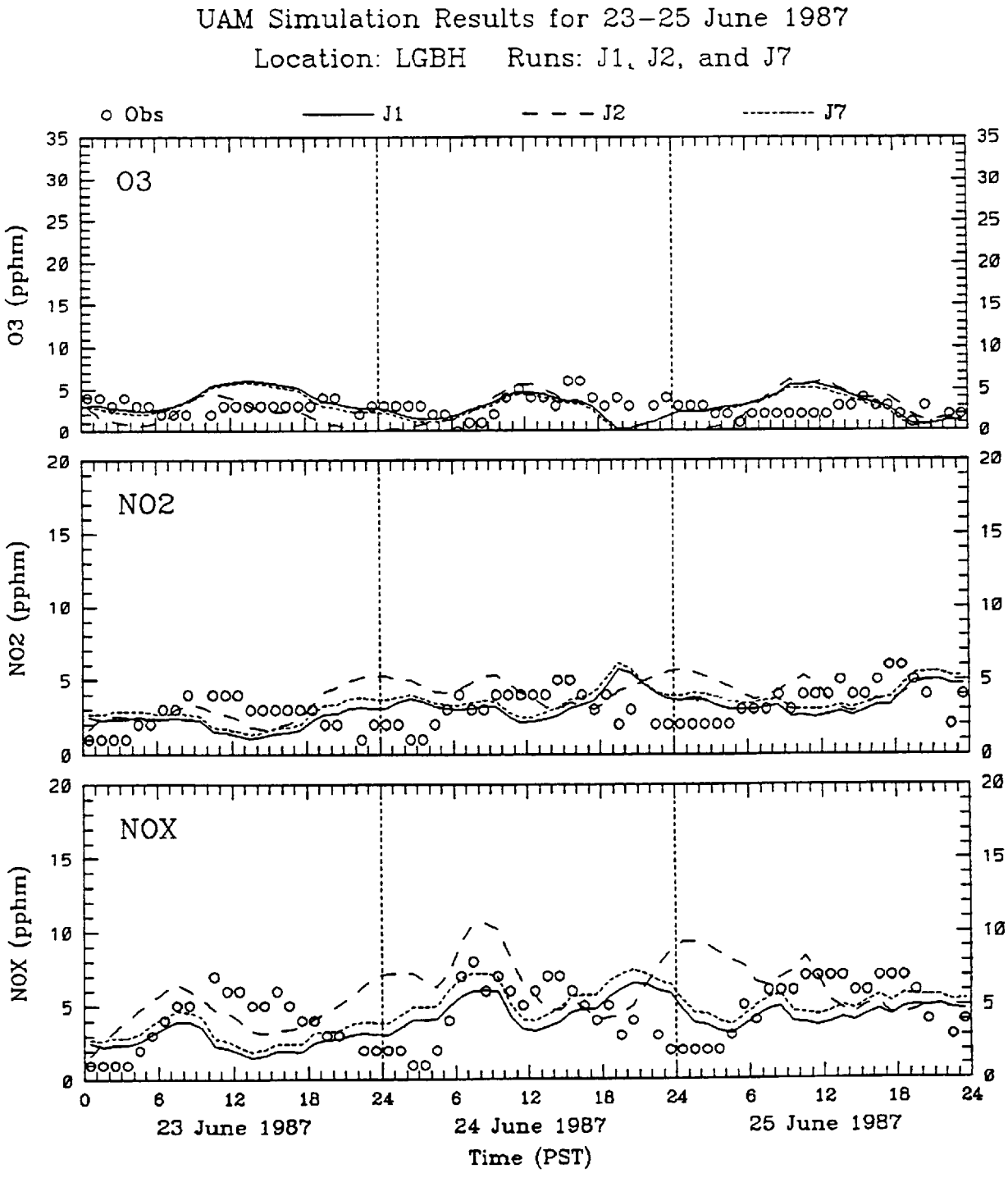


Figure 2-10(a). UAM simulation results at Long Beach

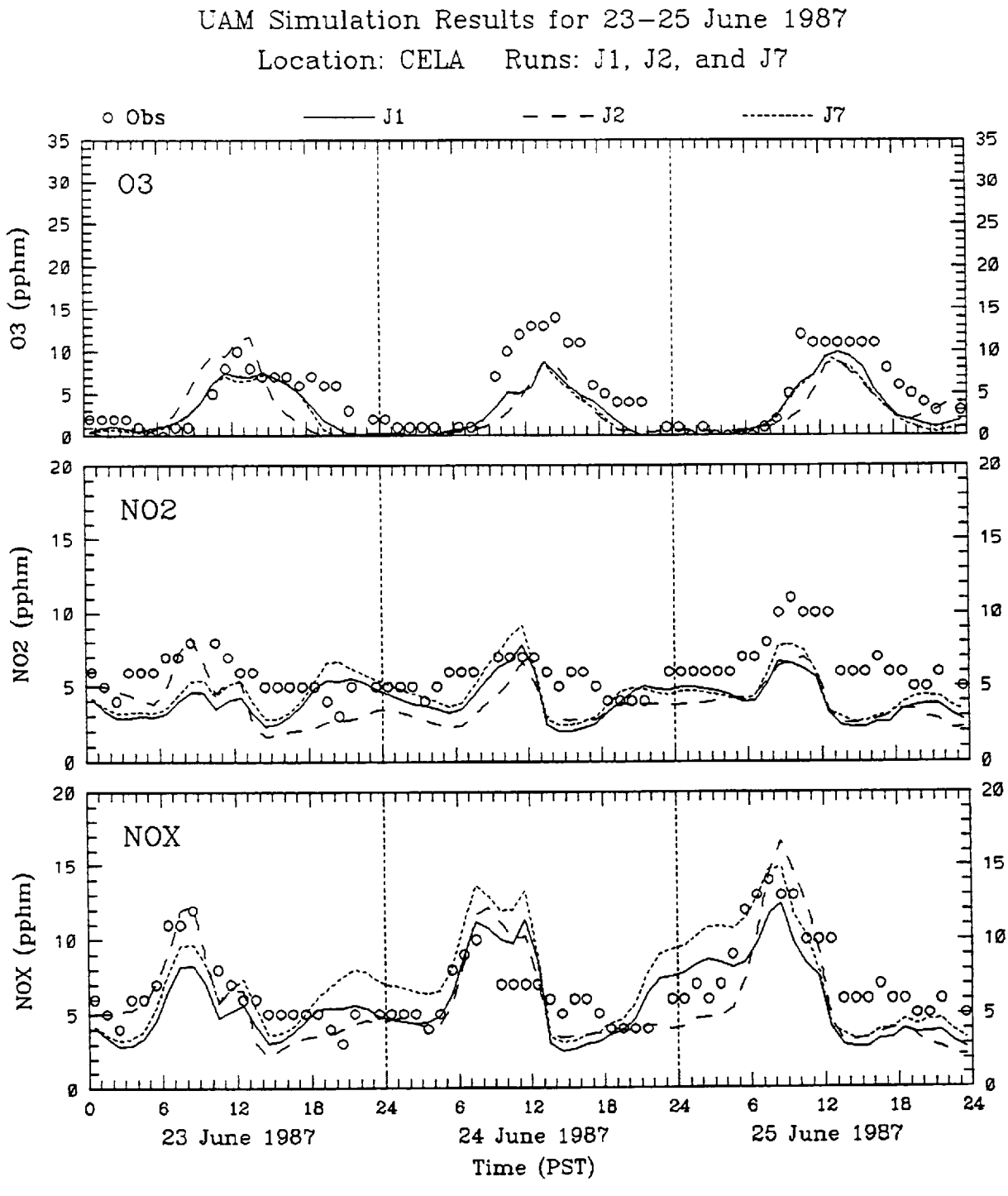


Figure 2-10(b). UAM simulation results at Los Angeles

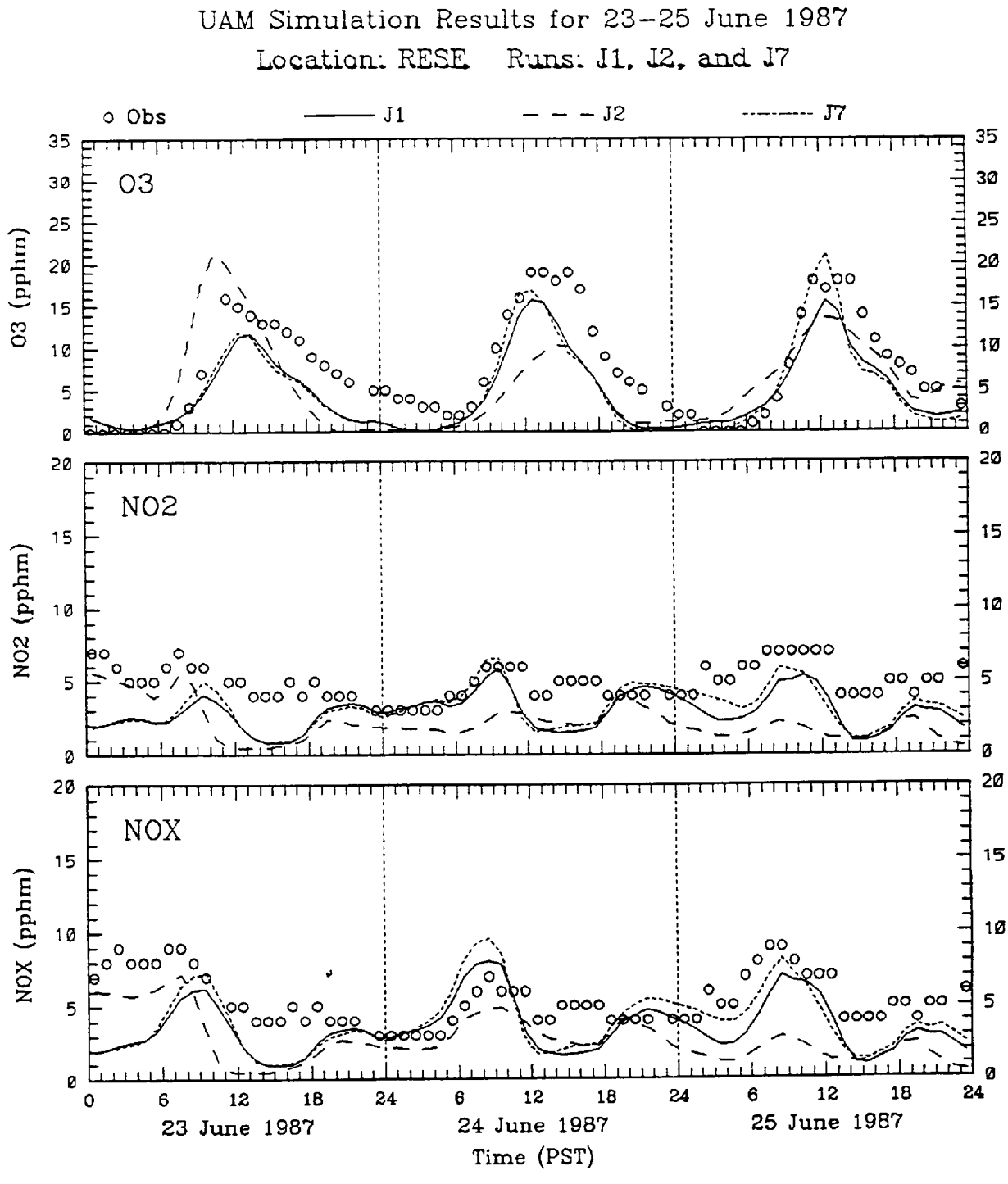


Figure 2-10(c). UAM simulation results at Reseda

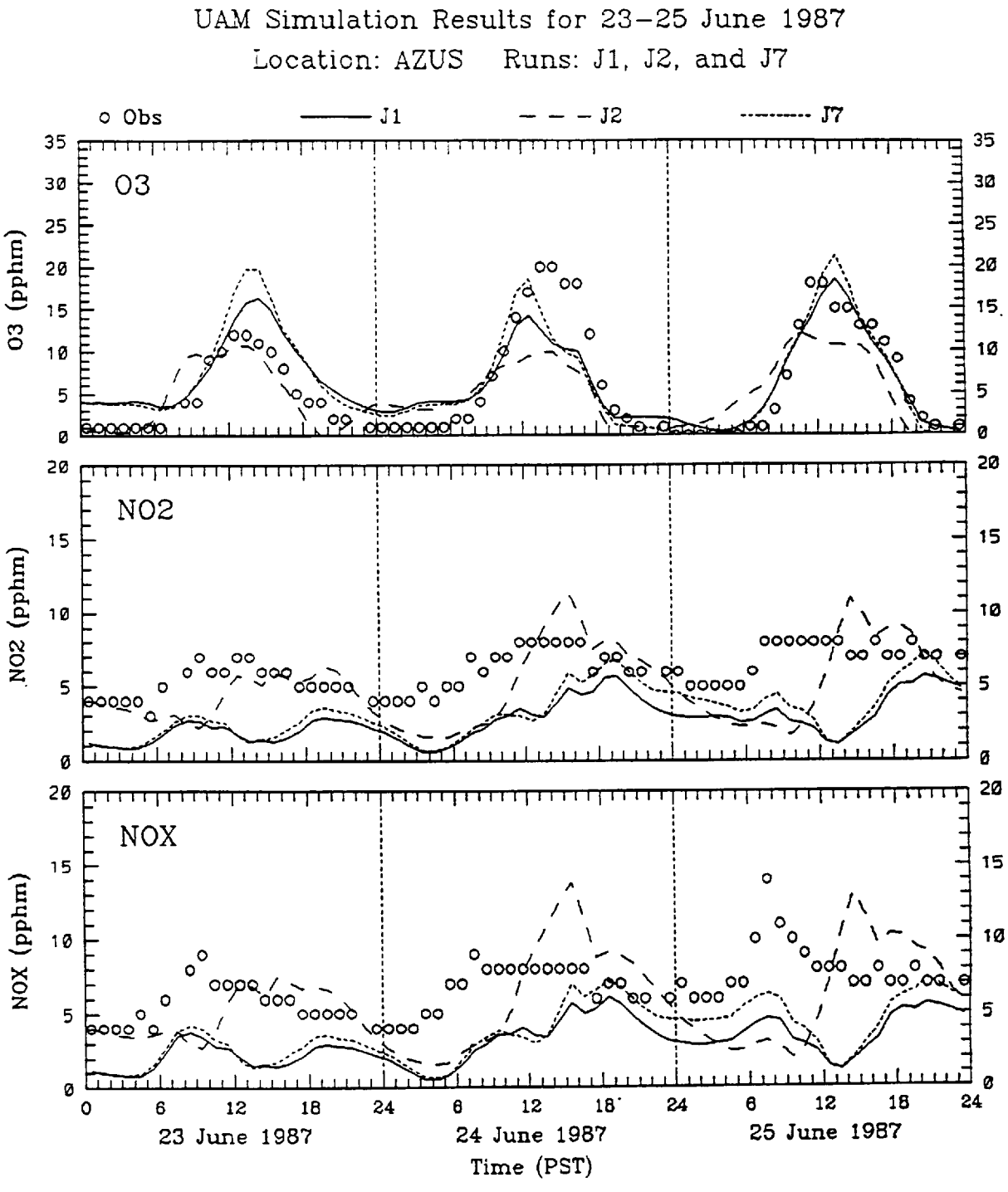


Figure 2-10(d). UAM simulation results at Azusa

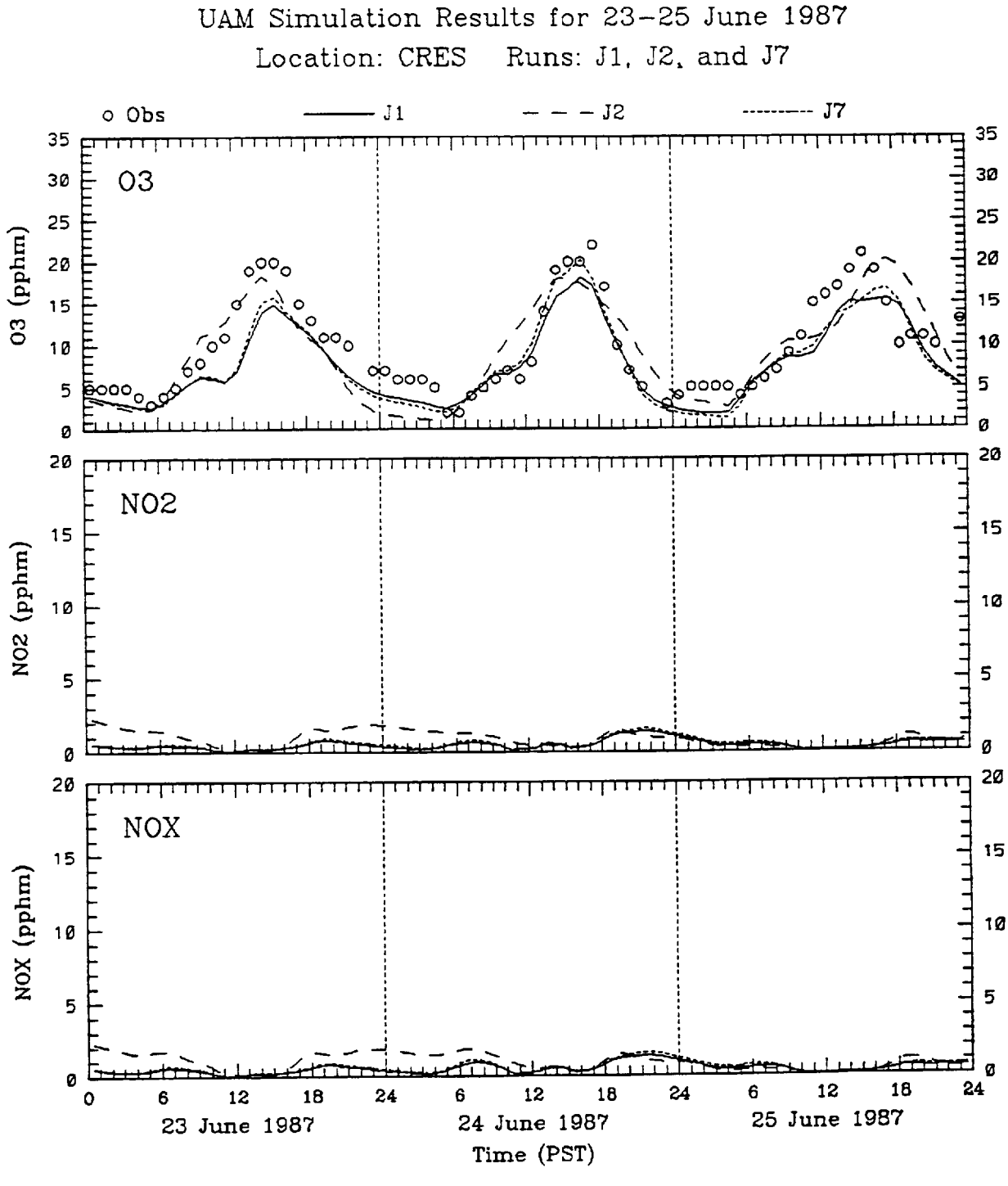


Figure 2-10(e). UAM simulation results at Crestline

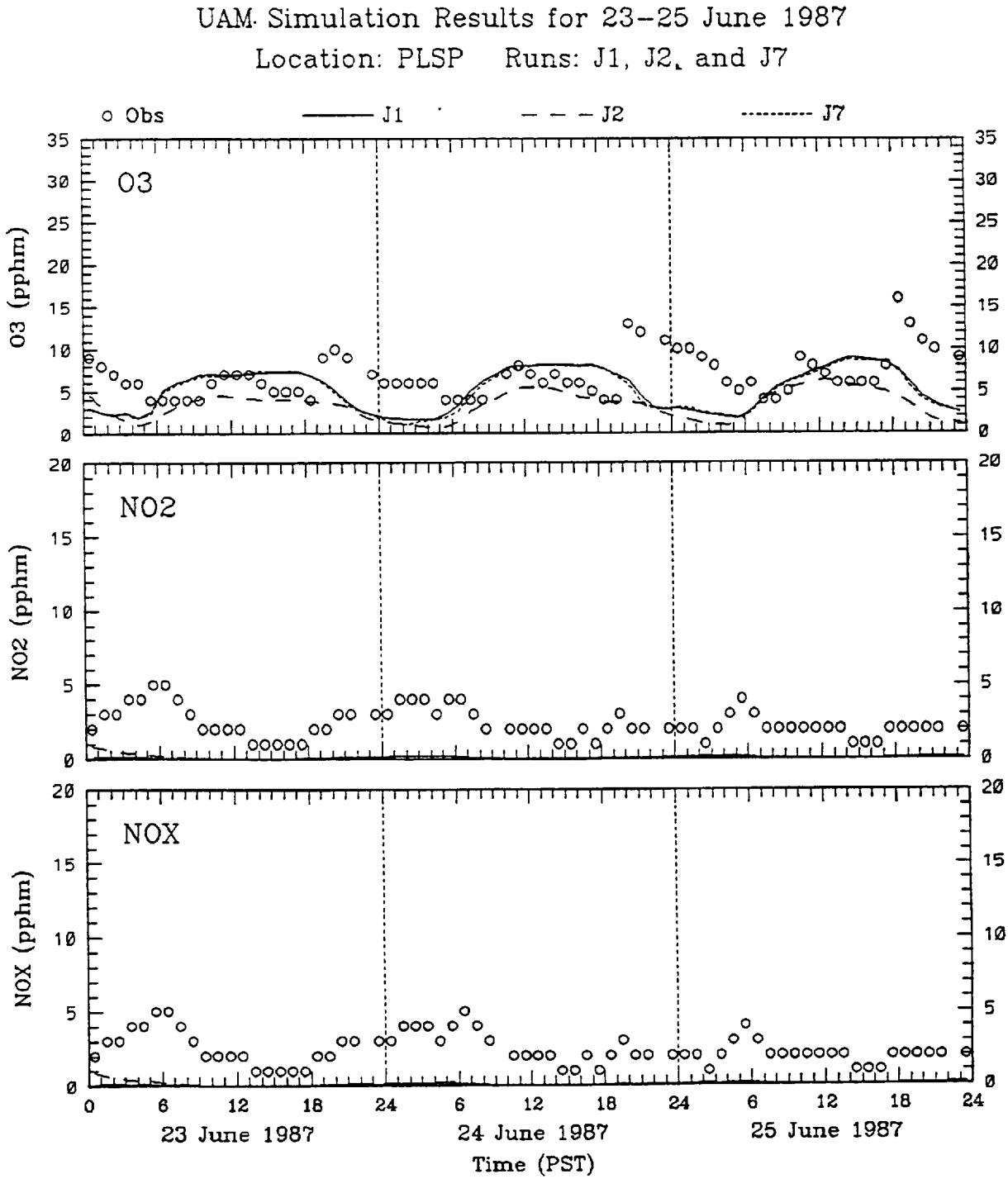


Figure 2-10(f). UAM simulation results at Palm Springs

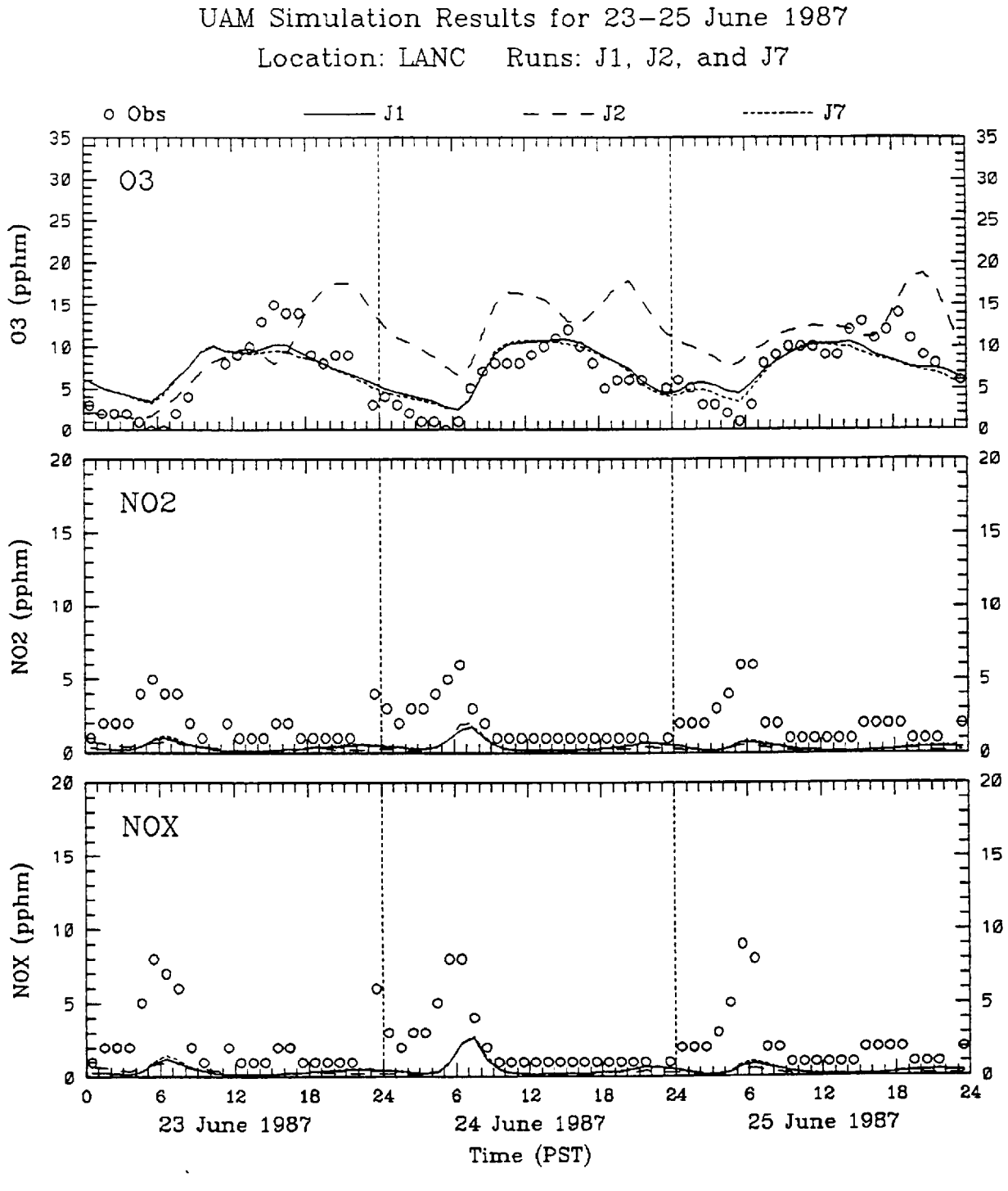


Figure 2-10(g). UAM simulation results at Lancaster

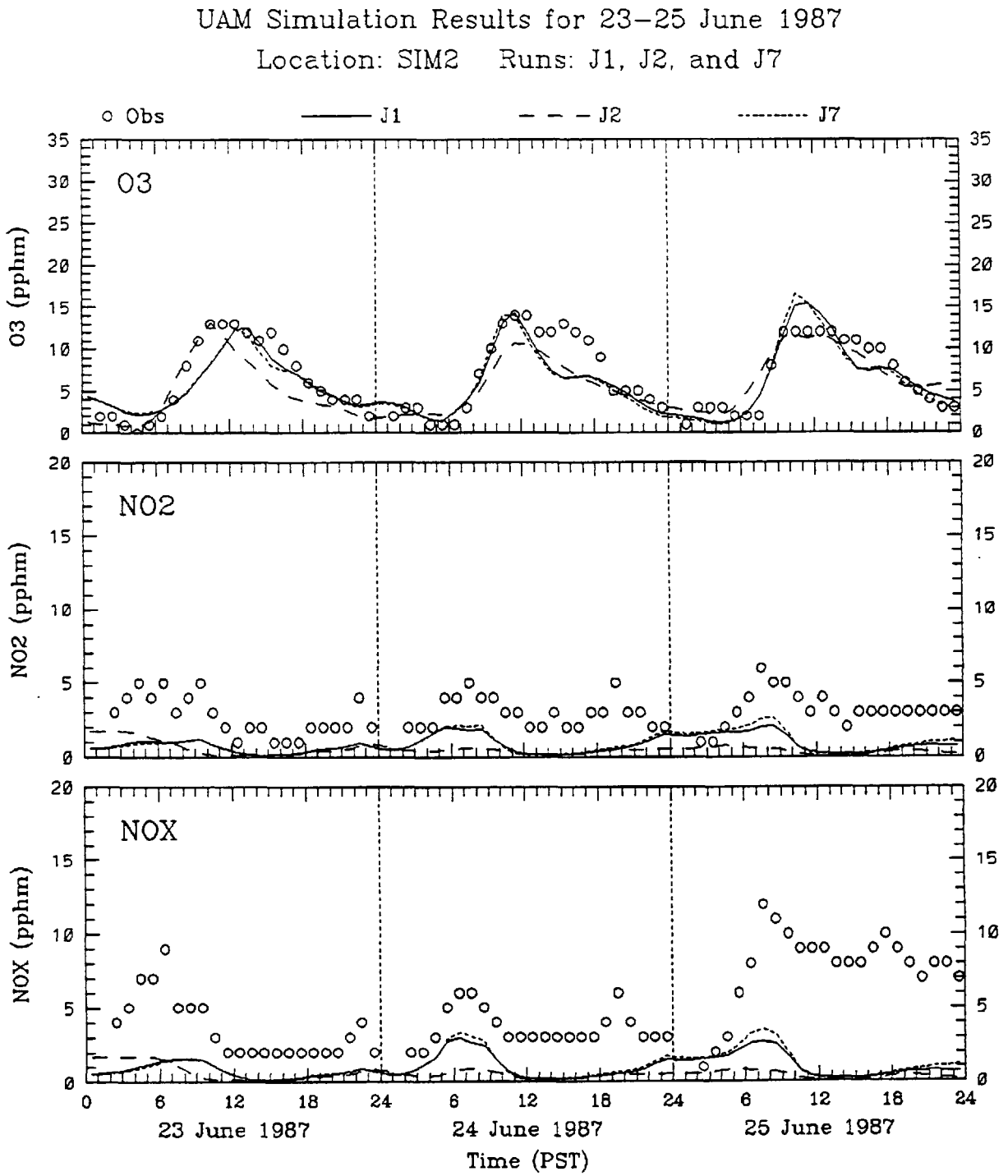


Figure 2-10(h). UAM simulation results at Simi Valley-Cochran

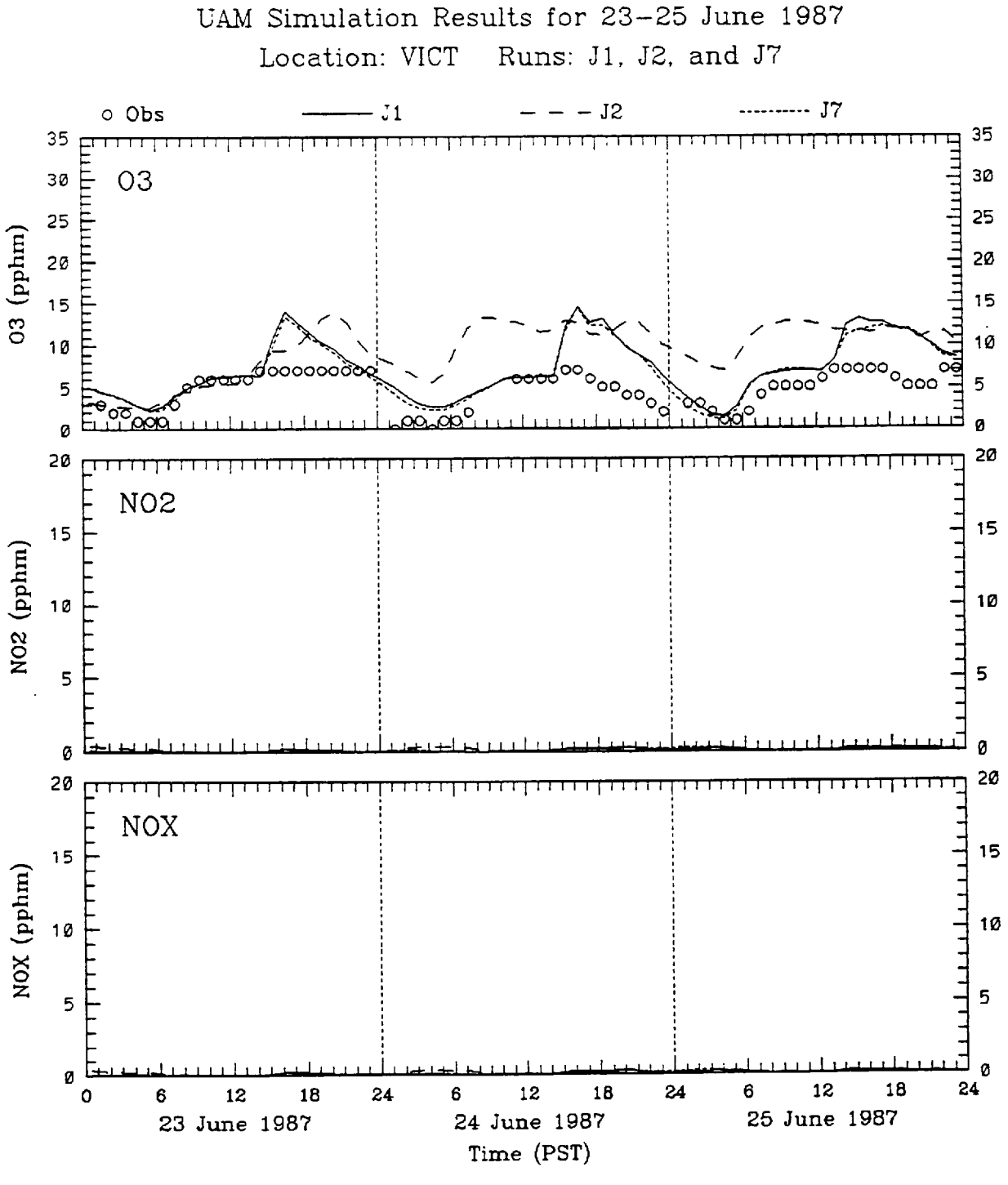


Figure 2-10(i). UAM simulation results at Victorville

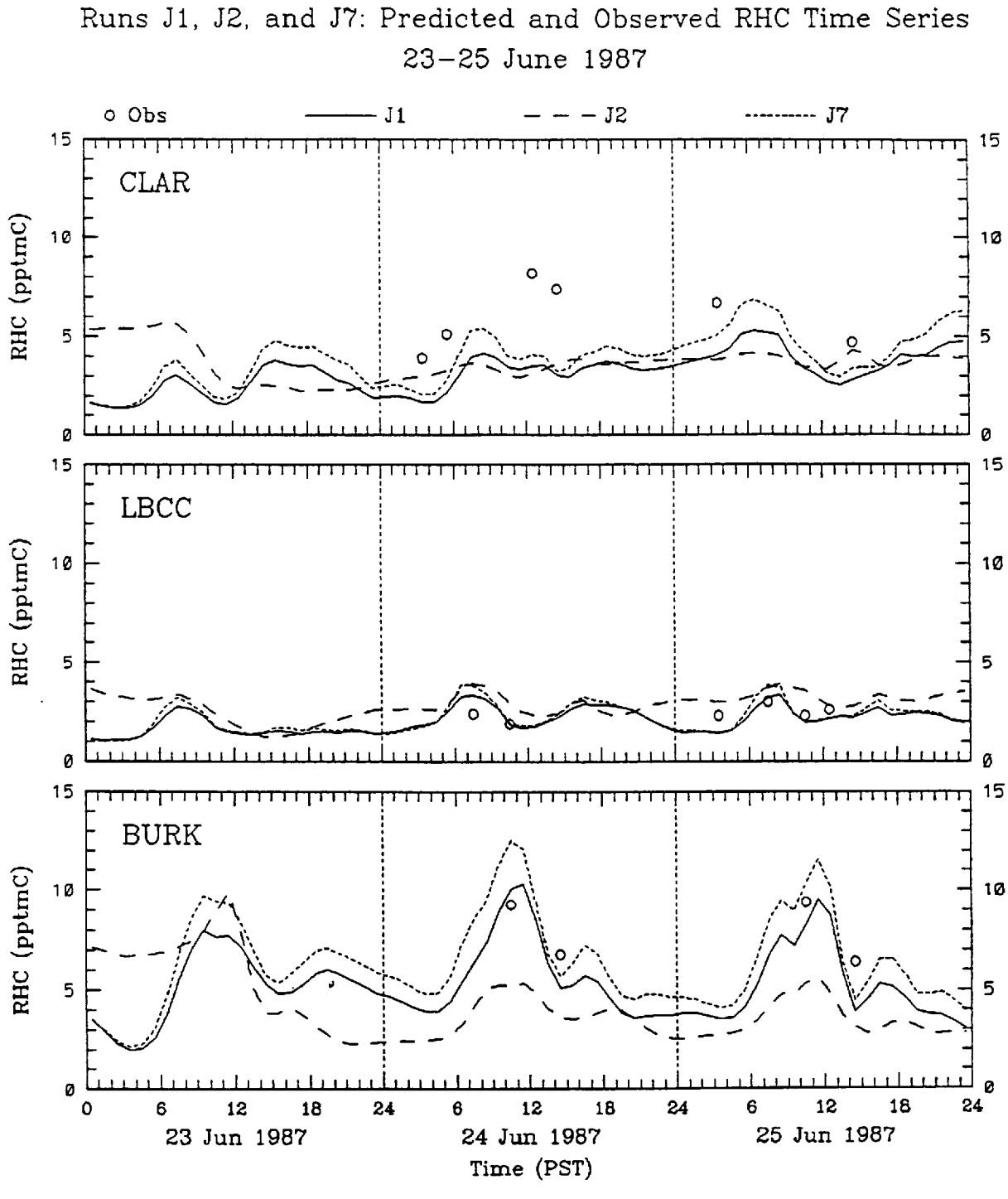


Figure 2-11(a). UAM simulation results for RHC (total reactive organic species) at Claremont College, Long Beach City College, and Burbank

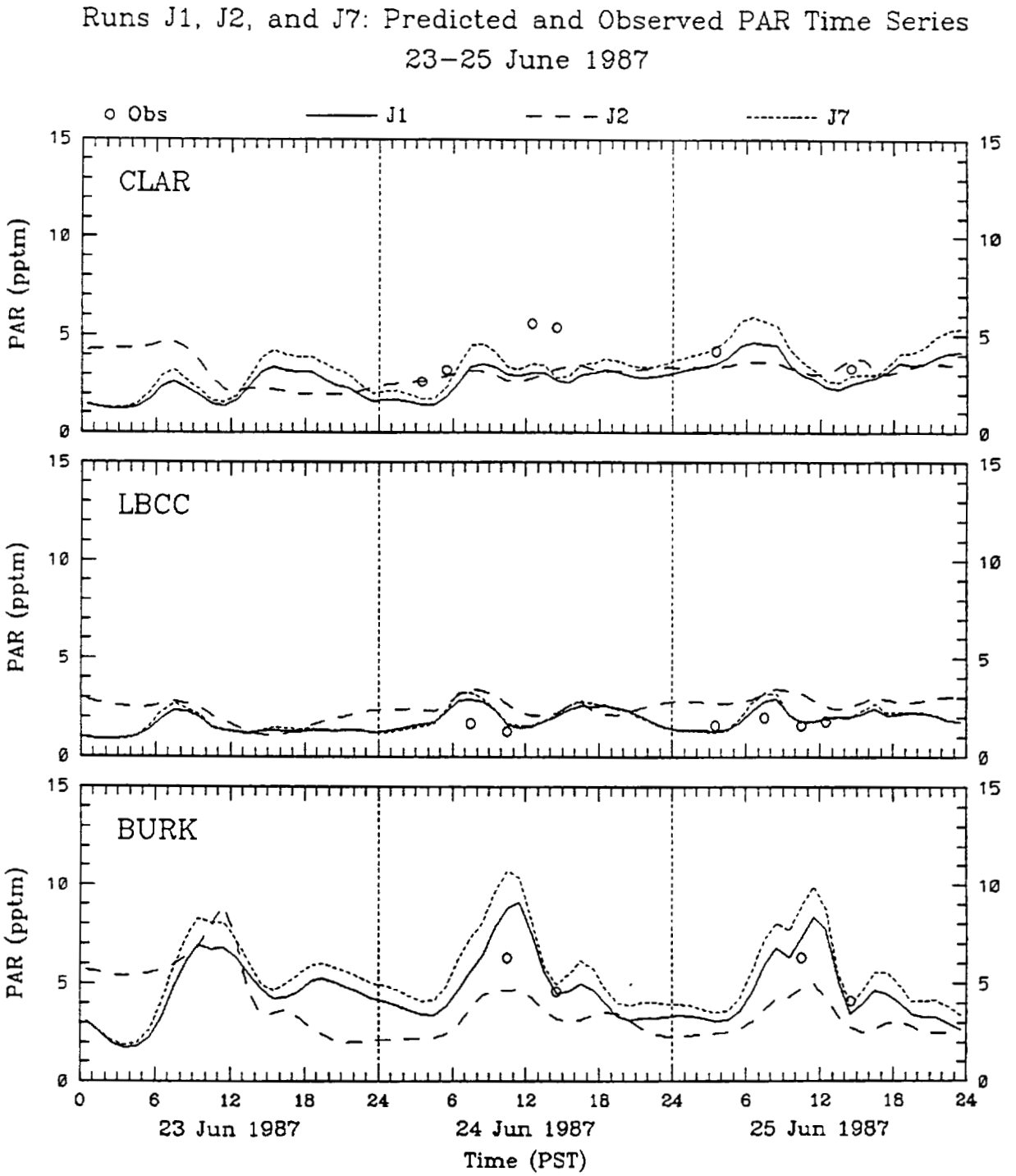


Figure 2-11(b). UAM simulation results for PAR (paraffinic carbon bonds) at Claremont College, Long Beach City College, and Burbank

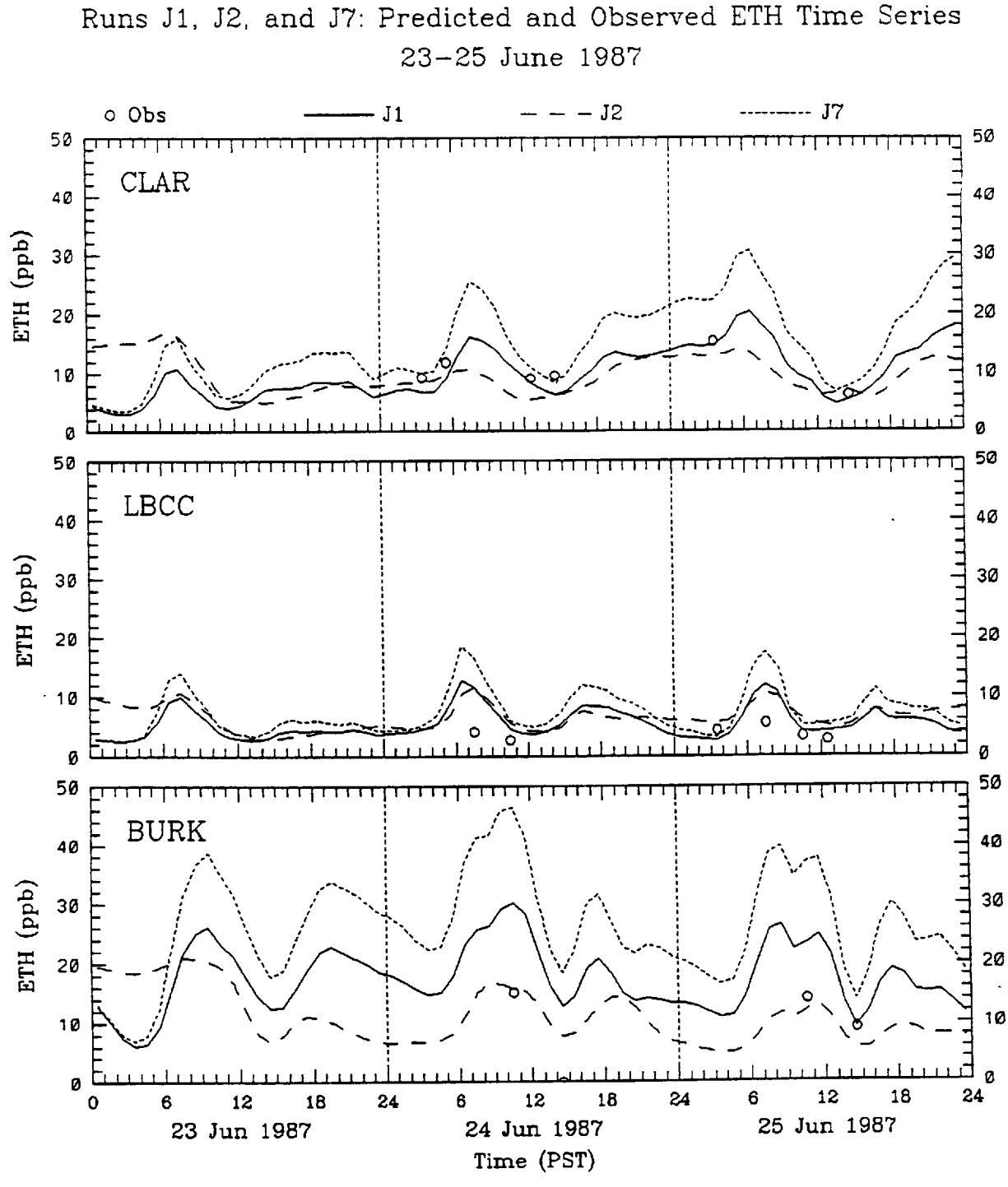


Figure 2-11(c). UAM simulation results for ETH (ethene) at Claremont College, Long Beach City College, and Burbank

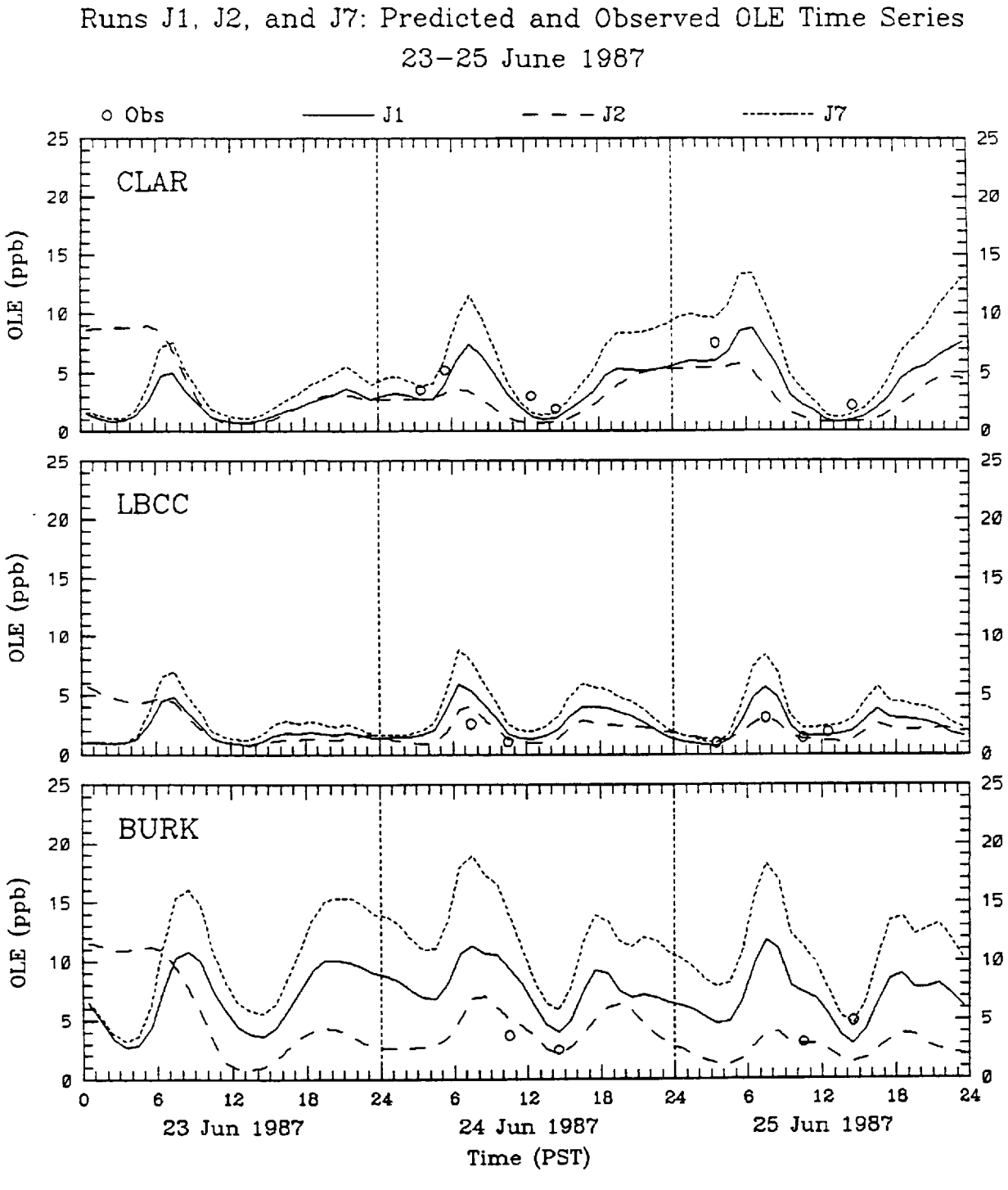


Figure 2-11(d). UAM simulation results for OLE (olefinic carbon bonds) at Claremont College, Long Beach City College, and Burbank

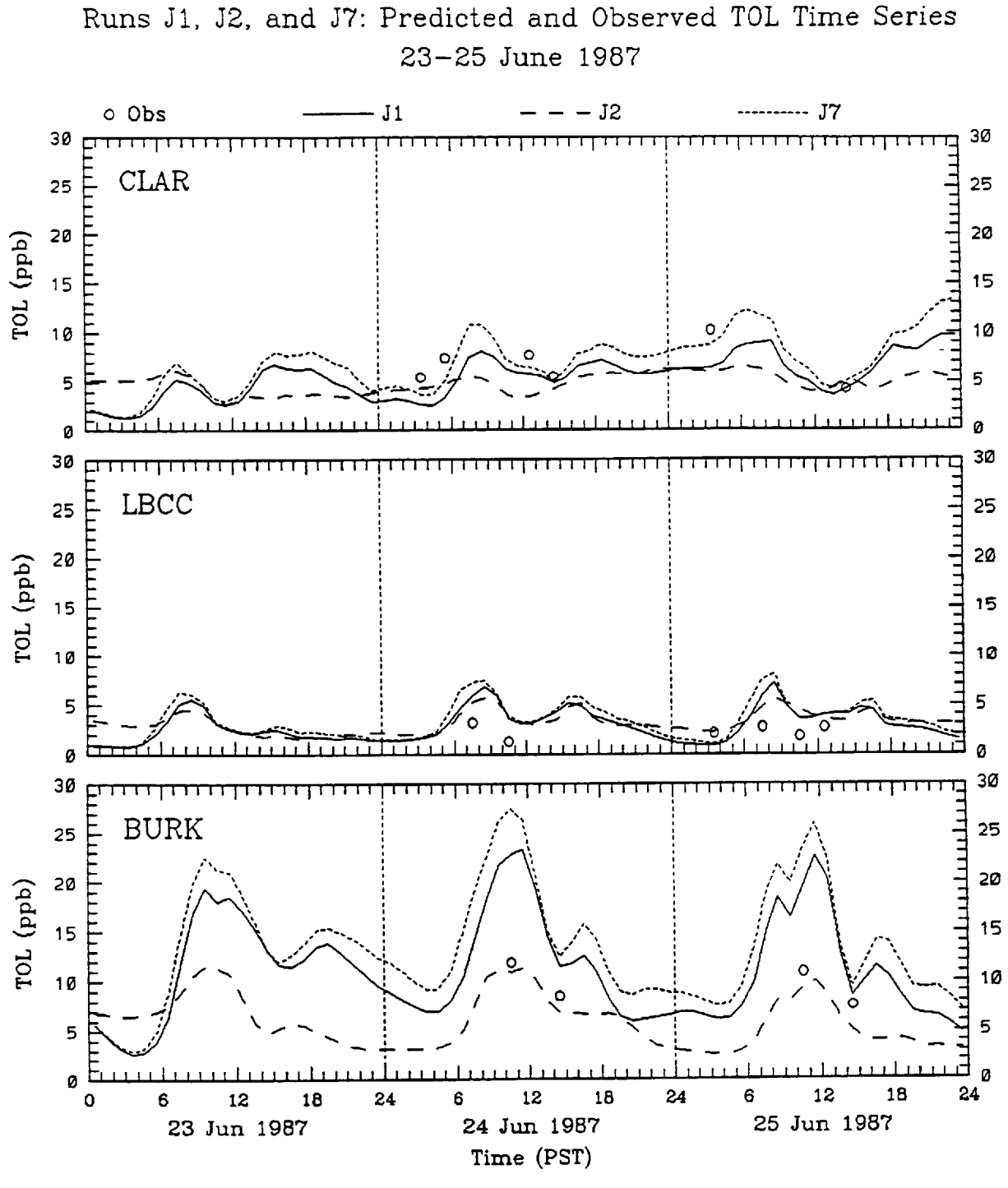


Figure 2-11(e). UAM simulation results for TOL (toluene) at Claremont College, Long Beach City College, and Burbank

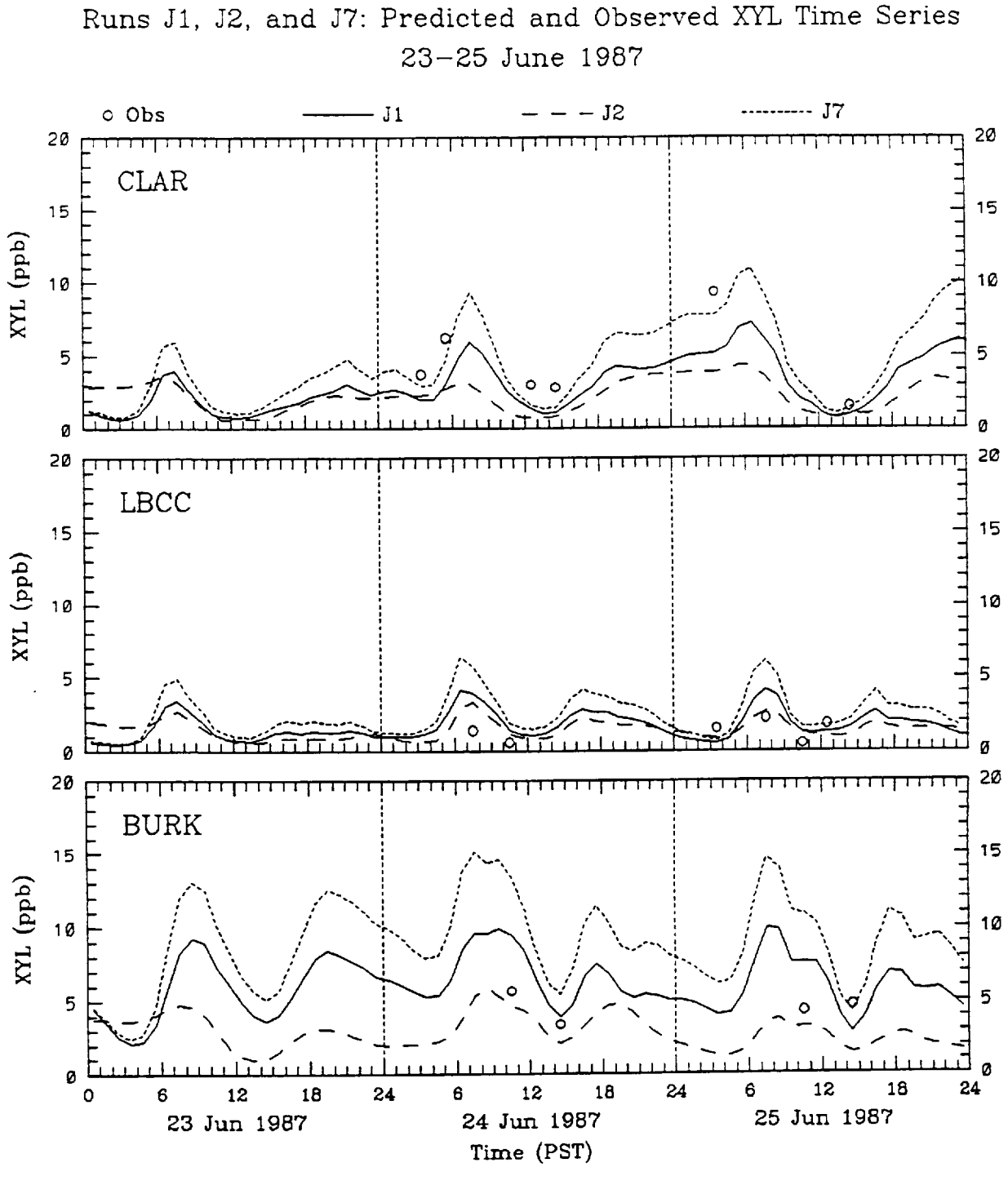


Figure 2-11(f). UAM simulation results for XYL (xylene) at Claremont College, Long Beach City College, and Burbank

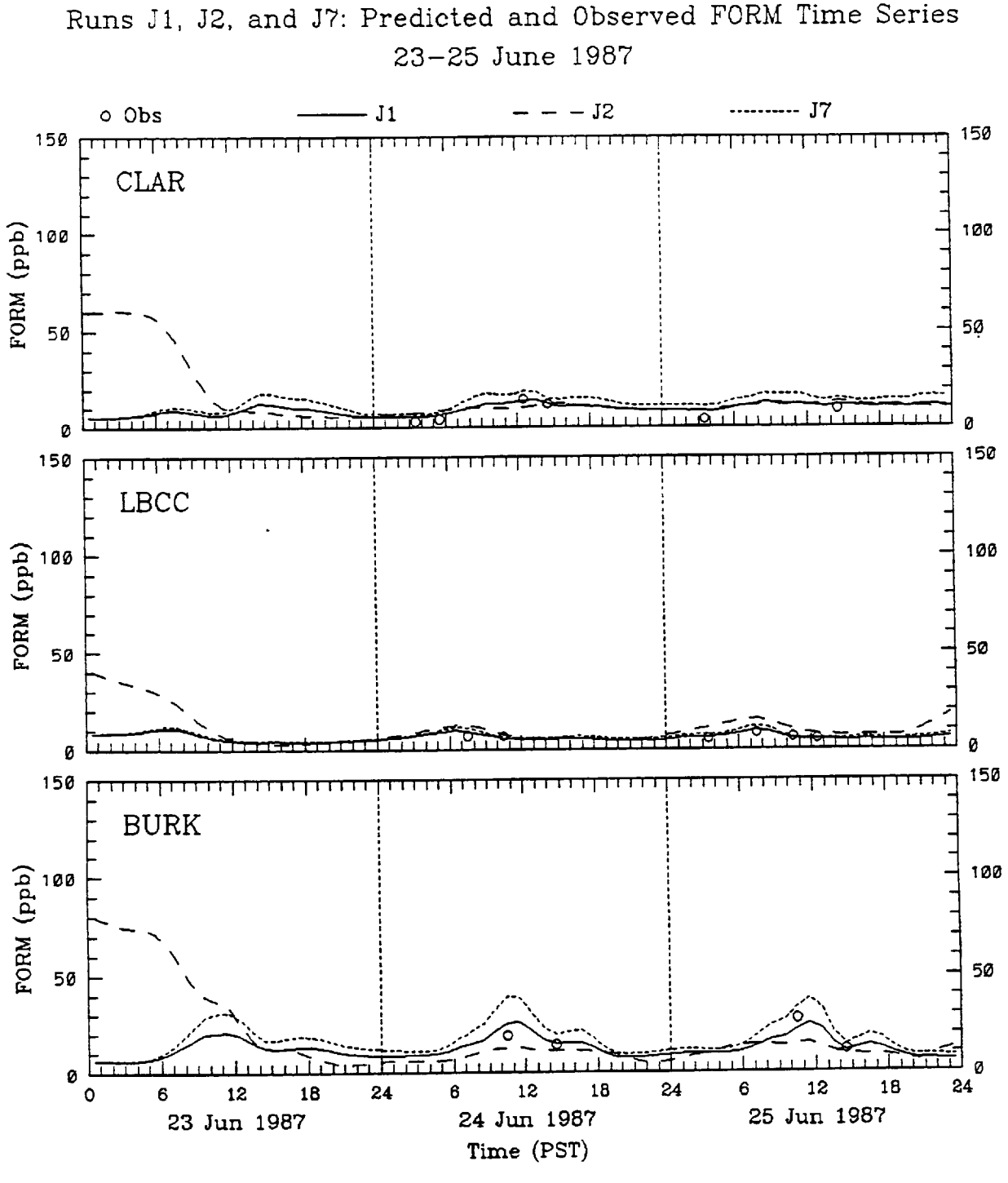


Figure 2-11(g). UAM simulation results for FORM (formaldehyde) at Claremont College, Long Beach City College, and Burbank

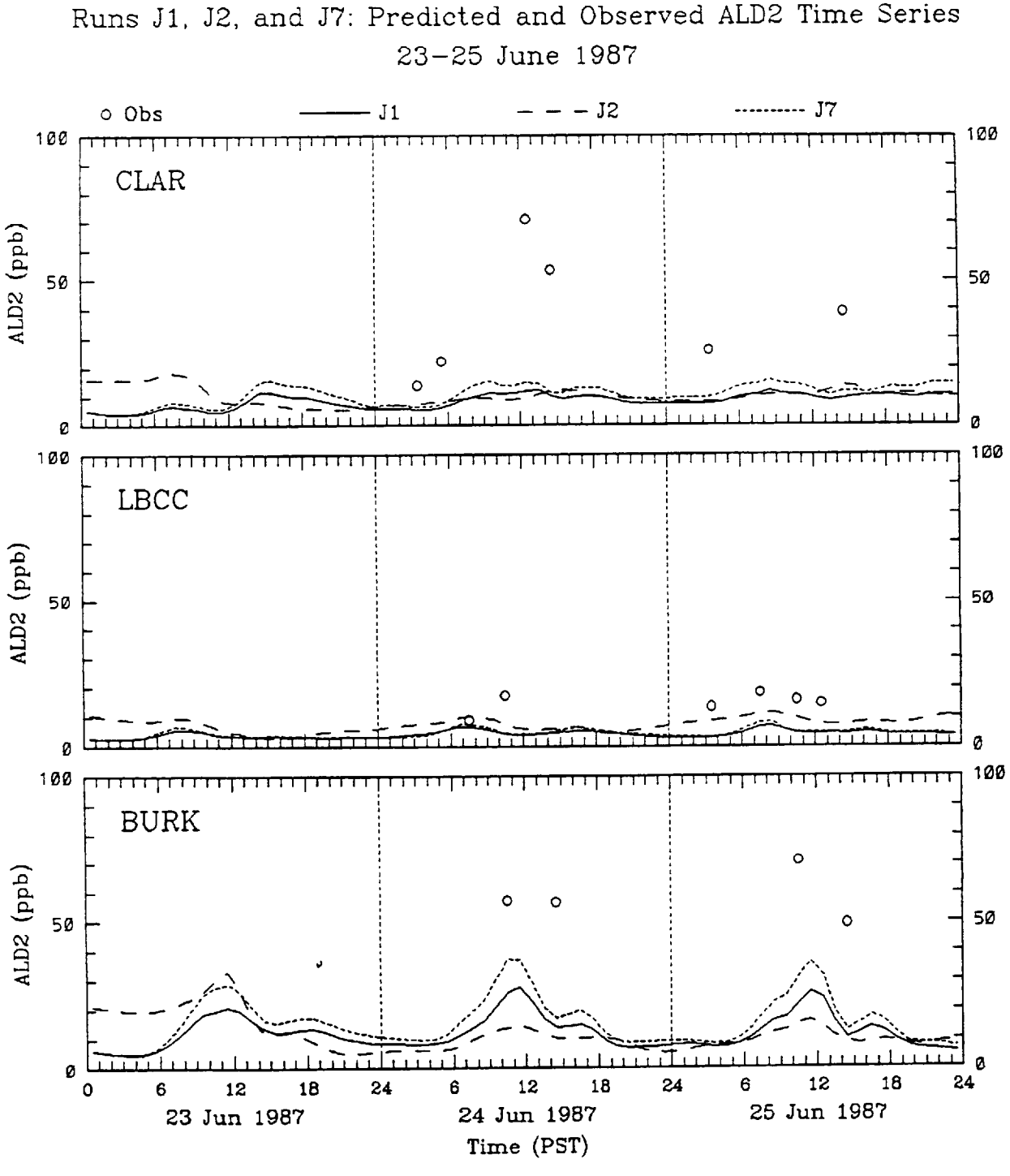


Figure 2-11(h). UAM simulation results for ALD2 (high molecular weight aldehydes) at Claremont College, Long Beach City College, and Burbank

Exhibit 2-1. Overall model performance measures for O_3 for Run J1

```
                Chemical Model Performance Evaluation
                        Run J1  June 1987

    Day = 23 June
 Species = O3
   Units = PPHM
                        Performance Measures
 ------------------------------------------------------------------------
 Cutoff = 8 PPHM

 Accuracy of Peak Estimation
 ---------------------------
Peak Estimation Accuracy (Paired in Time,Space)          ATS =  -32.79 %
Peak Estimation Accuracy (Paired in Space)               AS =  -32.79 %
Peak Estimation Accuracy (Paired in Time)                AT =  -24.55 %
Peak Estimation Accuracy (Unpaired)                      AU =   47.43 %
Average Accuracy Over All Stations (Paired in Space) A-MEAN =   27.94 %

Bias                                        Normalized Bias =  -18.96 %
                                                  Mean Bias =   -2.25 PPHM
Error                                      Normalized Error =   29.29 %
                                                Mean Error =    3.26 PPHM
Variance                                          Variance =   10.57 PPHM


    Day = 24 June
                        Performance Measures
 ------------------------------------------------------------------------
 Cutoff = 8 PPHM

 Accuracy of Peak Estimation
 ---------------------------
Peak Estimation Accuracy (Paired in Time,Space)          ATS =  -28.01 %
Peak Estimation Accuracy (Paired in Space)               AS =  -28.01 %
Peak Estimation Accuracy (Paired in Time)                AT =   -5.64 %
Peak Estimation Accuracy (Unpaired)                      AU =   68.41 %
Average Accuracy Over All Stations (Paired in Space) A-MEAN =   20.50 %

Bias                                        Normalized Bias =  -24.84 %
                                                  Mean Bias =   -3.26 PPHM
Error                                      Normalized Error =   29.77 %
                                                Mean Error =    3.79 PPHM
Variance                                          Variance =    9.61 PPHM


    Day = 25 June
                        Performance Measures
 ------------------------------------------------------------------------
 Cutoff = 8 PPHM

 Accuracy of Peak Estimation
 ---------------------------
Peak Estimation Accuracy (Paired in Time,Space)          ATS =  -27.61 %
Peak Estimation Accuracy (Paired in Space)               AS =  -25.32 %
Peak Estimation Accuracy (Paired in Time)                AT =   -9.17 %
Peak Estimation Accuracy (Unpaired)                      AU =   45.96 %
Average Accuracy Over All Stations (Paired in Space) A-MEAN =   22.88 %

Bias                                        Normalized Bias =   -9.74 %
                                                  Mean Bias =   -1.30 PPHM
Error                                      Normalized Error =   30.05 %
                                                Mean Error =    3.33 PPHM
Variance                                          Variance =   15.37 PPHM
```

Exhibit 2-2. Overall model performance measures for NO_2 for Run J1

```
                Chemical Model Performance Evaluation
                        Run J1  June 1987

    Day = 23 June
Species = NO2
  Units = PPHM
                        Performance Measures
-----------------------------------------------------------------------
Cutoff = 2 PPHM

Accuracy of Peak Estimation
---------------------------
Peak Estimation Accuracy (Paired in Time,Space)         ATS =  -34.86 %
Peak Estimation Accuracy (Paired in Space)               AS =  -32.94 %
Peak Estimation Accuracy (Paired in Time)                AT =  -28.37 %
Peak Estimation Accuracy (Unpaired)                      AU =   -9.84 %
Average Accuracy Over All Stations (Paired in Space) A-MEAN =   53.10 %

Bias                                        Normalized Bias =  -49.68 %
                                                  Mean Bias =   -2.23 PPHM
Error                                      Normalized Error =   57.58 %
                                                 Mean Error =    2.43 PPHM
Variance                                           Variance =    3.32 PPHM


    Day = 24 June
                        Performance Measures
-----------------------------------------------------------------------
Cutoff = 2 PPHM

Accuracy of Peak Estimation
---------------------------
Peak Estimation Accuracy (Paired in Time,Space)         ATS =  -34.79 %
Peak Estimation Accuracy (Paired in Space)               AS =  -13.81 %
Peak Estimation Accuracy (Paired in Time)                AT =   14.97 %
Peak Estimation Accuracy (Unpaired)                      AU =   47.81 %
Average Accuracy Over All Stations (Paired in Space) A-MEAN =   35.80 %

Bias                                        Normalized Bias =  -33.06 %
                                                  Mean Bias =   -1.67 PPHM
Error                                      Normalized Error =   48.22 %
                                                 Mean Error =    2.10 PPHM
Variance                                           Variance =    3.86 PPHM


    Day = 25 June
                        Performance Measures
-----------------------------------------------------------------------
Cutoff = 2 PPHM

Accuracy of Peak Estimation
---------------------------
Peak Estimation Accuracy (Paired in Time,Space)         ATS =  -40.13 %
Peak Estimation Accuracy (Paired in Space)               AS =  -39.28 %
Peak Estimation Accuracy (Paired in Time)                AT =   -4.41 %
Peak Estimation Accuracy (Unpaired)                      AU =   -4.41 %
Average Accuracy Over All Stations (Paired in Space) A-MEAN =   44.84 %

Bias                                        Normalized Bias =  -37.85 %
                                                  Mean Bias =   -2.04 PPHM
Error                                      Normalized Error =   51.48 %
                                                 Mean Error =    2.40 PPHM
Variance                                           Variance =    4.10 PPHM
```

Exhibit 2-3. Overall model performance measures for NO_x for Run J1

Chemical Model Performance Evaluation
Run J1 June 1987

Day = 23 June
Species = NOx
Units = PPHM

Performance Measures

Cutoff = 2 PPHM

Accuracy of Peak Estimation

Peak Estimation Accuracy (Paired in Time,Space)	ATS =	-90.15 %
Peak Estimation Accuracy (Paired in Space)	AS =	-75.01 %
Peak Estimation Accuracy (Paired in Time)	AT =	-75.05 %
Peak Estimation Accuracy (Unpaired)	AU =	12.21 %
Average Accuracy Over All Stations (Paired in Space)	A-MEAN =	56.35 %
Bias	Normalized Bias =	-45.72 %
	Mean Bias =	-2.55 PPHM
Error	Normalized Error =	57.88 %
	Mean Error =	2.89 PPHM
Variance	Variance =	7.02 PPHM

Day = 24 June

Performance Measures

Cutoff = 2 PPHM

Accuracy of Peak Estimation

Peak Estimation Accuracy (Paired in Time,Space)	ATS =	-83.36 %
Peak Estimation Accuracy (Paired in Space)	AS =	-74.06 %
Peak Estimation Accuracy (Paired in Time)	AT =	-51.11 %
Peak Estimation Accuracy (Unpaired)	AU =	3.23 %
Average Accuracy Over All Stations (Paired in Space)	A-MEAN =	41.04 %
Bias	Normalized Bias =	-26.78 %
	Mean Bias =	-1.76 PPHM
Error	Normalized Error =	50.47 %
	Mean Error =	2.57 PPHM
Variance	Variance =	8.07 PPHM

Day = 25 June

Performance Measures

Cutoff = 2 PPHM

Accuracy of Peak Estimation

Peak Estimation Accuracy (Paired in Time,Space)	ATS =	-76.55 %
Peak Estimation Accuracy (Paired in Space)	AS =	-76.55 %
Peak Estimation Accuracy (Paired in Time)	AT =	-46.26 %
Peak Estimation Accuracy (Unpaired)	AU =	12.47 %
Average Accuracy Over All Stations (Paired in Space)	A-MEAN =	51.67 %
Bias	Normalized Bias =	-35.30 %
	Mean Bias =	-2.42 PPHM
Error	Normalized Error =	52.75 %
	Mean Error =	3.03 PPHM
Variance	Variance =	8.73 PPHM

Exhibit 2-4. Overall model performance measures for O_3 for Run J2

```
                Chemical Model Performance Evaluation
                        Run J2  June 1987

    Day = 23 June
 Species = O3
   Units = PPHM
                        Performance Measures
 ------------------------------------------------------------------------
 Cutoff = 8 PPHM

 Accuracy of Peak Estimation
 ---------------------------
Peak Estimation Accuracy (Paired in Time,Space)         ATS =   -6.76 %
Peak Estimation Accuracy (Paired in Space)               AS =   -6.76 %
Peak Estimation Accuracy (Paired in Time)                AT =   10.64 %
Peak Estimation Accuracy (Unpaired)                      AU =  100.74 %
Average Accuracy Over All Stations (Paired in Space) A-MEAN =   24.02 %

Bias                                        Normalized Bias =  -13.79 %
                                                  Mean Bias =   -1.54 PPHM
Error                                      Normalized Error =   30.09 %
                                                 Mean Error =    3.19 PPHM
Variance                                          Variance =   15.78 PPHM


    Day = 24 June
                        Performance Measures
 ------------------------------------------------------------------------
 Cutoff = 8 PPHM

 Accuracy of Peak Estimation
 ---------------------------
Peak Estimation Accuracy (Paired in Time,Space)         ATS =  -47.53 %
Peak Estimation Accuracy (Paired in Space)               AS =  -46.01 %
Peak Estimation Accuracy (Paired in Time)                AT =  -15.05 %
Peak Estimation Accuracy (Unpaired)                      AU =   11.67 %
Average Accuracy Over All Stations (Paired in Space) A-MEAN =   23.88 %

Bias                                        Normalized Bias =  -20.35 %
                                                  Mean Bias =   -2.99 PPHM
Error                                      Normalized Error =   31.12 %
                                                  Mean Error =    4.04 PPHM
Variance                                          Variance =   16.99 PPHM


    Day = 25 June
                        Performance Measures
 ------------------------------------------------------------------------
 Cutoff = 8 PPHM

 Accuracy of Peak Estimation
 ---------------------------
Peak Estimation Accuracy (Paired in Time,Space)         ATS =  -11.01 %
Peak Estimation Accuracy (Paired in Space)               AS =   -5.89 %
Peak Estimation Accuracy (Paired in Time)                AT =    1.11 %
Peak Estimation Accuracy (Unpaired)                      AU =   11.59 %
Average Accuracy Over All Stations (Paired in Space) A-MEAN =   25.71 %

Bias                                        Normalized Bias =   -7.34 %
                                                  Mean Bias =   -1.17 PPHM
Error                                      Normalized Error =   32.61 %
                                                  Mean Error =    3.61 PPHM
Variance                                          Variance =   20.89 PPHM
```

Exhibit 2-5. Overall model performance measures for NO_2 for Run J2

```
                Chemical Model Performance Evaluation
                        Run J2  June 1987

    Day = 23 June
Species = NO2
  Units = PPHM
                        Performance Measures
-------------------------------------------------------------------------
Cutoff = 2 PPHM

 Accuracy of Peak Estimation
 ---------------------------
Peak Estimation Accuracy (Paired in Time,Space)          ATS =  -42.58 %
Peak Estimation Accuracy (Paired in Space)                AS =  -16.24 %
Peak Estimation Accuracy (Paired in Time)                 AT =    7.35 %
Peak Estimation Accuracy (Unpaired)                       AU =   29.97 %
Average Accuracy Over All Stations (Paired in Space) A-MEAN =   36.97 %

Bias                                          Normalized Bias =  -26.64 %
                                                    Mean Bias =   -1.19 PPHM
Error                                         Normalized Error =  41.66 %
                                                  Mean Error =    1.62 PPHM
Variance                                            Variance =    2.77 PPHM


    Day = 24 June
                        Performance Measures
-------------------------------------------------------------------------
 Cutoff = 2 PPHM

 Accuracy of Peak Estimation
 ---------------------------
Peak Estimation Accuracy (Paired in Time,Space)          ATS =  -19.86 %
Peak Estimation Accuracy (Paired in Space)                AS =   26.83 %
Peak Estimation Accuracy (Paired in Time)                 AT =   -2.95 %
Peak Estimation Accuracy (Unpaired)                       AU =   58.92 %
Average Accuracy Over All Stations (Paired in Space) A-MEAN =   37.77 %

Bias                                          Normalized Bias =  -24.09 %
                                                    Mean Bias =   -1.13 PPHM
Error                                         Normalized Error =  44.68 %
                                                  Mean Error =    1.84 PPHM
Variance                                            Variance =    3.74 PPHM


    Day = 25 June
                        Performance Measures
-------------------------------------------------------------------------
 Cutoff = 2 PPHM

 Accuracy of Peak Estimation
 ---------------------------
Peak Estimation Accuracy (Paired in Time,Space)          ATS =  -39.05 %
Peak Estimation Accuracy (Paired in Space)                AS =  -36.41 %
Peak Estimation Accuracy (Paired in Time)                 AT =   -6.76 %
Peak Estimation Accuracy (Unpaired)                       AU =   25.68 %
Average Accuracy Over All Stations (Paired in Space) A-MEAN =   47.11 %

Bias                                          Normalized Bias =  -31.91 %
                                                    Mean Bias =   -1.67 PPHM
Error                                         Normalized Error =  51.63 %
                                                  Mean Error =    2.32 PPHM
Variance                                            Variance =    4.88 PPHM
```

Exhibit 2-6 Overall model performance measures for NO_x for Run J2

```
                Chemical Model Performance Evaluation
                        Run J2  June 1987

    Day = 23 June
Species = NOx
  Units = PPHM
                        Performance Measures
 ------------------------------------------------------------------------
 Cutoff = 2 PPHM

 Accuracy of Peak Estimation
 ---------------------------
Peak Estimation Accuracy (Paired in Time,Space)         ATS =  -59.25 %
Peak Estimation Accuracy (Paired in Space)               AS =  -59.03 %
Peak Estimation Accuracy (Paired in Time)                AT =  -53.96 %
Peak Estimation Accuracy (Unpaired)                      AU =  194.90 %
Average Accuracy Over All Stations (Paired in Space) A-MEAN =   42.60 %

Bias                                        Normalized Bias =  -22.39 %
                                                  Mean Bias =   -1.24 PPHM
Error                                      Normalized Error =   43.41 %
                                                  Mean Error =    1.97 PPHM
Variance                                          Variance =    5.09 PPHM


    Day = 24 June
                        Performance Measures
 ------------------------------------------------------------------------
 Cutoff = 2 PPHM

 Accuracy of Peak Estimation
 ---------------------------
Peak Estimation Accuracy (Paired in Time,Space)         ATS =  -67.24 %
Peak Estimation Accuracy (Paired in Space)               AS =  -64.29 %
Peak Estimation Accuracy (Paired in Time)                AT =  -44.10 %
Peak Estimation Accuracy (Unpaired)                      AU =  230.07 %
Average Accuracy Over All Stations (Paired in Space) A-MEAN =   50.48 %

Bias                                        Normalized Bias =  -12.67 %
                                                  Mean Bias =    -.83 PPHM
Error                                      Normalized Error =   51.46 %
                                                  Mean Error =    2.45 PPHM
Variance                                          Variance =    9.02 PPHM


    Day = 25 June
                        Performance Measures
 ------------------------------------------------------------------------
 Cutoff = 2 PPHM

 Accuracy of Peak Estimation
 ---------------------------
Peak Estimation Accuracy (Paired in Time,Space)         ATS =  -58.74 %
Peak Estimation Accuracy (Paired in Space)               AS =  -58.74 %
Peak Estimation Accuracy (Paired in Time)                AT =  -44.72 %
Peak Estimation Accuracy (Unpaired)                      AU =  228.56 %
Average Accuracy Over All Stations (Paired in Space) A-MEAN =   48.96 %

Bias                                        Normalized Bias =  -26.29 %
                                                  Mean Bias =   -1.85 PPHM
Error                                      Normalized Error =   55.96 %
                                                  Mean Error =    3.02 PPHM
Variance                                          Variance =   11.04 PPHM
```

Exhibit 2-7 Subregional model performance measures for Run J1

Run J1, species: O3 (pphm), cutoff = 8 pphm

	Peak Acc. (%)		Bias (%)		Abs. Error (%)	
Region	Jun 24	Jun 25	Jun 24	Jun 25	Jun 24	Jun 25
T	20.	23.	-25.	-10.	30.	30.
A	17.	20.	-33.	-23.	33.	24.
B	29.	30.	-35.	0.	37.	26.
C	21.	15.	-30.	-21.	30.	23.
D	15.	20.	-19.	11.	25.	32.
E	36.	24.	-28.	-15.	31.	33.
F	38.	45.	-47.	-52.	47.	53.
G	9.	29.	13.	-12.	15.	16.
H	13.	23.	-25.	-19.	28.	28.
I	2.	6.	-31.	-23.	43.	32.

Run J1, species: NO2 (pphm), cutoff = 2 pphm

	Peak Acc. (%)		Bias (%)		Abs. Error (%)	
Region	Jun 24	Jun 25	Jun 24	Jun 25	Jun 24	Jun 25
T	36.	45.	-33.	-38.	48.	51.
A	18.	11.	-3.	-11.	38.	36.
B	19.	33.	-7.	-7.	33.	41.
C	6.	23.	-10.	-41.	28.	41.
D	48.	59.	-59.	-58.	60.	58.
E	--	--	--	--	--	--
F	95.	96.	-97.	-97.	97.	97.
G	71.	88.	-77.	-87.	77.	87.
H	51.	63.	-68.	-75.	68.	75.
I	--	--	--	--	--	--

Run J1, species: NOx (pphm), cutoff = 2 pphm

	Peak Acc. (%)		Bias (%)		Abs. Error (%)	
Region	Jun 24	Jun 25	Jun 24	Jun 25	Jun 24	Jun 25
T	41.	52.	-27.	-35.	50.	53.
A	38.	33.	-4.	-12.	37.	38.
B	12.	38.	12.	2.	39.	42.
C	26.	22.	3.	-35.	30.	36.
D	59.	63.	-61.	-61.	62.	62.
E	--	--	--	--	--	--
F	96.	96.	-97.	-97.	97.	97.
G	67.	90.	-75.	-86.	75.	86.
H	42.	69.	-67.	-78.	67.	78.
I	--	--	--	--	--	--

Exhibit 2-7. (Continued)

Run J1, species: RHC (pptm), cutoff = 2 pptm

	Peak Acc. (%)		Bias (%)		Abs. Error (%)	
Region	Jun 24	Jun 25	Jun 24	Jun 25	Jun 24	Jun 25
T	33.	11.	-29.	-25.	41.	26.
A	43.	7.	3.	-18.	28.	21.
B	18.	16.	-42.	-29.	42.	29.
C	11.	1.	-8.	-26.	17.	26.
D	35.	17.	-42.	-35.	53.	35.
E	--	--	--	--	--	--
F	--	--	--	--	--	--
G	--	--	--	--	--	--
H	--	--	--	--	--	--
I	--	--	--	--	--	--

Run J1, species: ETH (ppb), cutoff = 5 ppb

	Peak Acc. (%)		Bias (%)		Abs. Error (%)	
Region	Jun 24	Jun 25	Jun 24	Jun 25	Jun 24	Jun 25
T	119.	72.	19.	30.	51.	36.
A	245.	120.	71.	120.	71.	120.
B	4.	65.	33.	6.	88.	6.
C	101.	89.	101.	34.	101.	34.
D	80.	42.	-19.	6.	19.	20.
E	--	--	--	--	--	--
F	--	--	--	--	--	--
G	--	--	--	--	--	--
H	--	--	--	--	--	--
I	--	--	--	--	--	--

Run J1, species: FORM (ppb), cutoff = 2 ppb

	Peak Acc. (%)		Bias (%)		Abs. Error (%)	
Region	Jun 24	Jun 25	Jun 24	Jun 25	Jun 24	Jun 25
T	44.	49.	19.	17.	34.	26.
A	84.	92.	30.	15.	38.	21.
B	16.	8.	-10.	-9.	19.	9.
C	38.	9.	19.	-13.	19.	13.
D	14.	45.	26.	48.	43.	48.
E	--	--	--	--	--	--
F	--	--	--	--	--	--
G	--	--	--	--	--	--
H	--	--	--	--	--	--
I	--	--	--	--	--	--

Run J1, species: OLE (ppb), cutoff = 2 ppb

	Peak Acc. (%)		Bias (%)		Abs. Error (%)	
Region	Jun 24	Jun 25	Jun 24	Jun 25	Jun 24	Jun 25
T	106.	62.	19.	13.	57.	52.
A	128.	81.	109.	36.	109.	48.
B	4.	67.	-11.	-29.	47.	29.
C	206.	72.	105.	48.	105.	88.
D	95.	35.	-24.	-12.	28.	40.
E	--	--	--	--	--	--
F	--	--	--	--	--	--
G	--	--	--	--	--	--
H	--	--	--	--	--	--
I	--	--	--	--	--	--

Exhibit 2-7. (Concluded)

Run J1, species: PAR (pptm), cutoff = 2 pptm

	Peak Acc. (%)		Bias (%)		Abs. Error (%)	
Region	Jun 24	Jun 25	Jun 24	Jun 25	Jun 24	Jun 25
T	24.	23.	-17.	-1.	38.	17.
A	32.	47.	-24.	40.	24.	40.
B	14.	10.	-20.	-5.	32.	5.
C	45.	33.	19.	-1.	21.	16.
D	17.	13.	-25.	-12.	48.	15.
E	--	--	--	--	--	--
F	--	--	--	--	--	--
G	--	--	--	--	--	--
H	--	--	--	--	--	--
I	--	--	--	--	--	--

Run J1, species: TOL (ppb), cutoff = 2 ppb

	Peak Acc. (%)		Bias (%)		Abs. Error (%)	
Region	Jun 24	Jun 25	Jun 24	Jun 25	Jun 24	Jun 25
T	98.	79.	27.	25.	62.	45.
A	190.	110.	73.	29.	73.	59.
B	32.	111.	-5.	80.	46.	80.
C	96.	108.	63.	45.	63.	45.
D	30.	18.	10.	-14.	63.	14.
E	--	--	--	--	--	--
F	--	--	--	--	--	--
G	--	--	--	--	--	--
H	--	--	--	--	--	--
I	--	--	--	--	--	--

Run J1, species: ALD2 (ppb), cutoff = 10 ppb

	Peak Acc. (%)		Bias (%)		Abs. Error (%)	
Region	Jun 24	Jun 25	Jun 24	Jun 25	Jun 24	Jun 25
T	67.	64.	-74.	-72.	74.	72.
A	61.	57.	-73.	-71.	73.	71.
B	77.	78.	-82.	-78.	82.	78.
C	52.	64.	-65.	-74.	65.	74.
D	73.	63.	-73.	-71.	73.	71.
E	--	--	--	--	--	--
F	--	--	--	--	--	--
G	--	--	--	--	--	--
H	--	--	--	--	--	--
I	--	--	--	--	--	--

Run J1, species: XYL (ppb), cutoff = 2 ppb

	Peak Acc. (%)		Bias (%)		Abs. Error (%)	
Region	Jun 24	Jun 25	Jun 24	Jun 25	Jun 24	Jun 25
T	79.	44.	-27.	4.	40.	43.
A	161.	64.	0.	31.	0.	57.
B	6.	50.	-37.	-15.	37.	15.
C	75.	62.	40.	19.	40.	58.
D	78.	12.	-49.	-27.	49.	27.
E	--	--	--	--	--	--
F	--	--	--	--	--	--
G	--	--	--	--	--	--
H	--	--	--	--	--	--
I	--	--	--	--	--	--

Exhibit 2-8 Subregional model performance measures for Run J2

Run J2, species: O3 (pphm), cutoff = 8 pphm

	Peak Acc. (%)		Bias (%)		Abs. Error (%)	
Region	Jun 24	Jun 25	Jun 24	Jun 25	Jun 24	Jun 25
T	24.	26.	-20.	-7.	31.	33.
A	18.	30.	-28.	-29.	32.	30.
B	29.	30.	-38.	-22.	41.	35.
C	41.	24.	-51.	-21.	51.	23.
D	20.	24.	-14.	16.	24.	42.
E	31.	35.	-25.	-19.	33.	36.
F	69.	66.	-63.	-70.	63.	70.
G	34.	34.	64.	32.	64.	34.
H	13.	13.	-21.	-16.	22.	19.
I	2.	7.	-9.	2.	22.	17.

Run J2, species: NO2 (pphm), cutoff = 2 pphm

	Peak Acc. (%)		Bias (%)		Abs. Error (%)	
Region	Jun 24	Jun 25	Jun 24	Jun 25	Jun 24	Jun 25
T	38.	47.	-24.	-32.	45.	52.
A	20.	16.	-5.	-13.	43.	46.
B	21.	36.	4.	0.	33.	40.
C	31.	52.	-22.	-60.	34.	60.
D	42.	52.	-33.	-36.	42.	46.
E	--	--	--	--	--	--
F	94.	95.	-97.	-97.	97.	97.
G	66.	91.	-77.	-90.	77.	90.
H	60.	65.	-77.	-84.	77.	84.
I	--	--	--	--	--	--

Run J2, species: NOx (pphm), cutoff = 2 pphm

	Peak Acc. (%)		Bias (%)		Abs. Error (%)	
Region	Jun 24	Jun 25	Jun 24	Jun 25	Jun 24	Jun 25
T	51.	49.	-13.	-26.	51.	56.
A	39.	15.	-2.	-6.	49.	54.
B	43.	37.	35.	14.	50.	48.
C	46.	50.	2.	-56.	33.	56.
D	55.	56.	-34.	-37.	47.	49.
E	--	--	--	--	--	--
F	95.	95.	-97.	-97.	97.	97.
G	69.	94.	-78.	-90.	78.	90.
H	53.	72.	-74.	-85.	74.	85.
I	--	--	--	--	--	--

Exhibit 2-8. (Continued)

Run J2, species: RHC (pptm), cutoff = 2 pptm

	Peak Acc. (%)		Bias (%)		Abs. Error (%)	
Region	Jun 24	Jun 25	Jun 24	Jun 25	Jun 24	Jun 25
T	41.	35.	-34.	-13.	43.	34.
A	38.	22.	10.	21.	33.	26.
B	57.	43.	-63.	-50.	63.	50.
C	43.	41.	-45.	-47.	45.	47.
D	36.	40.	-37.	-34.	37.	34.
E	--	--	--	--	--	--
F	--	--	--	--	--	--
G	--	--	--	--	--	--
H	--	--	--	--	--	--
I	--	--	--	--	--	--

Run J2, species: ETH (ppb), cutoff = 5 ppb

	Peak Acc. (%)		Bias (%)		Abs. Error (%)	
Region	Jun 24	Jun 25	Jun 24	Jun 25	Jun 24	Jun 25
T	48.	30.	-13.	-5.	30.	35.
A	95.	92.	26.	92.	29.	92.
B	50.	2.	-28.	-26.	57.	26.
C	12.	7.	5.	-25.	5.	25.
D	28.	24.	-21.	-18.	21.	27.
E	--	--	--	--	--	--
F	--	--	--	--	--	--
G	--	--	--	--	--	--
H	--	--	--	--	--	--
I	--	--	--	--	--	--

Run J2, species: FORM (ppb), cutoff = 2 ppb

	Peak Acc. (%)		Bias (%)		Abs. Error (%)	
Region	Jun 24	Jun 25	Jun 24	Jun 25	Jun 24	Jun 25
T	55.	67.	12.	44.	46.	61.
A	104.	130.	49.	80.	49.	80.
B	37.	33.	-44.	-35.	44.	35.
C	32.	45.	-28.	-31.	28.	31.
D	20.	33.	26.	60.	50.	60.
E	--	--	--	--	--	--
F	--	--	--	--	--	--
G	--	--	--	--	--	--
H	--	--	--	--	--	--
I	--	--	--	--	--	--

Run J2, species: OLE (ppb), cutoff = 2 ppb

	Peak Acc. (%)		Bias (%)		Abs. Error (%)	
Region	Jun 24	Jun 25	Jun 24	Jun 25	Jun 24	Jun 25
T	58.	22.	-23.	-42.	42.	42.
A	59.	8.	59.	-29.	59.	29.
B	49.	7.	-54.	-51.	54.	51.
C	90.	32.	11.	-37.	25.	37.
D	47.	38.	-37.	-51.	37.	51.
E	--	--	--	--	--	--
F	--	--	--	--	--	--
G	--	--	--	--	--	--
H	--	--	--	--	--	--
I	--	--	--	--	--	--

Exhibit 2-8. (Concluded)

Run J2, species: PAR (pptm), cutoff = 2 pptm

	Peak Acc. (%)		Bias (%)		Abs. Error (%)	
Region	Jun 24	Jun 25	Jun 24	Jun 25	Jun 24	Jun 25
T	22.	30.	-26.	-9.	29.	32.
A	5.	73.	-19.	61.	19.	61.
B	41.	24.	-49.	-34.	49.	34.
C	25.	21.	-28.	-28.	28.	28.
D	20.	16.	-16.	-12.	22.	23.
E	--	--	--	--	--	--
F	--	--	--	--	--	--
G	--	--	--	--	--	--
H	--	--	--	--	--	--
I	--	--	--	--	--	--

Run J2, species: TOL (ppb), cutoff = 2 ppb

	Peak Acc. (%)		Bias (%)		Abs. Error (%)	
Region	Jun 24	Jun 25	Jun 24	Jun 25	Jun 24	Jun 25
T	40.	39.	-16.	-3.	33.	31.
A	69.	68.	28.	26.	28.	32.
B	40.	12.	-53.	-11.	53.	11.
C	5.	8.	-14.	-24.	14.	24.
D	24.	40.	-19.	-25.	32.	42.
E	--	--	--	--	--	--
F	--	--	--	--	--	--
G	--	--	--	--	--	--
H	--	--	--	--	--	--
I	--	--	--	--	--	--

Run J2, species: ALD2 (ppb), cutoff = 10 ppb

	Peak Acc. (%)		Bias (%)		Abs. Error (%)	
Region	Jun 24	Jun 25	Jun 24	Jun 25	Jun 24	Jun 25
T	70.	61.	-74.	-61.	74.	61.
A	56.	40.	-64.	-44.	64.	44.
B	86.	83.	-87.	-83.	87.	83.
C	75.	77.	-79.	-80.	79.	80.
D	77.	64.	-71.	-68.	71.	68.
E	--	--	--	--	--	--
F	--	--	--	--	--	--
G	--	--	--	--	--	--
H	--	--	--	--	--	--
I	--	--	--	--	--	--

Run J2, species: XYL (ppb), cutoff = 2 ppb

	Peak Acc. (%)		Bias (%)		Abs. Error (%)	
Region	Jun 24	Jun 25	Jun 24	Jun 25	Jun 24	Jun 25
T	29.	36.	-55.	-45.	55.	51.
A	9.	26.	-47.	-20.	47.	41.
B	50.	15.	-69.	-50.	69.	50.
C	3.	30.	-28.	-47.	28.	47.
D	37.	60.	-59.	-65.	59.	65.
E	--	--	--	--	--	--
F	--	--	--	--	--	--
G	--	--	--	--	--	--
H	--	--	--	--	--	--
I	--	--	--	--	--	--

Section 3

PHASE 2--IDENTIFICATION OF ALTERNATIVE BASE CASES

OBJECTIVE OF PHASE 2

The objective of Phase 2 activities was to examine the possibility of identifying alternative base cases that provided a level of Urban Airshed Model (UAM) performance for the June and August 1987 episodes that were comparable to the best achieved for each respective episode. If so, sensitivity studies were to be conducted in Phase 3 using the alternative base cases developed in Phase 2 to assess whether the choice of base case had a significant influence on UAM simulation results for hypothetical emission reduction strategies.

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 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 DESIGN

Run J1 (developed in Phase 1) for the June episode and Run A5 (the 26-28 August 1987 SCAQS episode with inputs developed by the CARB, including VOC emissions multiplied by a factor of 2.2) served as the points of departure for this study. Six additional simulations were conducted for candidate alternative base cases for the June episode. A simulation for the August 1987

SCAQS episode (Run A4) using inputs developed by the SCAQMD was also a candidate base case. Although the study team primarily focused on working with the June episode, it was recognized that there would be a need to examine the consistency of Phase 3 findings using a limited number of simulations for conditions other than the June SCAQS episode.

Model inputs were modified in an attempt to elucidate the possible influences of compensating errors. Previous modeling experience suggested that key model inputs included emissions, boundary concentrations, mixing heights, and wind speeds. Particular emphasis was placed on examining effects associated with the potential underestimation of VOC emissions. The candidate alternative base cases may be summarized as follows:

June episode

- Run J2--the SCAQMD simulation for the June SCAQS episode.
- Run J3--Run J2 modified by lowering VOC boundary concentration inputs by 15 percent and by increasing VOC emissions by a factor of 2.2 to preserve the total VOC loading in the modeling domain.
- Run J4--Run J1 modified by increasing VOC boundary values by 26 percent and using the nominal VOC emissions inputs (i.e., unscaled) to preserve the total VOC loading in the domain.
- Run J5--Run J1 modified by using the nominal (unscaled) VOC emissions and by decreasing the nominal mixing height and wind speed inputs by 32%. Reducing mixing heights and wind speeds by these amounts reduces the ventilation by 54%, which should offset the 54% reduction in VOC emissions from Run J1 (i.e., precursor concentrations for Run J5 should be comparable to those of Run J1).
- Run J6--Run J1 modified by scaling VOC emissions from major source categories by various factors (i.e., motor vehicles x 3; solvent usage x 1.5; biogenics x 1.5; industrial x 1.4; other sources x 2.4), which provides an overall increase of 2.2 times the nominal VOC emissions values; UAM results were similar to those of Run J1, which used a single scaling factor of 2.2 for all VOC sources.
- Run J7--Run J6 modified by reducing mixing heights by 20 percent and by increasing HONO emissions (previously set at zero) by 0.5 percent of NO_x emissions (as employed in

the CARB simulation for August); the purpose of lowering mixing heights was to reduce the NO_x underprediction bias noted in the other June simulations.

August episode

- Run A4--the UAM set-up for August developed by the SCAQMD using the nominal (unscaled) VOC emissions.

Table 3-1 summarizes the characteristics of the UAM simulations carried out in Phase 2. UAM simulation results were input to the MAPS software package developed by Alpine Geophysics for the calculation and display of various model performance measures.

PREPARATION OF MODEL INPUTS

Boundary Concentrations

Modifications to boundary concentration inputs for Runs J3 and J4 were developed by calculating the nominal mass flux of VOCs transported into the modeling domain. Changes in boundary values were made in a manner to offset the associated modification to VOC emissions, thus leaving the total VOC loading in the domain unchanged.

Wind and Mixing Heights

Modifications to wind and mixing height inputs were implemented by reducing all wind speed and mixing height inputs by 32 percent (for Run J5) and reducing all mixing height inputs by 20 percent (Run J7).

Emissions

A review of analyses of VOC/NO_x ratios for both UAM emissions and ambient data reported by Lurmann and Main (1992) indicates that VOC emissions may be underestimated by a factor of 2.2. To reconcile differences between the emissions estimates and the ambient data (assuming that NO_x emissions are approximately correct), we implemented the following methodology that has been employed in photochemical modeling work conducted by the Bay Area Air Quality

Table 3-1. Summary of alternative base case simulations

Run	Episode	Basic Model Setup	Emissions	Boundary Conditions	Mixing Heights	Wind Speeds
J1	June	API/SCE	VOC x 2.2	API/SCE	SCAQMD	API/SCE
J2	June	SCAQMD	VOC x 1.0	SCAQMD	SCAQMD	SCAQMD
J3	June	SCAQMD	VOC x 2.2	16 percent reduction in SCAQMD values for VOCs to offset use of increased VOC emissions	SCAQMD	SCAQMD
J4	June	API/SCE	VOC x 1.0	26 percent increase in API/SCE values for VOCs (an increase in VOC mass comparable to that achieved by multiplying VOC emissions by a factor of 2.2)	SCAQMD	API/SCE
J5	June	API/SCE	VOC x 1.0	API/SCE	lower SCAQMD values 32%	lower API/SCE values 32%
J6	June	API/SCE	various scaling factors for VOCs (motor vehicles x 3, solvent usage x 1.5, biogenics x 1.5, industrial x 1.4, other sources x 2.4)	API/SCE	SCAQMD	API/SCE
J7	June	API/SCE	various scaling factors for VOCs (motor vehicles x 3, solvent usage x 1.5, biogenics x 1.5, industrial x 1.4, other sources x 2.4); HONO emissions increased to 0.5% of NO_x emissions	API/SCE	lower SCAQMD values 20%	API/SCE
A4	August	SCAQMD	VOC x 1.0	SCAQMD	SCAQMD	SCAQMD
A5	August	CARB	VOC x 2.2	CARB	CARB	CARB

Management District. VOC emission correction factors were estimated for the following five major source categories:

- motor vehicles
- solvent usage
- biogenics
- industrial sources
- other sources (all other sources not indicated above)

Estimated bounds for the correction factors were established based on discussions with Dr. Philip Roth (Envair) and Mr. Fred Lurmann (Sonoma Technology Inc.):

• motor vehicles	2 to 4
• solvent usage	1 to 2
• biogenics	1 to 2
• industrial	1 to 1.6
• other sources	1.5 to 3

Estimates for the set of correction factors that provided an overall increase of 2.2 times the nominal VOC emissions loading were developed by trial and error, taking into account the relative contributions of each of the five source categories to the total reactive VOC emissions in the modeling domain. The results of this calculation were as follows:

• motor vehicles	3
• solvent usage	1.5
• biogenics	1.5
• industrial	1.4
• other sources	2.4

Note that obtaining a solution to this problem is facilitated by the fact that motor vehicles contribute a substantial portion of the VOCs in the domain. Thus, the factors for the other three categories are constrained to within a relatively narrow range.

ASSESSING THE EQUIVALENCE OF MODEL RESULTS

The identification and use of multiple base cases gives explicit recognition to an inability to distinguish preferences among a set of closely related model simulations. We term indistinguishable cases - i.e., those lying within a specified range of uncertainty - equivalent. However, we must stipulate equivalence: which simulations are equivalent and which are not. We may make this determination by comparing differences between simulations with a measure (or metric) derived from:

- knowledge of uncertainties in inputs. For example, the uncertainties associated with key inputs - or even one category of input, such as emissions - may serve as a lower bound for a metric used to ascertain distinguishability.
- knowledge of acceptable levels of uncertainty in model results. Given an ambient concentration level for O_3 of 240 ppb, a decision maker may specify that a bias (a component of uncertainty) should be no greater than 5 ppb. This assertion may serve as a starting point for developing a metric for determining equivalence in the context of our needs.

To develop a means for assessing the equivalence of the various model results, we calculated the metric, S_i, based on the following weighted combination of model performance characteristics:

$$S_i = W_b(B_{1i} + B_{2i}) + W_p(P_{1i} + P_{2i}) + W_{ae}(AE_{1i} + AE_{2i}) \qquad (1)$$

where

S_i is the calculated performance metric for pollutant i;

W_b, W_p, and W_{ae} are weighting factors associated with the normalized bias, average peak estimation accuracy, and normalized error, respectively;

B_{1i} and B_{2i} are the absolute values of the normalized bias (expressed as a percent) on days 1 and 2, respectively[1], as indicated in Tables 3-2 and 3-3;

P_{1i} and P_{2i} are the average peak estimation accuracy (expressed as a percent) on days 1 and 2, respectively; and

AE_{1i} and AE_{2i} are the normalized error (expressed as a percent) on days 1 and 2, respectively.

The weighting factors W_b, W_p, and W_{ae} were set to values of 3, 2, and 1, respectively, based on assumptions concerning the relative importance of the three errors. Values for S_i were calculated for both O_3 and NO_2. In addition, a combined metric considering both pollutants was also calculated in the following manner:

$$S_{O3+NO2} = 0.67\ S_{O3} + 0.33\ S_{NO2} \qquad (2)$$

O_3 results were given twice the weight of those for NO_2 because O_3 is of greater regulatory importance.

To develop a criterion for judging the equivalence of simulation results, we considered what level of uncertainty associated with the model results might be acceptable to decision makers. For example, given peak ambient concentrations for O_3 of 240 ppb, a decision maker might specify that the bias (a component of uncertainty) should be no greater than 5 ppb, or 2 percent (i.e., 5/240 x 100%). Similarly, the error in peak concentration estimation should also be no greater than 5 ppb, or 2 percent. For imprecision (i.e., normalized error), we assumed that, on the average, the results should be within 10 percent of the observations. If we insert these values into Eq. 2, then the associated performance metric is 40 (i.e., 3(2+2) + 2(2+2) + 1(10+10) = 40). That is, simulations with performance metrics that differ by no more than 40 would be judged equivalent. The values employed in this criterion calculation represent performance goals that

[1]Note that the designation day 1 and day 2 actually correspond to the second and third days of the multiday UAM simulation; results for the first simulation day are not considered since they may be significantly influenced by errors in the specification of initial conditions.

Table 3-2. Summary of UAM performance measures for O_3

Simulation	Peak Accuracy (%)		Bias (%)		Absolute Error (%)	
	Jun 24 Aug 27	Jun 25 Aug 28	Jun 24 Aug 27	Jun 25 Aug 28	Jun 24 Aug 27	Jun 25 Aug 28
J1	22	24	-23	-10	31	30
J2	24	33	-11	8	39	39
J3	22	35	-1	11	28	39
J4	38	31	-41	-29	42	34
J5	43	40	-47	-40	48	43
J6	22	23	-22	-9	30	30
J7	22	27	-18	-7	31	31
A4	24	31	-6	3	24	32
A5	28	39	-9	5	36	45

Table 3-3. Summary of UAM performance measures for NO_2

Simulation	Peak Accuracy (%)		Bias (%)		Absolute Error (%)	
	Jun 24 Aug 27	Jun 25 Aug 28	Jun 24 Aug 27	Jun 25 Aug 28	Jun 24 Aug 27	Jun 25 Aug 28
J1	36	43	-32	-37	48	51
J2	38	47	-24	-32	45	52
J3	36	48	-28	-36	47	54
J4	36	45	-31	-34	46	48
J5	40	39	13	3	49	44
J6	36	45	-33	-38	48	52
J7	33	42	-23	-29	48	48
A4	39	45	-4	4	58	58
A5	25	40	-13	-6	36	38

may be difficult to achieve in actual practice. Nevertheless, they provide a means for discriminating among a set of model runs such as those developed in this study.

As noted at the beginning of this section, a criterion for establishing equivalence could also be developed considering the uncertainty in model inputs. These uncertainties may range from 10 to 30 percent or more for various model inputs and certainly would yield an equivalence criterion less stringent than that noted above based on assumed acceptable levels of uncertainty in model results.

DISCUSSION OF RESULTS

Figures 3-1, 3-2, and 3-3 summarize the calculated performance metrics for O_3, NO_2, and the combination of both O_3 and NO_2, respectively. Note that the horizontal grid spacing on these graphics is 40, corresponding to the equivalence criterion cited above. Table 3-4 summarizes the equivalences that exist among runs (i.e., performance metrics differ by no more than 40 among all runs in a particular tier). The tier 1 group has the best performance, tier 2 next, etc.

From the combined O_3 and NO_2 results given in Table 3-4, Runs J1, J2, J3, J6, and J7 for the June episode are judged equivalent by the criterion cited above. Results for O_3 are consistent with the combined (O_3 and NO_2) results, but the equivalences for NO_2 are somewhat different. The two August simulations are not judged equivalent for either O_3 or NO_2 but the combined results do indicate equivalence.

For the purposes of this study, we recommended that preference be given to the selection of base cases that are expected to provide the greatest variation in model results for the emission reduction scenarios to be investigated in Phase 3. Runs J1, J2, and J7 provided considerable differences in the treatment of emissions, meteorological, and boundary concentration inputs and were recommended for use in the June sensitivity simulations. Runs A4 and A5 were deemed suitable candidates for studying sensitivity issues using the August episode. Appendices C and D provide time series displays showing estimated and measured values at air monitoring locations

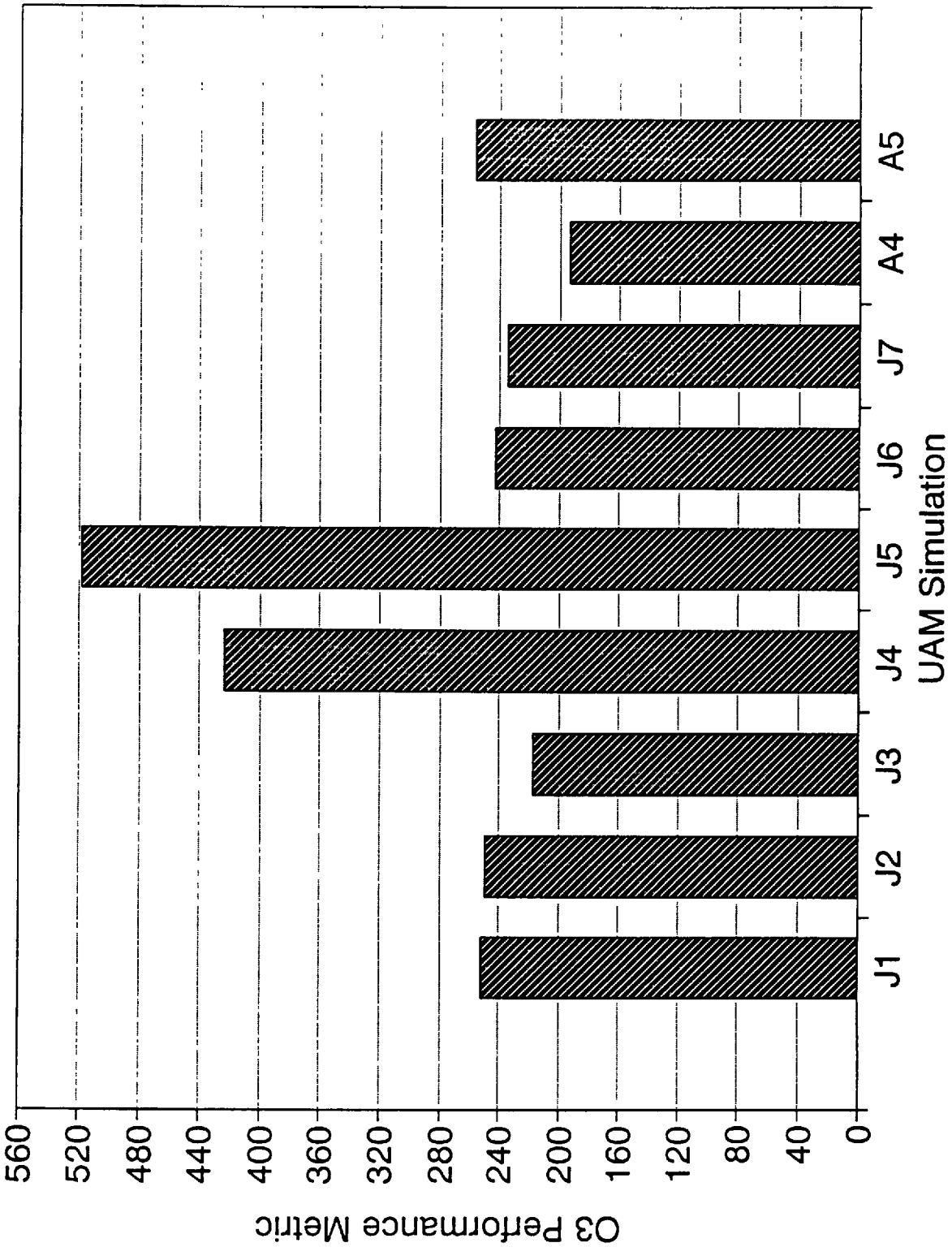


Figure 3-1. Summary of performance metrics for O_3.

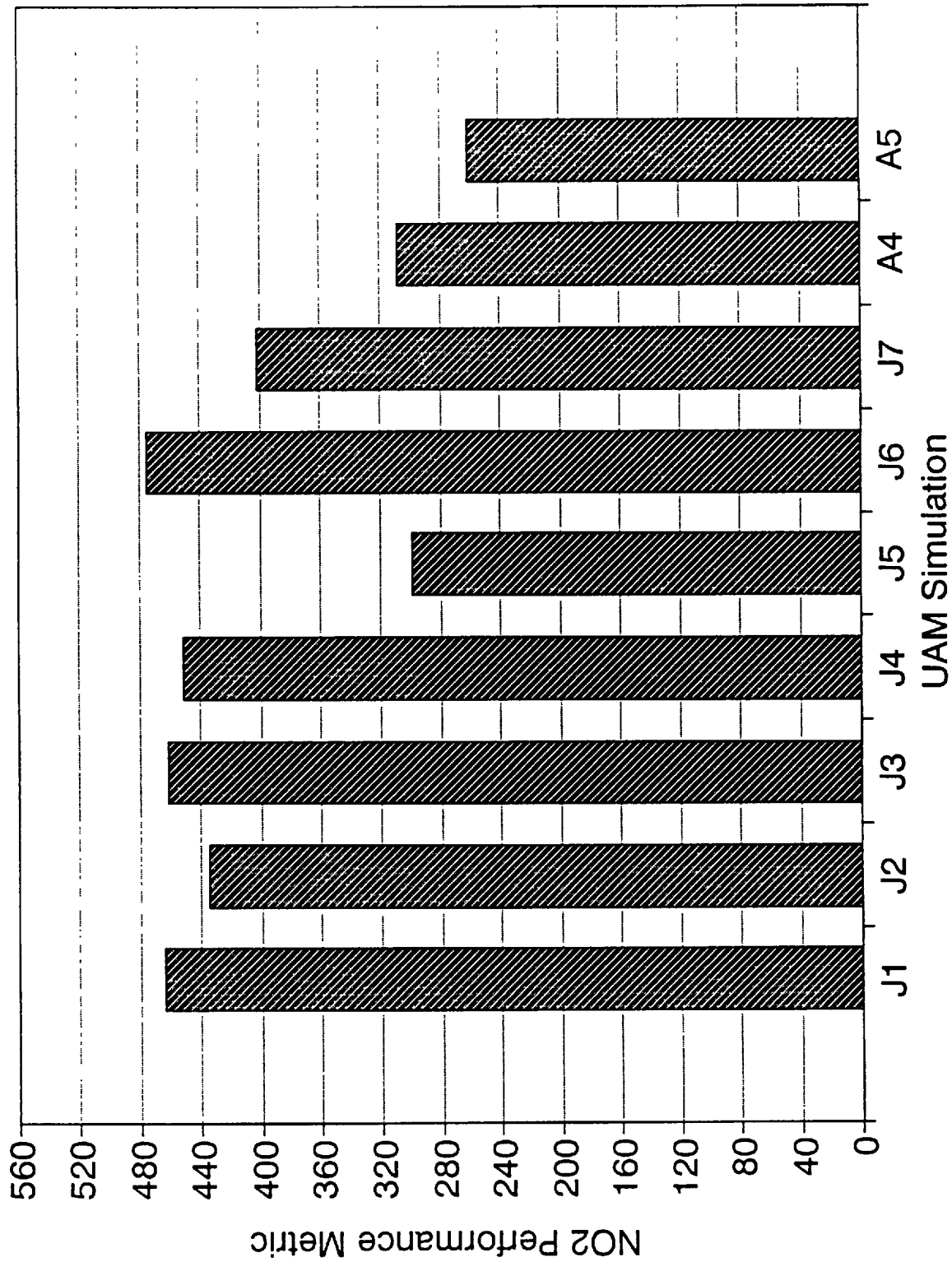


Figure 3-2. Summary of performance metrics for NO_2.

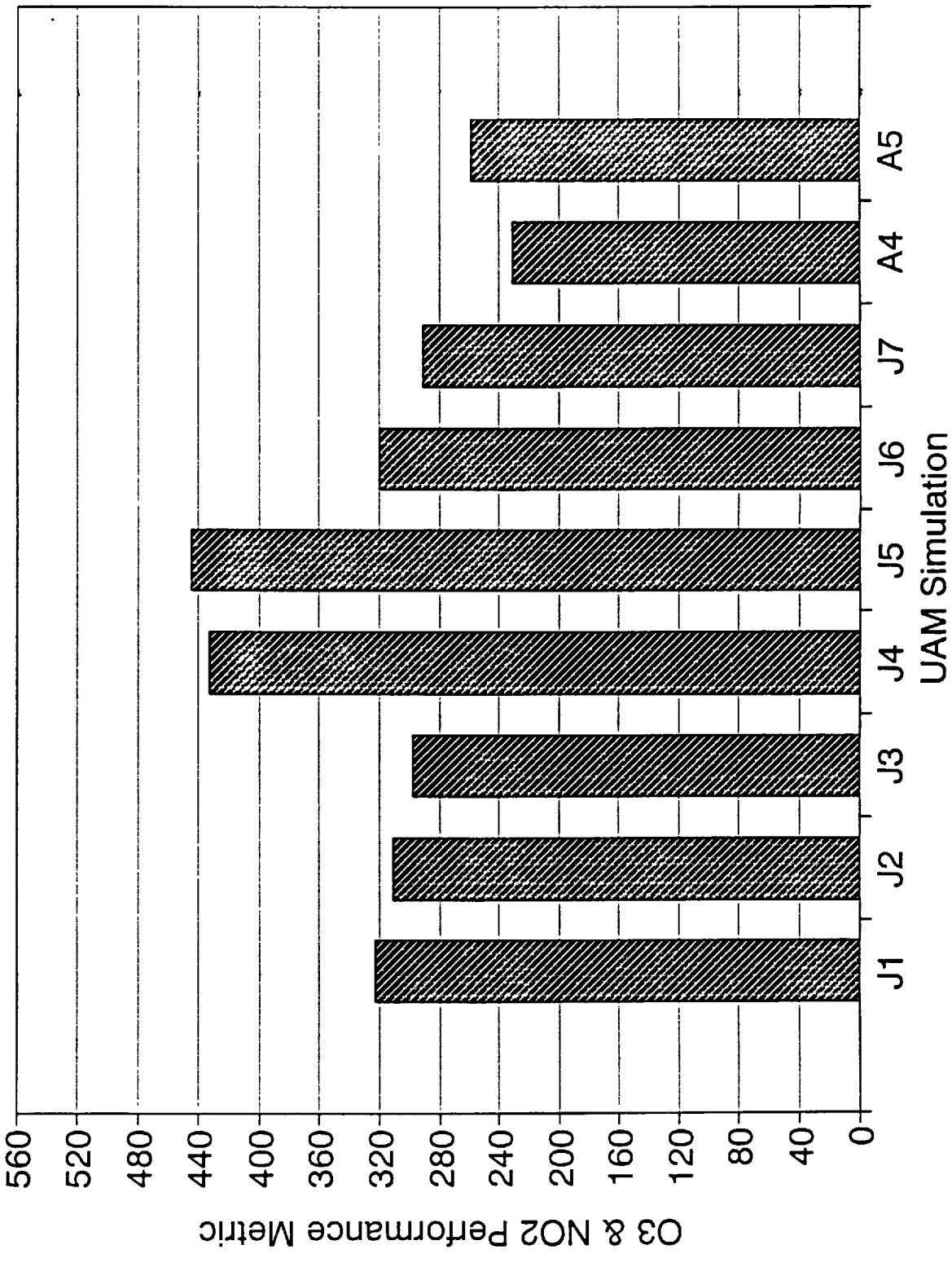


Figure 3-3. Summary of performance metrics for combined O_3 and NO_2 results.

Table 3-4. Summary of equivalences among simulations (i.e., performance metrics differ by no more than 40)

Tier	O_3	NO_2	O_3 & NO_2
	June		
1	J3,J7,J6,J2,J1	J5	J7,J3,J2,J6,J1
2	J4	J7,J2	J4,J5
3	J5	J2,J4,J3,J1	
4		J4,J3,J1,J6	
	August		
1	A4	A5	A4,A5
2	A5	A4	

for O_3, NO_2, and VOCs for the J1, J2, and J7 simulations. Similar displays showing results for the simulations of the August episode (i.e., Runs A4 and A5) are provided in Appendices E and F.

KEY FINDINGS

Candidate alternative base cases for both the June and August SCAQS episodes have been identified, differing in primarily in the treatment of VOC emissions, boundary values, mixing heights, and wind velocity. An objective methodology has been implemented to assess the equivalence of candidate alternative base cases. Five simulations for the June SCAQS episode (Runs J1, J2, J3, J6, and J7) and two simulations for the August SCAQS episode (Runs A4 and A5) were judged equivalent. It was recommended that Runs J1, J2, and J7, as well as Runs A4 and A5 be employed in Phase 3 sensitivity studies.

Section 4

PHASE 3--CONDUCT OF SENSITIVITY STUDIES

OBJECTIVES OF PHASE 3

The primary objective of the Phase 3 activities was to ascertain whether the choice of base case has a significant influence on UAM simulation results for hypothetical emission reduction strategies[1]. If the model exhibits significant sensitivity to the choice of base case, particular attention needs to be given to any interpretation of results concerned with emission control strategy assessment.

STUDY DESIGN

To develop initial information concerning the sensitivity of UAM results to the choice of base case, we carried out simulations for two hypothetical emission reduction scenarios using three of the June runs developed in Phase 2. These base cases were selected because they were expected to provide the greatest variability in UAM results. Specifically, we employed the conditions of Run J2 (the UAM set-up developed by the SCAQMD employing nominal VOC emissions estimates), Run J1 (the UAM set-up developed in this study with all VOC emission sources scaled by a factor of 2.2), and Run J7 (the UAM set-up developed in this study using different scaling factors to increase VOC emissions for five major source groupings). Simulations were conducted using inputs for each of the three base cases with emissions modified in the following manner:

- Scenario 1--a 50 percent reduction in all anthropogenic VOC emissions, and
- Scenario 2--a 50 percent reduction in VOC emissions and a 25 percent reduction in NO_x emissions from all anthropogenic sources.

[1]Note that 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.

Two additional emission reduction scenarios were examined using the J1 and J2 base cases, namely

- Scenario 3--a 25 percent reduction of NO_x emissions from all anthropogenic sources, and
- Scenario 4--a 50 percent reduction of NO_x emissions from all stationary sources emitted aloft in the UAM.

Finally, to provide some insight into the consistency of the findings for other meteorological conditions, two simulations were conducted for the August 1987 SCAQS episode, namely

- Scenario 5--a 50 percent reduction of VOC emissions and a 25 percent reduction of NO_x emissions from all anthropogenic sources using the original SCAQMD simulation for the August episode (Run A4, with nominal VOC emissions estimates) and the CARB simulation for the August episode (Run A5, with VOC emissions multiplied by a factor of 2.2).

PREPARATION OF MODEL INPUTS

Most UAM inputs for the sensitivity studies were the same as those employed in the alternative base case simulations. However, changes were made to both the emissions and initial and boundary concentration inputs. In the latter case, initial and boundary inputs were changed to reflect the conditions associated with the altered emissions rates. In particular, base case initial and boundary concentration inputs for VOC and NO_x (in excess of natural background values) were scaled in proportion to the changes in emissions for these species. Thus, it was assumed that emission sources in the SoCAB contributed directly to that portion of the initial and boundary precursor concentrations in excess of background values, and thus, as emissions changed, so would the initial and boundary concentrations. Ideally, changes in initial and boundary concentrations for O_3 and other secondary pollutants would be derived based on the application of a larger-scale model or modeling results for upwind air basins. In the absence of such results, sensitivity simulations could be conducted using both present input concentrations and background concentrations to determine what influence these inputs have on the results. For the

simulations reported herein, a conservative approach was taken. That is, no changes were made to the existing inputs for O_3 and other secondary species.

DISCUSSION OF RESULTS

To assess the UAM results, we have produced graphical displays comparing the estimated concentrations at air monitoring locations for each emission reduction scenario (i.e., time series plots), as well as spatial maps illustrating the differences in maximum hourly-averaged concentrations for each simulation day. In the following discussion and the attached figures, we employ the following designations for the three base cases and six sensitivity simulations:

- Runs J1, J2, and J7 denote the June base case simulations, as described previously;
- Runs A4 and A5 denote the August base case simulations;
- Runs J8, J9, and J10 denote simulations for which inputs were derived from the J1, J2, and J7 base cases, respectively, with anthropogenic VOC emissions reduced by 50 percent;
- Runs J11, J12, and J13 denote simulations for which inputs were derived from the J1, J2, and J7 base cases, respectively, with anthropogenic VOC emissions reduced by 50 percent and NO_x emissions reduced by 25 percent;
- Runs J14 and J15 denote simulations for which inputs were derived from the J1 and J2 base cases, respectively, with anthropogenic NO_x emissions reduced by 25 percent;
- Runs J16 and J17 denote simulations for which inputs were derived from the J1 and J2 base cases, respectively, with NO_x emissions from elevated sources reduced by 50 percent; and
- Runs A6 and A7 denote simulations for which inputs were derived from the A4 and A5 base cases, respectively, with anthropogenic VOC emissions reduced by 50 percent and NO_x emissions reduced by 25 percent;

Various graphical displays were generated to assist in the analysis of the sensitivity results, including:

- spatial maps illustrating the difference in peak O_3 and NO_2 concentrations in each grid cell for each of the last two simulation days;
- spatial maps illustrating the maximum one-hour O_3 and NO_2 concentration in each grid cell for each of the last two simulation days;
- spatial maps illustrating the percentage change in peak O_3 and NO_2 concentrations from base case values in each grid cell for each of the last two simulation days;
- spatial maps illustrating the difference in percentage reductions of peak O_3 and NO_2 concentrations associated with two simulations for each of the last two simulation days; and
- time series plots at all air monitoring stations for both O_3 and NO_2 concentrations.

For the purpose of this presentation, we have selected a few of these graphics for use in illustrating the key findings. Note that all figures are presented at the end of this section.

Scenario 1--50 Percent Reduction in VOC Emissions (June Episode)

Figures 4-1 through 4-3 show the spatial distribution of maximum estimated O_3 concentrations for the J1, J2, and J7 base cases, respectively, on 25 June, the last day of each simulation. Note that the highest estimated concentrations for J1 and J7 are located in the northwestern portion of the modeling domain in the vicinity of Newhall. Estimated concentrations in this area are significantly larger than the observed values, suggesting that problems still exist in the specification of meteorological and/or emissions inputs in this and immediately upwind areas. Complex wind convergence phenomena occurring in this area may not be adequately treated using the diagnostic wind model employed to develop UAM meteorological input fields. Thus, we have ignored these modeling results for this analysis. In contrast, the peak estimated concentration in the eastern portion of the modeling domain is reasonably consistent among the three base cases (ranging from 26.8 to 28.9 pphm). These values are about 3 to 5 pphm greater than the highest observation reported at a monitoring location situated a few grid cells to the north of where the highest estimated values occur.

Figure 4-4 depicts the change in maximum estimated O_3 concentrations on 25 June resulting from a 50 percent reduction of anthropogenic VOC emissions using conditions derived from the J1 base case (i.e., a comparison of Run J1 and J8 results). Figures 4-5 and 4-6 provide similar results for Runs J9 and J10 using the J2 and J7 base cases, respectively. Figures 4-7 through 4-9 show the corresponding percentage changes in maximum O_3 concentrations. Note that this level of VOC control leads to lower estimated O_3 concentrations in almost all portions of the domain.

To assist in comparing spatial results derived from different base cases, we have developed displays that show the difference in values. Figure 4-10 is a display of the difference in percentage reductions of maximum estimated O_3 concentrations for the 50 percent VOC reduction scenario for simulations derived from the J1 and J2 base cases. For example, if Run J8 yielded a 30 percent reduction in O_3 relative to Run J1 for a particular grid cell and Run J9 gave a 40 percent reduction relative to Run J2, then the difference of 10 percent (40 percent - 30 percent = 10 percent) would be displayed in Figure 4-10 for that grid cell. An examination of Figure 4-10 indicates that differences in percentage reductions in maximum estimated O_3 for results derived from the J1 base case are from 10 to 30 percent greater than the corresponding reductions derived from the J2 base case in areas between Pasadena and Lancaster, between Pomona and Hesperia, and the area to the east of Victorville (see Figure 2-3 for the locations of these sites). In other areas, the J1-based reductions can be 10 to 30 percent less than J2-based results. Figures 4-11 and 4-12 illustrate differences in results between the other combinations of the three base cases.

The differences in results shown in Figures 4-10 and 4-12 may be attributable to differences in wind fields employed in the alternative base cases. Recall that base cases J1 and J7 employ one set of wind inputs, and base case J2 uses another. Some of the greatest differences in results noted in Figures 4-10 and 4-12 occur in areas of large spatial gradients in the concentration field. The effects of emission reductions in such locations can give rise to significant differences in results (e.g., the percentage change in the peak O_3 for a particular grid cell).

Table 4-1 summarizes the influence of the choice of alternative base case on the regional peak O_3 concentration in the eastern portion of the modeling domain. Note that we did not consider the influence on the peak concentration in the western portion of the domain for the reasons cited earlier. For 50 percent anthropogenic VOC emissions control, the percent reductions in peak O_3 levels ranged from 31 to 42 percent on June 24 and from 28 to 31 percent on June 25 for the three alternative June base cases.

Scenario 2--50 Percent Reduction of VOC Emissions and 25 Percent Reduction in NO_x Emissions (June Episode)

Figures 4-13 through 4-15 depict the change in peak O_3 concentration on 25 June resulting from a 50 percent reduction in VOC emissions and a 25 percent reduction in NO_x emissions for the J1, J2, and J7 base case modeling conditions, respectively. The corresponding percentage changes in maximum estimated O_3 concentrations on 25 June are shown in Figures 4-16 through 4-18. This combination of emission reductions also helps to reduce maximum estimated O_3 levels. However, a comparison of the corresponding figures for Scenarios 1 and 2 (e.g., Figures 4-7 and 4-16) indicates that over most of the domain, the addition of NO_x controls reduces the effectiveness of the VOC-only control scenario. This can be more readily seen in Figures 4-19 through 4-24, which illustrates the change in maximum estimated O_3 concentrations for Runs J11, J12, and J13 (i.e., the combination of VOC and NO_x reductions) relative to Runs J8, J9, and J10 (i.e., only VOC reductions).

A comparison of results derived from the J1 and J7 base cases (see Figure 4-11) indicates that over much of the region, the differences in estimated O_3 percentage reductions do not differ by more than 10 percent. That is, the J1- and J7-derived results provide similar estimates of O_3 percentage reductions for the VOC control scenario. In contrast, the effectiveness of the VOC control scenario derived from the J2 base case can differ significantly from that indicated by the other two base cases in some areas of the domain.

Table 4-1. The influence of choice of alternative base case on peak O_3 concentration in the eastern portion of the modeling domain for various hypothetical emission reduction scenarios.

Percent Emission Reduction[1]		Percent Reduction in Peak O_3 Concentration									
		Base Cases									
		J1		J2		J7		A4		A5	
VOC	NO_x	Jun 24	Jun 25	Jun 24	Jun 25	Jun 24	Jun 25	Aug 27	Aug 28	Aug 27	Aug28
50	0	42	31	31	31	40	28				
50	25	27	23	30	31	21	28	5	18	38	40
0	25	14	13	2	-3						
0	50[2]	1	1	0	0						

Notes:

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).

To complement the spatial displays, we have generated graphics illustrating the estimated O_3 concentrations as a function of time at each air monitoring location. Figure 4-25 shows the estimated O_3 concentrations for the three base cases and the observed values for 23-25 June 1987 at Reseda, Glendora, and Redlands. The purpose of this figure is to show how well the estimated concentrations agree with observations. Note that VOC emissions inputs used in Runs J1 and J7 are 2.2 times the values employed in Run J2.

Figures 4-26 through 4-28 show the time series of estimated concentrations for the three base cases and two associated emission reduction scenarios at Reseda, Glendora, and Redlands, respectively. In general, the J1- and J7-derived results suggest that the VOC control scenario will yield greater reductions in O_3 than the corresponding J2-derived results. Similarly, the J1- and J7-derived results indicate that NO_x controls will be more counterproductive in helping to reduce O_3 than is otherwise suggested by the corresponding J2-derived results.

Table 4-1 summarizes how the choice of alternative base case influences the peak O_3 concentration in the eastern portion of the modeling domain. The reduction in peak concentration ranges from 21 to 30 percent on 24 June and from 23 to 31 percent on 25 June for the three alternative June base cases. The J2 base case (UAM inputs developed by the SCAQMD) yields somewhat greater percentage reductions in the peak concentration than either the J1 or J7 base cases (UAM inputs developed in this study).

Scenario 3--25 Percent Reduction of NO_x Emissions (June Episode)

Figures 4-29 through 4-32 depict the change in maximum estimated O_3 concentrations on 25 June resulting from a 25 percent reduction of anthropogenic NO_x emissions using conditions derived from the J1 and J2 base cases. For the J1 base case, this level of NO_x control leads to higher estimated O_3 concentrations in coastal and central portions of the basin as well as in the San Fernando and San Gabriel Valleys. Some decreases in peak O_3 were estimated in the eastern portions of the modeling domain. For the J2 base case, a smaller increase in O_3 is estimated in the eastern San Fernando Valley and a greater increase in the Glendora area.

An examination of Figure 4-33 indicates that large differences in percentage changes in maximum estimated O_3 for results derived from the J1 and J2 base cases occur in the San Fernando and eastern San Gabriel and Pomona Valley areas.

Table 4-1 summarizes how the choice of alternative base case influences the peak O_3 concentration in the eastern portion of the modeling domain. The reduction in peak concentration ranges from 2 to 14 percent on 24 June and from -3 to 2 percent on 25 June for the two alternative June base cases. The J1 base case (UAM inputs developed in this study) indicates that NO_x controls will exhibit some influence on peak O_3 in the eastern portion of the domain, whereas the J2 base case yields only a very small (about 2 to 3 percent) influence on this peak concentration.

Scenario 4--50 Percent Reduction in Elevated NO_x Emissions (June Episode)

Figures 4-34 through 4-37 illustrate the changes in maximum estimated O_3 concentrations on 25 June resulting from a 50 percent reduction of NO_x emissions from elevated sources using conditions derived from the J1 and J2 base cases. Control of NO_x emissions from elevated sources generally leads to increases in peak O_3 levels in the central basin and San Fernando Valley areas and very modest (i.e., less than 2 percent) benefits in the eastern portions of the domain. Figure 4-38 provides a comparison of results derived from the J1 and J2 base cases. Differences in results using the two base cases differed by as much as 9 to 16 percent in the area northeast of Long Beach and portions of the San Fernando and San Gabriel Valleys.

The influence on peak O_3 in the eastern portion of the domain is summarized in Table 4-1. As indicated above, this control scenario has little influence on the peak O_3 concentration.

Scenario 5--50 Percent Reduction of VOC Emissions and 25 Percent Reduction of NO_x Emissions (August Episode)

A comparison of simulation results for Scenarios 2 and 5 provides an indication of the consistency of the findings of this investigation for different meteorological conditions. Figures 4-39 through

4-44 show maximum estimated O_3 concentrations and the change in peak O_3 levels on 28 August resulting from a 50 percent reduction in VOC emissions and a 25 percent reduction in NO_x emissions for the A4 and A5 base cases. The corresponding changes in O_3 concentrations for 25 June are shown in Figures 4-13, 4-14, 4-16, and 4-17. Note in comparing results that the J2 and A4 base cases were developed by the SCAQMD. The SCAQMD base case yields results that indicate O_3 levels will increase over a significant portion of the coastal and central basin areas in response to the imposition of the hypothetical VOC and NO_x controls. Figure 4-45 illustrates that there are significant differences in the estimated percentage changes in peak O_3 over large areas for the two August base cases.

Table 4-1 provides a means of comparing the influence of both the June and August base cases on peak O_3 in the eastern portion of the modeling domain. The percent reductions in peak concentration range from 5 to 38 percent for 27 August and from 18 to 40 percent for 28 August.

SUMMARY OF KEY FINDINGS

The alternative base cases employed in this study produced significant differences in estimates of the air quality benefits associated with hypothetical emission control scenarios. All base cases yielded lower estimated O_3 concentrations resulting from a 50 percent reduction in anthropogenic VOC emissions. The percentage reduction of the peak O_3 in the eastern portion of the modeling domain for particular simulation days ranged from 21 to 30 percent and 21 to 31 percent for 24 and 25 June, respectively, and ranged from 5 to 38 percent and from 18 to 40 percent for 27 and 28 August, respectively. For the scenario in which anthropogenic VOC and NO_x emissions were reduced by 50 and 25 percent, respectively, two of the alternative June base cases indicated that the additional NO_x control would be counterproductive (i.e., would yield a smaller reduction in the peak O_3 concentration than was estimated for the case where only VOC emissions were reduced). The third June base case indicated that there would be essentially no change to the estimated peak O_3 level in the eastern portion of the domain. 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 O_3 (i.e., a 13 to 14 percent reduction), whereas a second

alternative base case yielded very little change in the peak concentration (i.e., about 2 to 3 percent). 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 O_3 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 O_3 values ranged from 9 to 16 percent.

Alternative base case studies provide a lower bound estimate on the uncertainty that attends modeling estimates of the air quality benefits associated with future year emission control plans. Such uncertainties may have significant implications for how much control is implemented in an area, which in turn can have important ramifications for the associated control costs.

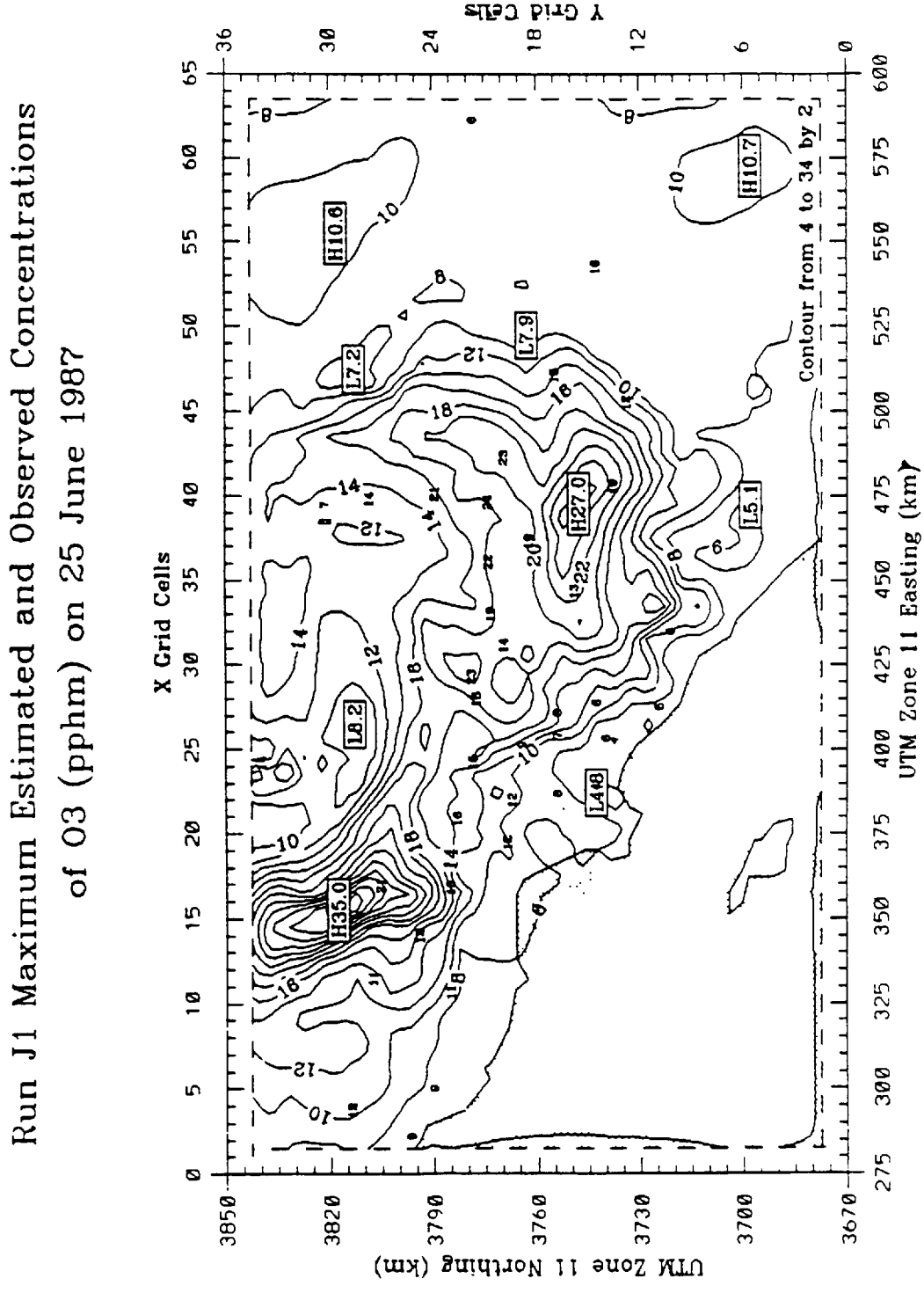


Figure 4-1. Maximum estimated and observed O_3 concentrations (pphm) on 25 June 1987 for Run J1

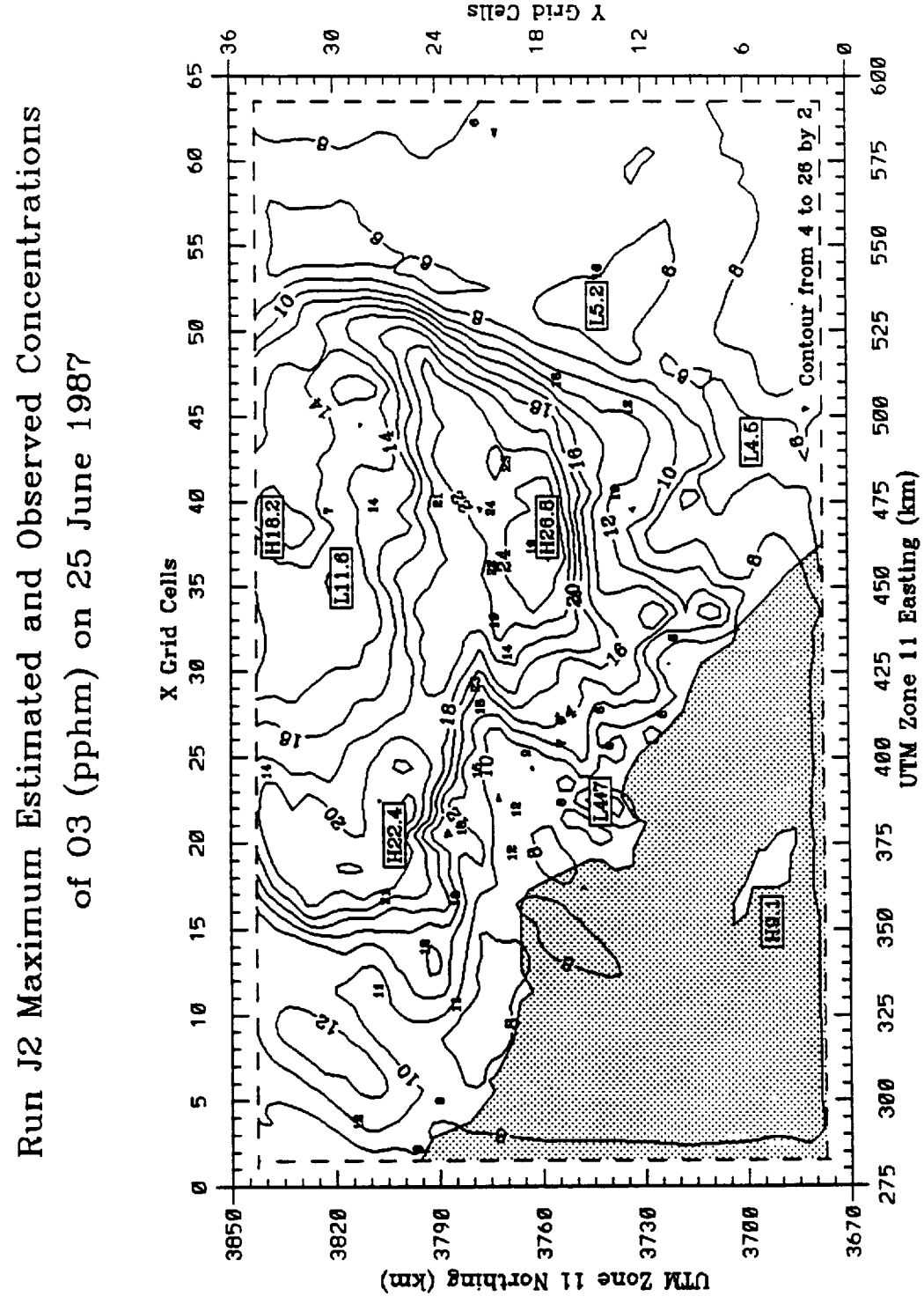


Figure 4-2. Maximum estimated and observed O_3 concentrations (pphm) on 25 June 1987 for Run J2

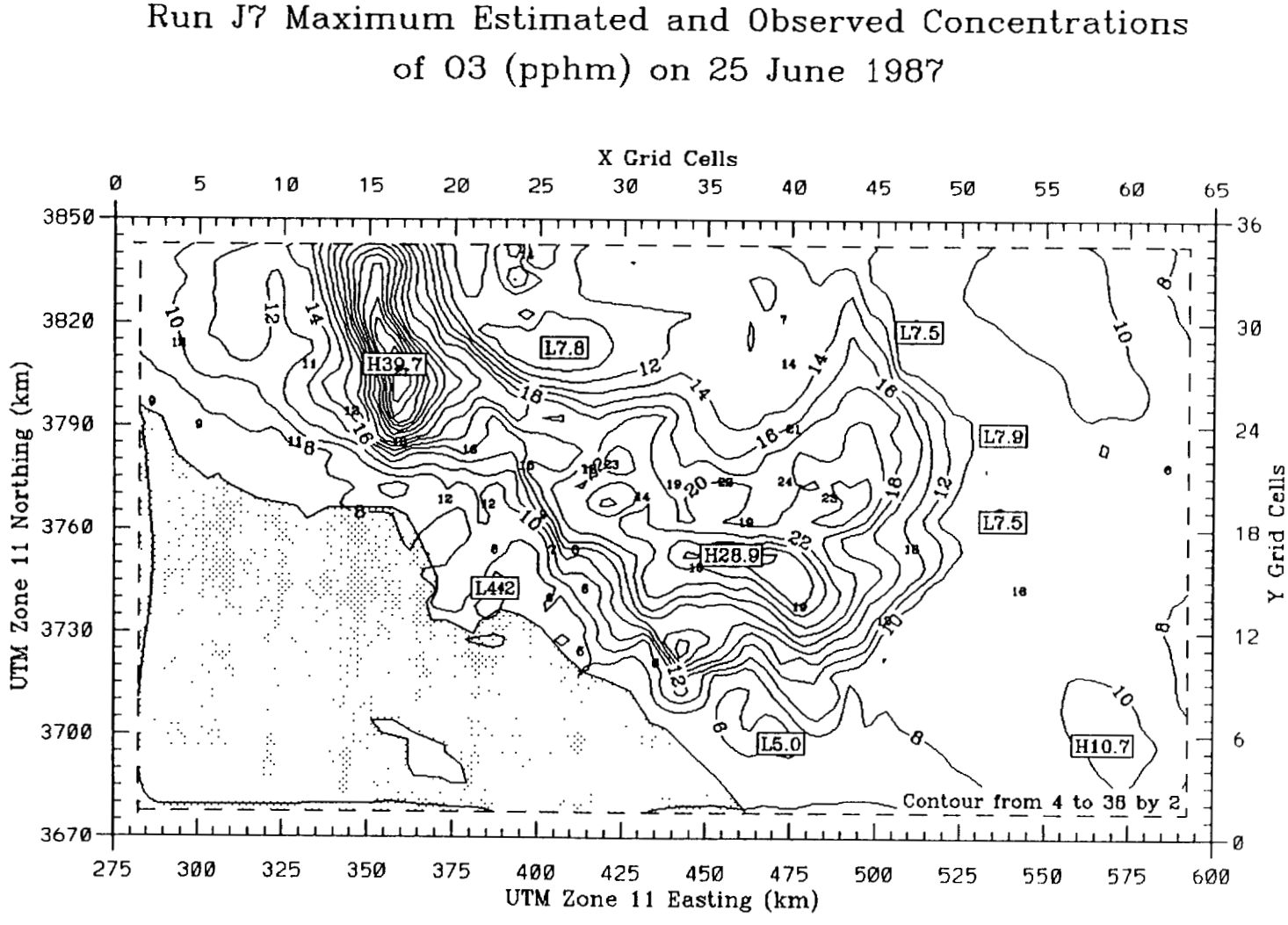


Figure 4-3. Maximum estimated and observed O_3 concentrations (pphm) on 25 June 1987 for Run J7

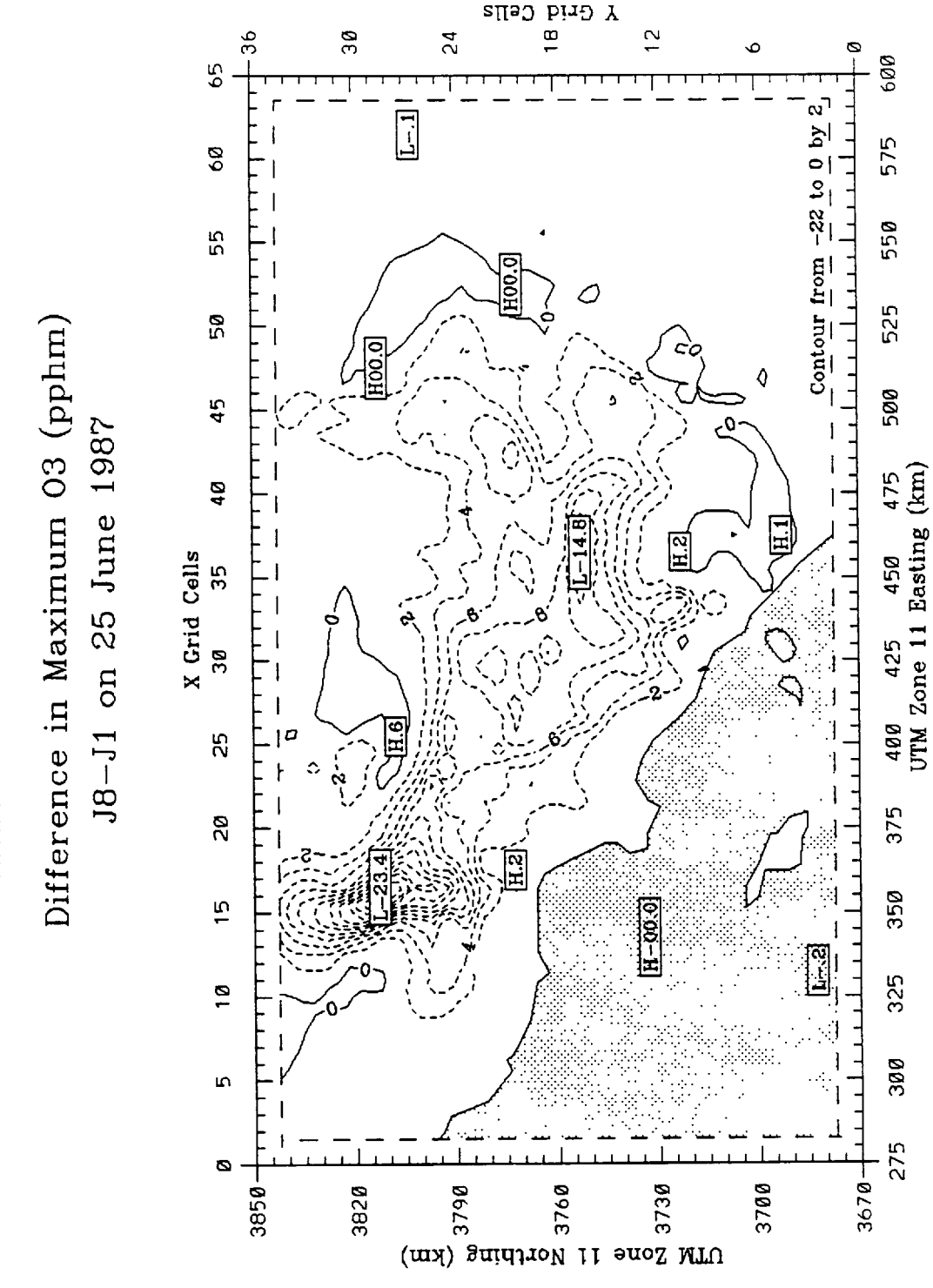


Figure 4-4. Difference in estimated maximum O_3 concentrations (pphm) [Run J8 - Run J1] on 25 June

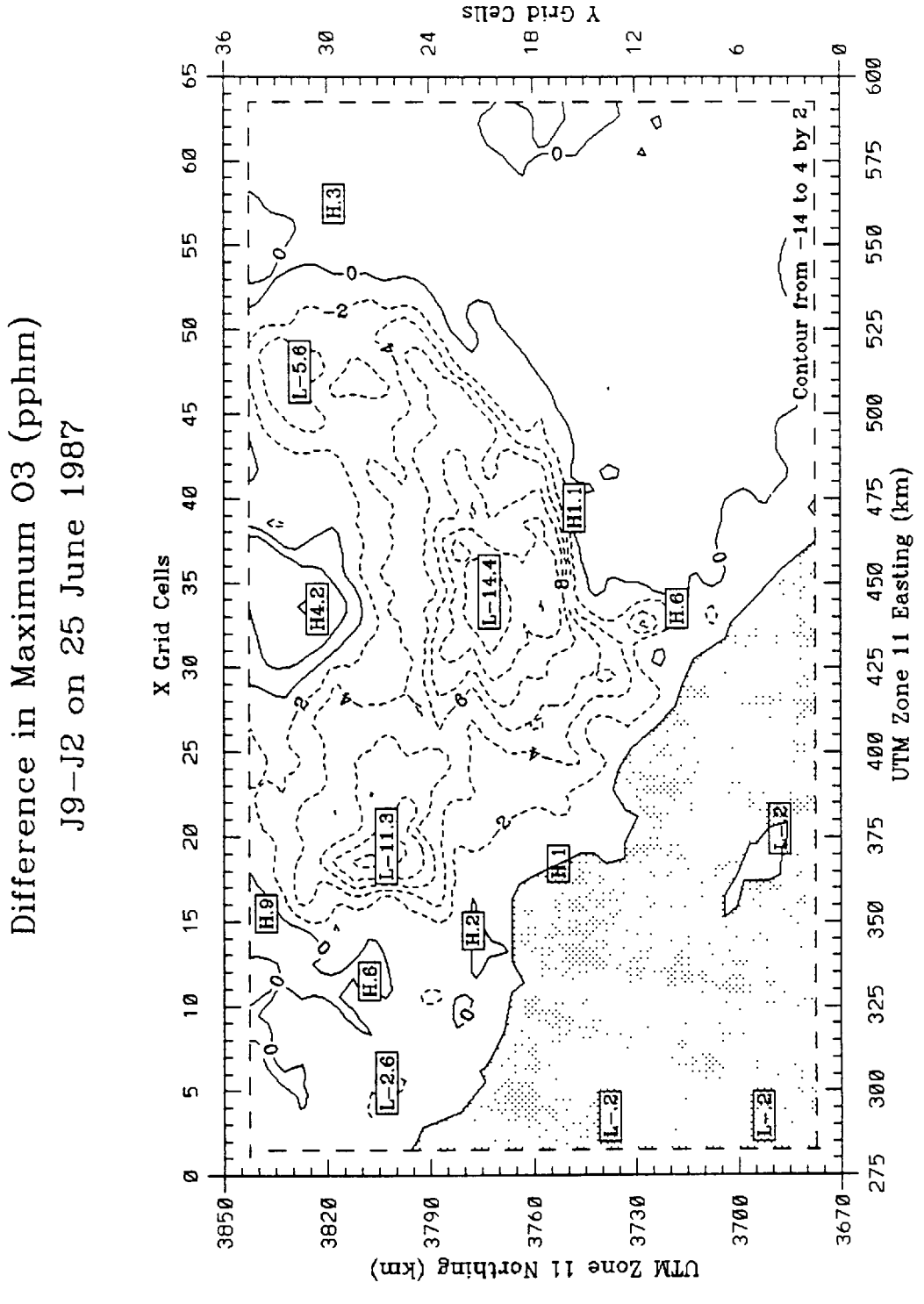


Figure 4-5. Difference in estimated maximum O_3 concentrations (pphm) [Run J9 - Run J2] on 25 June

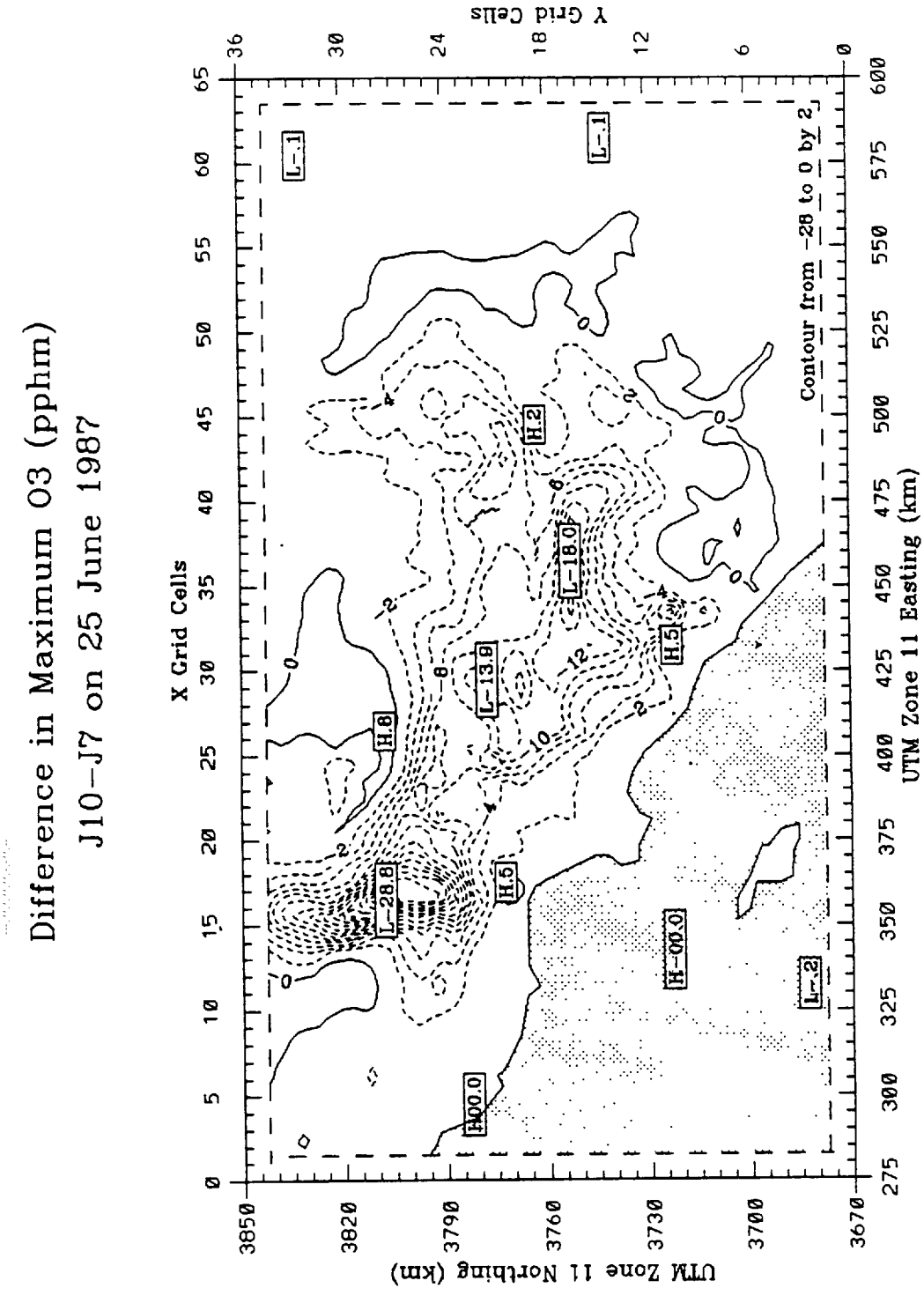


Figure 4-6. Difference in estimated maximum O_3 concentrations (pphm) [Run J10 - Run J7] on 25 June

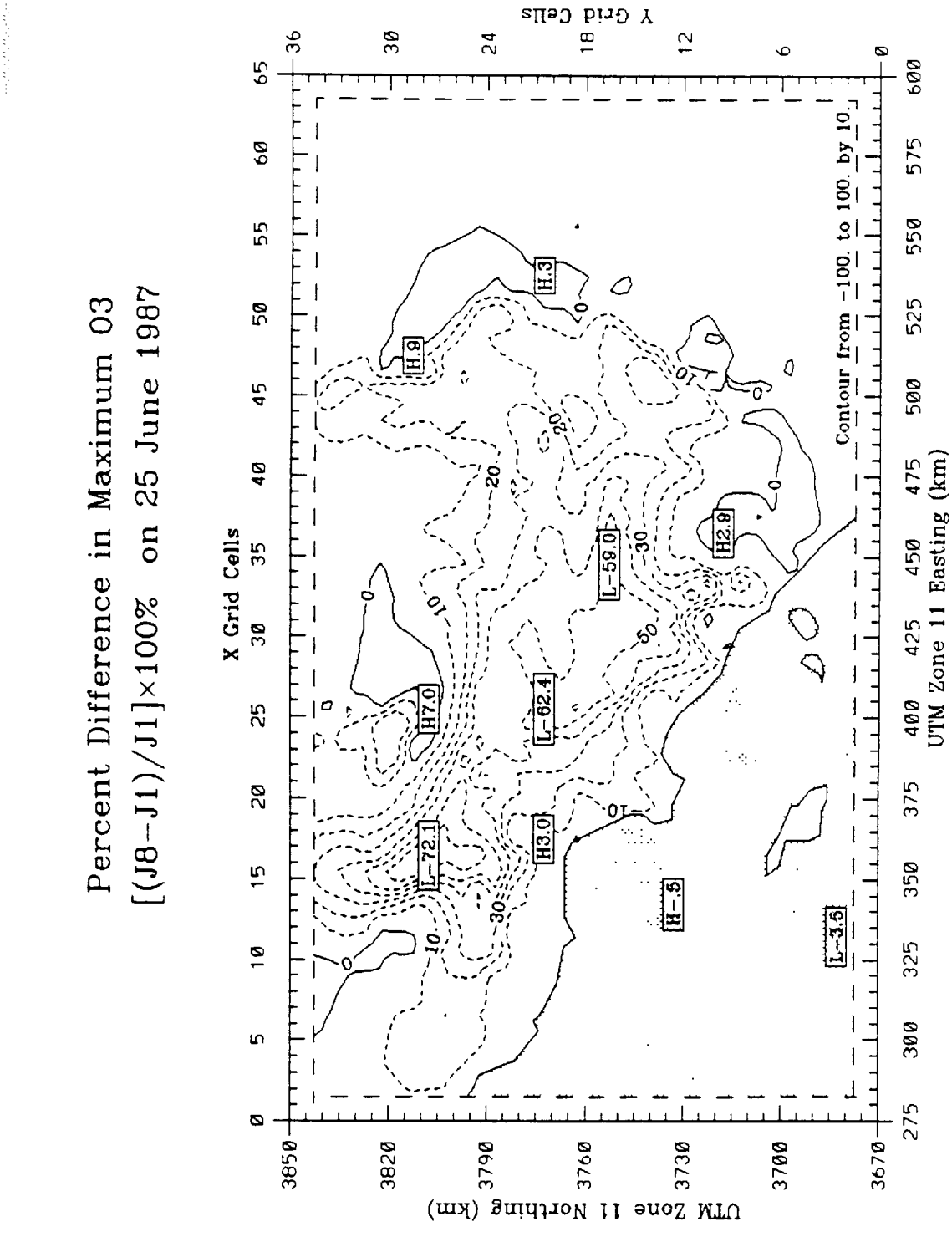


Figure 4-7. Percent difference in estimated maximum O_3 concentrations [(J8 - J1)/J1 x 100%] on 25 June

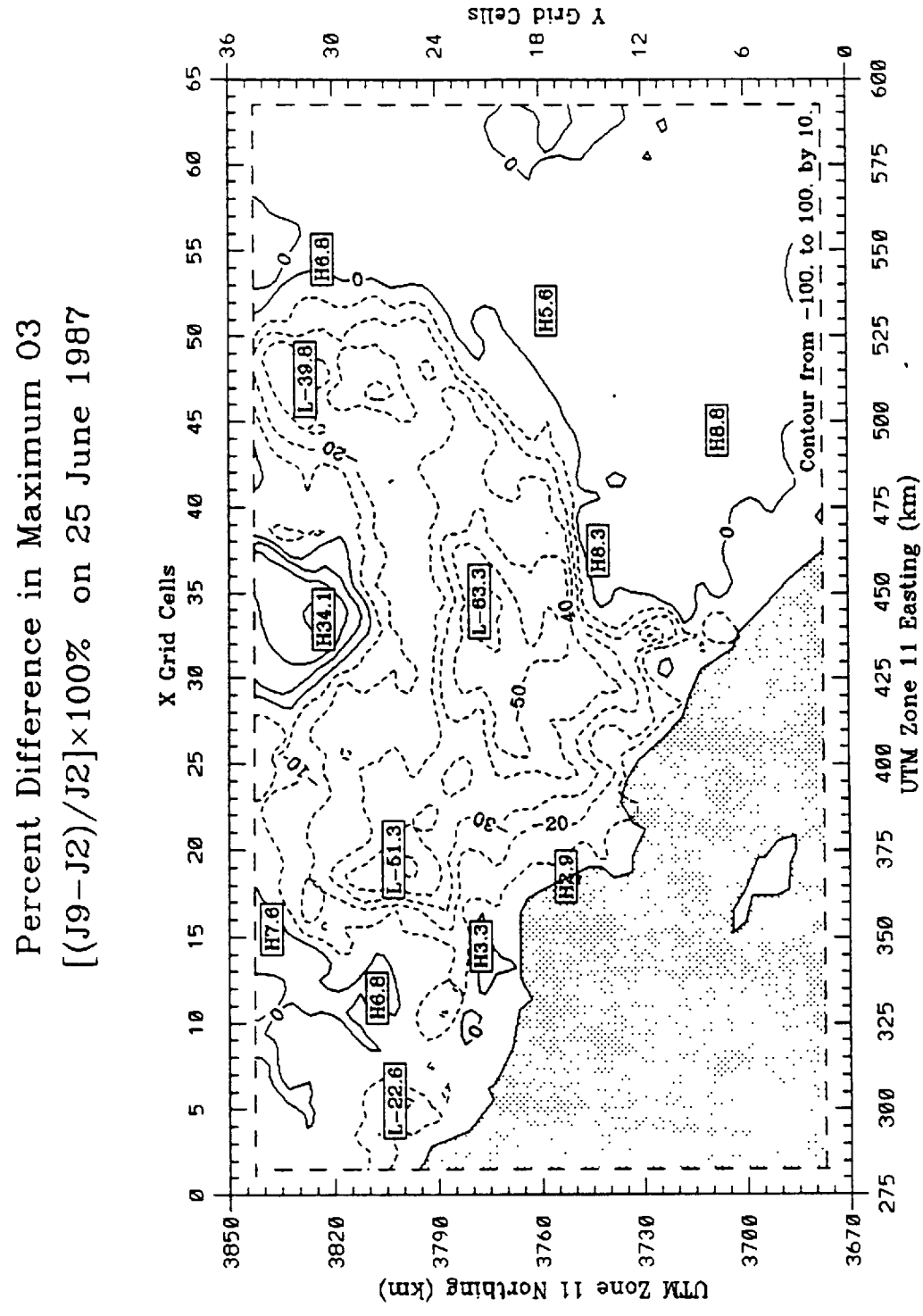


Figure 4-8. Percent difference in estimated maximum O_3 concentrations [(J9 - J2)/J2 x 100%] on 25 June

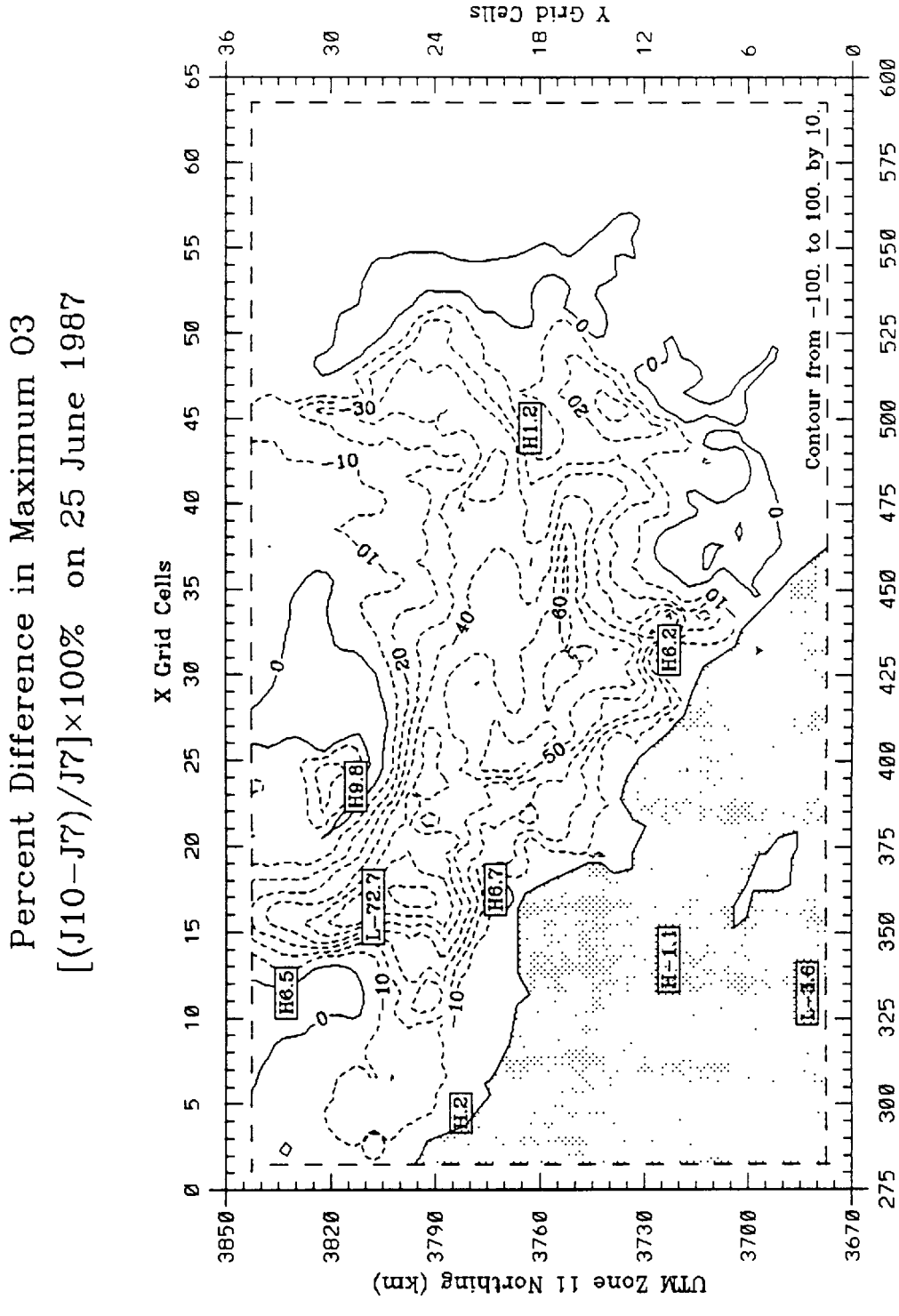


Figure 4-9. Percent difference in estimated maximum O_3 concentrations [(J10 - J7)/J7 x 100%] on 25 June

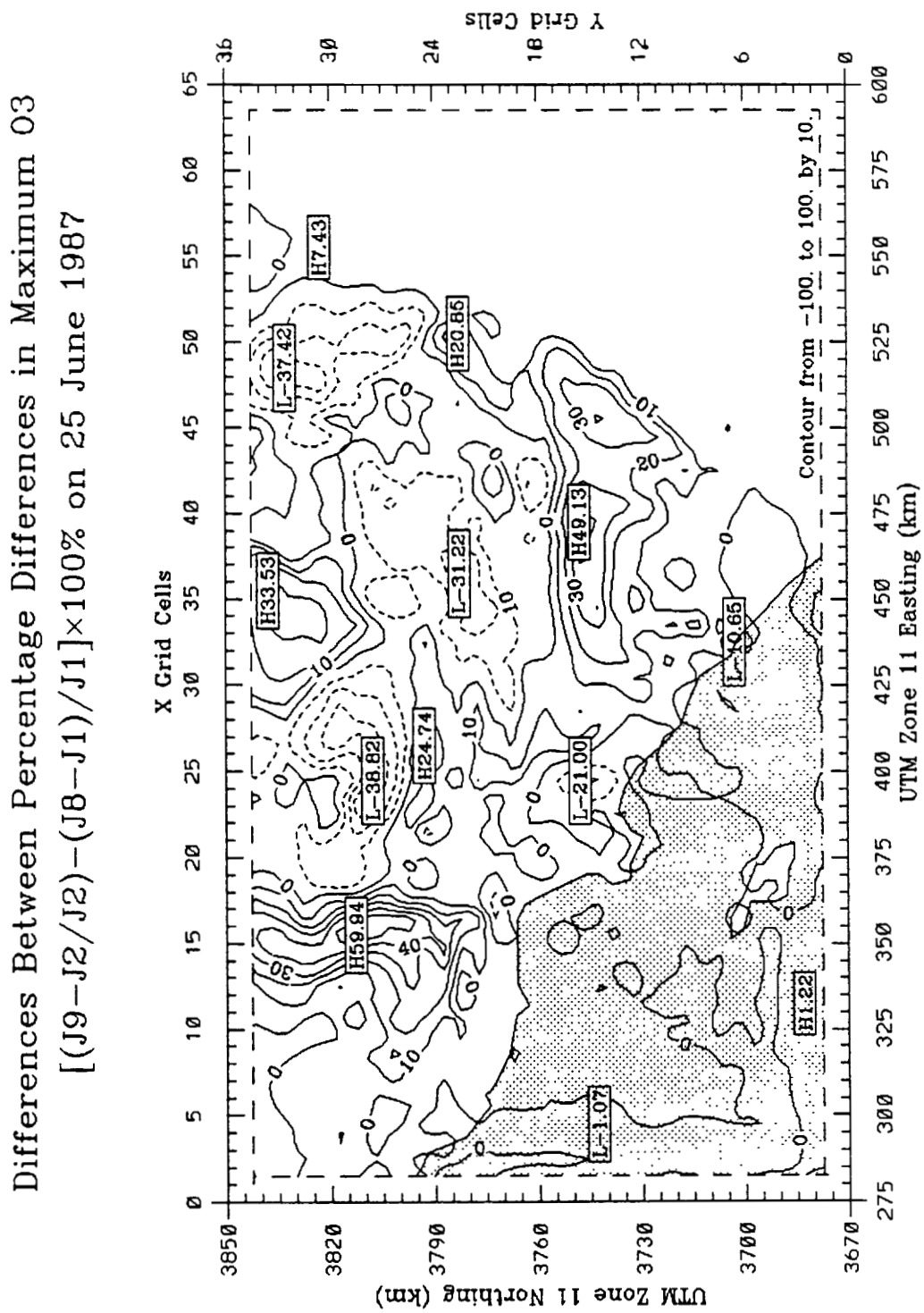


Figure 4-10. Differences in percentage changes in estimated maximum O_3 concentrations [{(J9 - J2)/J2 - (J8 - J1)/J1} x 100%] on 25 June

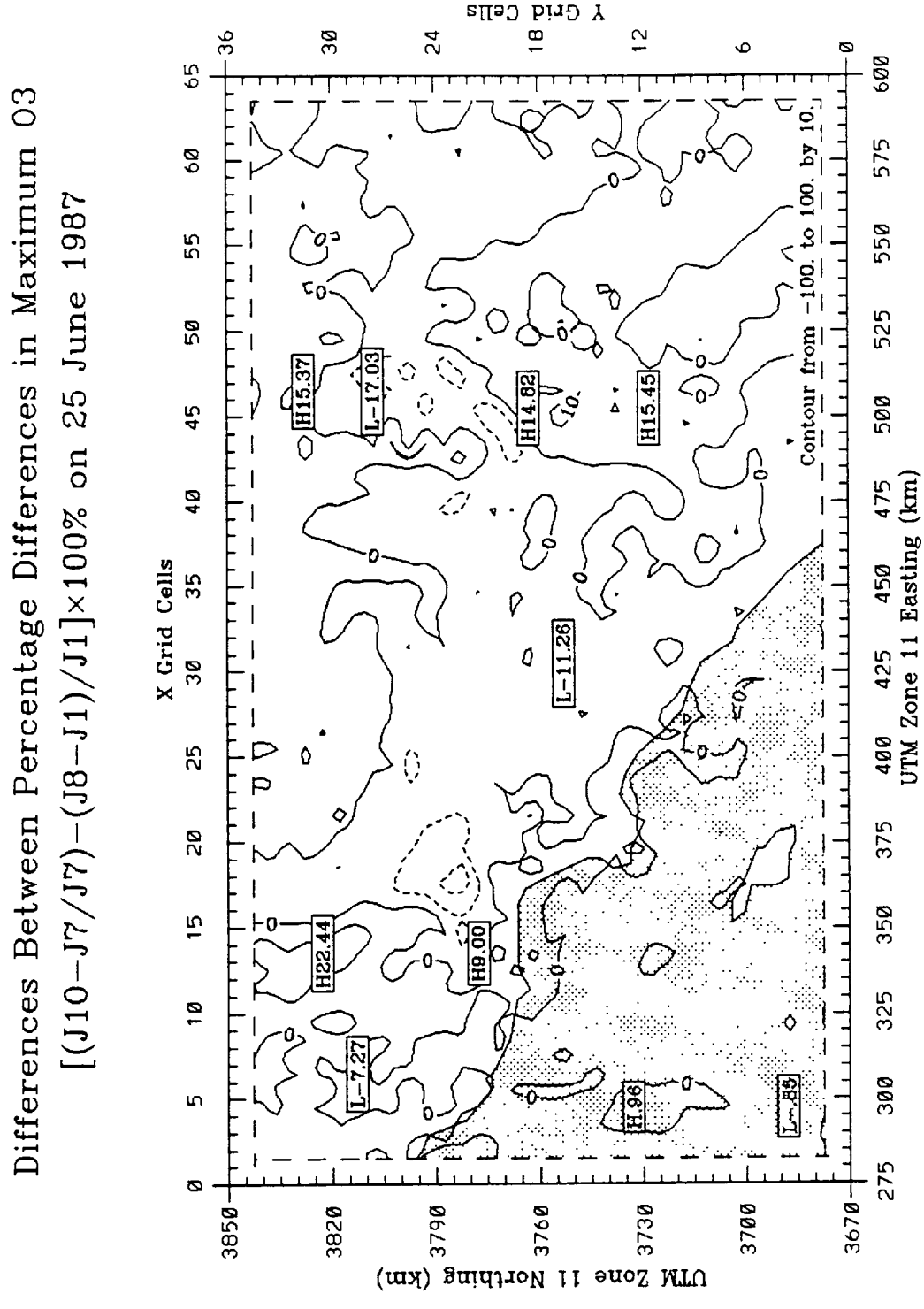


Figure 4-11. Differences in percentage changes in estimated maximum O_3 concentrations [{(J10 - J7)/J7 - (J8 - J1)/J1} x 100%] on 25 June

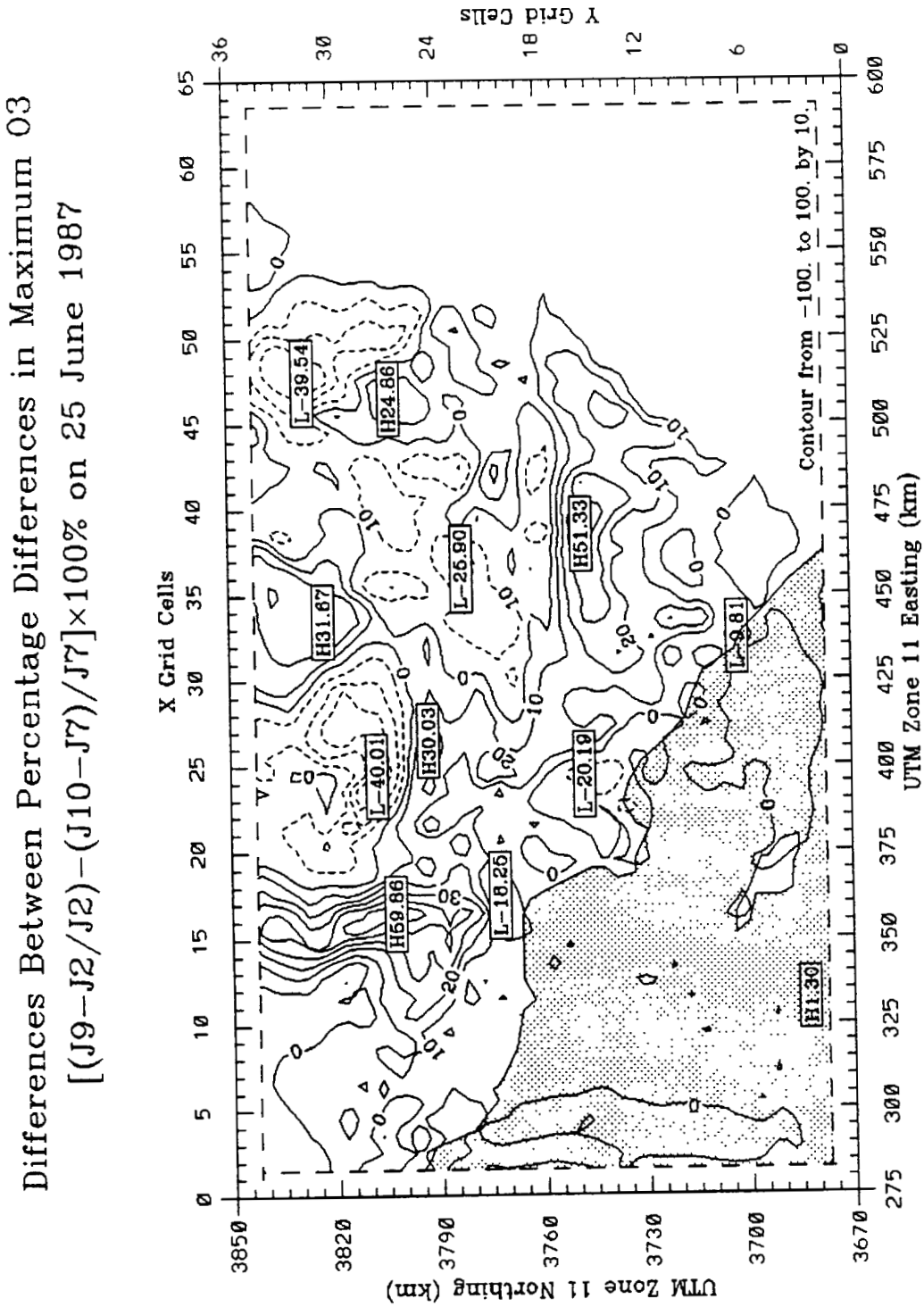


Figure 4-12. Differences in percentage changes in estimated maximum O_3 concentrations [{(J9 - J2)/J2 - (J10 - J7)/J7} x 100%] on 25 June

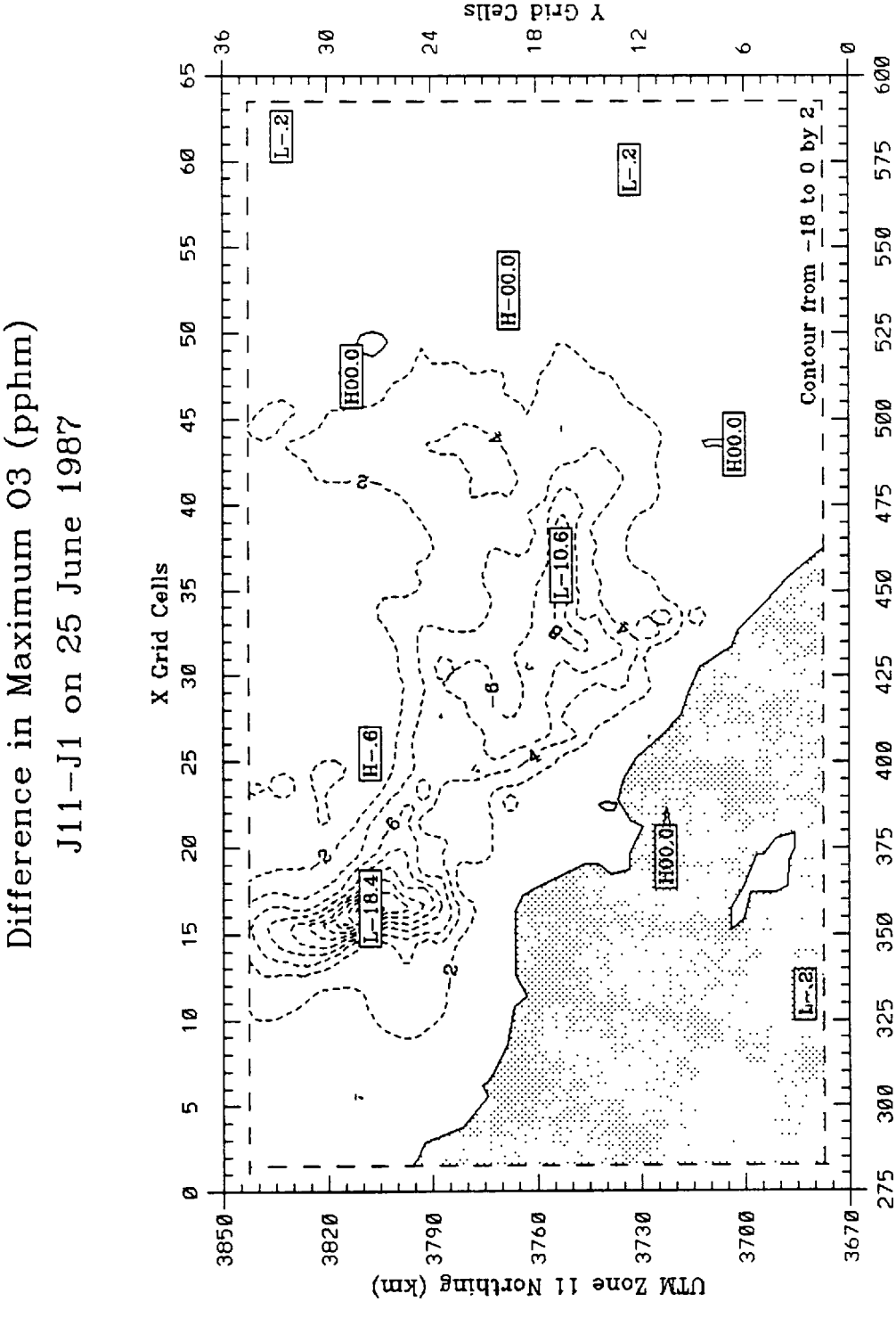


Figure 4-13. Difference in estimated maximum O_3 concentrations (pphm) [Run J11 - Run J1] on 25 June

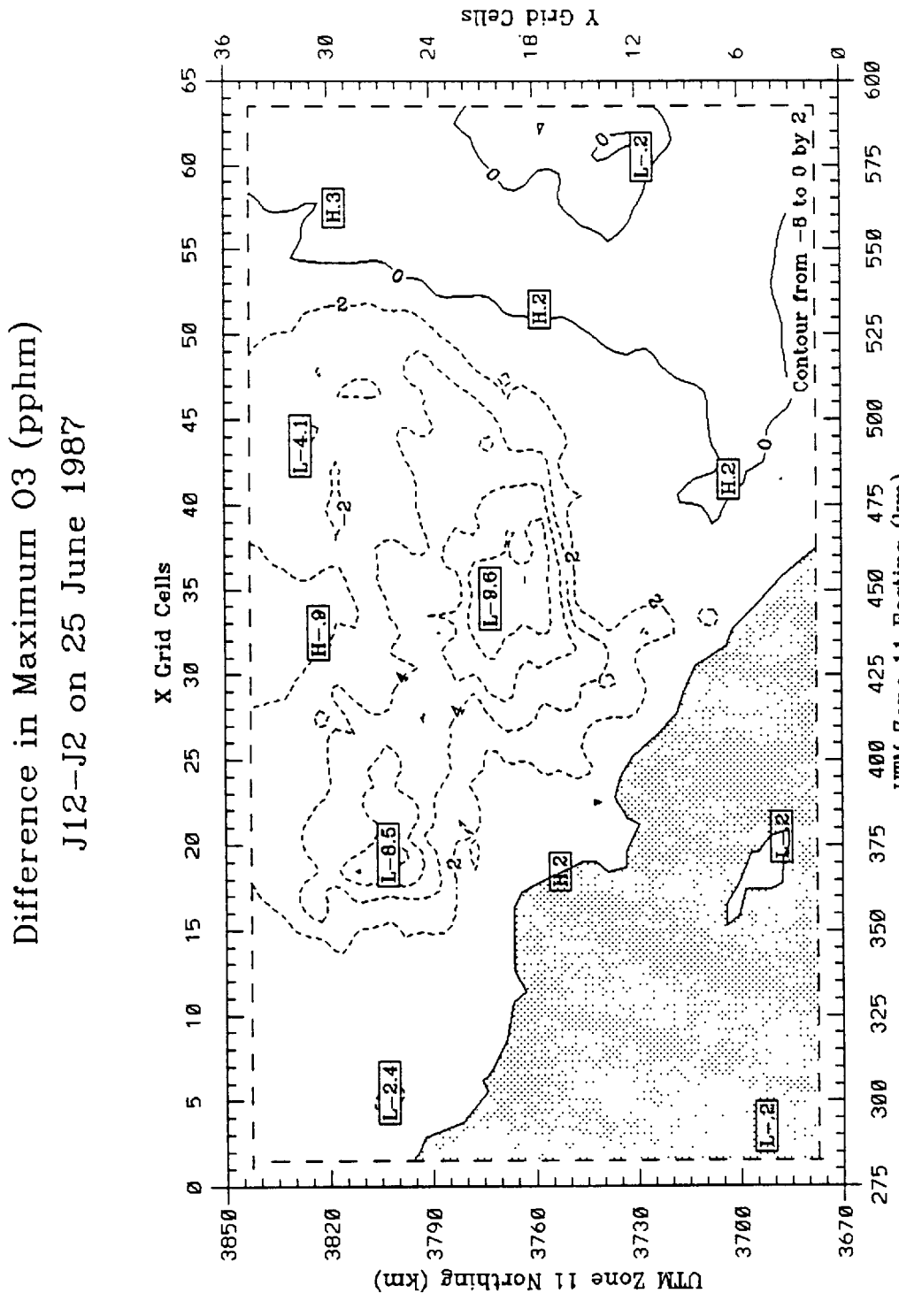


Figure 4-14. Difference in estimated maximum O_3 concentrations (pphm) [Run J12 - Run J2] on 25 June

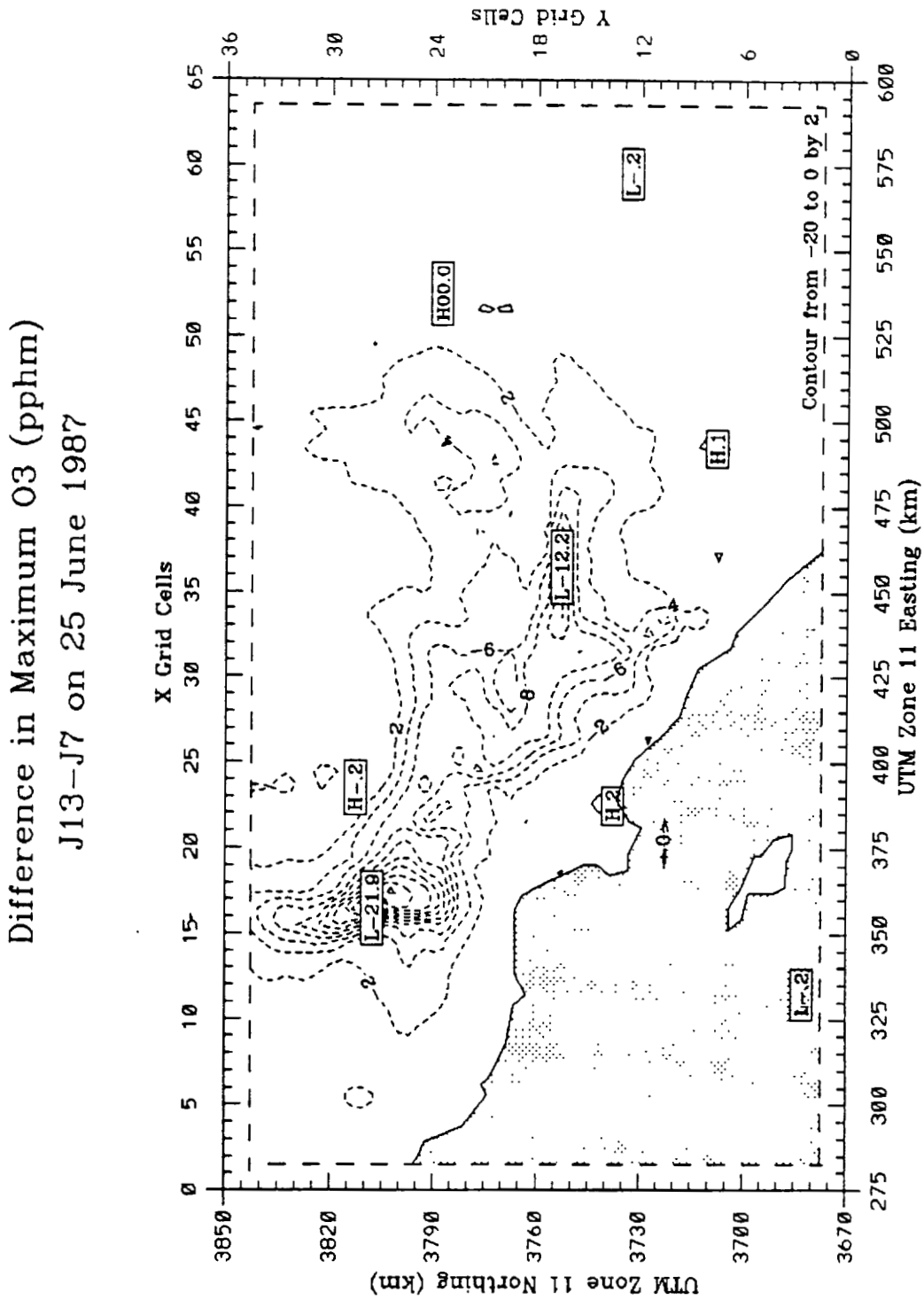


Figure 4-15. Difference in estimated maximum O_3 concentrations (pphm) [Run J13 - Run J7] on 25 June

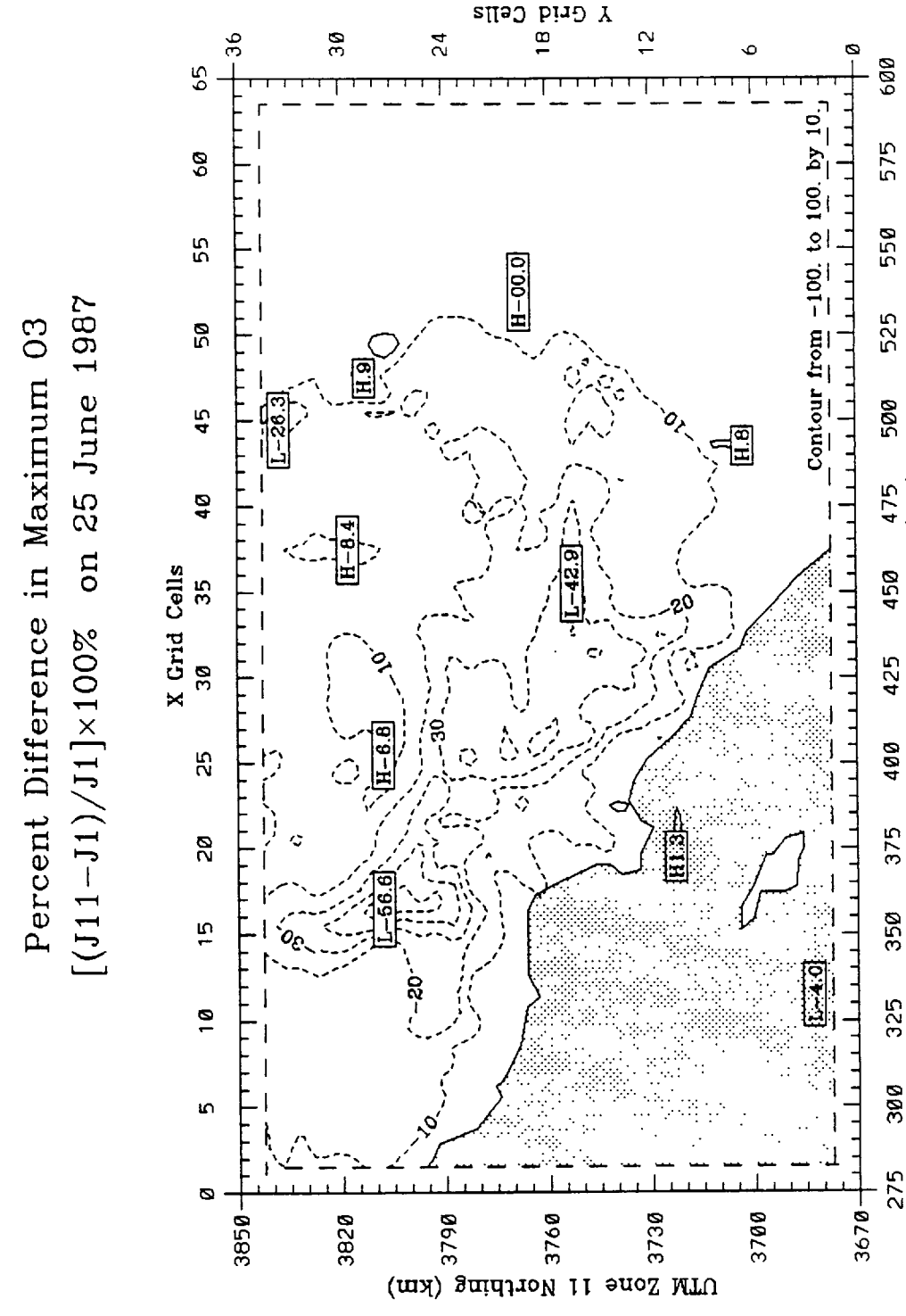


Figure 4-16. Percent difference in estimated maximum O_3 concentrations [(J11 - J1)/J1 x 100%] on 25 June

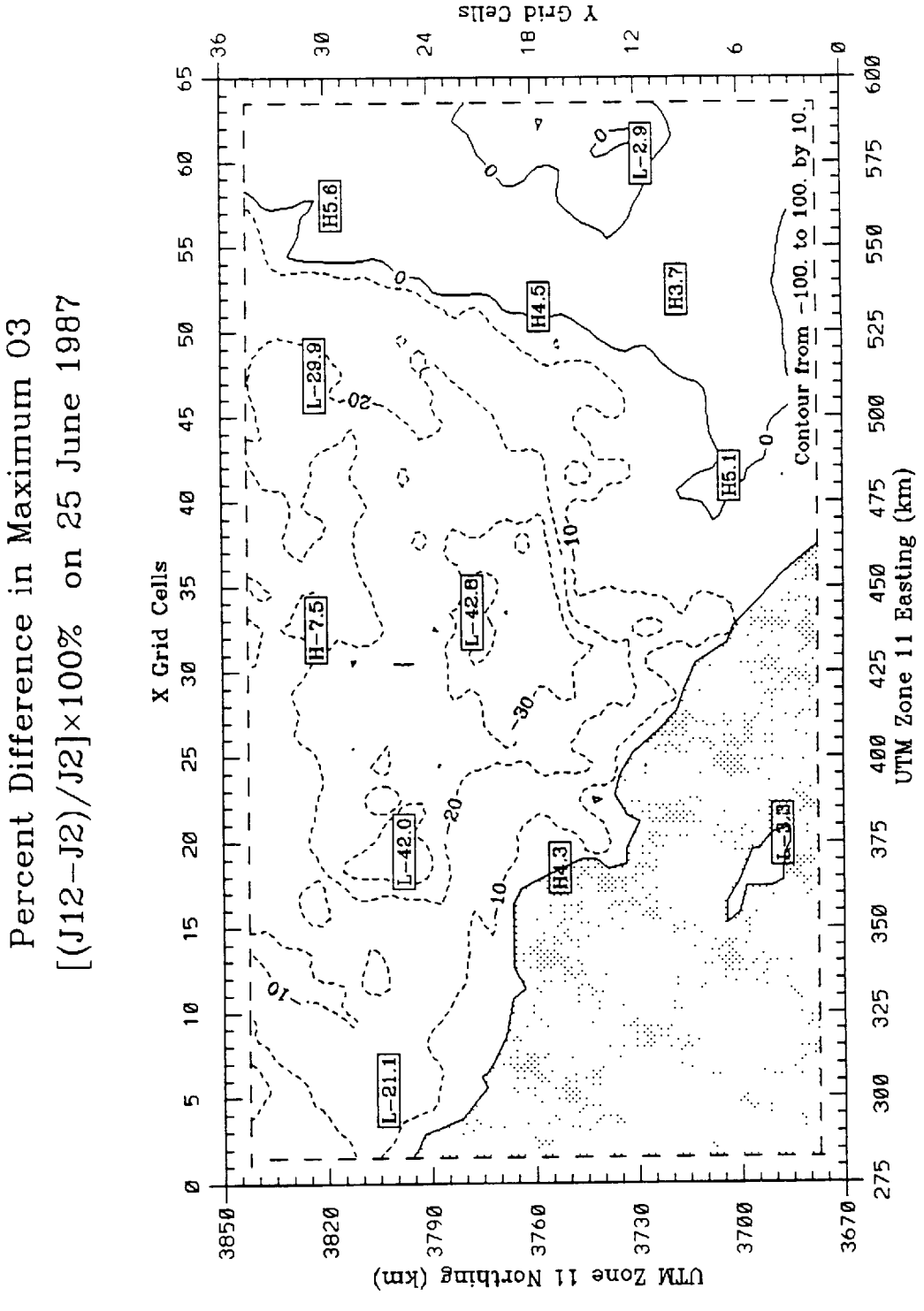
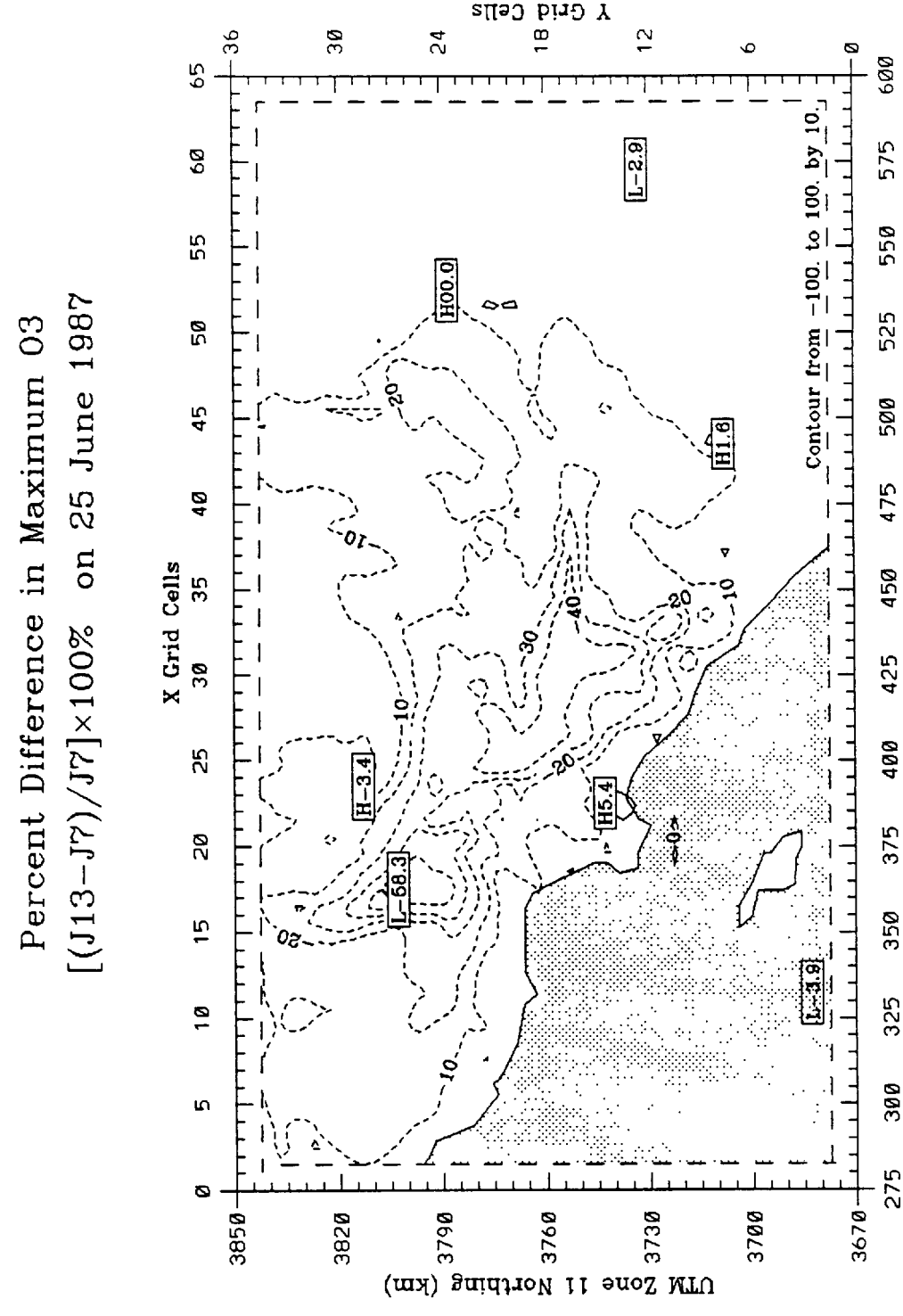


Figure 4-17. Percent difference in estimated maximum O_3 concentrations [(J12 - J2)/J2 x 100%] on 25 June



Dashed contours indicate values less than zero

Figure 4-18. Percent difference in estimated maximum O_3 concentrations [(J13 - J7)/J7 x 100%] on 25 June

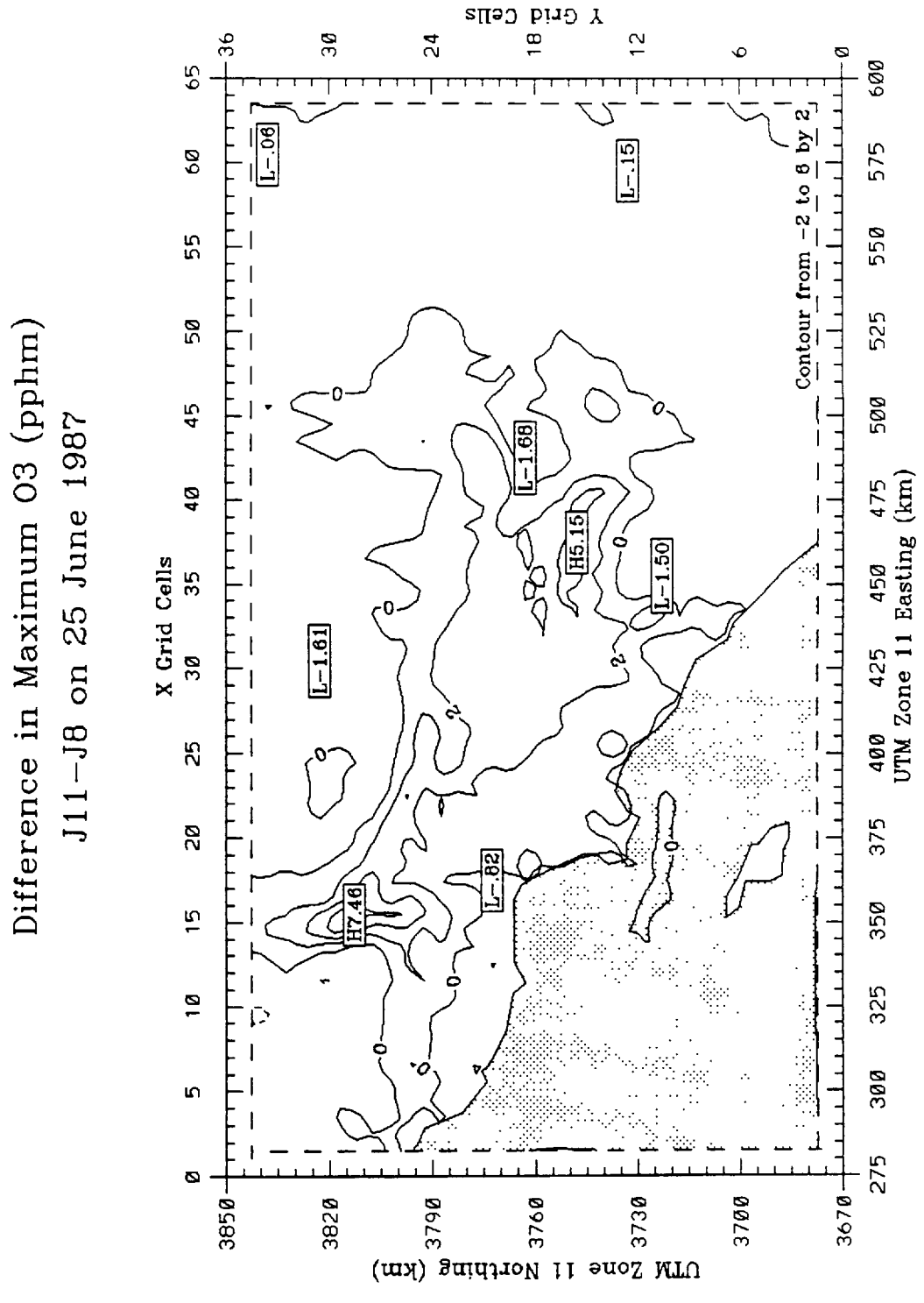


Figure 4-19. Difference in estimated maximum O_3 concentrations (pphm) [Run J11 - Run J8] on 25 June

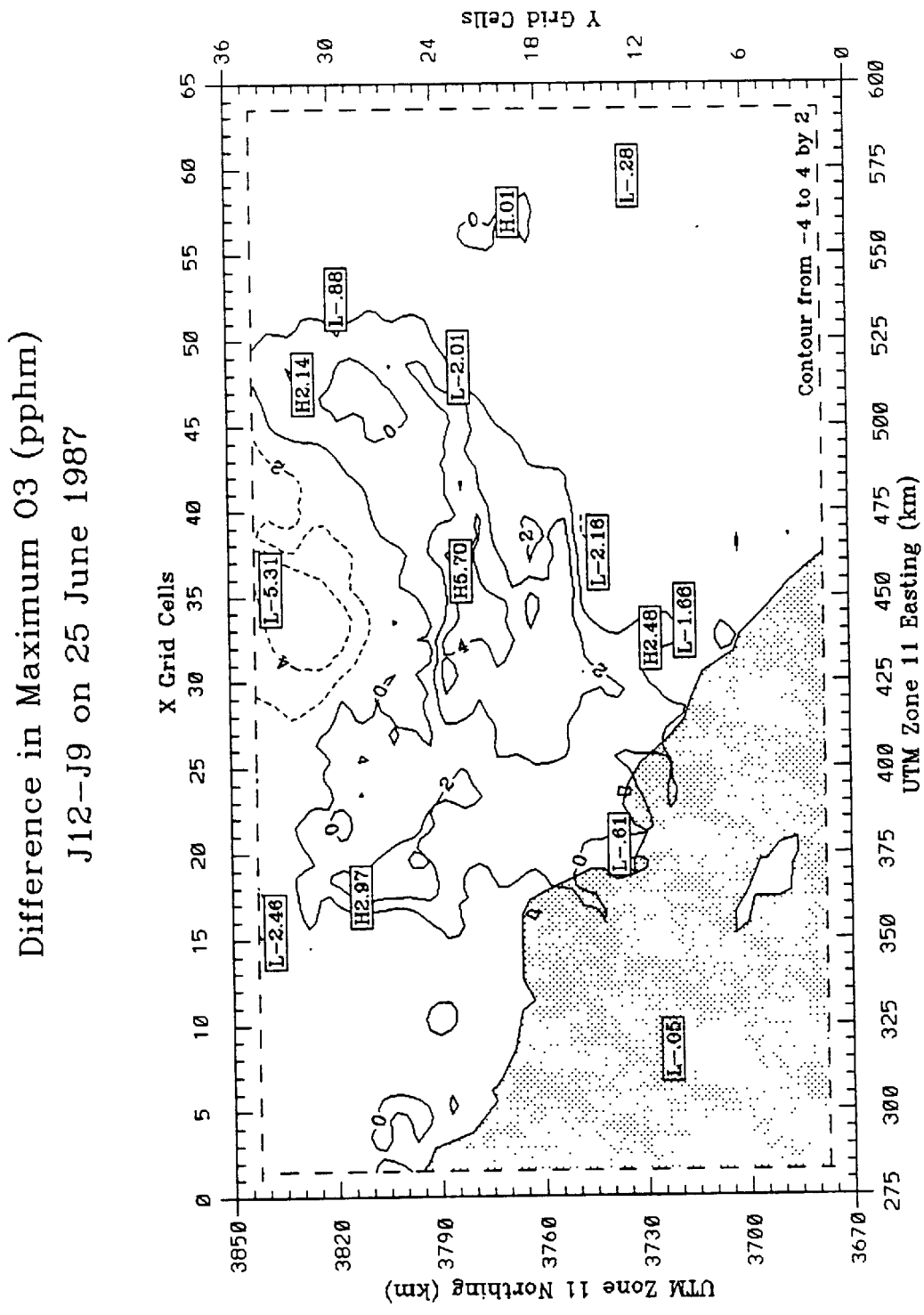


Figure 4-20. Difference in estimated maximum O_3 concentrations (pphm) [Run J12 - Run J9] on 25 June

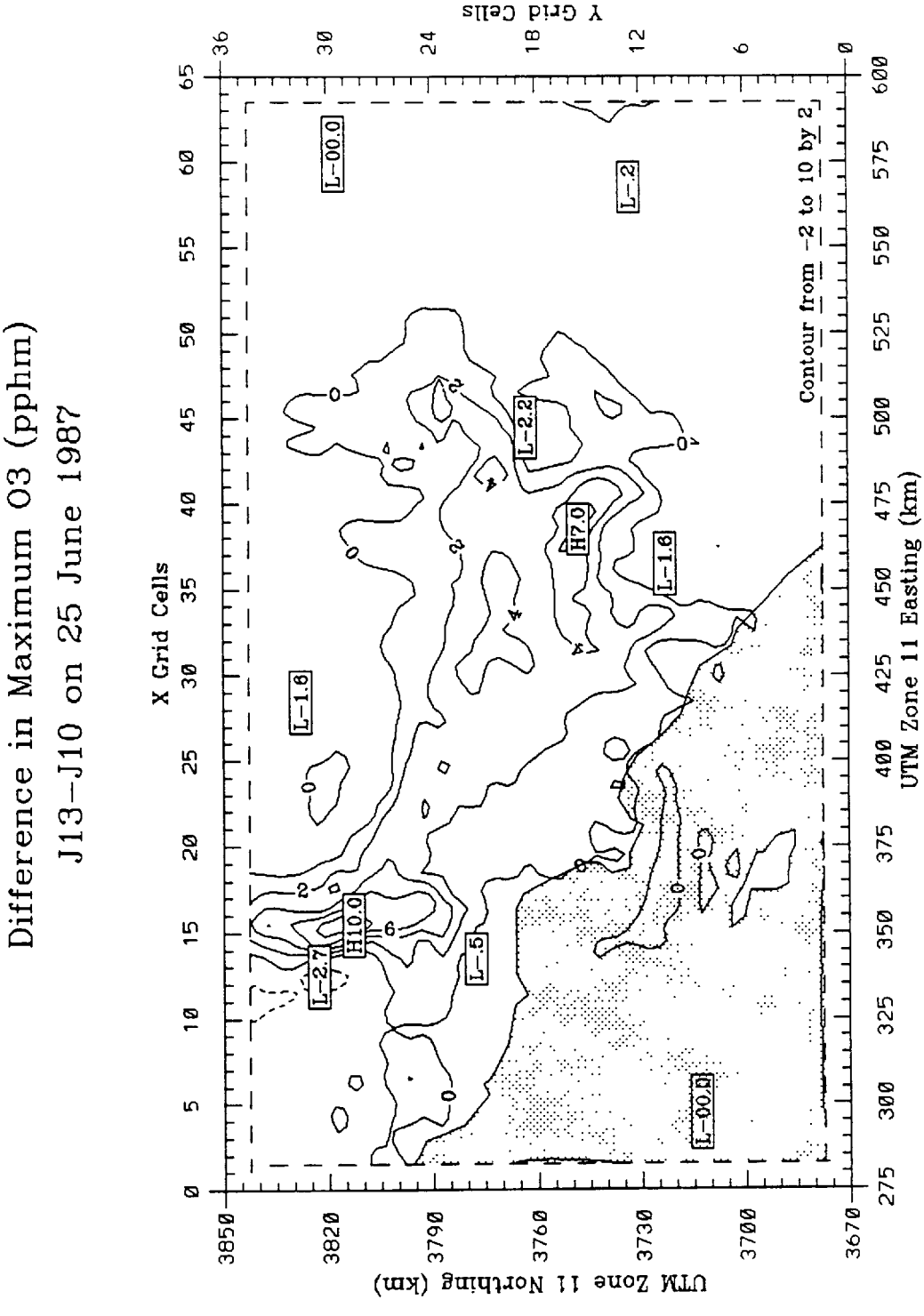
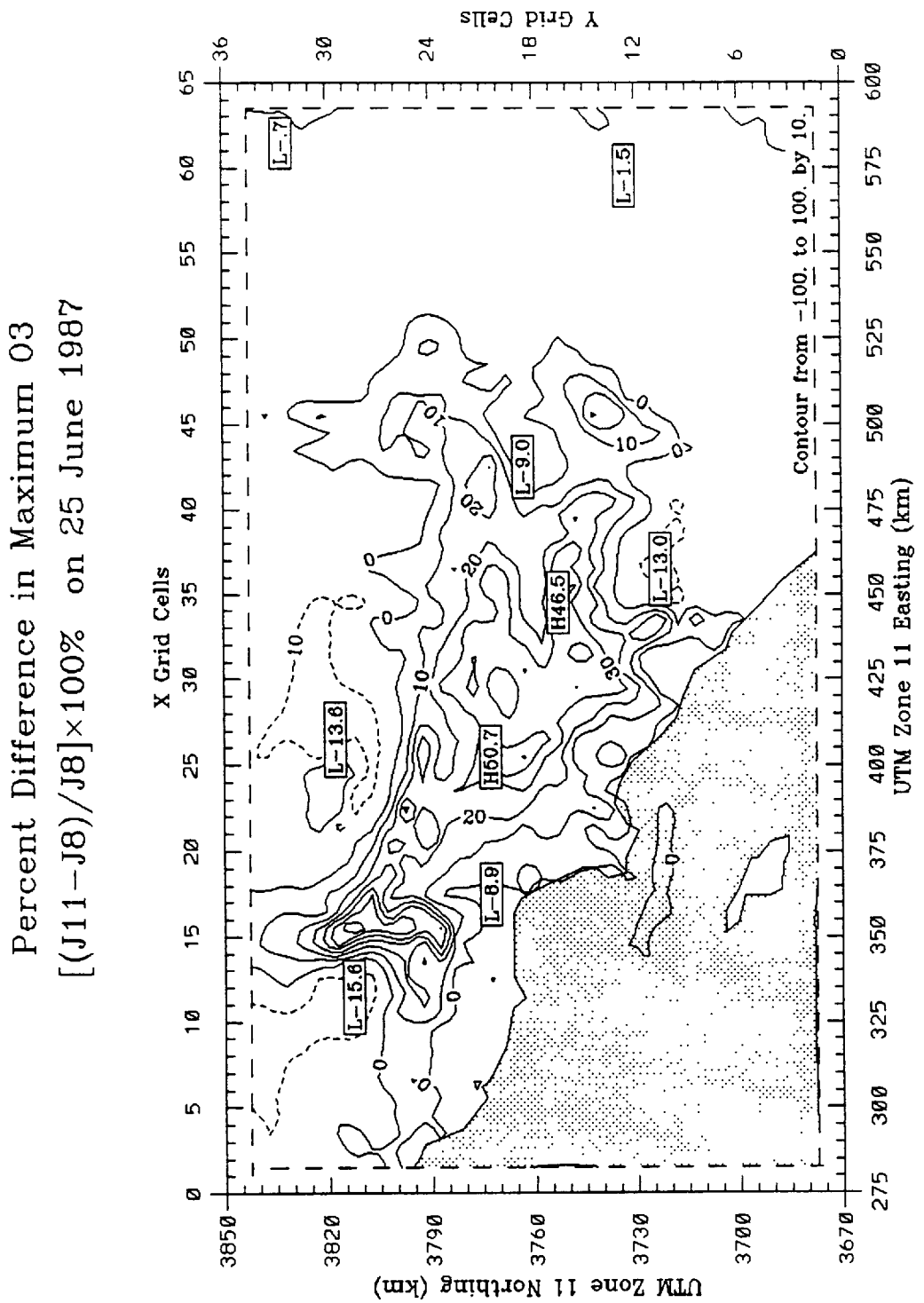


Figure 4-21. Difference in estimated maximum O_3 concentrations (pphm) [Run J13 - Run J10] on 25 June



Dashed contours indicate values less than zero

Figure 4-22. Percent difference in estimated maximum O_3 concentrations [(J11 - J8)/J8 x 100%] on 25 June

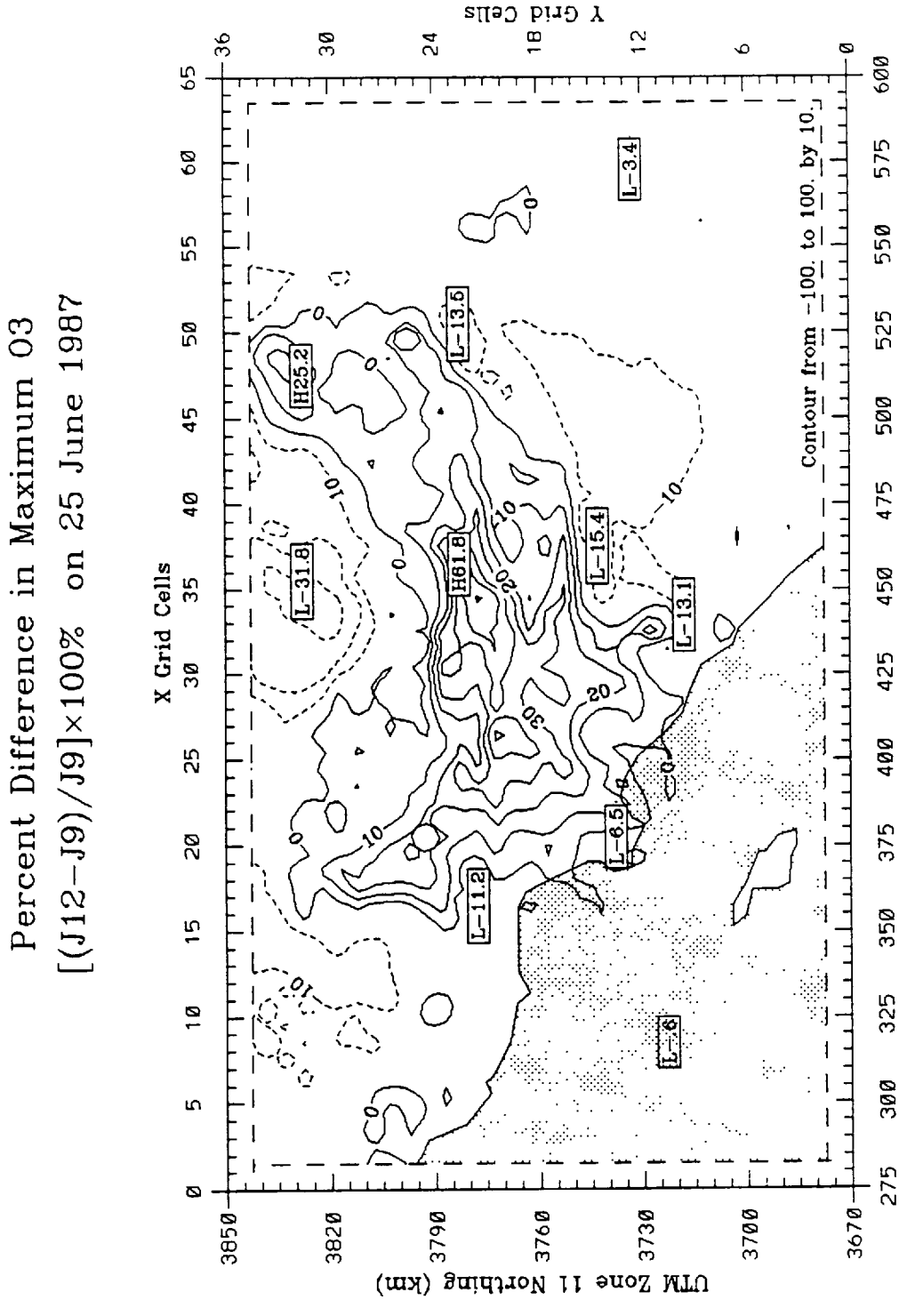


Figure 4-23. Percent difference in estimated maximum O_3 concentrations [(J12 - J9)/J9 x 100%] on 25 June

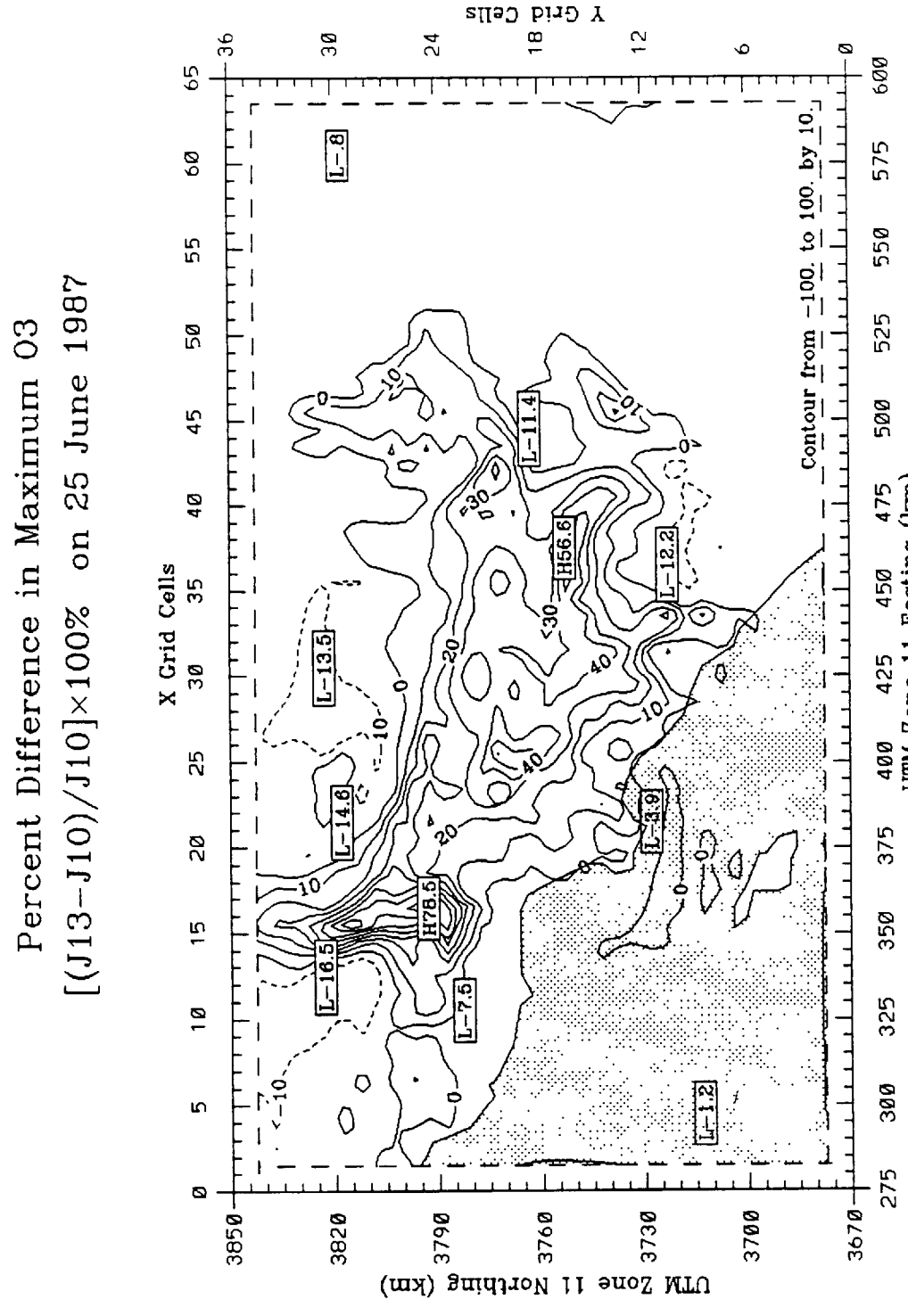


Figure 4-24. Percent difference in estimated maximum O_3 concentrations [(J13 - J10)/J10 x 100%] on 25 June

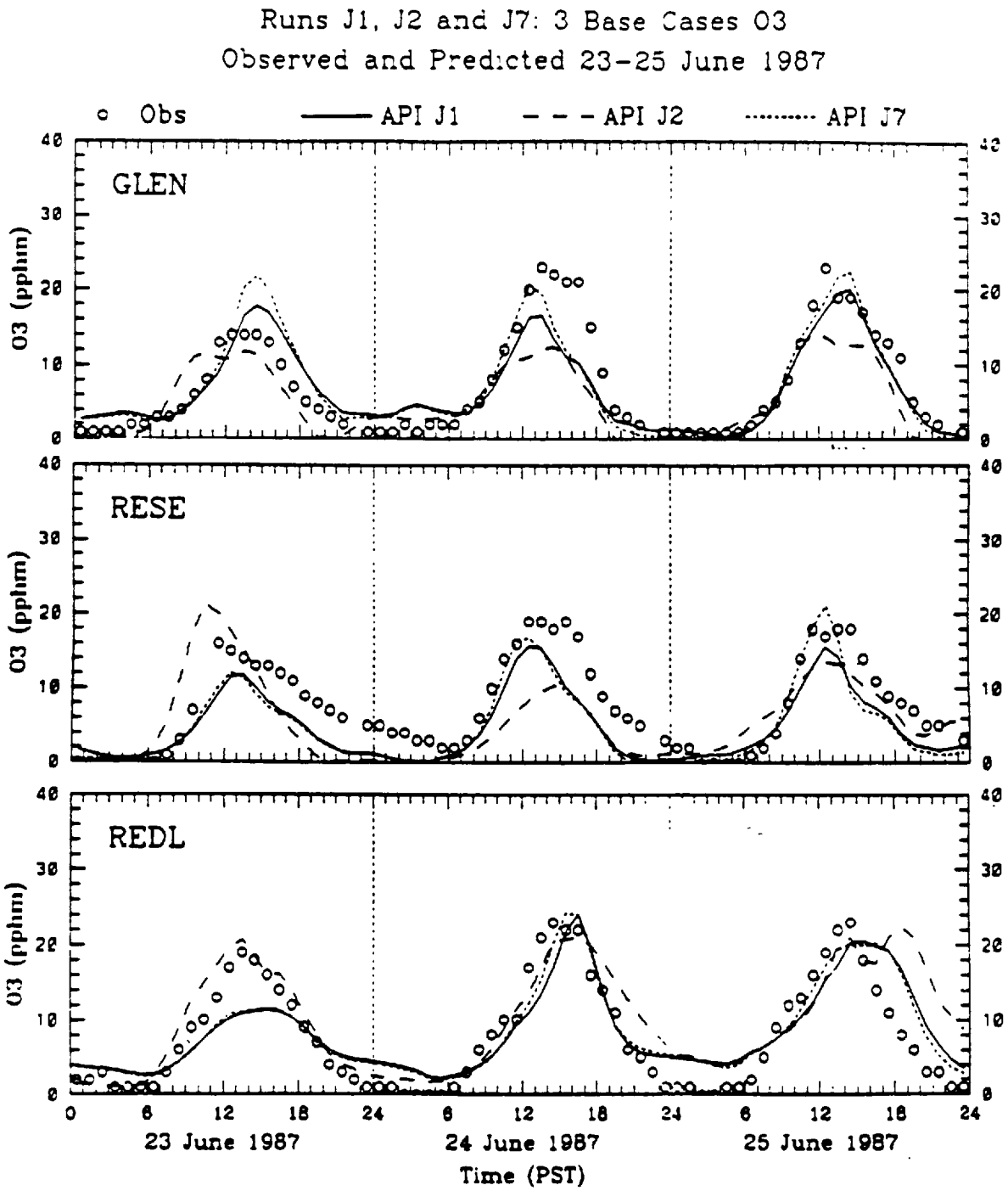
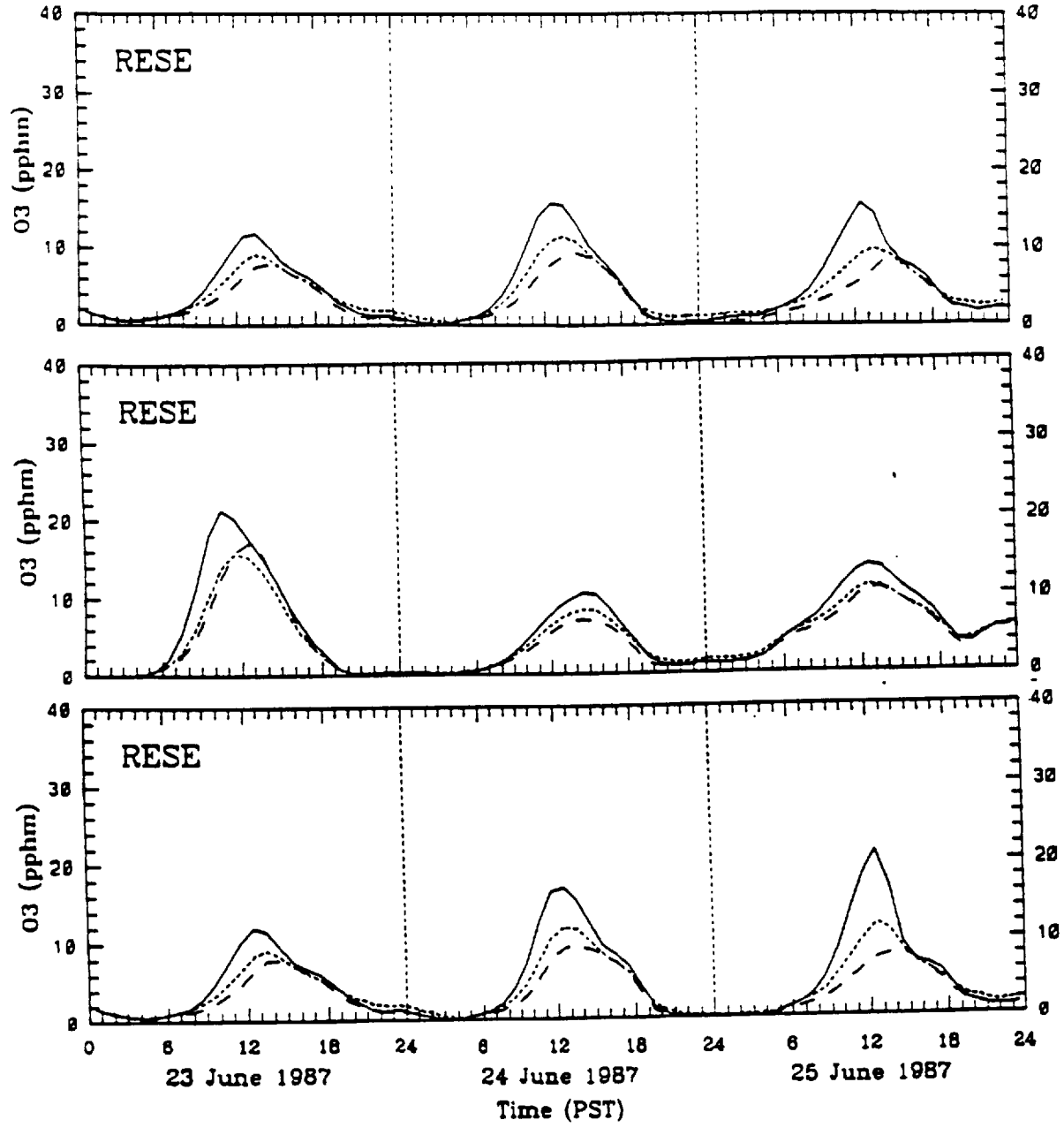
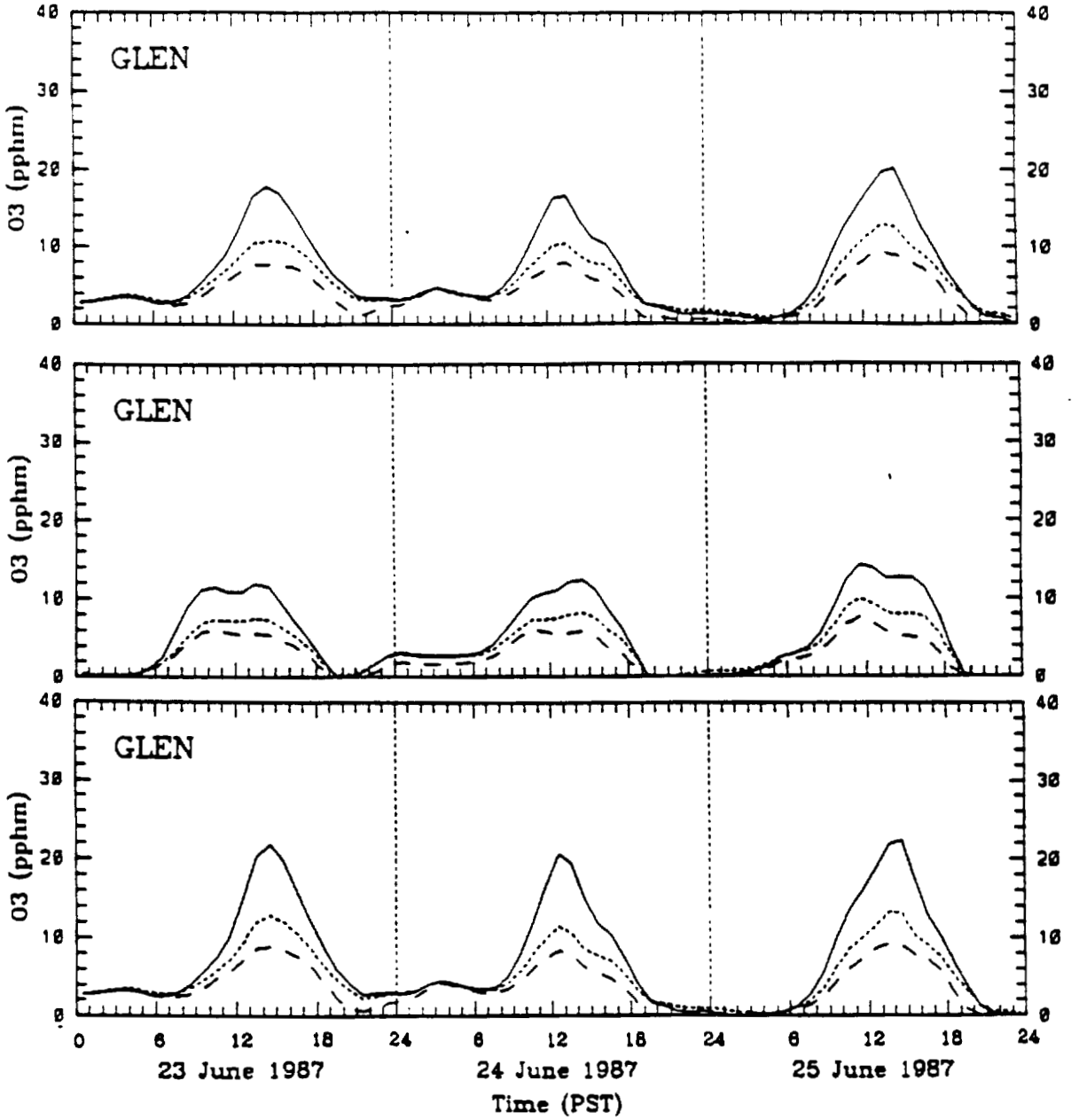


Figure 4-25. Estimated and observed O_3 concentrations (pphm) at Glendora, Reseda, and Redlands on 23-25 June 1987 for Runs J1, J2, and J7



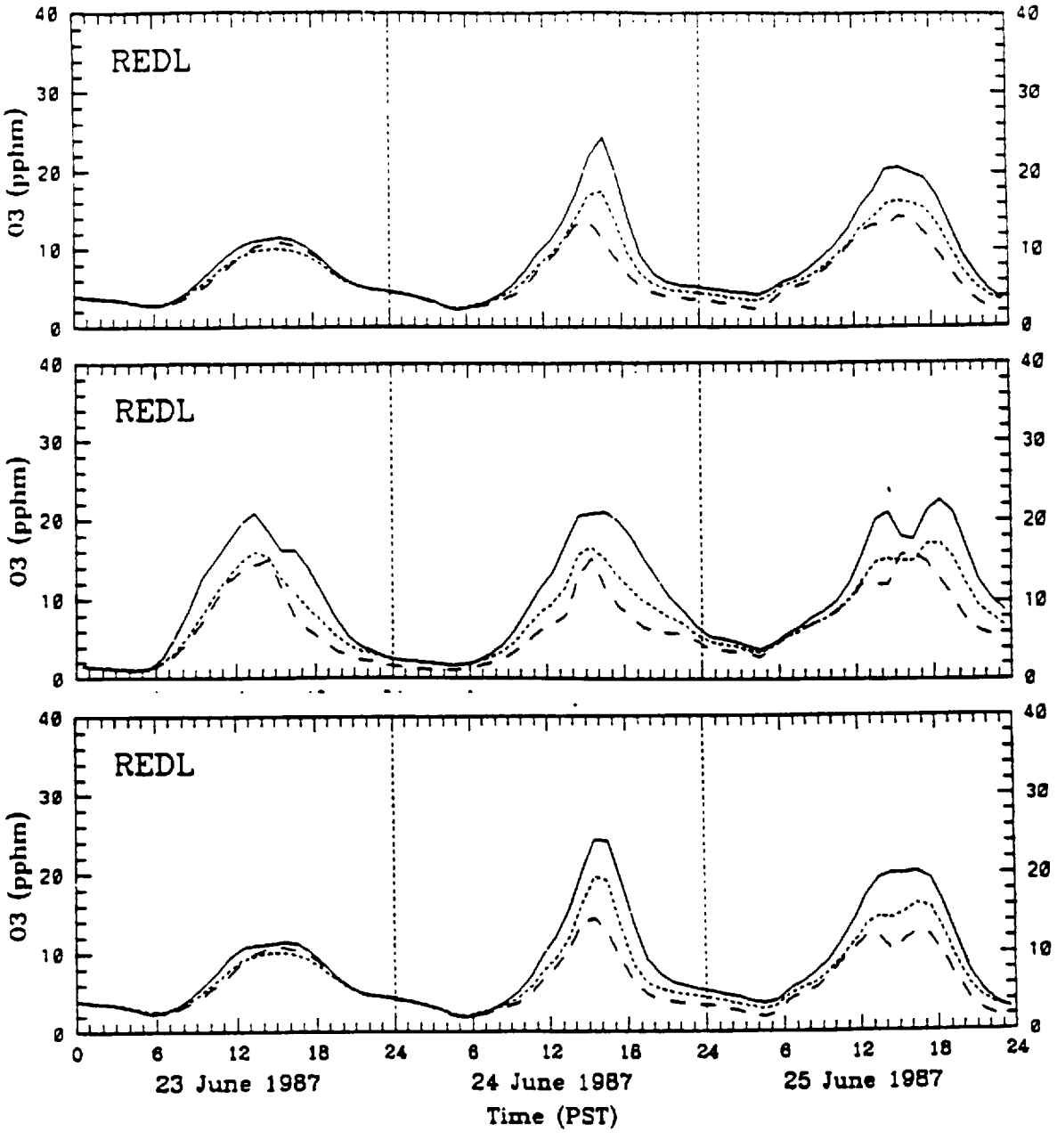
Lines: base case (solid), 50% VOC reduction (dashed), 50% VOC and 25% NO_x reductions (dotted)
Base Cases: top panel (J1), middle panel (J2), bottom panel (J7)

Figure 4-26. O_3 time series for Reseda



Lines: base case (solid), 50% VOC reduction (dashed), 50% VOC and 25% NO_x reductions (dotted)
Base Cases: top panel (J1), middle panel (J2), bottom panel (J7)

Figure 4-27. O_3 time series for Glendora



Lines: base case (solid), 50% VOC reduction (dashed), 50% VOC and 25% NO_x reductions (dotted)
Base Cases: top panel (J1), middle panel (J2), bottom panel (J7)

Figure 4-28. O_3 time series for Redlands

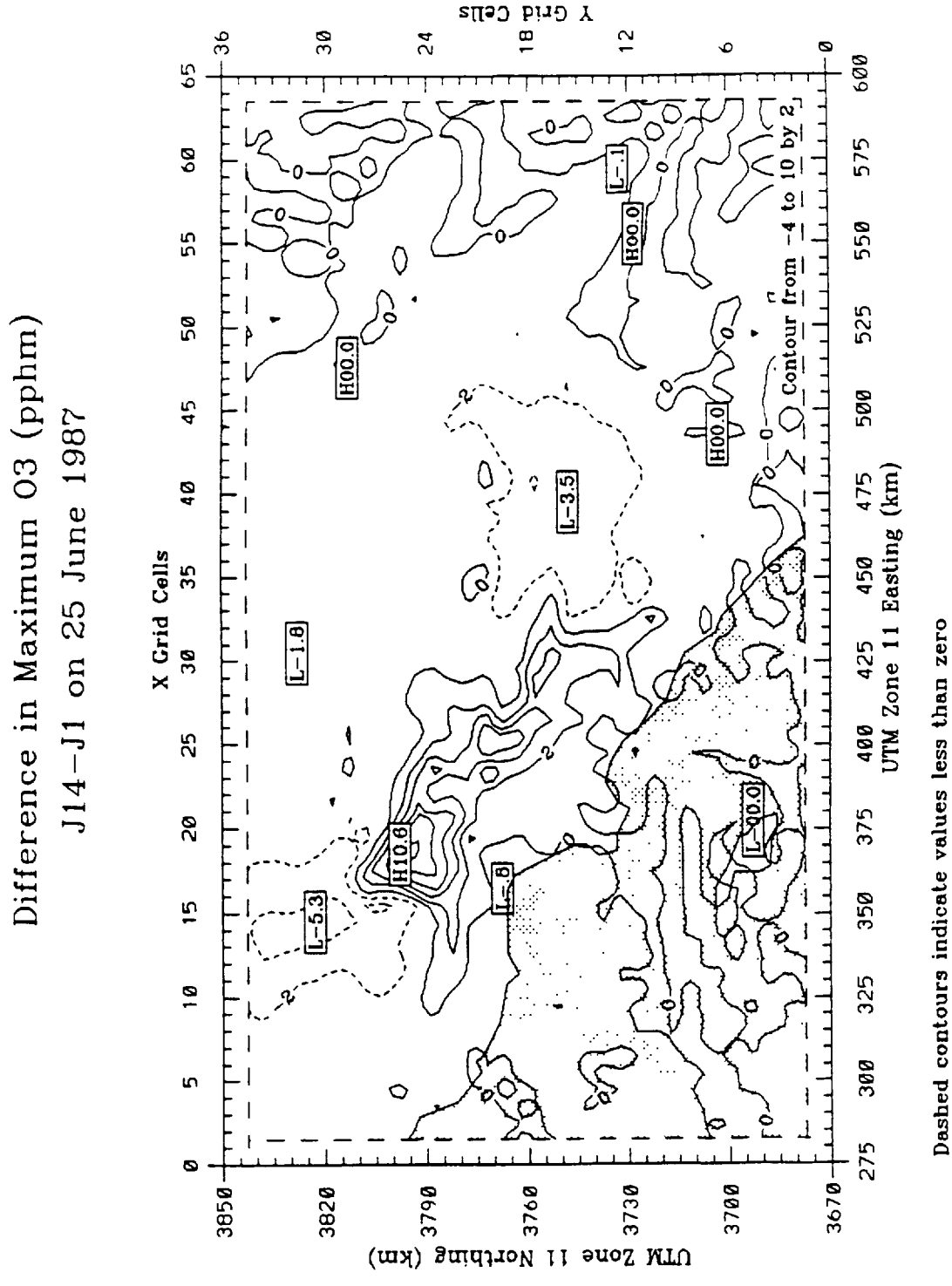


Figure 4-29. Difference in estimated maximum O_3 concentrations (pphm) [Run J14 - Run J1] on 25 June

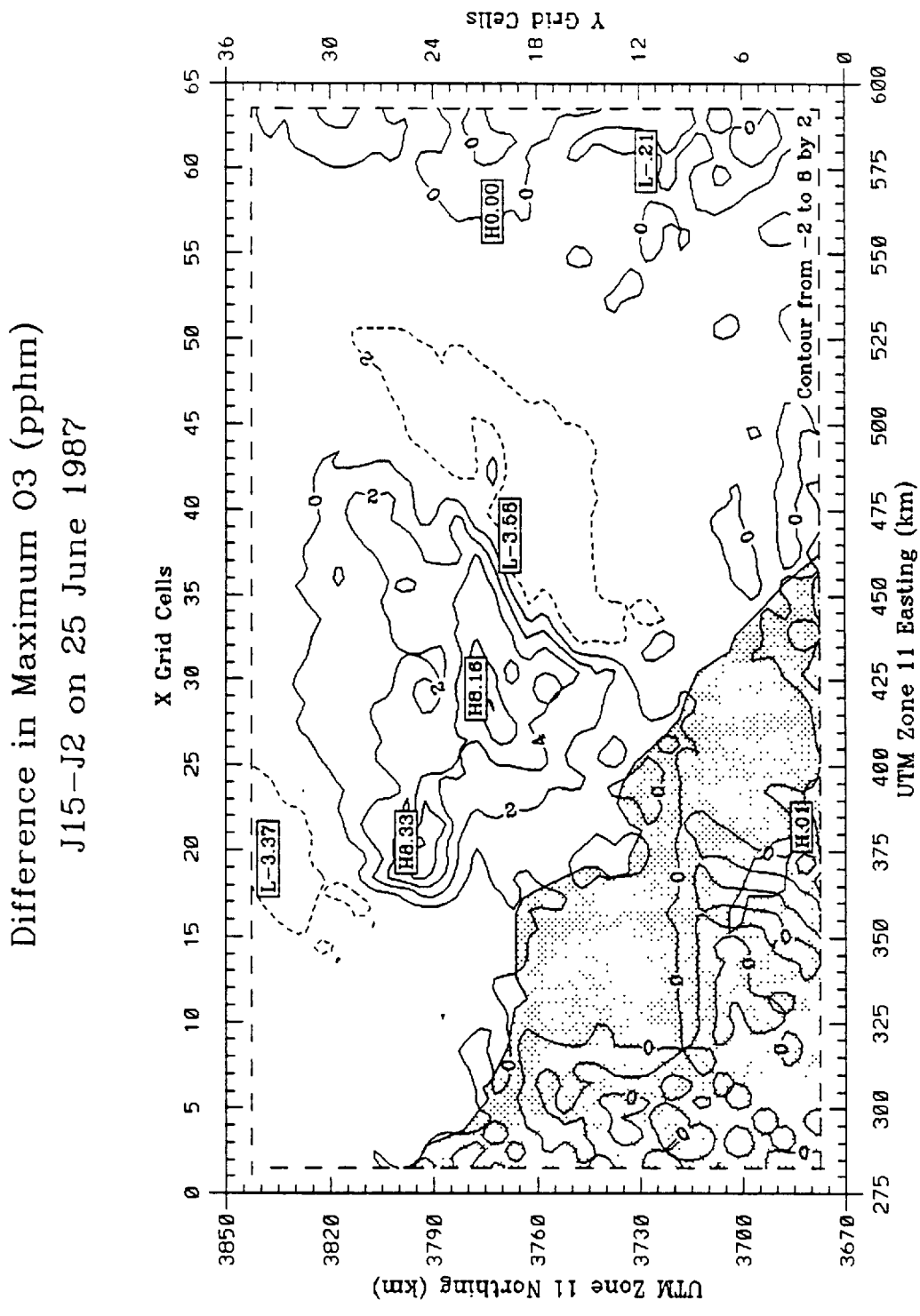


Figure 4-30. Difference in estimated maximum O_3 concentrations (pphm) [Run J15 - Run J2] on 25 June

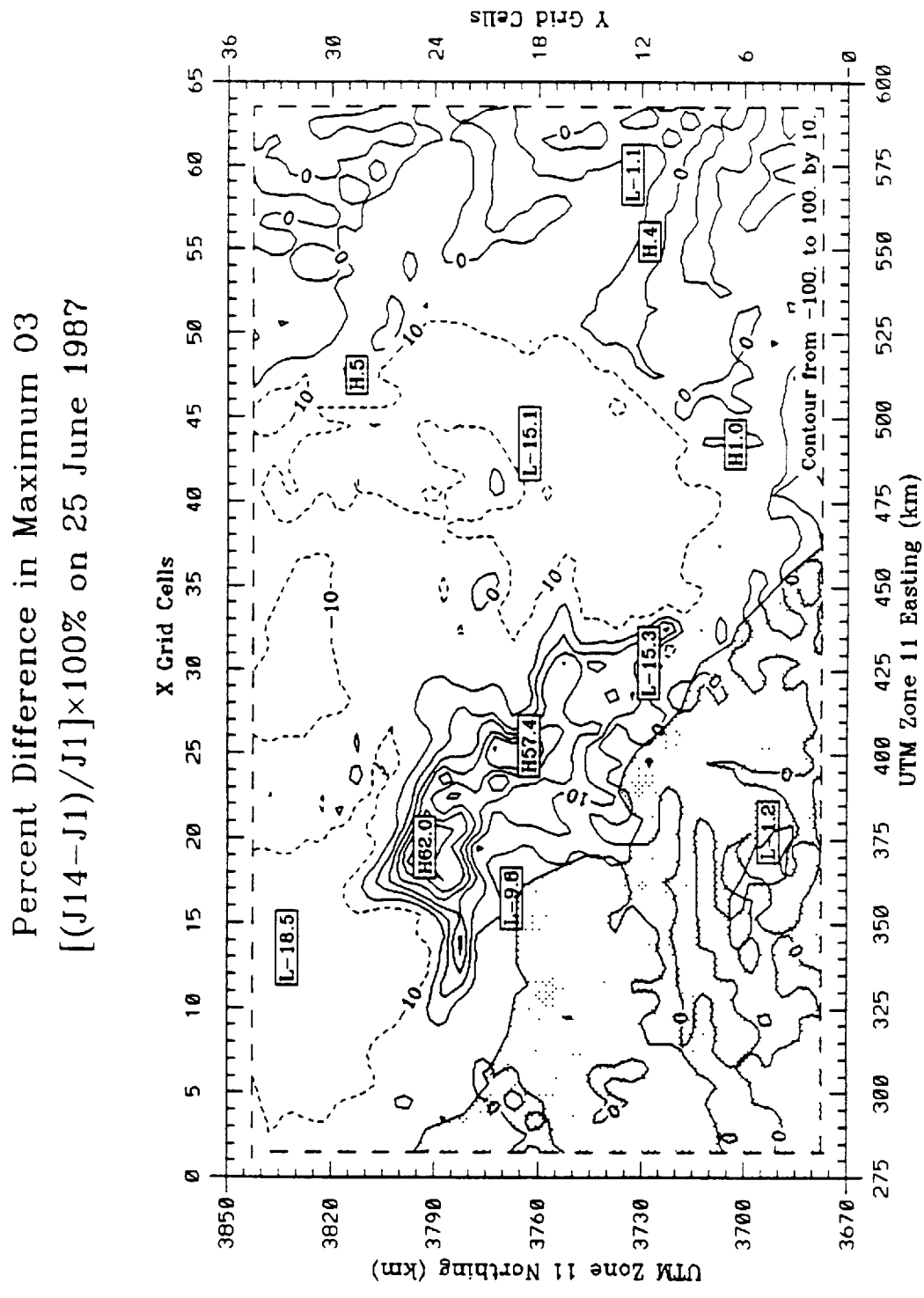


Figure 4-31. Percent difference in estimated maximum O_3 concentrations [(J14 - J1)/J1 x 100%] on 25 June

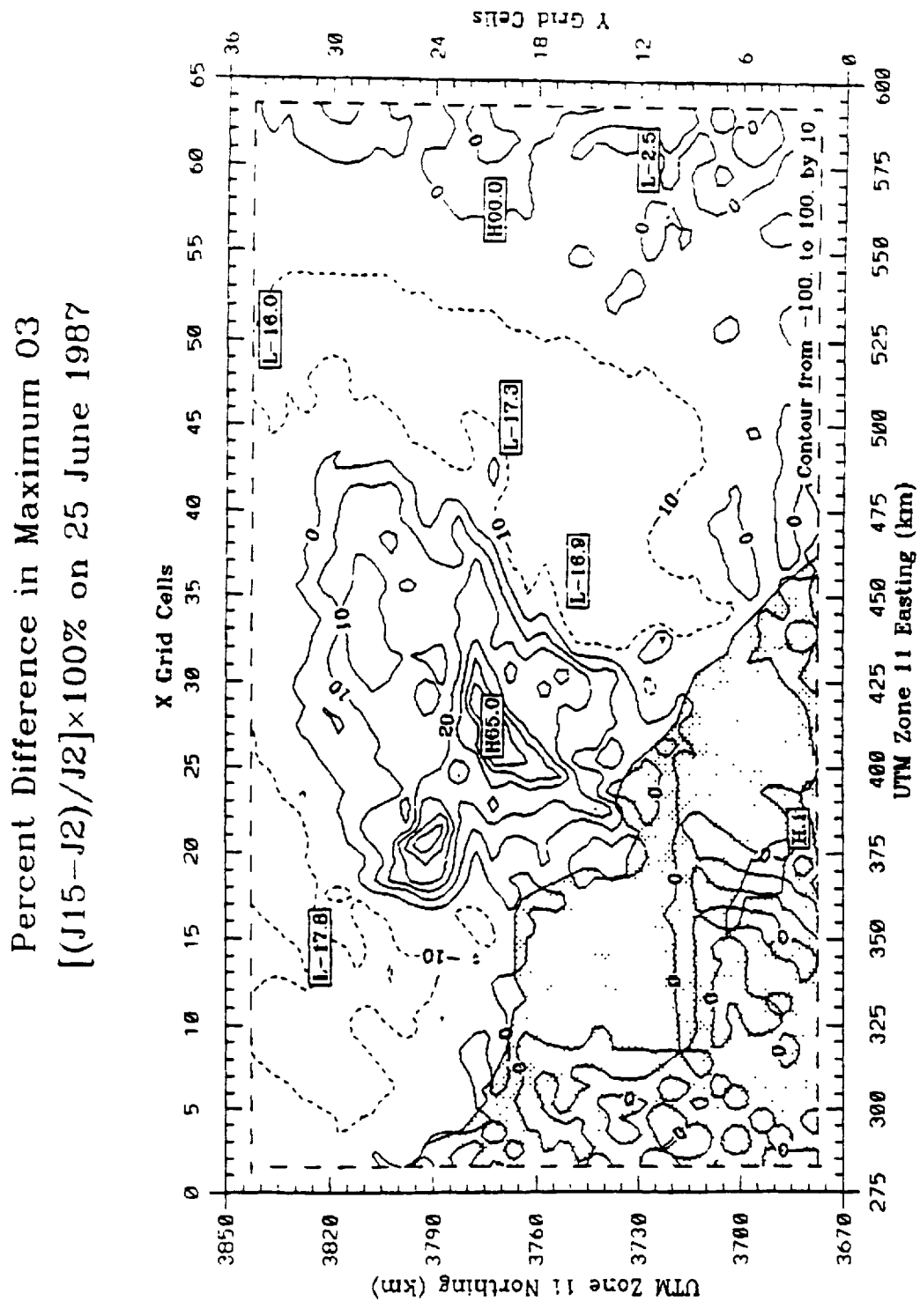


Figure 4-32. Percent difference in estimated maximum O_3 concentrations [(J15 - J2)/J2 x 100%] on 25 June

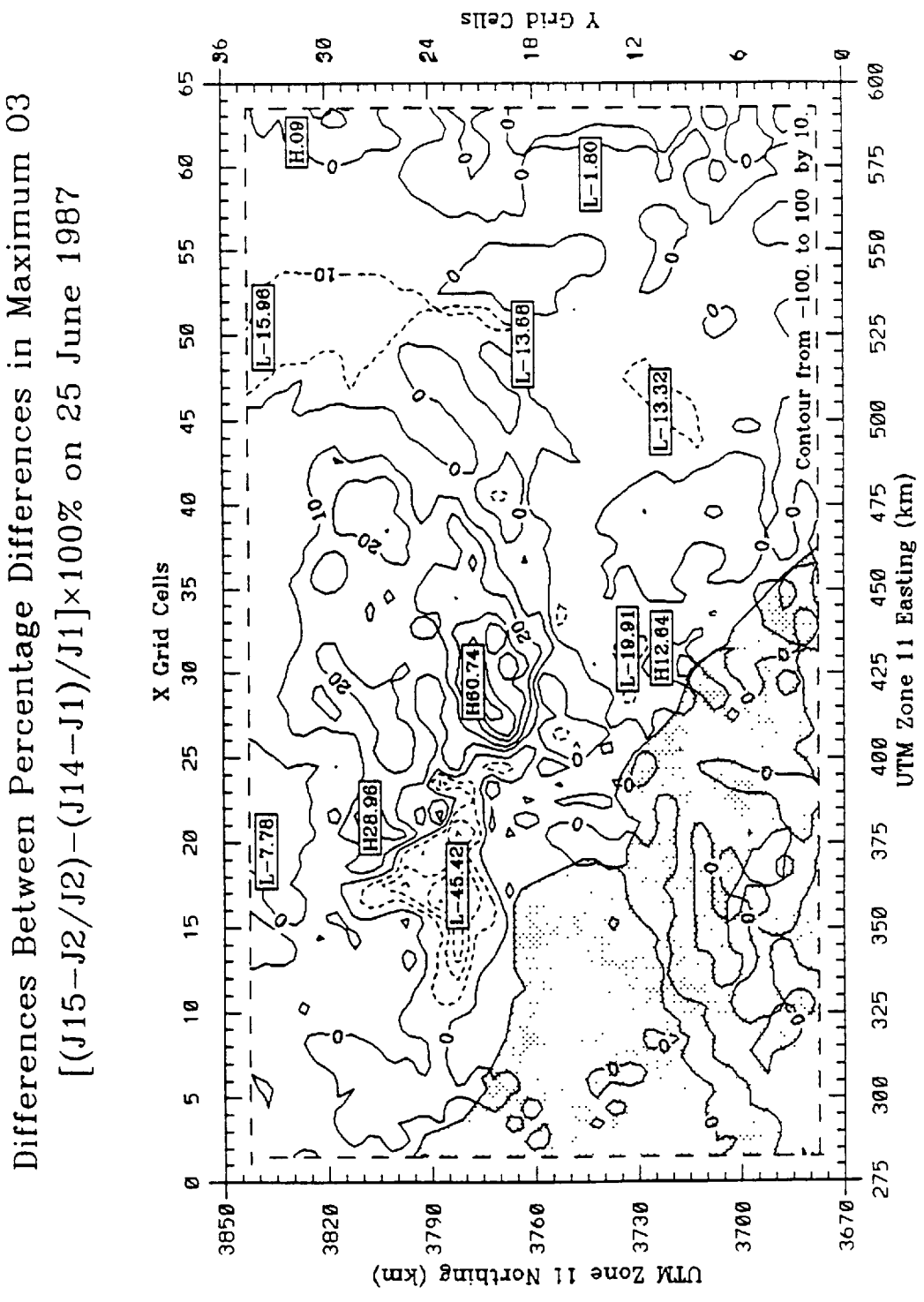


Figure 4-33. Differences in percentage changes in estimated maximum O_3 concentrations [{(J15 - J2)/J2 - (J14 - J1)/J1} x 100%] on 25 June

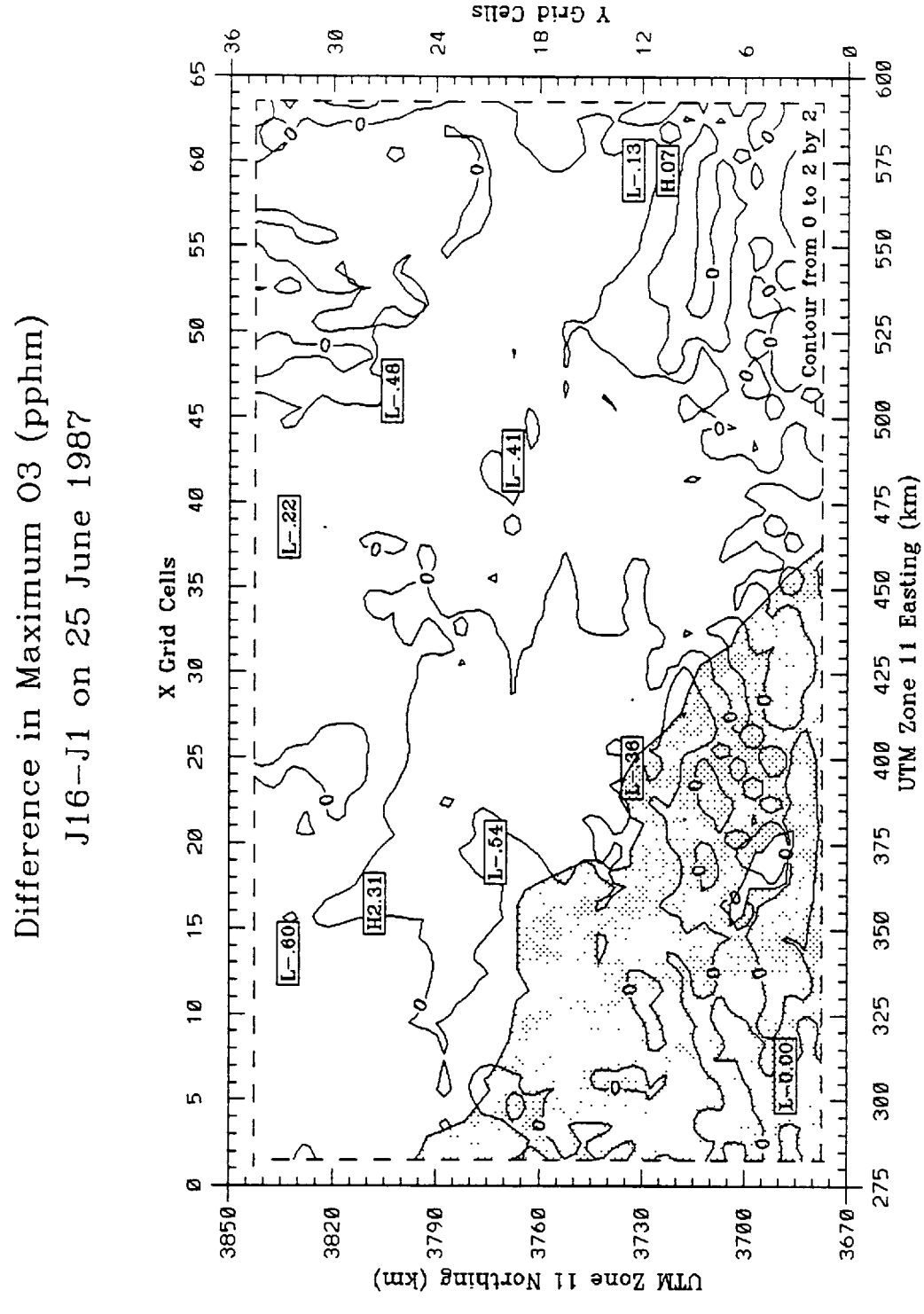


Figure 4-34. Difference in estimated maximum O_3 concentrations (pphm) [Run J16 - Run J1] on 25 June

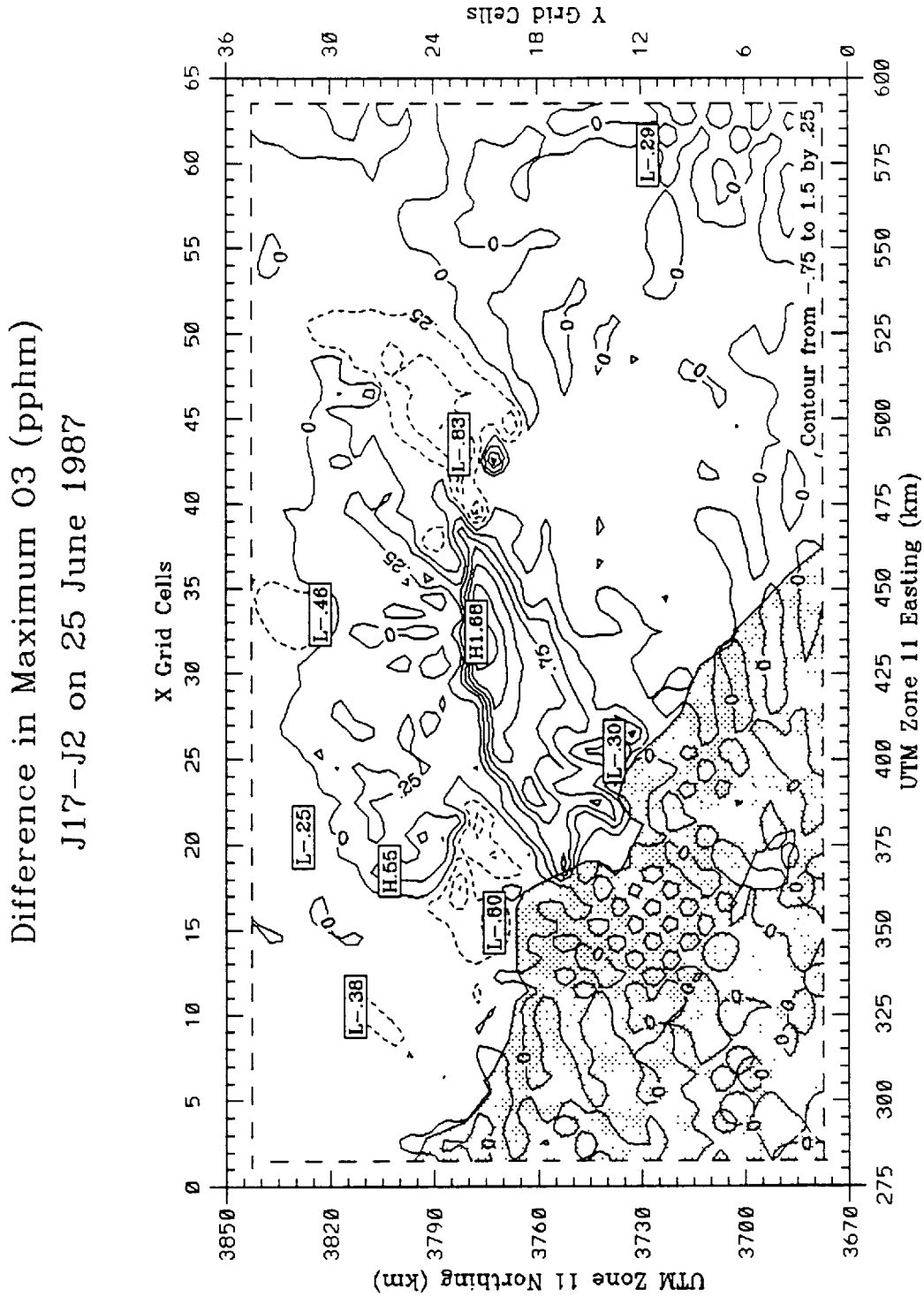


Figure 4-35. Difference in estimated maximum O_3 concentrations (pphm) [Run J17 - Run J2] on 25 June

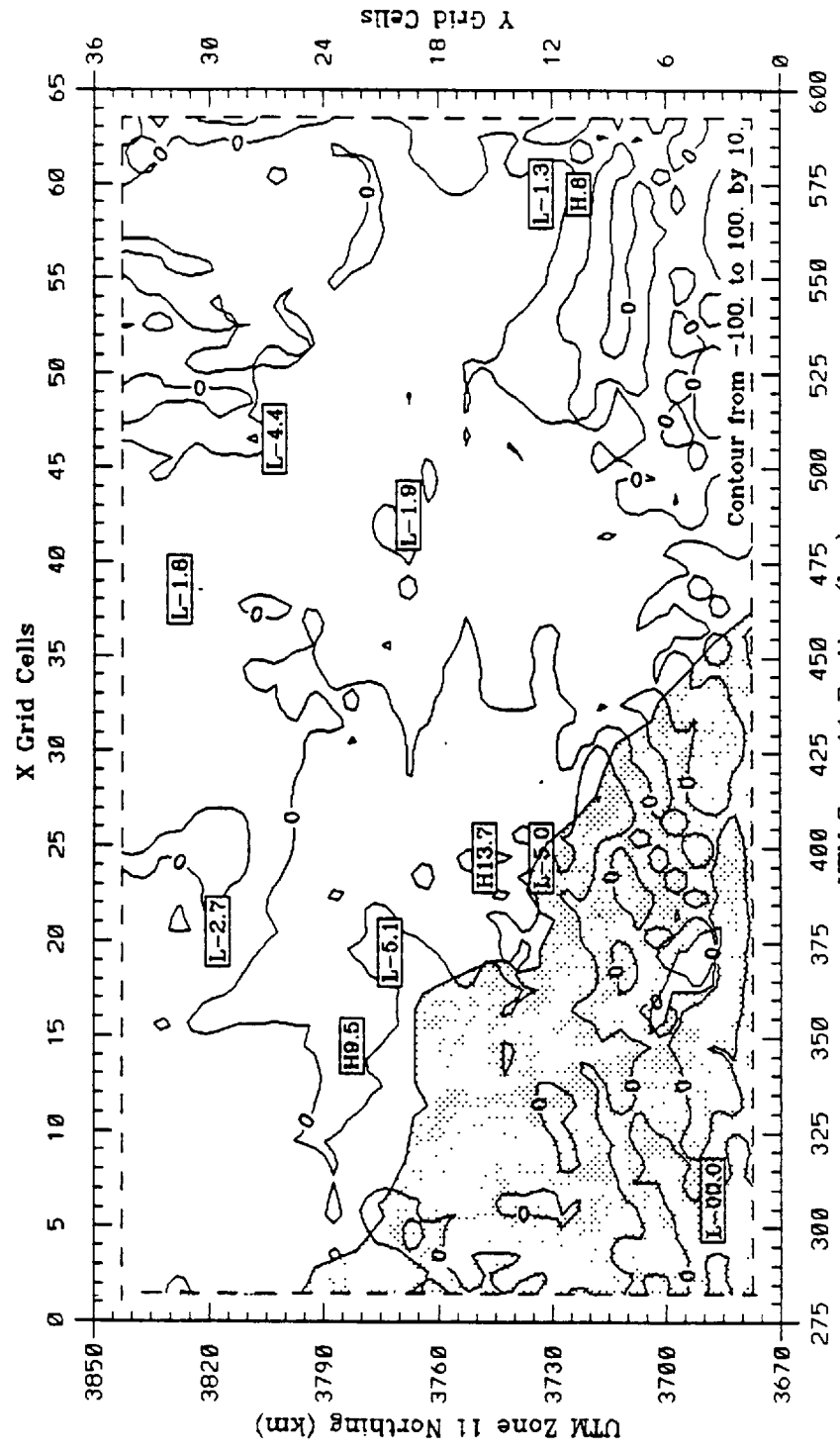


Figure 4-36. Percent difference in estimated maximum O_3 concentrations [(J16 - J1)/J1 x 100%] on 25 June

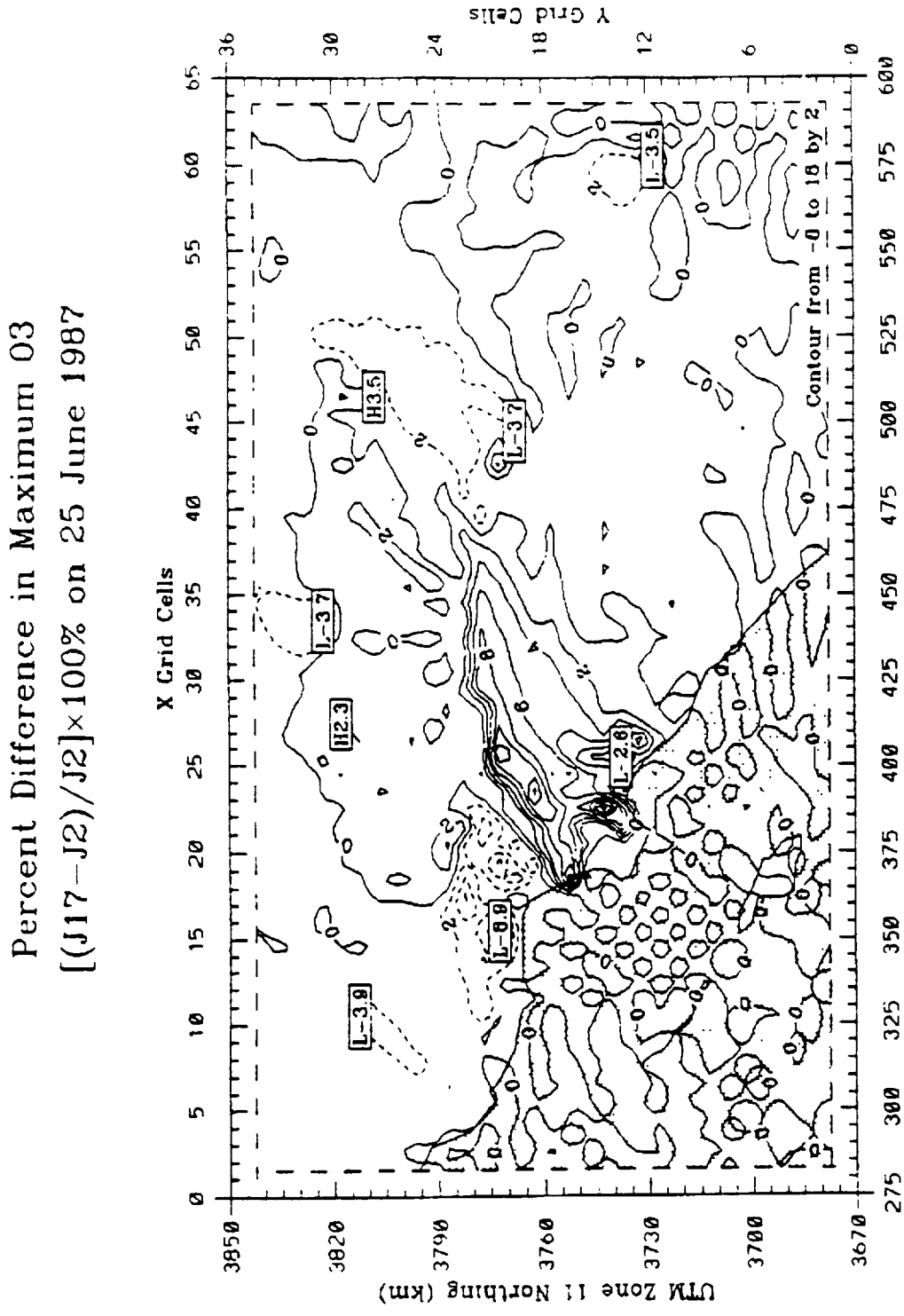


Figure 4-37. Percent difference in estimated maximum O_3 concentrations [(J17 - J2)/J2 x 100%] on 25 June

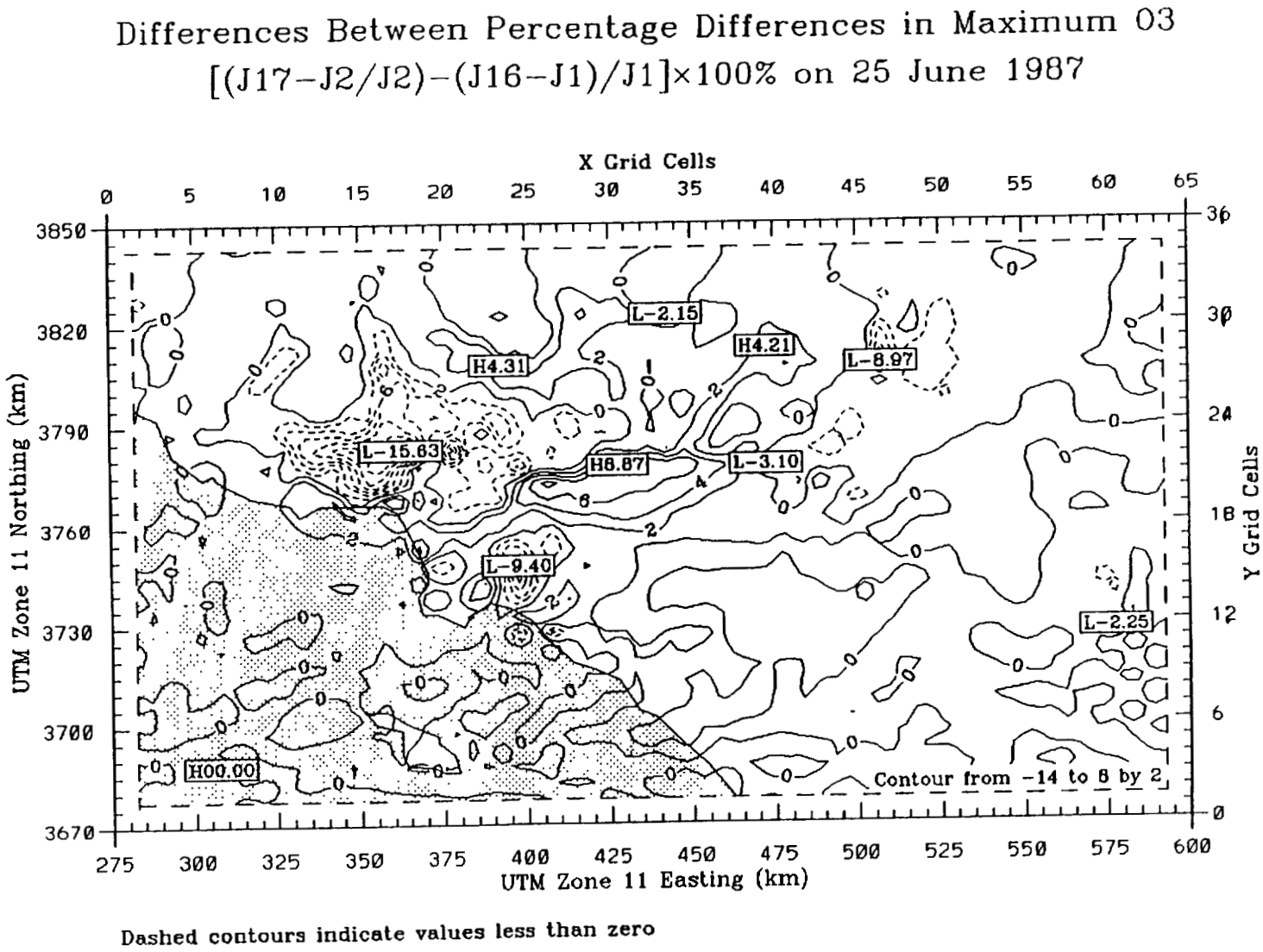


Figure 4-38. Differences in percentage changes in estimated maximum O_3 concentrations [{(J17 - J2)/J2 - (J16 - J1)/J1} x 100%] on 25 June

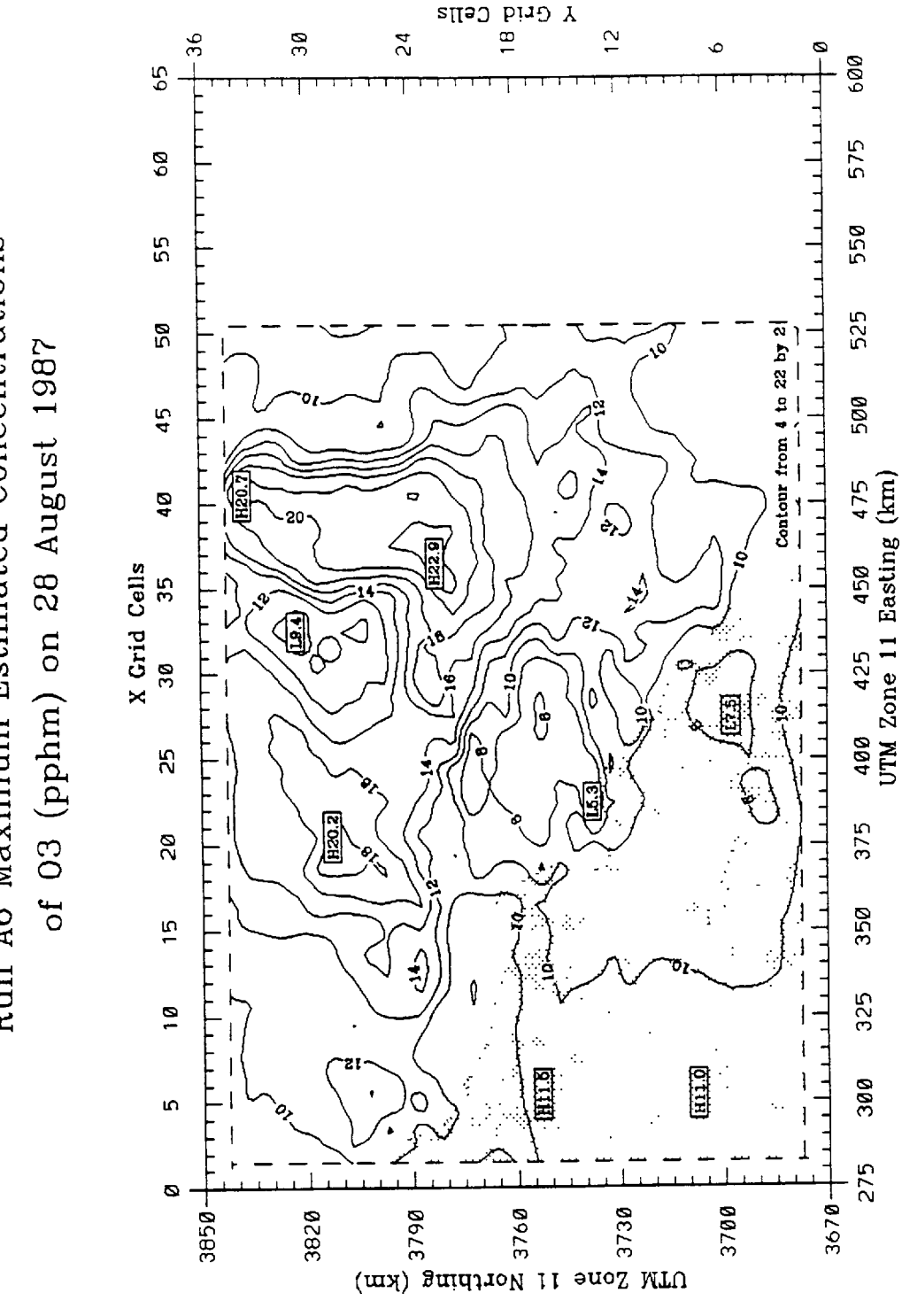


Figure 4-39. Maximum estimated and observed O_3 concentrations (pphm) on 28 August 1987 for Run A6

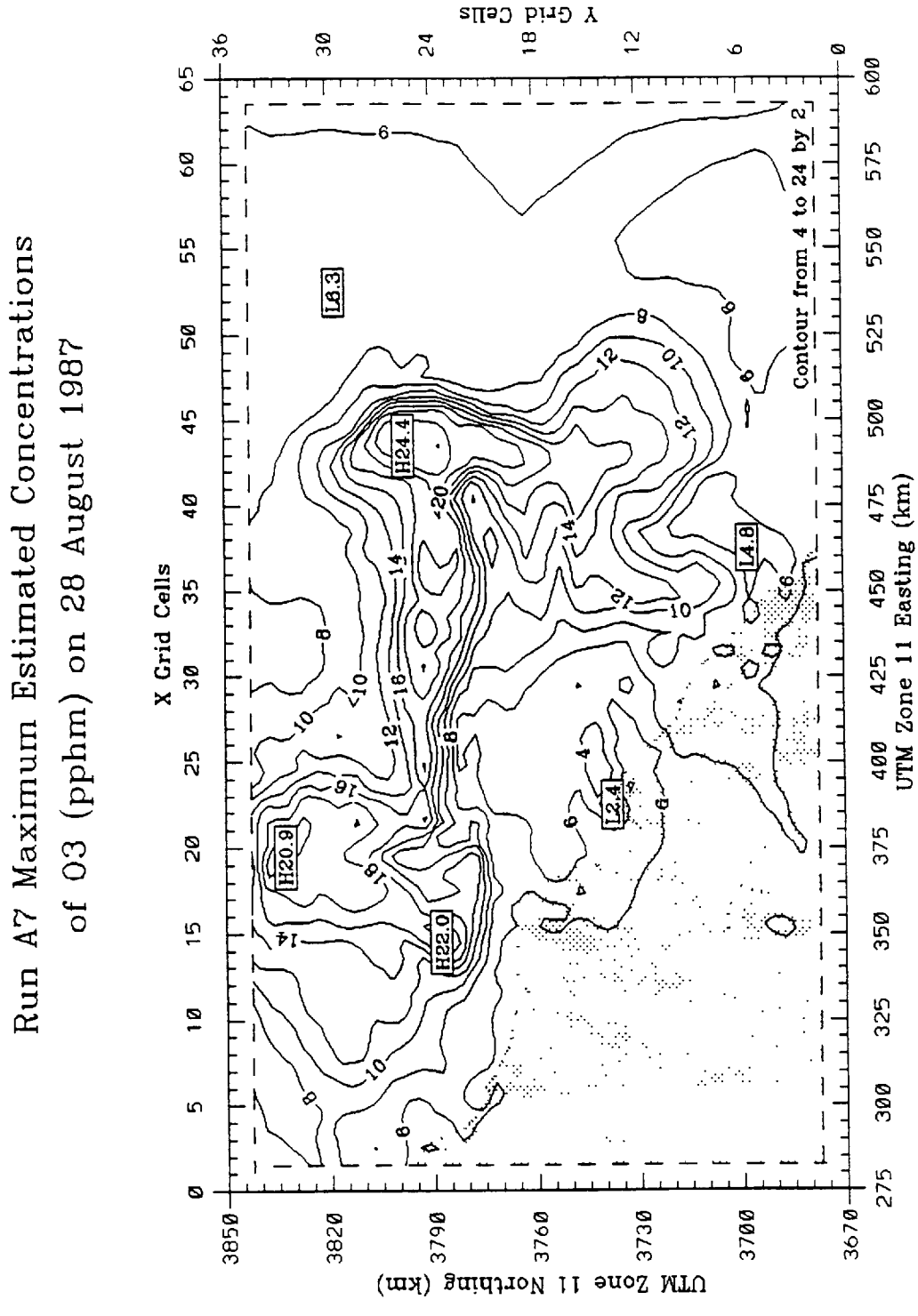


Figure 4-40. Maximum estimated and observed O_3 concentrations (pphm) on 28 August 1987 for Run A7

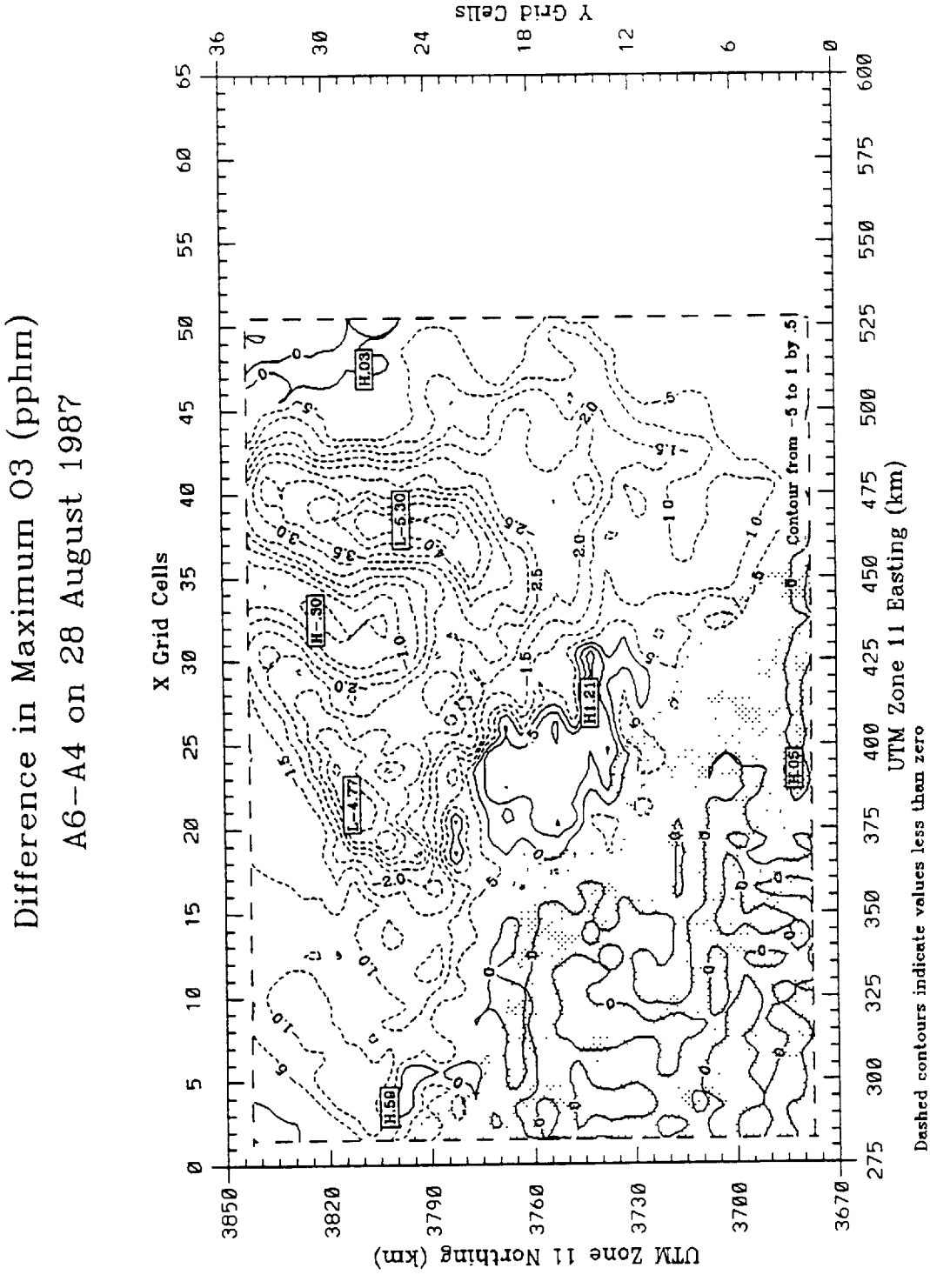


Figure 4-41. Difference in estimated maximum O_3 concentrations (pphm) [Run A6 - Run A4] on 28 August

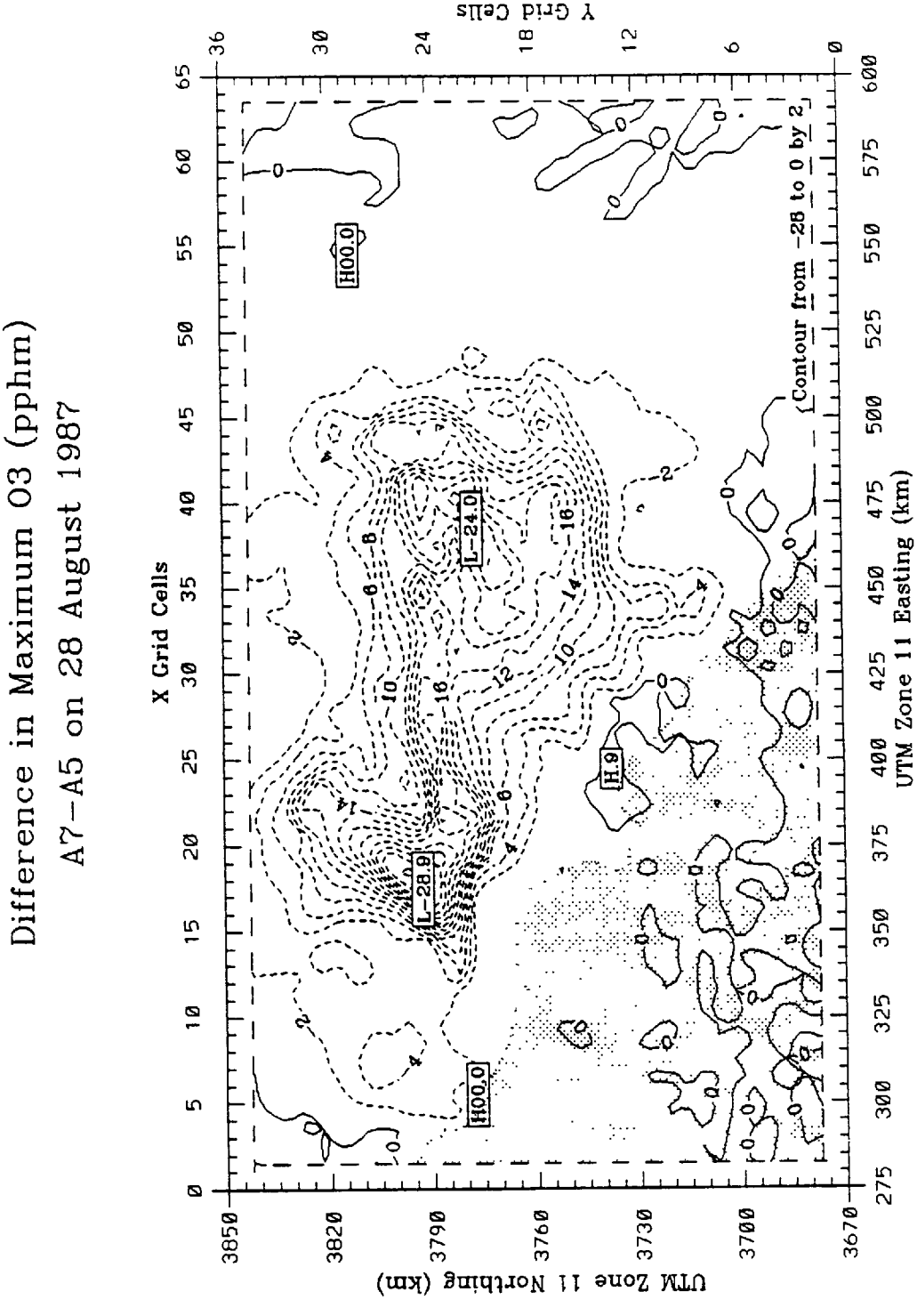


Figure 4-42. Difference in estimated maximum O_3 concentrations (pphm) [Run A7 - Run A5] on 28 August

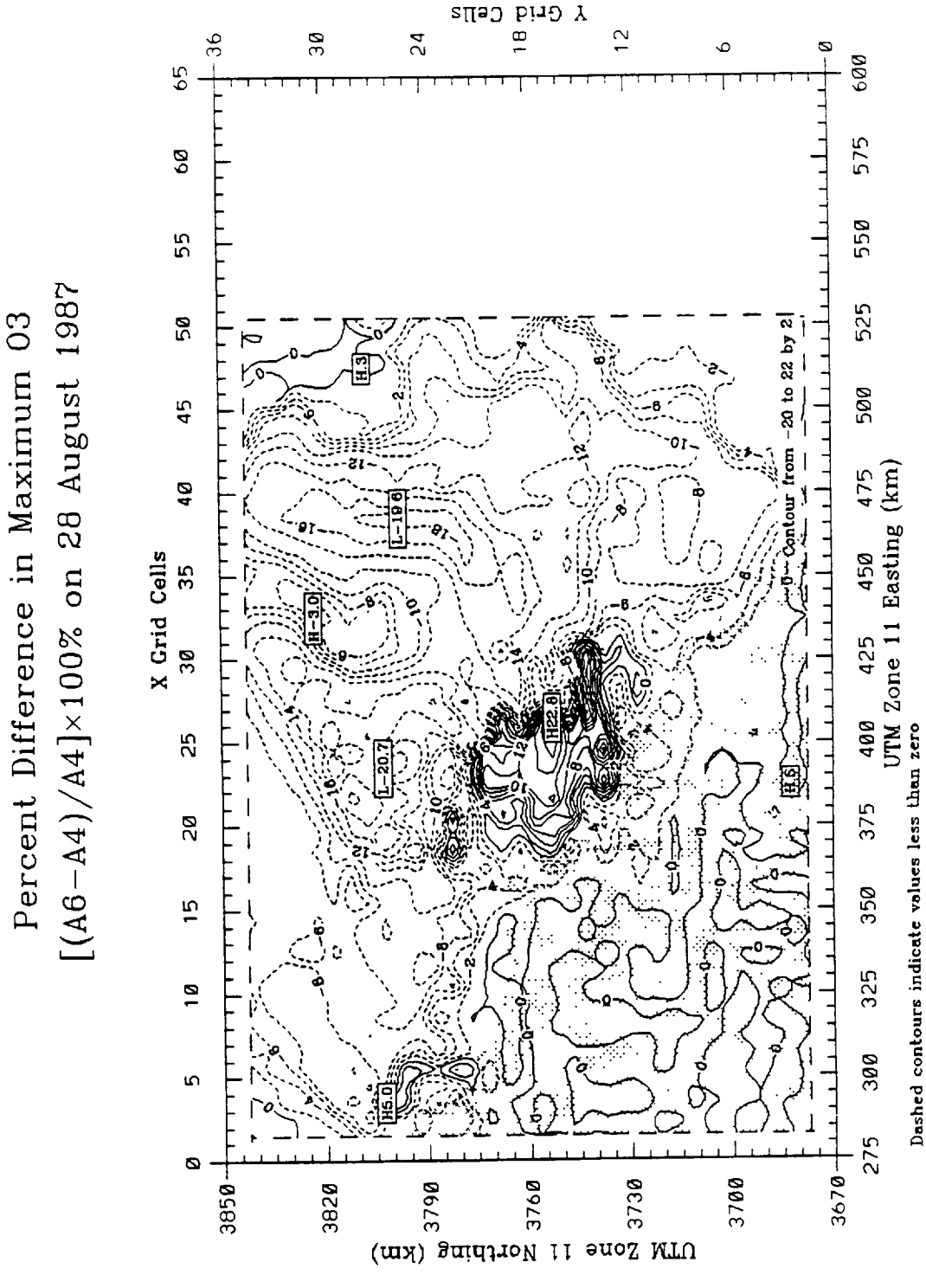


Figure 4-43. Percent difference in estimated maximum O_3 concentrations [(A6 - A4)/A4 x 100%] on 28 August

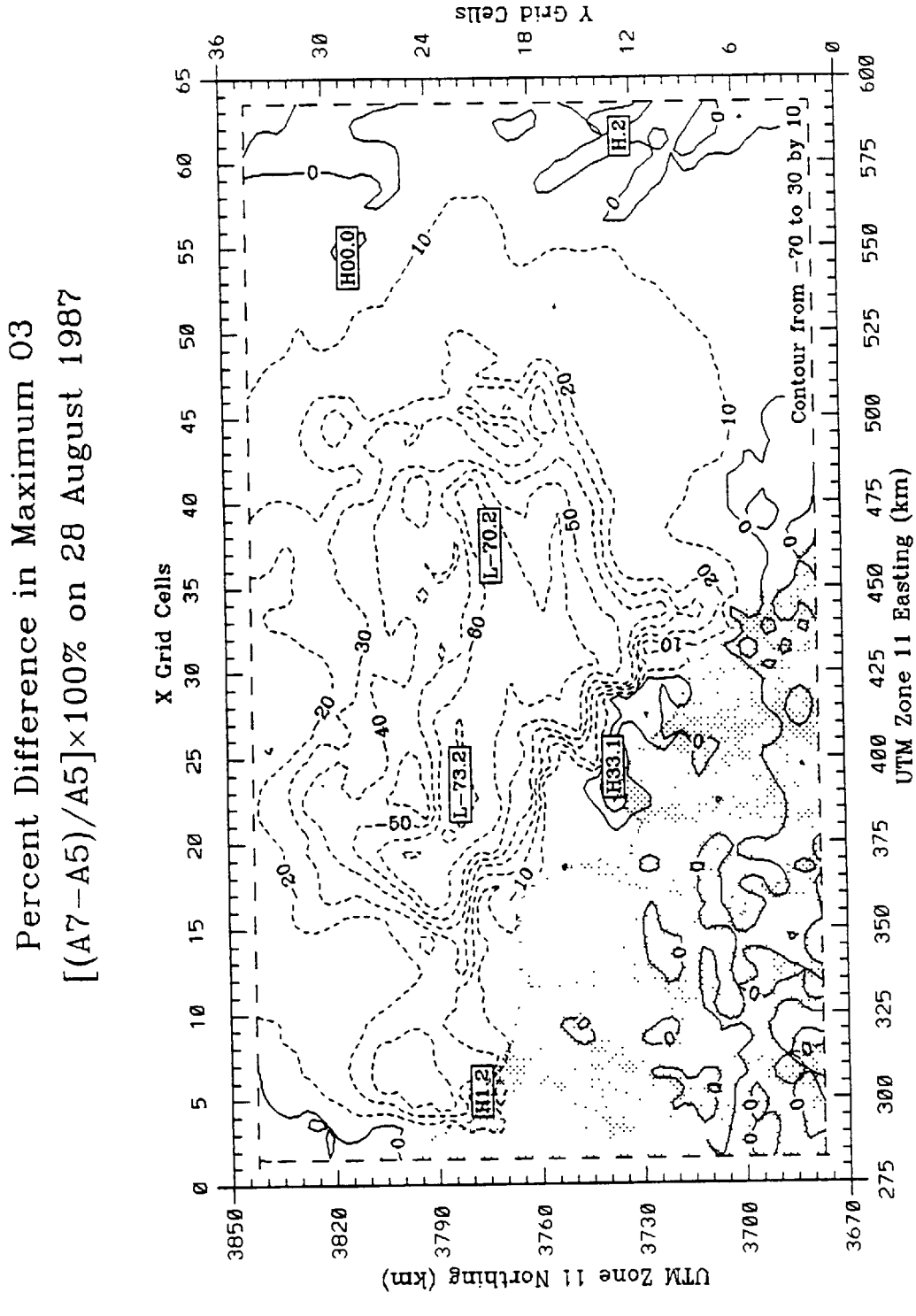


Figure 4-44. Percent difference in estimated maximum O_3 concentrations [(A7 - A5)/A5 x 100%] on 28 August

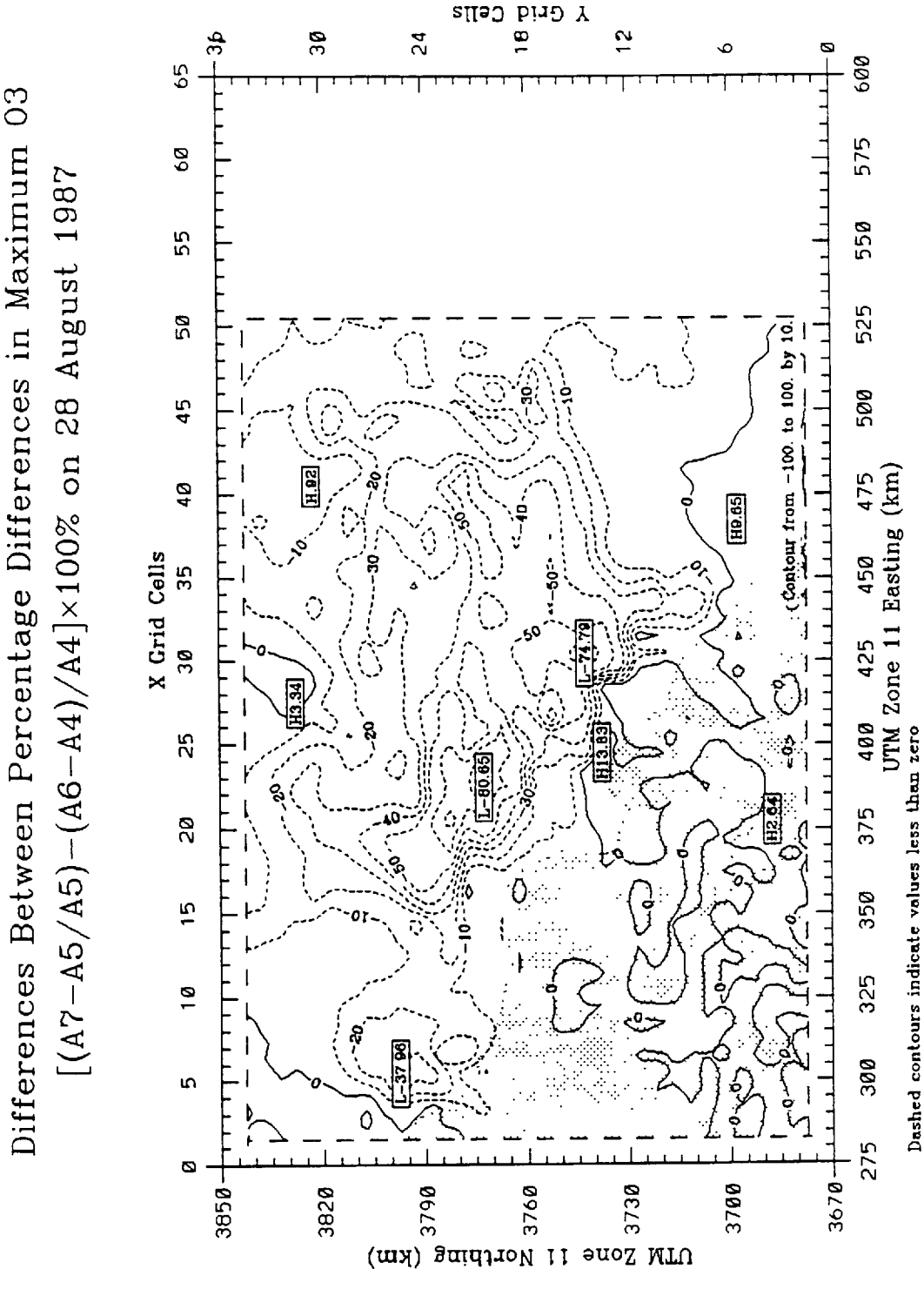


Figure 4-45. Differences in percentage changes in estimated maximum O_3 concentrations [{(A7 - A5)/A5 - (A6 - A4)/A4} x 100%] on 28 August

Section 5
IMPLICATIONS FOR REGULATORY MODELING

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

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 O_3 and NO_2. 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 O_3 fields, i.e., the decreases in estimated O_3 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 O_3 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 O_3 concentrations. For 24 June, the estimated reductions in peak O_3 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 O_3 concentration than was estimated for the case where VOC emissions alone were reduced). The third June base case yielded peak O_3 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 O_3 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 O_3 (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 O_3 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 O_3 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 O_3 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 O_3 episodes occurring in June and August of 1987 indicated that the model was not replicating important features of the O_3 concentration field, including the relatively high peak concentrations reported at inland monitoring stations and the formation of an extensive layer of high O_3 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 O_3 formation aloft to the extent indicated by available measurements. Moreover, the model generated O_3 concentrations in an area north of the San Fernando Valley that were much higher than the observations. The accuracy of VOC and NO_2 estimates was poorer than that for O_3, 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 O_3 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

[1]For 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 O_3 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 O_3 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 O_3 that are somewhat smaller than 10 percent or greater than 15 percent.

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 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 O_3 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 O_3 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 O_3 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 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 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.

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American Petroleum Institute
1220 L Street, Northwest
Washington, D.C. 20005

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The Importance of Using Alternative Base Cases in Photochemical Modeling

Appendices

STEP
Strategies for Today's Environmental Partnership

American Petroleum Institute
1220 L Street, Northwest
Washington, D.C. 20005

STEP
Strategies for Today's Environmental Partnership

One of the most significant long-term trends affecting the future vitality of the petroleum industry is the public's concerns about the environment. Recognizing this trend, API member companies have developed a positive, forward looking strategy called STEP: Strategies for Today's Environmental Partnership. This program aims to address public concerns by improving our industry's environmental, health and safety performance; documenting performance improvements; and communicating them to the public. The foundation of STEP is the API Environmental Mission and Guiding Environmental Principles.

API ENVIRONMENTAL MISSION AND GUIDING ENVIRONMENTAL PRINCIPLES

The members of the American Petroleum Institute are dedicated to continuous efforts to improve the compatibility of our operations with the environment while economically developing energy resources and supplying high quality products and services to consumers. The members recognize the importance of efficiently meeting society's needs and our responsibility to work with the public, the government, and others to develop and to use natural resources in an environmentally sound manner while protecting the health and safety of our employees and the public. To meet these responsibilities, API members pledge to manage our businesses according to these principles:

- To recognize and to respond to community concerns about our raw materials, products and operations.
- To operate our plants and facilities, and to handle our raw materials and products in a manner that protects the environment, and the safety and health of our employees and the public.
- To make safety, health and environmental considerations a priority in our planning, and our development of new products and processes.
- To advise promptly, appropriate officials, employees, customers and the public of information on significant industry-related safety, health and environmental hazards, and to recommend protective measures.
- To counsel customers, transporters and others in the safe use, transportation and disposal of our raw materials, products and waste materials.
- To economically develop and produce natural resources and to conserve those resources by using energy efficiently.
- To extend knowledge by conducting or supporting research on the safety, health and environmental effects of our raw materials, products, processes and waste materials.
- To commit to reduce overall emission and waste generation.
- To work with others to resolve problems created by handling and disposal of hazardous substances from our operations.
- To participate with government and others in creating responsible laws, regulations and standards to safeguard the community, workplace and environment.
- To promote these principles and practices by sharing experiences and offering assistance to others who produce, handle, use, transport or dispose of similar raw materials, petroleum products and wastes.

The Importance of Using Alternative Base Cases in Photochemical Modeling

Appendices

Health and Environmental Sciences Department

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PREPARED UNDER CONTRACT BY:

STEVEN REYNOLDS, HARVEY MICHAELS, AND PHILIP ROTH
ENVAIR
12 PALM AVENUE
SAN RAFAEL, CA 94901

T.W. TESCHE AND DENNIS MCNALLY
ALPINE GEOPHYSICS
P.O. BOX 2059
CRESTED BUTTE, CO 81224

LUANN GARDNER AND GREG YARWOOD
SYSTEMS APPLICATIONS INTERNATIONAL
101 LUCAS VALLEY ROAD
SAN RAFAEL, CA 94903

JULY 1994

American
Petroleum
Institute

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APPENDIX A

Final Report

PROTOCOL FOR A STUDY TO IMPROVE URBAN AIRSHED MODEL PERFORMANCE AND TO ASSESS MODEL SENSITIVITY TO ALTERNATIVE BASE CASES

Prepared for

American Petroleum Institute
1220 L Street, Northwest
Washington, DC 20005

Prepared by

Steven D. Reynolds

Envair
12 Palm Avenue
San Rafael, California 94901

26 August 1992

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Section 1

INTRODUCTION

As part of its Air Modeling Research Study, the American Petroleum Institute (API) is sponsoring an investigation to assess the potential importance of compensatory errors in photochemical model results. Partial funding for this activity is also being provided by the Southern California Edison Company (SCE). Specifically, an effort will be made to determine whether alternative base case conditions can be identified which yield model results consistent with the highest level of performance achievable with an available data base. That is, uncertainties in model inputs may be sufficiently large to allow construction of alternative base cases that produce comparable model performance. Assuming that such alternative base cases can be constructed, a key issue is whether significant differences in calculated air quality improvements may arise in simulations of emission reduction strategies. Of particular concern would be a situation wherein the preference for VOC vs. NO_x control is dependent on the choice of the base case.

A second goal of the API study is to develop a better understanding of the relationship between model performance and the quality of the data base available for use in preparing model inputs. Such information is needed to better specify the types and amounts of meteorological, emissions, and air quality data needed to adequately support regulatory applications of photochemical models.

To achieve these two key objectives, a series of Urban Airshed Model (UAM) sensitivity studies is planned based on existing model applications to the South Coast Air Basin (SoCAB). In concept, simulations of episodes that occurred during the conduct of the 1987 Southern California Air Quality Study (SCAQS) provide the most suitable point of departure for the investigations since the SCAQS data base contains a variety of supplemental meteorological and air quality measurements. However, a review of UAM performance for O_3 episodes occurring in June and August of 1987 indicates that some improvement to the representation of atmospheric processes is needed prior to undertaking the proposed modeling study. The information contained in the SCAQS data base will be used to identify alternative

base cases and to establish UAM input files based on different assumptions concerning data availability.

This study is being carried out by API's Air Modeling Research Team (API-AMRT), consisting of the consortium of Envair, Alpine Geophysics, and Sonoma Technology Inc. and their subcontractor Systems Applications International. Technical oversight for these activities is being provided by API's Air Modeling Task Force (API-AMTF) and Vince Mirabella of SCE.

Discussions involving members of the API-AMTF and the California Air Resources Board (CARB) 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 API-AMRT and CARB personnel would work together in trying to resolve UAM performance problems and in studying model sensitivity issues of common interest. This protocol discusses key technical and administrative issues and describes the activities to be carried out by the participants. Note that this protocol does not address activities associated with the second API objective (i.e., the study of the amounts and types of data needed to support UAM regulatory applications). These activities will be pursued separately by the API-AMRT.

STRUCTURE OF THE STUDY

The proposed study will be carried out in three phases:

- Phase 1--improve model performance
- Phase 2--identify alternative base cases
- Phase 3--conduct sensitivity studies

The technical work to be conducted in each phase is discussed in Sections 2, 3, and 4, respectively. Issues concerning schedule and communications are presented in Sections 5 and 6, respectively.

PARTICIPANTS AND THEIR RESPONSIBILITIES

The proposed study will be conducted by the API-AMRT. California Air Resources Board staff will cooperate with the API-AMRT and will carry out several tasks which will contribute to this study. Oversight for the industry-sponsored activities will be provided by the API-AMTF and by SCE. The responsibilities of each participant may be summarized as follows:

API Air Modeling Task Force

API's Air Modeling Task Force will provide technical oversight for the activities of the API-AMRT. The Task Force will also work with CARB project oversight personnel to address pertinent administrative matters as may arise during the course of the study. Howard Feldman of API will serve as the primary point of contact for such administrative matters as may require the attention of API. Kenneth Steinberg (Exxon) and Charles Schleyer (Mobil Research and Development Corporation) will serve as the primary points of contact for the Task Force.

Southern California Edison

Vince Mirabella of SCE will work with the API Air Modeling Task Force to provide technical oversight for the industry-sponsored activities.

API Air Modeling Research Team

The API-AMRT will assume lead responsibility for the following activities:

- diagnosing and rectifying UAM performance problems that arise in the June 1987 episode;
- identifying alternative base cases and conducting associated UAM simulations for the June 1987 episode;
- performing UAM sensitivity studies for a series of hypothetical emissions reduction plans using the June 1987 meteorological conditions; assessing differences in UAM results associated with the alternative base cases;

- documenting the results of work conducted by the API-AMRT, including diagnostic and model improvement activities, as well as model sensitivity results; and

- interpreting and documenting the findings of the joint API-AMRT and CARB activities for API.

Steven Reynolds of Envair will assume responsibility for directing the day-to-day technical activities of the API-AMRT and will serve as the primary point of contact for interactions with CARB technical staff. Philip Roth of Envair will provide overall administrative oversight and will critically review proposed work plans, progress, and reports. T. W. Tesche, Fred Lurmann, and LuAnn Gardner will direct the technical efforts of Alpine Geophysics, Sonoma Technology Inc., and Systems Applications International, respectively.

California Air Resources Board

The CARB will assume lead responsibility for the following activities:

- diagnosing and rectifying UAM performance problems that arise in the August 1987 episode;

- identifying alternative base cases and conducting associated UAM simulations for the August 1987 episode;

- performing UAM sensitivity studies for a series of hypothetical emissions reduction plans using the August 1987 meteorological conditions; assessing differences in UAM results associated with the alternative base cases; and

- documenting the work conducted by CARB, including the results of diagnostic and model improvement activities, as well as model sensitivity results.

Kit Wagner will serve as CARB's primary point of contact for technical matters. Terry McGuire will serve as the point of contact for administrative issues.

Section 2

PHASE 1--IMPROVE MODEL PERFORMANCE

The API-AMRT has obtained UAM input and output files for the 23-25 June 1987 episode and has been able to adequately replicate simulation results provided by the South Coast Air Quality Management District (SCAQMD). The CARB modeling team has been engaged in studies using the August episode. In Phase 1, the API-AMRT will attempt to identify shortcomings in existing simulations for the June episode, and the CARB modeling team will perform similar studies for the August episode. Particular attention will be given to assuring that efforts to diagnose and rectify model performance problems are scientifically sound and justified and will not be viewed as merely "tuning" exercises.

OBJECTIVES OF THE PHASE 1 WORK

The specific objectives of Phase 1 activities may be summarized as follows:

- identify and prioritize UAM performance problems in existing simulations for the June and August 1987 SCAQS episodes;
- diagnose the possible causes of UAM performance problems;
- identify appropriate modifications to model inputs; and
- 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 will be designed to reduce the discrepancies between model estimates and observed air quality levels where these can be logically defended based on sound scientific principles through (preferably) analyses of relevant, site-specific data. Four principles will govern the model improvement activities:

- any changes to the model or its inputs must be fully documented, both in hard copy and magnetic media where appropriate;

- any changes to the model or its inputs must 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;

- all proposed changes to the model or its inputs will be subject to review by all participants; and

- if scientific differences of opinion arise, a specific effort will be made to reach a consensus on all proposed input modifications; resolution of any residual issues will worked out through joint discussions involving API, SCE and CARB project oversight personnel.

To help assure that the proposed diagnostic and model improvement activities will not be viewed as a "tuning" exercise, the API-AMRT and CARB modeling teams will prepare a technical memorandum describing the proposed modifications to existing inputs for the June and August episodes for review and comments by API, SCE, and CARB project oversight personnel prior to evaluating model performance.

TYPES OF IMPROVEMENTS SOUGHT AND PRIORITY

For the UAM simulation of the 23-25 June 1987 episode using inputs developed by the SCAQMD, the model exhibits a tendency to underestimate O_3 concentrations by 24 to 32 percent. Peak O_3 concentrations are also underestimated at several monitoring stations where relatively high concentrations were reported (e.g., Azusa, Banning, Burbank, Glendale, Pasadena, and Reseda). Hourly-averaged NO and NO_2 concentrations also tend to be underestimated by 31 to 48 percent and 24 to 32 percent, respectively.

For the UAM simulation of the 26-28 August 1987 episode using SCAQMD inputs, the O_3 results exhibit little overall bias, with absolute discrepancies ranging from 15 to 27 percent of the measured values. While the overall bias may be small, there is a tendency to overpredict

during the late afternoon through the night and into the midmorning period at several stations. Correspondingly, there is a tendency to underpredict during the middle of the day when the highest O_3 values are reported. Significant discrepancies exist between estimated and measured peak O_3 concentrations at several stations (e.g., Glendale, HESP, CRES, Pasadena, Pico Rivera, and VICT). Hourly-averaged NO_2 concentrations also tend to be underestimated by 2 to 21 percent.

The types of improvements to model performance and their priority are as follows (highest priority listed first):

- reduce biases in relatively high or peak O_3 values
- reduce biases in O_3, NO, and NO_2 results on a subregional basis
- improve timing and spatial alignment of peak O_3 values

INITIAL PLANS FOR DIAGNOSIS/IMPROVEMENT ACTIVITIES

Based on discussions with CARB concerning the experience they have gained in simulating the August episode and considering the findings of pertinent analyses of the SCAQS data base, the study team will identify specific model inputs that are candidates for modification. In cases where improvements to the treatment of certain inputs will involve the expenditure of significant effort, the potential importance of such input modifications will be initially assessed through the conduct of coarse sensitivity studies. That is, we will modify the magnitude and spatial and temporal characteristics of the inputs, as appropriate, to roughly "bound" the potential change in the input(s) of interest. The study team will perform the requisite UAM sensitivity simulations and analyze the results and provide a recommendation concerning whether further effort should be expended to better quantify the inputs in question. Improved treatments will be developed for those inputs identified in the coarse sensitivity analyses that are expected to have a significant influence on model results (subject to the availability of sufficient funding or personnel time to perform the work). To the extent possible, the importance of groups of input changes will be examined to minimize the number

of required computer simulations. Examples of "potential" improvements in the treatment of model inputs currently under consideration include:

Emissions

The following analysis will be given the highest priority relative to emissions-related concerns:

- Modify the existing base case emissions inputs to correct for biases. The Bay Area Air Quality Management District (BAAQMD) has recently been involved in a study to develop a set of acceptable "correction factors" to be applied to their emissions inventory. Correction factors have been developed for four major categories of sources: motor vehicles, general area (population based emissions), biogenics, and low point sources (permitted sources with less than 50m plume rise). The study team will review the methodology developed by the BAAQMD, the Van Nuys tunnel study, and the results of pertinent SCAQS ambient NMOG and NO_x data analyses reported by Sonoma Technology Inc. to identify a suitable methodology for specifying correction factors to be applied to the existing SoCAB emissions inputs.

Mobile Source Emissions

The following analyses will be given lower priority relative to emissions-related concerns. Note that it may not be feasible to conduct detailed assessments of the following issues within the tight time frame of this study. If necessary, the study team will attempt to develop bounds for the possible influences on emissions and carry out associated UAM sensitivity tests.

- Take into account the spatial distribution of vehicle ages, which are likely to be distributed in a manner similar to the socioeconomic distribution of the population. Attempt to develop spatially varying estimates of the vehicle age distribution using the SmogCheck data base, which provides information concerning vehicle age and vehicle registration address (namely, postal zip code).

- Include the temporal distribution of emissions as a function of location. Some commuters travel significant distances from outlying areas to the central part of the basin. The resulting emissions occur earlier in outlying areas and later in the central basin. The current temporal distribution is most representative of conditions in the central basin. In the proposed work, examine traffic count data collected in outlying and central basin areas to assess the potential importance of this effect and to provide a means of estimating revised temporal distribution functions.

- Flatten and broaden temporal distributions. Of particular concern in the current inventory is the sharp drop-off in vehicle emissions in the evening, especially in suburban and shopping areas. Again, examine readily available traffic count data in suburban areas to quantify this effect.

- Include an improved treatment of the magnitude and temporal distribution of truck emissions. It is expected that truck operations are conducted on a schedule that differs from that of automobiles. In addition, the fraction of the vehicle mix represented by trucks varies in space; trucks are more likely to be operated in selected corridors and areas of the basin. Note that truck operations are not considered in the regional transportation models employed in the SoCAB. In the proposed work, review procedures and associated data bases used to estimate truck emissions. Attempt to identify improved means for quantifying these emissions.

- Include an improved treatment of the magnitude and temporal distribution of bus emissions. Similar comments to those cited above for trucks.

- Update speciation profiles (i.e., the composition of organic species emitted from various source categories). CARB recognizes that the motor vehicle speciation profiles are out of date. It is recommended that they be updated using results from the auto/oil program and recent vehicle test data collected by the CARB.

Solar Energy Inputs

- Lower photolysis rates about 15% to 20%. Gery has developed recent information on quantum yields, which was used in developing photolysis rates for UAM simulations. The values chosen were picked from an array of results that considered variations in elevation, O_3 column, UV albedo, and turbidity. It appears that the current values may be applicable to an elevation of about 1400 meters. Review the current specification of photolysis rates in light of the specific conditions being simulated. Develop improved estimates of these inputs based on the findings of this review.

- Account for effects of aerosol formation and cloud cover on photolysis rates. These influences on photolysis rates are assumed to be spatially invariant. The validity of the assumption and its potential influence on O_3 formation need to be examined for the episodes of interest. Day specific cloud cover and aerosol data will be examined to determine areas of the basin where attenuated photolysis rates should be employed.

Wind Field Inputs

- Examine how well the model represents the formation of pollutant layers aloft. Roberts and Main (1992) have conducted analyses of the SCAQS data and noted the existence of significant quantities of O_3 in stable layers aloft over the SoCAB during the June and August episodes. However, it appears that the UAM does not adequately simulate the formation of O_3 in such layers. Diagnostic studies will be carried out to determine whether the current wind field and mixing height inputs support the development of pollutant layers aloft. If not, recommendations for alterations to model inputs will be developed.

- Consider the development of meteorological fields using a prognostic model with four dimensional data assimilation and compare results with those of the prognostic and diagnostic model used by the SCAQMD. Note that the District

used different wind modeling techniques in preparing meteorological inputs for the June and August episodes. A review of existing wind fields developed using prognostic and diagnostic approaches has indicated significant differences in the calculated flow fields in certain parts of the modeling domain.

It is important to understand that significant effort may be required to develop meteorological fields using a prognostic model. Furthermore, there is limited experience in the application of these advanced models to support the preparation of inputs for photochemical models. Thus, there is a risk that the prognostic models may not perform adequately in their initial application to the SoCAB. Rectifying such problems would require further diagnostic and evaluative studies. Careful consideration will need to be given to the expected level of improvement in photochemical model performance and the associated project costs. Efforts to look at wind field inputs must be balanced with the potential need to examine the other inputs cited in this section.

In the proposed study, the study team will review existing diagnostic and prognostic wind model results for the SoCAB, characterize the similarities and differences in the wind velocity and mixing height fields, and identify any needed improvements to such input fields. We will also review previous photochemical model sensitivity studies to estimate whether the expected changes in meteorological inputs are likely to yield a significant improvement in the photochemical model's performance. If it appears that it would be beneficial to pursue the prognostic modeling activity, we will develop further information concerning the scope of work, costs, and potential risks. This assessment will be completed by 1 September 1992. We will solicit authorization from API, SCE, and CARB project oversight personnel prior to the expenditure of significant project resources in the prognostic modeling activity.

Boundary Concentration Inputs

- Modify ambient concentration values at the top boundary to better emulate observed conditions. Diagnostic analyses should also include the calculation of pollutant fluxes through the horizontal and vertical boundaries of the modeling domain and comparisons of these fluxes with the emissions values for the various O_3 precursors. Such analyses may also be performed for selected subregions of the modeling domain. Analyses of concentration data collected aloft in the SoCAB will be used in conjunction with any available air quality data collected during the modeling periods to prepared revised boundary concentration inputs.

The topics discussed above should be viewed as an initial list of modeling concerns; this list may be truncated, expanded, and modified in accordance with what is learned in the early simulations. The API-AMRT and CARB modeling teams will prepare technical memoranda describing the proposed changes to model inputs for the June and August episodes, respectively. API, SCE, and CARB project oversight personnel will have an opportunity to review and to provide comments on the proposed input modifications.

API-AMRT Activities

Specific tasks to be carried out by the API-AMRT are as follows:

Task API 1.1--Obtain the inputs and outputs for CARB's current base case run for the August 1987 SCAQS episode. Replicate CARB's base case simulation for the August episode on the API-AMRT's computer system. It is expected that CARB staff will carry out all prescribed runs using the August episode; however, the API-AMRT may wish to duplicate some runs or carry out others apart from CARB's efforts. This activity is intended to assure that the API-AMRT can simulate both the June and August episodes and carry out any sensitivity or alternative base case runs of interest.

Task API 1.2--Obtain pertinent air quality and meteorological measurements for 23-25 June 1987 contained in the SCAQS data base. Review available reports documenting analyses of the SCAQS data. Identify and prioritize UAM performance problems for

the June episode. Identify appropriate modifications to model inputs and document proposed changes in a technical memorandum. Carry out a full evaluation of the predictive performance of the UAM for the June episode and assess the adequacy of performance using the procedures and criteria cited in Section 2.6. To the extent feasible, this effort will build on work carried out to date by the SCAQMD and CARB. The API-AMRT will coordinate their evaluation activities with those of CARB and will maintain frequent communications concerning progress and findings.

Task API 1.3--Prepare a written report documenting the model improvement activities for the June episode. Submit copies of the draft report to the API Air Modeling Task Force, SCE, and CARB for review and comments. Revise the final report based on comments provided by the reviewers.

CARB Activities

Specific tasks to be carried out by the CARB modeling team are as follows:

Task CARB 1.1--Obtain and review the inputs and outputs for the API-AMRT's base case run for the June 1987 episode. It is expected that the API-AMRT will carry out all prescribed runs using the June episode; however, CARB may wish to duplicate some runs or carry out others apart from the API-AMRT's efforts. This activity is intended to assure that CARB personnel can simulate both the June and August episodes and carry out any sensitivity or alternative base case runs of interest.

Task CARB 1.2--Identify and prioritize UAM performance problems for the August episode. Identify appropriate modifications to model inputs and document proposed changes in a technical memorandum. Carry out a full evaluation of the predictive performance of the UAM for the August episode and assess the adequacy of performance using the procedures and criteria cited in Section 2.6. This effort will build on work carried out to date by CARB. The CARB modeling team will coordinate their evaluation activities with those of the API-AMRT and will maintain frequent communications concerning progress and findings.

Task CARB 1.3--Prepare a written report documenting the model improvement activities for the August episode. Submit copies of the draft report to the API-AMRT, API Air Modeling Task Force, and SCE for review and comments. Revise the final report based on comments provided by the reviewers.

NUMBER OF COMPUTER SIMULATIONS

Recognizing that diagnostic and model improvement activities can be consumptive of personnel time and computational resources, an effort will be made to minimize the number of diagnostic/improvement iterations required to achieve adequate model performance. Specific steps to be implemented include:

- assessing the potential importance of modifications to selected inputs through use of coarse sensitivity studies, and developing improved treatments only for those inputs that are expected to have a significant influence (say, 5-10 ppb or more for O_3) on model results. To the extent possible, the importance of groups of input changes will be examined to minimize the number of required computer simulations.

- analyzing UAM simulation results for one episode prior to conducting a similar simulation for the second episode.

- simulating only a portion of the full episode period whenever possible (e.g., running the model for the first two days of a three-day simulation period).

Considering the labor and computational resources currently available to support the Phase 1 activities and assuming that no prognostic meteorological modeling is carried out, the API and CARB modeling teams will each be able to perform a total of about 10 full UAM simulations for the June and August 1987 episodes, respectively. If prognostic meteorological modeling is conducted, it will be necessary to carefully examine the budget for Phase 1, including the number of UAM simulations that can be supported. API, SCE, and CARB project oversight personnel are advised that significant costs may be incurred in implementing a prognostic meteorological modeling study for the SoCAB.

PROCEDURES AND CRITERIA FOR JUDGING ACCEPTABLE PERFORMANCE

Model evaluation procedures will be based on those recommended by Tesche et al. (1990). Both statistical and graphical comparisons of calculated and measured O_3 and precursor concentrations will be performed for each episode, with particular attention given to the second and third days of each episode period. The following eleven numerical measures will be used to characterize model performance:

- relative error--the ratio of the maximum one-hour averaged calculated concentration and the maximum one-hour measured concentration (unpaired in space or time);

- paired peak estimation accuracy--the discrepancy between the magnitude of the measured peak one-hour concentration and the calculated concentration at the same time and location (calculated as the estimated peak concentration minus the peak measured concentration);

- temporally-paired peak estimation accuracy--the discrepancy between the highest measured concentration at a monitoring station and the highest calculated concentration occurring within the block of nine grid cells immediately surrounding the monitoring location;

- spatially-paired peak estimation accuracy--the discrepancy between the magnitude of the measured peak one-hour average concentration and the highest one-hour concentration calculated at the same location within three hours (either before or after);

- unpaired peak estimation accuracy--the discrepancy between the magnitude of the peak one-hour average measured concentration (considering all stations) and the highest calculated values anywhere in the modeling domain;

- average station peak estimation accuracy--the average value of the spatially-paired peak estimation accuracy measures;

- mean bias error--the average signed deviation of the concentration residuals (estimated minus measured) for all pairs of measured and estimated concentrations above specified threshold values;

- mean normalized bias error--the average signed normalized deviation of the concentration residuals ([estimated minus measured]/[measured]) for all pairs of measured and estimated concentrations above specified threshold values;

- mean absolute gross error--the average unsigned deviation of the concentration residuals (|estimated minus measured|) for all pairs of measured and estimated concentrations above specified threshold values;

- mean absolute normalized gross error--the average unsigned deviation of the concentration residuals (|estimated minus measured|/measured) for all pairs of measured and estimated concentrations above specified threshold values; and

- standard deviation of residual distribution--the standard deviation of all pairs of estimated and measured concentrations above specified threshold values.

Graphical representations of model performance will include:

- accuracy plots--displays depicting the five peak concentration accuracy measures and a single display summarizing the peak estimation accuracy at all monitoring stations;

- time series plots--displays showing the hourly measured and estimated concentrations at each monitoring station, as well as the maximum and minimum estimated concentrations within one and two grid cells of the station location at each hour;

- ground level isopleths--spatial displays showing the estimated and measured concentrations at selected hours during the simulation, as well as similar displays depicting the maximum estimated and measured values;

- scatterplots--displays of estimated and measured values, including visual aids showing the perfect correlation line and domains wherein the estimates are within a factor of two of the measurements;

- bias and error plots--displays showing bias vs. concentration, gross error vs. concentration, bias vs. time of day, and gross error vs. time of day.

Numerical and graphical assessments of bias, accuracy, and error measures will be performed for both O_3 and its precursors (primarily NO, NO_2, and VOCs). Displays of residuals plotted against selected variables will also be employed to provide insights concerning the possible causes of poor model performance. Other diagnostic analyses may include mass flux calculations, comparisons of ambient measurements and VOC and NO_x emissions inputs, and assessments of how well model estimates agree with available pollutant measurements collected aloft.

Criteria for judging acceptable model performance are provided in CARB photochemical modeling guidance (CARB, 1990). Minimum acceptable performance standards for the current study will be those associated with Class B performance, which represent a level of O_3 performance typical of the better model performances seen to date. However, the API-AMRT and CARB modeling teams will strive to meet a more stringent set of standards (summarized below) that provide much greater assurance that the model is adequately simulating the important atmospheric and emissions processes associated with the June and August episodes. In conducting the model performance improvement activities, the modeling teams will attempt to achieve as many of the more stringent goals as possible. Note that achievement of the more stringent standards may only be possible using "best estimate" emissions inputs (i.e., emissions values corrected for biases). Model performance will be deemed inadequate if any of the Class B performance standards are not achieved. Thus, the

performance standards for the joint API-CARB modeling study may be summarized as follows:

- the model's overall performance--for the entire modeling domain and duration of the simulation--meets the following criteria:
  - peak prediction accuracy (unpaired in space and time): the goal is $\leq \pm 5\%$, and the minimum acceptable performance is $\leq \pm 20\%$;
  - bias (paired in space and time): the goal is $\leq \pm 5\%$, and the minimum acceptable performance is $\leq \pm 15\%$; and
  - gross error (paired in space and time): the goal is $\leq 25\%$, and the minimum acceptable performance is $\leq 35\%$
- the model's subregional performance for all important subregions meets the following criteria:
  - bias (paired in space and time): the goal is $\leq 5\%$, and the minimum acceptable performance is $\leq \pm 30\%$; and
  - gross error (paired in space and time): the goal is $\leq 25\%$, and the minimum acceptable performance is $\leq 40\%$.

If any of the Class B performance standards are not achieved, then the API-AMRT and CARB modeling teams will assess the need to conduct further diagnostic analyses. Final determination of the adequacy of model performance will rest with API, SCE, and CARB project oversight personnel.

Section 3

PHASE 2--IDENTIFY ALTERNATIVE BASE CASES

OBJECTIVES OF THE PHASE 2 WORK

The specific objectives of the Phase 2 activities may be summarized as follows:

- identify plausible alternative conditions that might define an acceptable base case;
- identify alternative base cases that provide a level of UAM performance comparable to that of the reference cases for the June and August 1987 episodes.

INITIAL PLAN FOR IDENTIFYING ALTERNATIVE BASE CASES

The API-AMRT and CARB study teams will carry out a careful, thoughtful assessment of the base cases developed in Phase 1. Based on this assessment, plausible alternative conditions that might define an acceptable base case will be defined. These alternatives will be documented in a technical memorandum and will be submitted to API, SCE, and CARB project oversight personnel for review and comment. Based on discussions with API, SCE, and CARB project oversight personnel, a simulation plan will be developed for examining alternative base cases. This plan will include a protocol for developing or modifying alternative "potential" base cases, using information gained from simulations carried out to date. That is, the protocol will provide general guidance on how, for example, an alternative base case might be modified (if appropriate), based on what was learned from the prior simulations.

Alternative "potential" base cases might include:

- a reference base case - the June and August 1987 UAM simulations developed in Phase 1, or an agreed upon alternative, and,

for example, assuming that VOC and CO emissions are underestimated and that NO_x emissions are relatively unbiased,

- increased boundary conditions to compensate for underestimated VOC emissions;
- reduced wind speeds and mixing heights to compensate for underestimated VOC emissions;
- increased boundary conditions combined with reduced wind speeds and mixing heights to compensate for underestimated VOC emissions;
- increased VOC emissions, in an attempt to minimize or eliminate emissions bias (50% increase);
- increased VOC emissions, in an attempt to minimize or eliminate emissions bias (100% increase); and
- a best attempt to eliminate bias - increased VOC emissions (by an amount to be estimated based on the results of prior runs), combined with altered boundary conditions, wind speeds and mixing heights, as warranted.

Specific alternatives will be developed in this phase of the study. Recommendations will be summarized in a technical memorandum and provided to CARB, API and SCE for review and comments. The study team will modify the recommendations, as appropriate, based on discussions with and comments from all study participants.

API-AMRT Activities

Specific tasks to be carried out by the API-AMRT may be summarized as follows:

Task API 2.1--Develop a simulation plan for alternative base cases. Work with the CARB modeling team to define plausible alternative conditions that may serve to define alternative base cases for the June 1987 episode. Prepare a technical memorandum documenting these alternatives for the June episode and submit to API, SCE, and CARB project oversight personnel for review and comment. Based on discussions with API, SCE, and CARB project oversight personnel, develop a

simulation plan for examining alternative base cases. This plan will include a protocol for developing or modifying alternative "potential" base cases, using information gained as the simulations are carried out. Submit protocol to all participants for their review and comments, and revise the protocol as appropriate.

Task API 2.2--Carry out simulations. The API-AMRT will perform the series of proposed simulations for the June 1987 episode, including test simulations, diagnostic analyses, revised simulations, and comparative analyses. The API-AMRT will maintain frequent communications with the CARB modeling team concerning the findings.

Task API 2.3--Work with the CARB modeling team to analyze and document the results of the alternative base case simulations. The API-AMRT will document the findings of simulations for the June 1987 episode in a technical memorandum and provide copies to all participants for review and comments.

CARB Activities

Task CARB 2.1--Develop a simulation plan for alternative base cases. Work with the API-AMRT modeling team to define plausible alternative conditions that may serve to define alternative base cases. Prepare a technical memorandum documenting these alternatives for the August episode and submit to API, SCE, and CARB project oversight personnel for review and comment. Based on discussions with API, SCE, and CARB project oversight personnel, develop a simulation plan for examining alternative base cases. This plan will include a protocol for developing or modifying alternative "potential" base cases, using information gained as the simulations are carried out. Submit protocol to all participants for their review and comments, and revise the protocol as appropriate.

Task CARB 2.2--Carry out simulations. The CARB modeling team will perform the series of proposed simulations for the August 1987 episode, including test simulations,

diagnostic analyses, revised simulations, and comparative analyses. The CARB modeling team will maintain frequent communications with the API-AMRT concerning the findings.

Task CARB 2.3--Work with the API-AMRT to analyze and document the results of the alternative base case simulations. The CARB modeling team will document the findings of simulations for the August 1987 episode in a technical memorandum and provide copies to all participants for review and comments.

Section 4

PHASE 3--CONDUCT SENSITIVITY STUDIES

OBJECTIVE OF THE PHASE 3 WORK

The primary objective of the Phase 3 activities is to ascertain 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.

SPECIFICATION OF HYPOTHETICAL EMISSION REDUCTION SCENARIOS

The API-AMRT and CARB modeling teams will be able perform a combined total of about 12 UAM simulations. Assuming that three alternative base cases are identified in Phase 2, it will be possible to study two hypothetical emission reduction scenarios (i.e., 3 base cases x 2 emission scenarios x 2 episodes = 12 UAM runs).

We suggest that the initial emission reduction scenario[1] represent an across-the-board 50 percent reduction in both VOC and NO_x emissions from all anthropogenic sources in the study area. UAM simulations would be conducted for up to three alternative base cases for both the June and August episodes (i.e., six UAM simulations). The API-AMRT and CARB modeling teams will prepare a technical memorandum summarizing the results of this first round of sensitivity runs. Recommendations will also be provided concerning the specifications for the second set of simulations. These simulations might involve a different mix of across-the-board VOC and NO_x emission reductions (i.e., the same reduction applied to all anthropogenic sources for a particular pollutant), or might include simple reductions applied to different categories of sources. The final specifications will be developed based on comments and suggestions provided by CARB, API, and SCE project oversight personnel.

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[1]Note that only hypothetical emission reduction scenarios will be examined in this study. It is 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.

PREPARATION OF MODEL INPUTS

Most UAM inputs for the sensitivity studies will be the same as those employed in the alternative base case simulations. However, changes will be made to both the emissions and initial and boundary concentration inputs. In the latter case, initial and boundary inputs will be changed to reflect the conditions associated with the altered emissions rates.

The API-AMRT and CARB modeling teams will implement straightforward, across-the-board reductions to VOC and NO_x emissions. Emission reductions may be applied to major categories of sources (e.g., mobile, area, and/or large point sources).

Base case initial concentration inputs for VOC and NO_x (in excess of natural background values) will be scaled in proportion to the changes in emissions for these species. Consideration will also be given to a similar scaling of boundary concentrations to the extent these inputs appear to be directly influenced by anthropogenic emissions in the SoCAB. The API-AMRT and CARB modeling teams will work together to develop a consistent procedure for modifying all base case initial and boundary concentration inputs (including O_3).

PLANS FOR PHASE 3 WORK

API-AMRT Activities

Task API 3.1--Develop recommendations for hypothetical emissions reduction plans. The API-AMRT will work with the CARB modeling team to develop final specifications for the hypothetical emission reduction plans. The simulations that derive will be used in assessing the differences in possible outcomes among the alternative base cases. The plan will also discuss procedures for reducing boundary and initial conditions. The API-AMRT will prepare a technical memorandum summarizing the simulation plans for the June episode and provide copies to API, CARB, and SCE for review and comment.

Task API 3.2--Carry out emissions reduction simulations for the June episode. The API-AMRT will analyze the UAM results and work with CARB personnel to interpret

the findings. The results and findings will be summarized in a brief report, which will be submitted to API, SCE, and CARB for review and comment.

Task API 3.3--Prepare a synthesis report and journal paper. The API-AMRT will prepare a synthesis report (incorporating the written materials prepared in Task API 3.2) discussing objectives of the work, findings and implications for the use of UAM in developing SIPs and AQMPs. The API-AMRT will also prepare a journal paper documenting in detail the work carried out and the findings of the study. The API-AMRT will work with CARB modeling personnel to coordinate the joint or separate submittal of journal papers.

CARB Activities

Task CARB 3.1--Develop recommendations for hypothetical emissions reduction plans. The CARB modeling team will work with the API-AMRT to develop final specifications for the hypothetical emission reduction plans. The plan will also discuss procedures for reducing boundary and initial conditions. A technical memorandum will be prepared summarizing the simulation plans for the August episode and copies will be provided to API, CARB, and SCE project oversight personnel for review and comment.

Task CARB 3.2--Carry out emissions reduction simulations for the August episode. The CARB modeling team will analyze the UAM results and work with the API-AMRT to interpret the findings. The results and findings will be summarized in a brief report, which will be submitted to API, SCE, and CARB project oversight personnel for review and comment.

Task CARB 3.3--Prepare a synthesis report and journal paper. The CARB modeling team will prepare a synthesis report (incorporating the written materials prepared in Task CARB 3.2) discussing objectives of the work, findings and implications for the use of UAM in developing SIPs and AQMPs. The CARB modeling team may also prepare a journal paper documenting in detail the work carried out and the findings of

the study. The CARB modeling team will work with the API-AMRT to coordinate the joint or separate submittal of journal papers.

Section 5

SCHEDULE

The participants recognize that timely completion of the proposed work is essential to assure its utilization in ongoing and planned UAM regulatory applications. Thus, the technical activities will be conducted in accordance with the following schedule:

Phase 1--improve model performance	1 July-30 September 1992[2]
Phase 2--identify alternative base cases	15 September-15 October 1992
Phase 3--conduct sensitivity studies	1 October-31 December 1992

The API-AMRT and CARB study teams will discuss the status of technical activities on a regular basis during the course of the investigations. Problems in adhering to the schedule cited above will be brought to the attention of the all participants as soon as they become known. In the event that one group cannot adhere to the prescribed schedule, the other group may find it necessary to modify their planned activities, as needed to achieve their technical objectives in a timely manner.

[2]CARB staff will attempt to adhere to the 30 September deadline for the Phase 1 work. However, all study participants are advised that the ability of CARB staff to meet this deadline may be precluded by other ongoing work to be conducted during the July-September time frame.

Section 6

COMMUNICATIONS

Frequent communications among the study teams will be required to assure that the proposed technical activities are carried out in a coordinated, efficient manner. Issues of particular importance include the sharing of information, meetings, and documentation of the work.

SHARING INFORMATION

The API-AMRT and CARB study teams agree to perform the proposed activities in an open manner and further agree to freely share the results of all work carried out in Phases 1 through 3. Specific types of information to be shared include:

- all UAM input and output files
- all preprocessor input and output files
- hard copy graphical displays of model results
- the findings of analyses and interpretations of model results
- technical memoranda and reports documenting the work carried out

The participants recognize that the proposed study is likely to generate a significant volume of information, especially as may be contained in UAM-related input and output files. Transfer of such information can involve significant amounts of labor and computer resources. Thus, the participants agree to limit requests for voluminous information to that essential to the achievement of their technical objectives. Any problems arising in the sharing of information will be resolved through discussions involving key API, SCE, and CARB project oversight personnel.

MEETINGS

Formal meetings involving the API-AMRT, API Air Modeling Task Force, SCE, and CARB will be held at key project milestones to discuss the progress and findings of the study and plans for subsequent activities. These meetings and the key topics will be as follows:

- Formal Meeting 1--to discuss the activities and findings of diagnostic and model improvement efforts carried out in Phase 1; plans for identifying alternative base cases in Phase 2 and conducting model sensitivity studies in Phase 3 will also be discussed; to be held on or about 15 October 1992.

- Formal Meeting 2--to discuss the overall findings of Phases 2 and 3 of the study; to be held in early February 1993.

Informal meetings involving the API-AMRT and CARB modeling teams will be held on a more frequent basis to promote the exchange of information and coordination of technical activities. These meetings and the key topics will be as follows:

- Informal Meeting 1--to discuss Phase 1 planned activities, including the results of previous diagnostic analyses and proposed approaches for improving model performance; to be held on or about 8 July 1992.

- Informal Meeting 2--to discuss interim findings of the Phase 1 activities and subsequent plans for further diagnostic and model improvement activities; to be held on or about 1 September 1992.

- Informal Meeting 3--to discuss the findings of Phase 2 efforts to identify alternative base cases (note that plans for Phase 2 activities will be discussed during Formal Meeting 1); to be held on or about 3 November 1992.

- Informal Meeting 4--to discuss interim findings of Phase 3 efforts involving the influence of alternative base cases on the results for hypothetical emissions reduction scenarios; to be held on or about 1 December 1992.

Steven Reynolds will assume lead responsibility for arranging the meetings. The meetings will be held on dates and at locations to be mutually agreed upon by all participants.

Telephone conference calls involving key members of the API-AMRT and CARB modeling teams will be held to further promote the timely exchange of information and the coordination of technical efforts. Topics to be covered will include the status and findings of ongoing technical activities, plans for upcoming activities, and identified problem areas and suggestions for their resolution. Steven Reynolds will be responsible for developing an agenda for each call. In general, the conference calls will be held on a weekly basis and no less frequently than biweekly. The duration of such calls will range from 10 to 60 minutes, depending on the amount of information that needs to be discussed.

REPORTING

The API-AMRT and CARB agree to provide timely written documentation of the work carried out for the proposed joint study. Technical reports will be prepared upon completion of Phases 1, 2, and 3 by both the API-AMRT and CARB study teams. These reports will include a description of the technical approach and analyses of the results. Draft reports will be distributed to all participants in accordance with the following schedule:

- Draft Phase 1 report — 30 September 1992
- Draft Phase 2 report — 1 November 1992
- Draft Phase 3 report — 15 January 1993

The participants agree to review and to provide written comments on the draft reports within three weeks of receipt. Final reports, incorporating responses to the comments, will be completed three weeks subsequent to the receipt of the comments and distributed to all participants.

The API and CARB study teams may individually elect to present the findings of their respective work at suitable conferences or to publish their respective work in technical

journals, in either case giving proper acknowledgement to the work of the other participants. In lieu of, or in addition to the above, specific consideration will be given during the course of the study to the preparation of one or more joint publications if deemed appropriate by mutual agreement of all participants.

REFERENCES

CARB, 1990. "Technical Guidance Document: Photochemical Modeling", California Air Resources Board, Sacramento, California.

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Tesche, T.W., et al., 1990. "Improvement of Procedures for Evaluating Photochemical Models", Contract No. A832-103, California Air Resources Board, Sacramento, California.

APPENDIX B

Appendix B

REVISION OF MODEL INPUTS

This appendix discusses modifications made to the existing UAM inputs for the June 1987 SCAQS episode. 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

SIMULATION STARTING TIME

A possible explanation for the inability of the model to adequately simulate the formation of the highly polluted air mass aloft was that precursors had already begun to accumulate aloft prior to 23 June (the original starting time for the June simulation). Thus, we initiated the new simulation at midnight on 22 June. This decision required the study team to develop a complete set of UAM inputs for 22 June.

VERTICAL GRID HEIGHT AND RESOLUTION

The original top of the modeling region was set at 1000 m. As shown in Figure 2-3, this places the top of the grid in the immediate vicinity of the layer of high O_3 concentrations aloft. To allow the model to simulate the formation and transport of pollutants within this layer, we increased the top of the region to 1500 m. In mountainous areas, the top of the region was increased (above the 1500 m value) as needed to maintain a minimum vertical grid domain depth of 800 m. In addition, we also increased the number of vertical grid levels from five to nine. An examination of Figure 2-3 indicates that significant vertical concentration gradients exist aloft. An increased number of grid levels was specified to provide the model with finer vertical grid resolution than

would otherwise be available using five levels. In addition, the increased number of grid layers provided a better opportunity to represent wind shear effects. Upon finding that the model did not adequately represent the formation of the O_3 layer aloft, we reverted to the use of six vertical grid levels to help reduce the computing burden in Phase 2 and 3 simulations. An analysis of simulation results using both nine and six levels indicated that there was little influence on estimated ground-level concentrations.

WIND FIELDS AND MIXING HEIGHTS

Efforts to improve the representation of wind fields for the June episode are discussed in the report by Tesche and McNally (1992). In their assessment of the wind fields developed by the SCAQMD, they found that the computed wind velocities differed from the observations in the eastern portions of the modeling domain, especially to the east of Palm Springs. Of particular concern was that O_3 and precursors were being transported out of the modeling domain at a greater rate than actually occurred during the June episode. Basically, the District's winds carried O_3 and precursors out of the eastern part of the domain, whereas the wind observations in this area suggested that the flow was easterly, thus keeping these pollutants within the modeling region.

In an attempt to improve the representation of pollutant transport, a complete set of wind fields for 22-25 June 1987 were developed using the Diagnostic Wind Model, as documented in the report by Tesche and McNally (1992). A subsequent analysis of estimated and observed wind speeds for each hour indicated the existence of a bias. To remove this wind speed bias, we developed a set of gridded "correction factors". For the region below the mixing height, we calculated the ratio of the observed wind speed to the estimated wind speed on an hour-by-hour basis at each measurement location (except the Los Alamitos site because exceptionally high wind speeds were reported there). For each hour, these ratio values were spatially mapped to the modeling grid using Poisson smoothing; boundary values were established using the region-wide mean ratio value specified at pseudo-sites situated at 20 km intervals along the boundary. The

mean values were calculated using only those data for which the ratio of estimate to measured values was greater than .25 and less than 4.0.

Above the mixing height, a single correction factor was generated for all cells and for all days since data were too limited to justify any greater detail. Means were calculated as described in the previous paragraph.

The District's mixing heights were used for June 23, 24, and 25. For June 22, unsmoothed temperatures, ground elevations, and two temperature soundings (at 5 am and 11 am at Loyola Marymount College) were combined to generate mixing heights using the Holzworth technique. Before 5 am, the 5 am sounding was used; if the base of the elevated inversion was estimated to be above 1475 m (the top of the sounding), the mixing height was set at 1500 m. After 11 am, the 11 am sounding was used, but if the inversion base height was estimated to be above 1000 m (the top of the sounding), the mixing height was again set at 1500 m. Between 5 am and 11 am, mixing heights were calculated using the two soundings, followed by a temporal linear interpolation. Mixing heights were set to a minimum of 100 m in the mountains between 9 am and 9 pm. Mixing heights in desert areas were set to 50 m between midnight and 5 am. A minimum height of 50 m was applied to all other places and times. The results were then passed three times through a one-cell-radius smoothing routine. Finally, beginning at 7 pm on 22 June, the mixing heights were gradually forced to conform with the District's estimated values at midnight on 23 June.

INITIAL AND BOUNDARY CONCENTRATIONS

Initial concentration values for 22 June were assumed to be the same as those originally specified for June 23, with the exception suitable modifications were made to encompass the increased number of vertical grid levels. A key objective of starting the simulation on June 22 was to obtain better estimates of gridded concentrations on June 23 (rather than trying to specify these values through initial conditions using the available data); in any event, the results on 24 and 25 June (the

days of greatest interest) are not likely to be sensitive to the initial values specified 48 hours earlier in the simulation.

Interpretation of the sparse data to support the estimation of concentrations along the lateral and top boundaries was guided by suggestions provided by Main *et al.* (1991), namely: (1) O_3 concentrations aloft are generally higher than at the surface, (2) RHC values should be either independent of height or decrease with height, (3) an attempt should be made to use day- or episode-specific values, rather than average values, and (4) temporal resolution should be no finer than one day.

For the boundary concentrations specified at the top of the domain, significant differences exist between the values used in this study and those employed by the SCAQMD. In particular, the District's RHC[1] values varied spatially from 500 to 1,000 ppbC; this spatial pattern was held fixed over the three days. In this study, we set RHCs spatially constant at 60 ppbC on 23 June 23 and 100 ppbC on 24 and 25 June. The choice of these values was based on aircraft measurements at 1500 m for these days reported by Main *et al.* (1991). The O_3 boundary value was set to a constant of 100 ppb in the District's base case. In this study, O_3 was spatially constant, but set at 70 ppb on 22 and 23 June, at 80 ppb on 24 June, and at 100 ppb on 25 June. No changes were made to the District's boundary concentration inputs for the other species.

Significant differences exist in the boundary values specified along the lateral boundaries of the domain. The District's RHCs vary from 100 to 550 ppbC, usually with higher values aloft. In this study, RHCs above the mixing height were set at 60 ppbC on 22 and 23 June, and at 100 ppbC on 24 and 25 June. Below the mixing height, they were assumed constant at 110 ppbC. The O_3 boundary values were set to 50 ppb below the mixing height on all days. Above the mixing height, they were set to 70 ppb on 22 and 23 June, to 80 ppb on 24 June, and to 100 ppb on 25 June.

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[1]RHC refers to the sum of all reactive organic species.

Concentrations on lateral boundaries were chosen based on analyses of data reported at monitoring stations near the boundary of the modeling domain. These stations included Anacapa Island and Casitas Pass on the west, Lancaster and Barstow on the north, Joshua Tree and Twenty-Nine Palms on the east, and Oceanside, Escondido, and Del Mar on the south.

PHOTOLYSIS RATES

New values for the photolysis rates (*J* values) for 5 key photolysis reactions in the UAM were recalculated for conditions specific to the June SCAQS episode using the photolysis rate preprocessor incorporated in the UAM-V model. The photolysis reactions of concern are:

k_1	NO_2	→	$O(^3P)$
k_9	O_3	→	$O(^1D)$
k_{38}	FORM	→	radicals
k_{39}	FORM	→	molecules
k_{45}	ALD2	→	radicals

Rates for other photolysis reactions in the UAM were not recalculated, although they were altered by the change to k_1 since they are determined through ratios to k_1.

The UAM-V preprocessor generates a look-up table of photolysis rates for varying solar zenith angles and altitudes as a function of solar flux, albedo, turbidity, and O_3 column density, using wavelength-resolved absorption cross-section and quantum yield data for each photolysis reaction. Inputs to the preprocessor are:

- the extraterrestrial solar flux — a parameterization of the brightness of the sun at the top of the atmosphere (Fröhlich and Wehrli, 1983).
- surface UV-albedo over the modeling domain — the fraction of ultraviolet light reflected from the earth's surface.

- turbidity for the modeling domain — the optical extinction due to aerosol scattering and absorption. An aerosol loading representative of urban air (optical depth 0.2) is utilized (Schippnick and Green, 1982).

- total O_3 column density over the modeling domain — in Dobson Units (DU).

- the wavelength resolved absorption cross-section, $\sigma(\lambda)$, for each species undergoing photolysis. Current data: NO_2 (NASA, 1990), HCHO (Cantrell *et al.*, 1990; Rogers, 1990), O_3 (Molina and Molina, 1986), ALD2 (Martinez *et al.*, 1992).

- the wavelength-resolved quantum yield, $\phi(\lambda)$, for each photolysis process. Current data: NO_2 (Gardner, Sperry and Calvert, 1987), HCHO (Calvert, 1980), $O_3 \rightarrow O(^1D)$ (NASA, 1990), ALD2 (IUPAC, 1989).

The first four inputs above are combined to calculate the wavelength resolved actinic flux, $I(\lambda)$ ($280 \text{ nm} < \lambda < 420 \text{ nm}$), as a function of the solar zenith angle and altitude (Schippnick and Green, 1982; Green, Cross and Smith, 1980). The photolysis rates are then obtained by performing an integration over the triple product $I \cdot \sigma \cdot \phi$ at 1 nm wavelength intervals:

$$J_n = \int_{\lambda_{min}}^{\lambda_{max}} I_n(\lambda) \cdot \sigma_n(\lambda) \cdot \phi_n(\lambda) \, d\lambda$$

The result is a look-up table of photolysis rates for 10 solar zenith angles and 11 heights above sea level.

The specification of representative conditions for the June 1987 SCAQS episode may be summarized as follows:

- O_3 column--Values for the O_3 column over the SoCAB were obtained from Nimbus 7 Satellite TOMS data (NSSDC, 1991). The satellite passes over the area at about mid-day and records the O_3 column at 1.5° longitude by 1° latitude resolution, giving a total of nine values over the SCAQS modeling domain for each day. The average O_3 column over all nine cells over the 4 day period was 334 DU. The second highest and second lowest values observed in any one cell were 345 and 324 DU.

- Altitude--Since the UAM does not include provisions to represent the variation of photolysis rates with altitude, characteristic values for the modeling domain must be

specified. Since much of the terrain in the SCAQS domain is situated above the 300 m msl, photolysis rates for 980 m above sea level were used in the simulations reported herein.

- UV albedo--Peterson (1976) recommended an average UV albedo of 0.05. Jeffries and Sexton (1987) argue that more recent measurements suggest that this value should be larger, and recommend a value of 0.08. A realistic upper limit for the UV albedo is probably 0.1.

To examine the sensitivity of photolysis estimates to assumptions concerning values for the O_3 column and UV albedo, calculations were performed for the following three conditions:

	O_3 column	UV albedo
best estimate	334 DU	0.08
lower bound	345 DU	0.05
upper bound	324 DU	0.1

The results of these calculations are plotted in Figures B-1 through B-5; also included are the default values from the UAM and the calculations of Jeffries and Sexton (1987). Note that the calculated "best estimate" values are for an altitude of 980 m above sea level, whereas the values from the UAM and Jeffries and Sexton are for an altitude of 640 m. Of the five reactions studied, NO_2 photolysis is virtually insensitive to the O_3 column, whereas O_3 photolysis is most sensitive to the O_3 column; thus the range in these calculations for NO_2 is indicative of changing the albedo from 0.05 to 0.1, whereas the range in the calculations for O_3 is indicative of the change in albedo plus the change in O_3 column from 324 to 345 DU.

The best estimate photolysis rates calculated here are generally smaller than those currently utilized in the UAM. The largest differences are for the photolysis of formaldehyde (FORM), for which updated sources for the absorption cross-section have been used. The revised rates for formaldehyde are about 20 percent smaller than the nominal UAM estimates. Excluding FORM

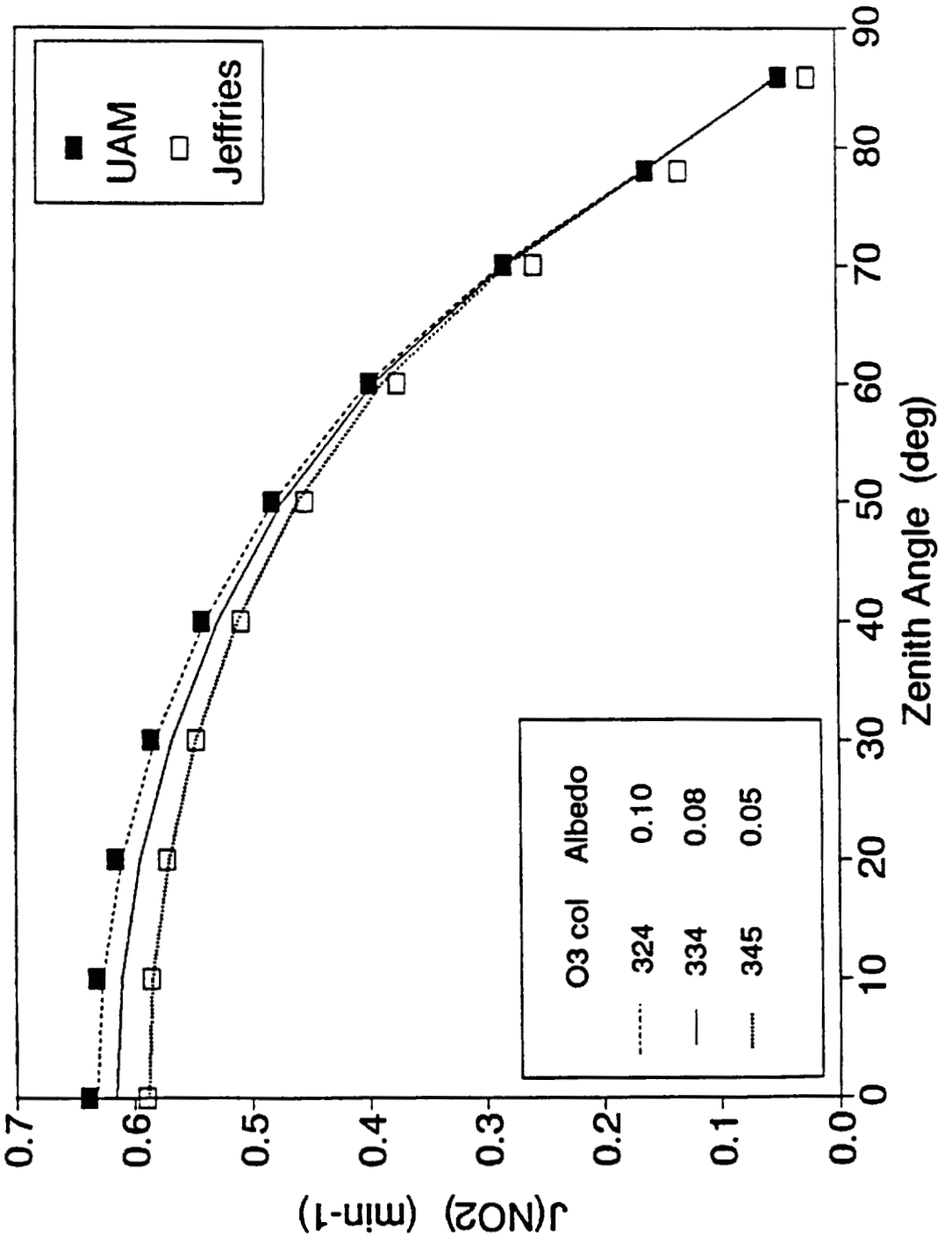


Figure B-1. Comparison of rates for NO_2 photolysis for the SoCAB on 22-25 June 1987. (Comparisons include UAM default values, values estimated by Jeffries and Sexton (1987), and values calculated in this study assuming various settings for the O_3 column and UV albedo.)

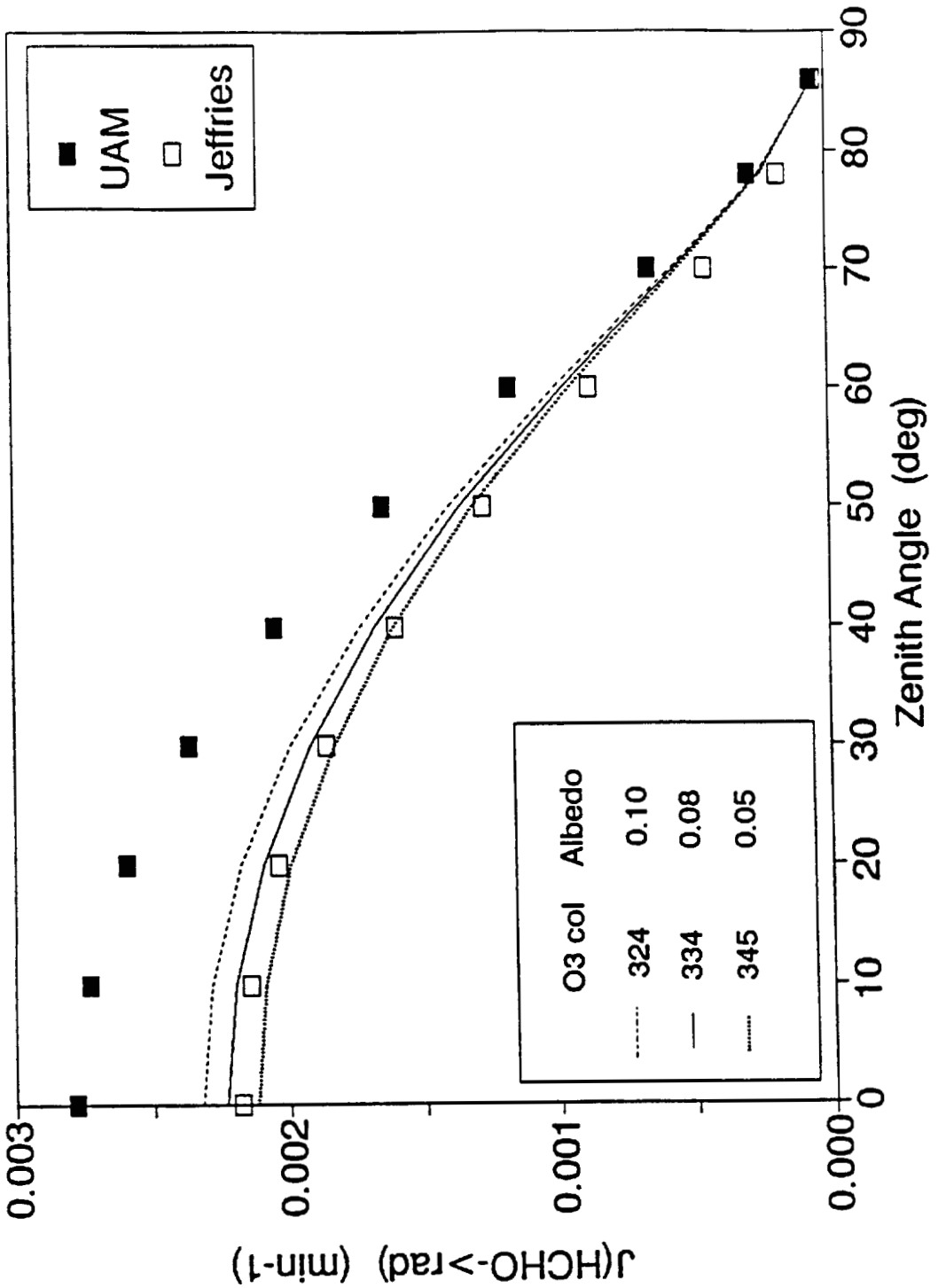


Figure B-2. Comparison of rates for HCHO photolysis to radicals for the SoCAB on 22-25 June 1987. (Comparisons include UAM default values, values estimated by Jeffries and Sexton (1987), and values calculated in this study assuming various settings for the O_3 column and UV albedo.)

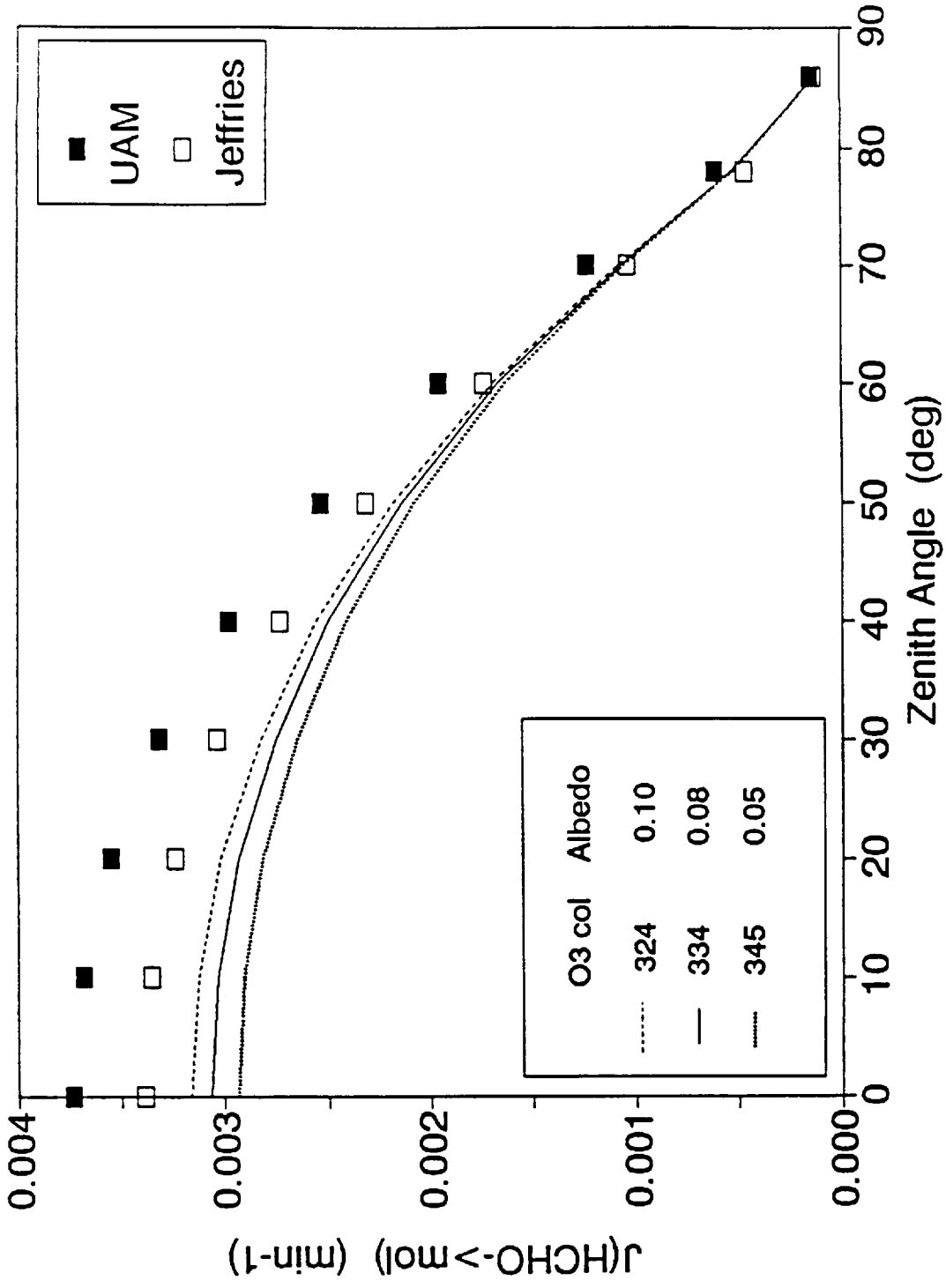


Figure B-3. Comparison of rates for HCHO photolysis to molecules for the SoCAB on 22-25 June 1987. (Comparisons include UAM default values, values estimated by Jeffries and Sexton (1987), and values calculated in this study assuming various settings for the O_3 column and UV albedo.)

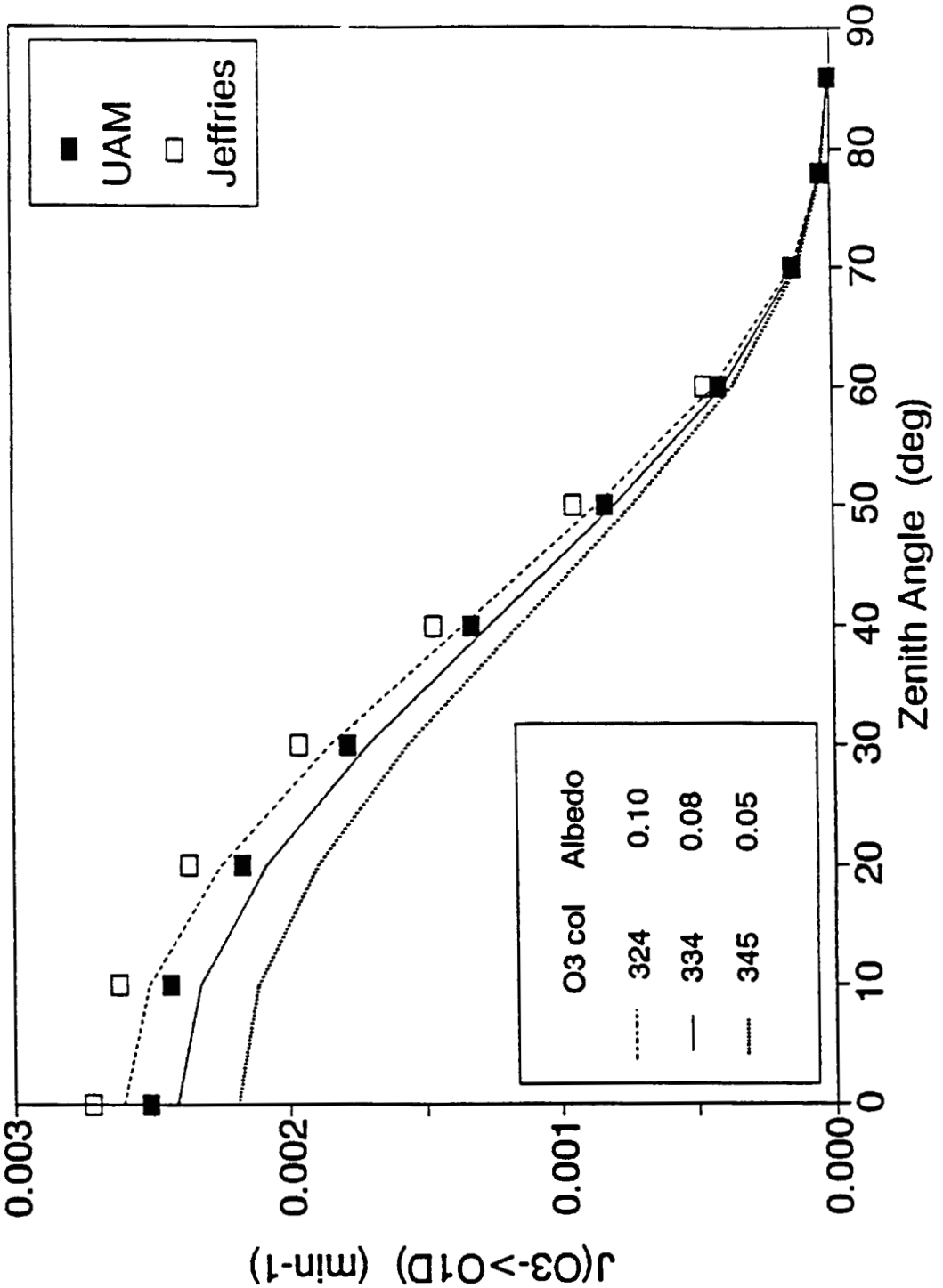


Figure B-4. Comparison of rates for O_3 photolysis to O(1D) for the SoCAB on 22-25 June 1987. (Comparisons include UAM default values, values estimated by Jeffries and Sexton (1987), and values calculated in this study assuming various settings for the O_3 column and UV albedo.)

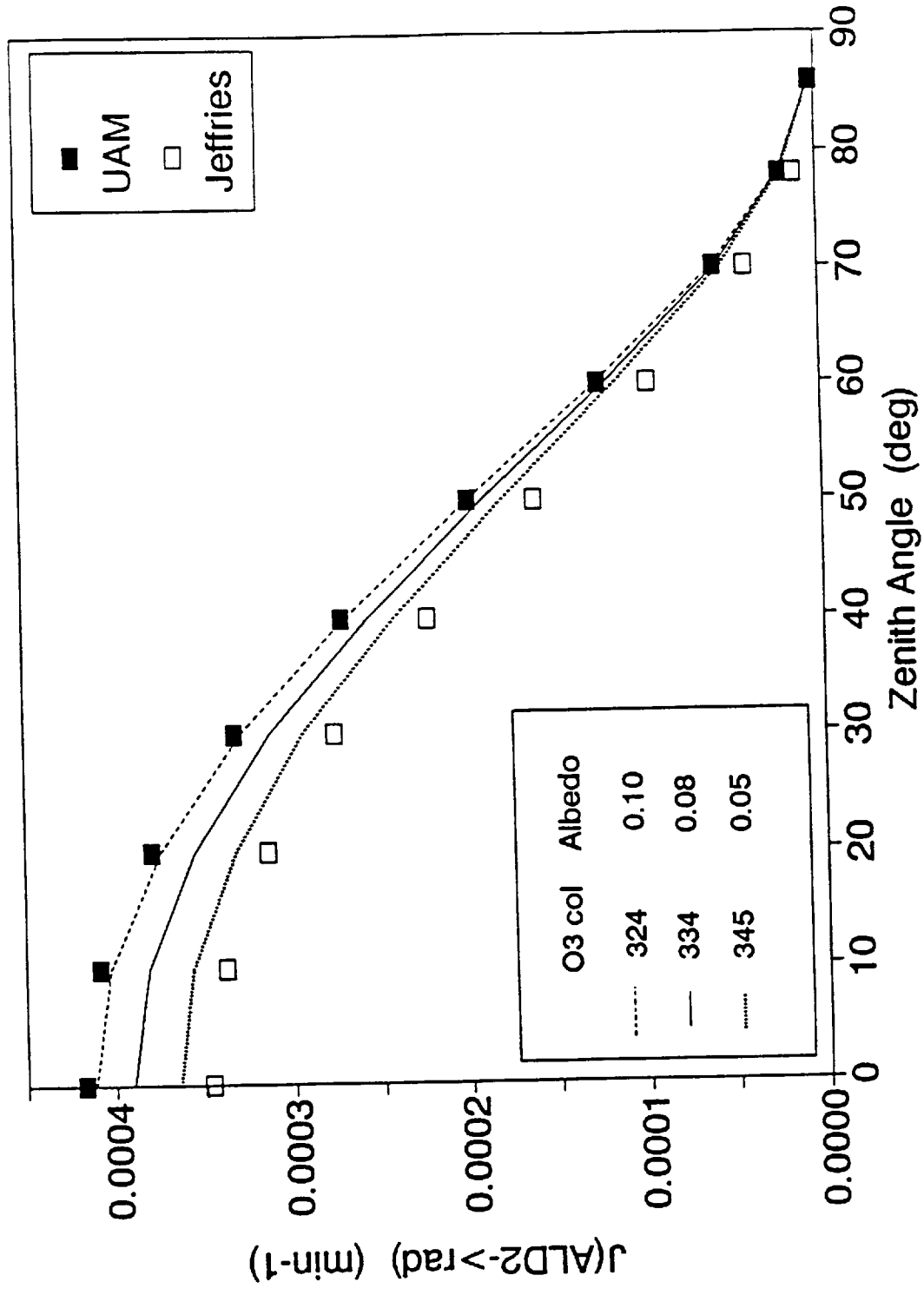


Figure B-5. Comparison of rates for ALD2 photolysis to radicals for the SoCAB on 22-25 June 1987. (Comparisons include UAM default values, values estimated by Jeffries and Sexton (1987), and values calculated in this study assuming various settings for the O_3 column and UV albedo.)

photolysis, agreement with the UAM values is best for NO_2 photolysis and poorest for O_3 and ALD2 photolysis. This is almost certainly because the UAM photolysis rates were calculated for an O_3 column of 300 DU compared to the best estimate for the June SCAQS episode of 334 DU. In fact, seasonal average O_3 column data for 30° North suggest that an O_3 column of 300 DU would be typical for the SoCAB in the summer months. Caution should be exercised in using the photolysis rates estimated herein for conditions other than those present during the June 1987 SCAQS episode.

EMISSIONS

A consequence of including an additional "ramp-up" day (i.e., 22 June) was the need to develop suitable emissions inputs. We calculated average ambient temperatures for each hour on 22 and 23 June and found that none of the hourly values differed by more than 2.5 °C; the daily average temperatures on 22 and 23 June were 20.1 and 19.8 °C, respectively. Considering the small differences in ambient temperatures, we assumed that emissions estimates for 22 June were equivalent to those of 23 June.

Initial model simulations for the June episode using revised inputs as described in the previous sections in conjunction with nominal emissions estimates yielded results that significantly underestimated measured O_3 concentrations. This finding was also noted by CARB in their work with the August SCAQS episode. Use of inputs that understate precursor emissions was thought to partially contribute to this bias in model O_3 estimates.

As noted in a recent National Research Council report (NRC, 1991),

> "Ambient monitoring data from many urban and rural areas of the United States, along with data from roadside motor vehicle emissions tests, tunnel studies, and remote sensing studies of on-road vehicle exhaust, show that current inventories underestimate VOC and carbon monoxide (CO) emissions by large margins."

The authors of the NRC report also noted that an assessment of recent photochemical modeling experience indicates that the models tend to underestimate O_3 concentrations. That some model results have not exhibited even larger tendencies to underestimate O_3 concentrations has been attributed to the possible use of input values that have compensated for the underestimates in VOC emissions (e.g., the use of artificially high VOC boundary concentrations). To achieve the objectives of the current study, it was important that we employ accurate emissions estimates.

To identify an objective means for adjusting the nominal emissions estimates, we examined the findings of Lurmann and Main (1992), who have carried out analyses of gridded VOC and NO_x emissions data to ascertain their consistency with ambient data collected during the SCAQS field program. In particular, comparisons were made using average emissions within 15 x 15 km grids encompassing each SCAQS air monitoring site for the 6-8 am period and the 7-8 am ambient measurements. They found that the average VOC/NO_x ratios in the emissions inventory were 54 and 39 percent lower than ambient ratios in the summer and fall, respectively. Average CO/NO_x ratios in the emissions inventory were 43 and 38 percent lower than ambient ratios in the summer and fall, respectively. They noted that discrepancies between ambient and emissions inventory ratios were similar to those found in the SCAQS tunnel study, wherein CO and VOC estimates from EMFAC7E were 56 and 52 percent lower than measured emission rates in the Van Nuys Tunnel, whereas NO_x emissions estimates and measurements were in close agreement.

Based on the results cited above, it appeared that VOC emissions were underestimated and that NO_x emissions were unbiased. Using data collected at eight sites, the average ambient VOC/NO_x ratio was 8.9, and the average VOC/NO_x ratio in the emissions inventory was found to be 4.1. Thus, we estimated that VOC emissions were underestimated by a factor of 2.2 (i.e., 8.9/4.1 = 2.2). To adjust the emissions inputs, we multiplied all VOC emissions by a factor of 2.2.

APPENDIX C

Appendix C

O_3, NO_2, AND NO_x SIMULATION RESULTS FOR 23-25 JUNE 1987

This appendix contains time series plots showing estimated and measured concentrations for Runs J1, J2, and J7 for 23-25 June 1987. Each display illustrates the estimated and measured concentrations for O_3, NO_2, and NO_x at an air monitoring station. The figures are organized by subregion as indicated below:

- Region A--Coastal Region

  Anaheim (ANAH)
  Costa Mesa (COST)
  El Toro (TORO)
  Long Beach (LGBH)
  Long Beach City College (LBCC)
  Los Alamitos (LSAL)
  West Los Angeles (WSLA)

- Region B--Central Basin

  La Habra (LAHB)
  Los Angeles (CELA)
  Lynnwood (LYNN)
  Pasadena (PASA)
  Pico Rivera (PICO)
  Whittier (WHIT)

- Region C--San Fernando Valley

  Burbank (BURK)
  Reseda (RESE)

- Region D--Eastern Region

  Azusa (AZUS)
  Fontana (FONT)
  Glendora (GLEN)
  Norco (NORC)
  Pomona (POMA)

Redlands (REDL)
Riverside-Rubidoux (RIVR)
Rubidoux (RUBI)
San Bernardino (SNBD)
Upland (UPLA)

- Region E--Basin Rim

  Banning (BANN)
  Crestline (CRES)
  Hemet (HEME)
  Perris (PERI)

- Region F--Far Eastern Region

  Palm Springs (PLSP)
  29 Palms (29PL)

- Region G--Lancaster

  Lancaster (LANC)

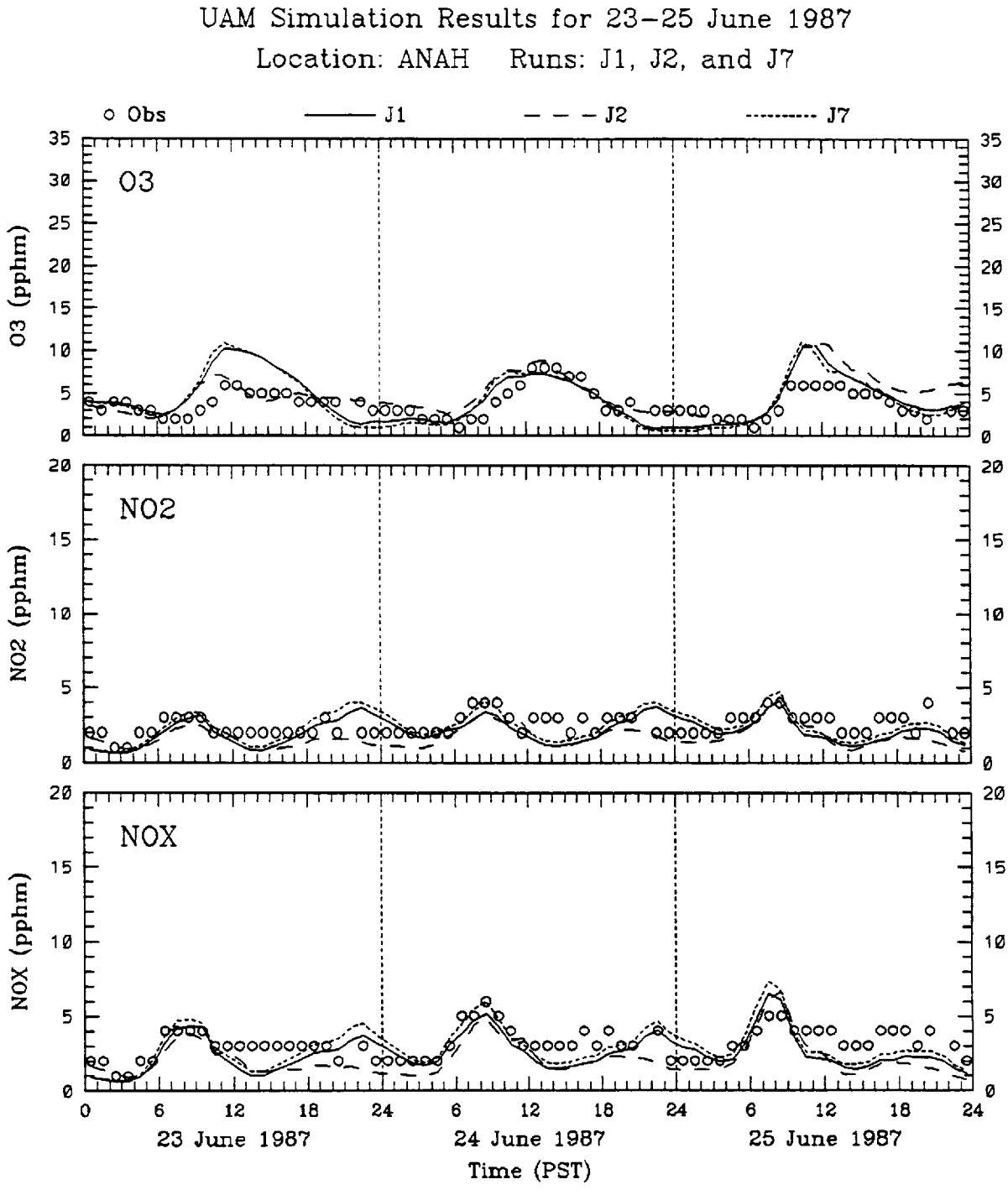
- Region H--Ventura County

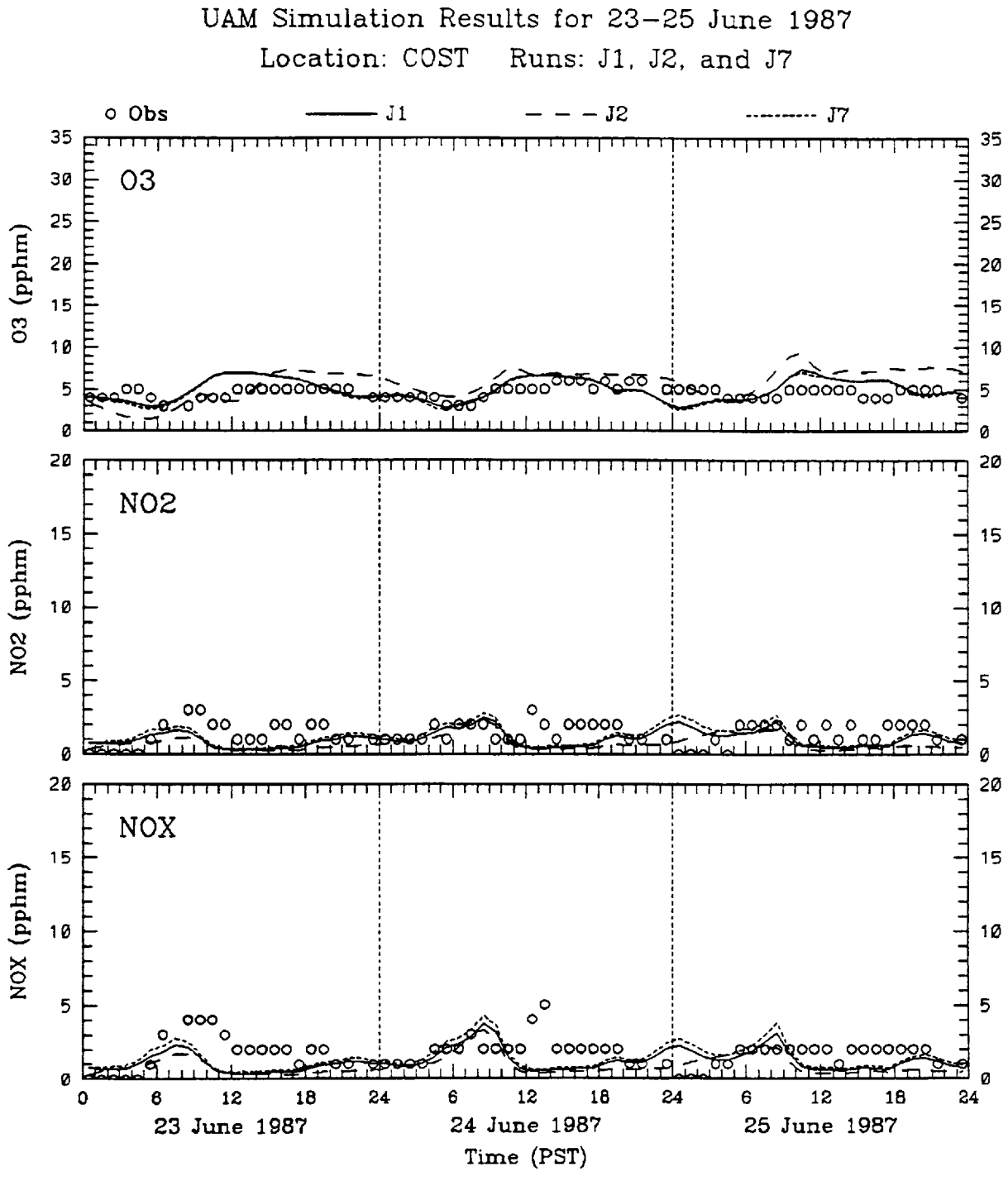
  El Rio-Rio Mesa H.S. (ERIO)
  Ojai (OJAI)
  Piru-2SW (PRU2)
  Simi Valley-Cochran (SIM2)
  Thousand Oaks-Windsor (OAKS)
  Ventura-Emma Wood (EMMA)

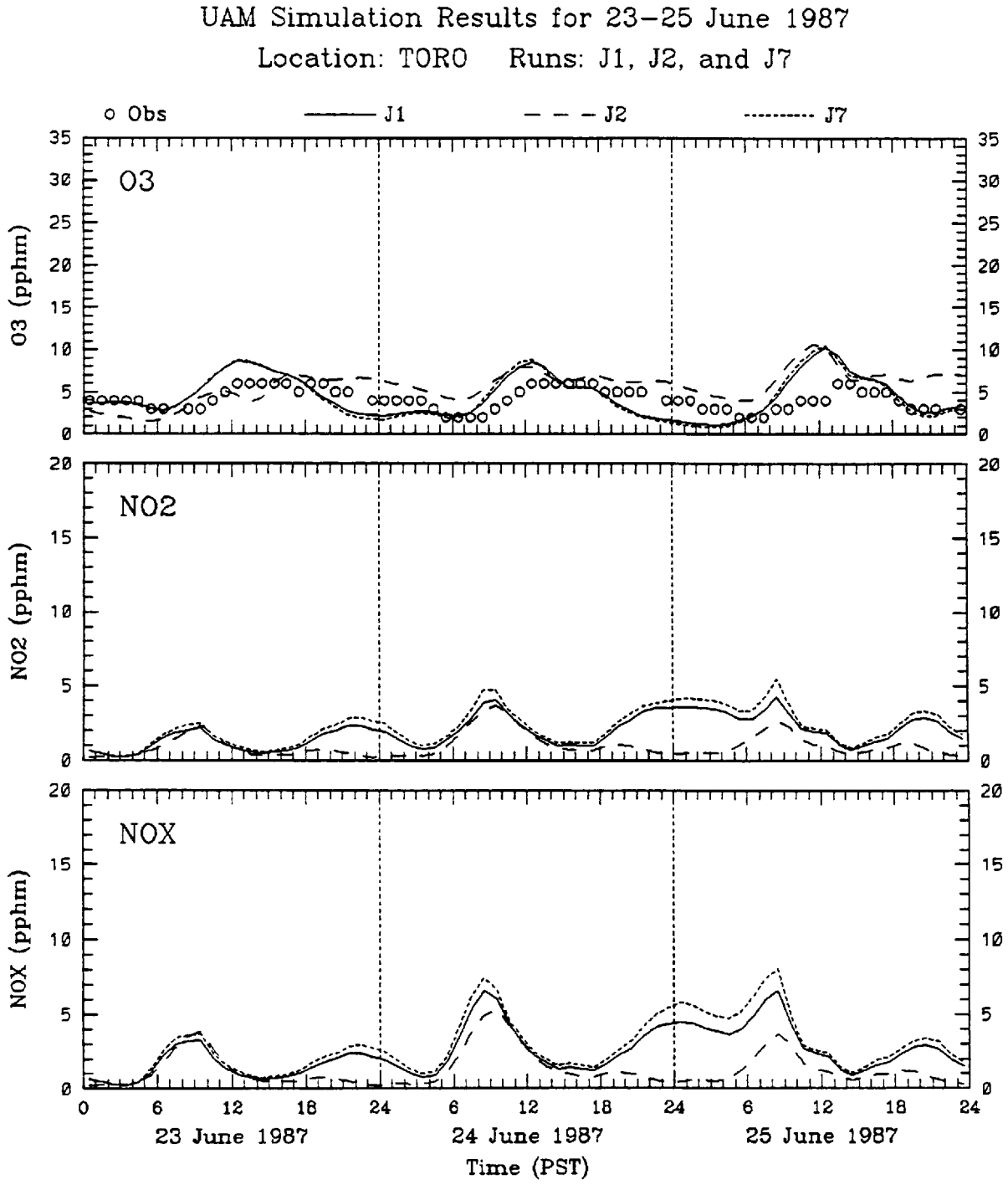
- Region I--Victorville and Hesperia

  Hesperia (HESP)
  Victorville (VICT)

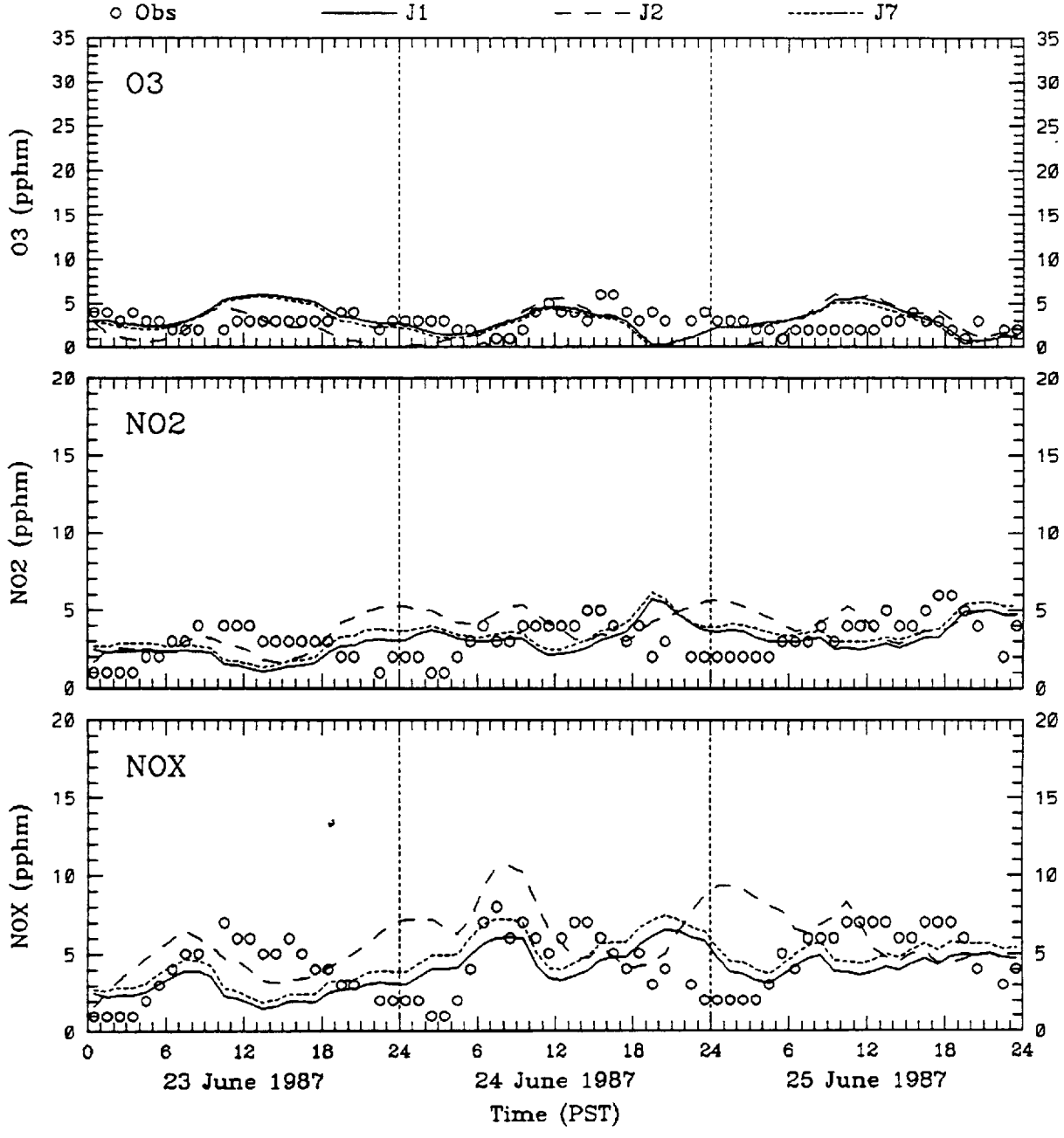
Figure 2-1 in Section 2 shows the locations of these air monitoring stations.



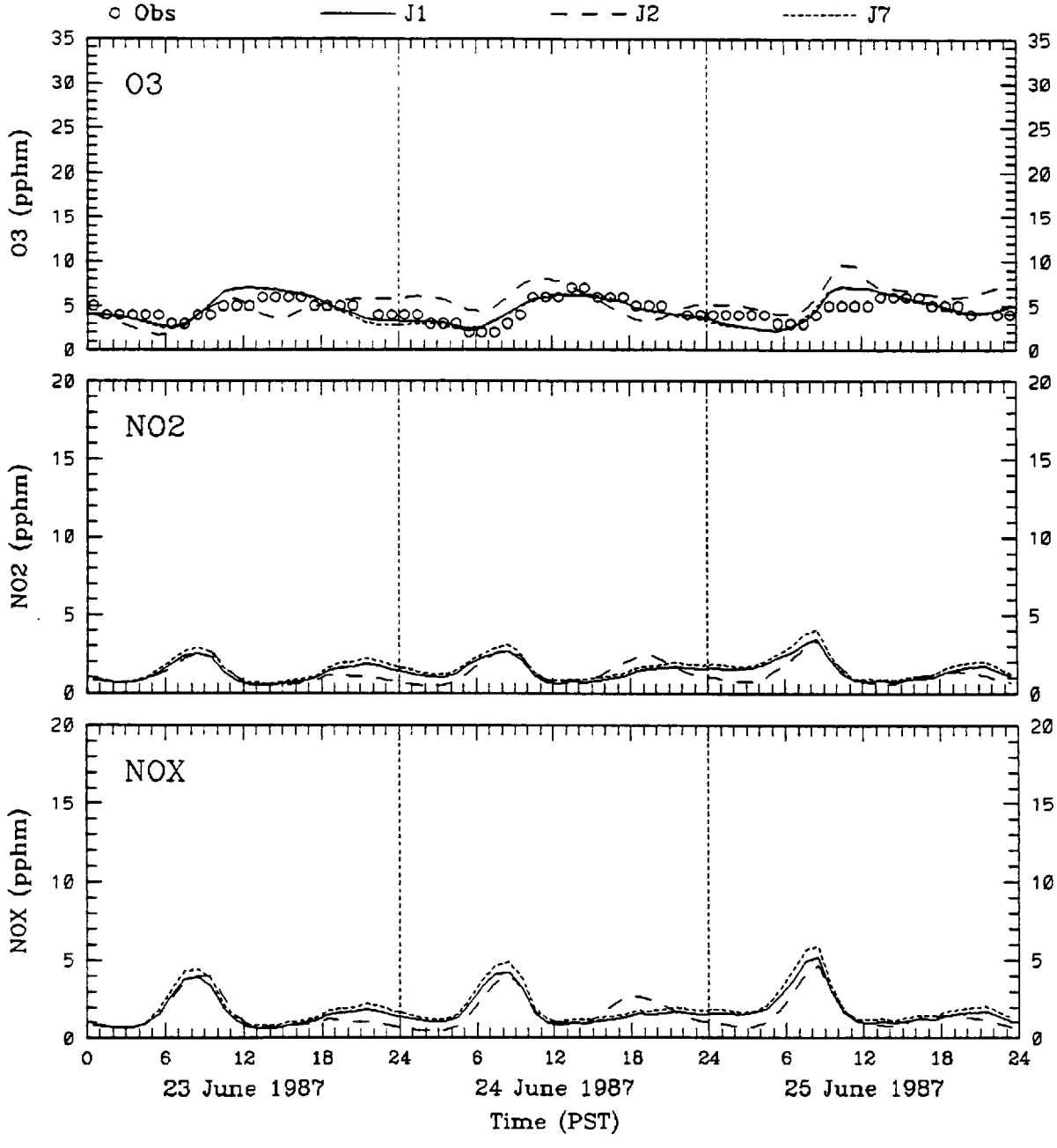


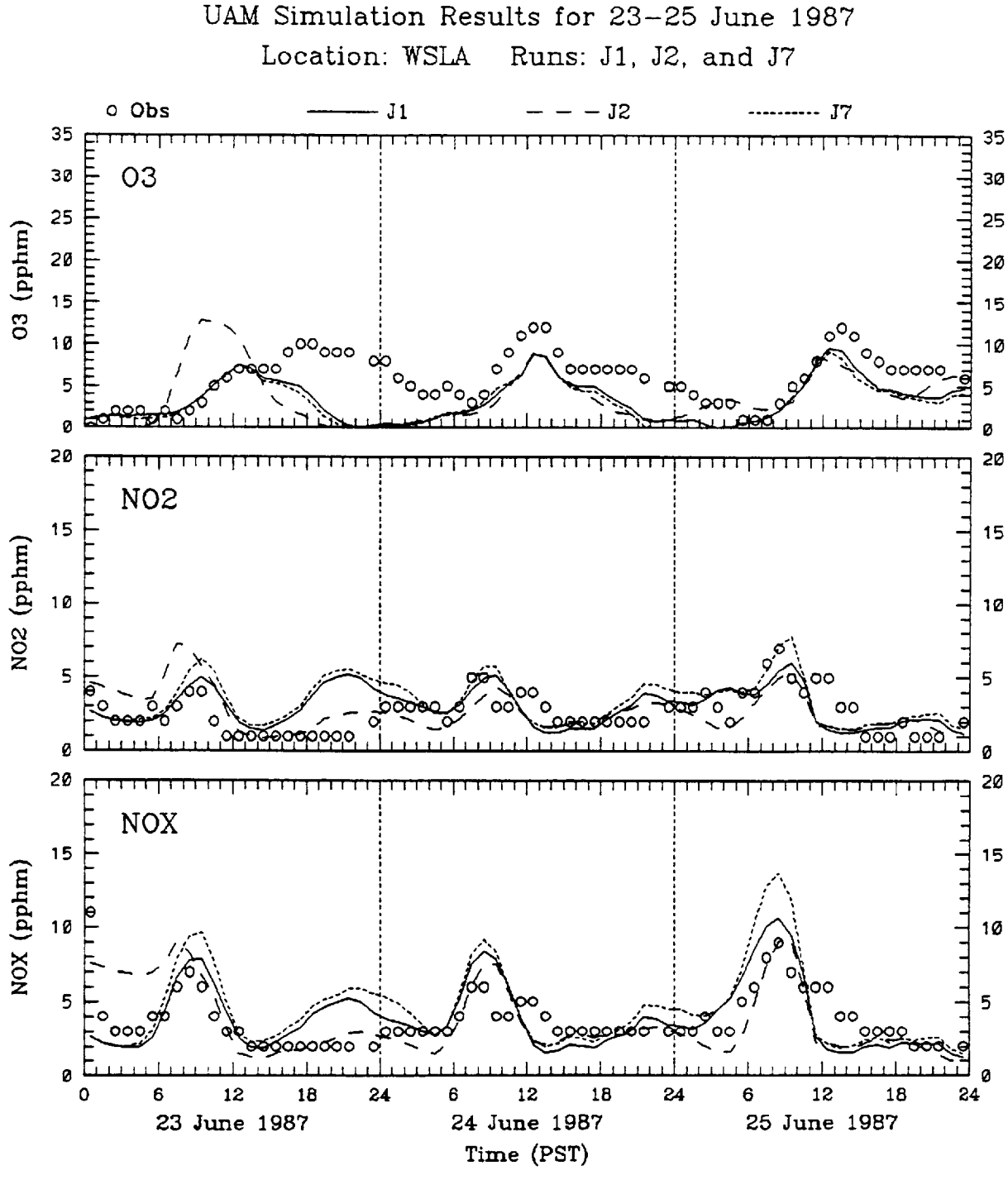


UAM Simulation Results for 23–25 June 1987
Location: LGBH Runs: J1, J2, and J7

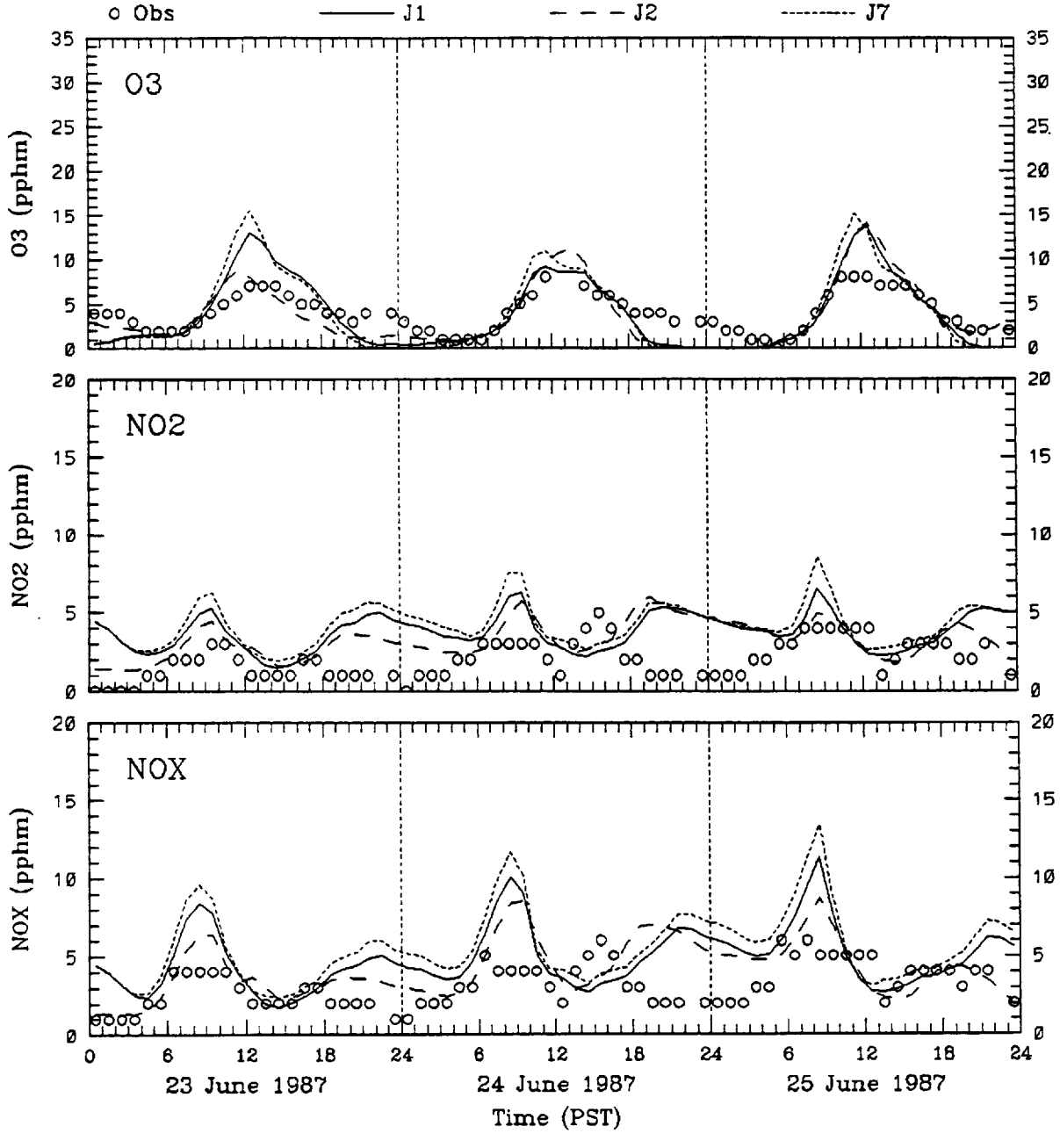


UAM Simulation Results for 23–25 June 1987
Location: LSAL Runs: J1, J2, and J7

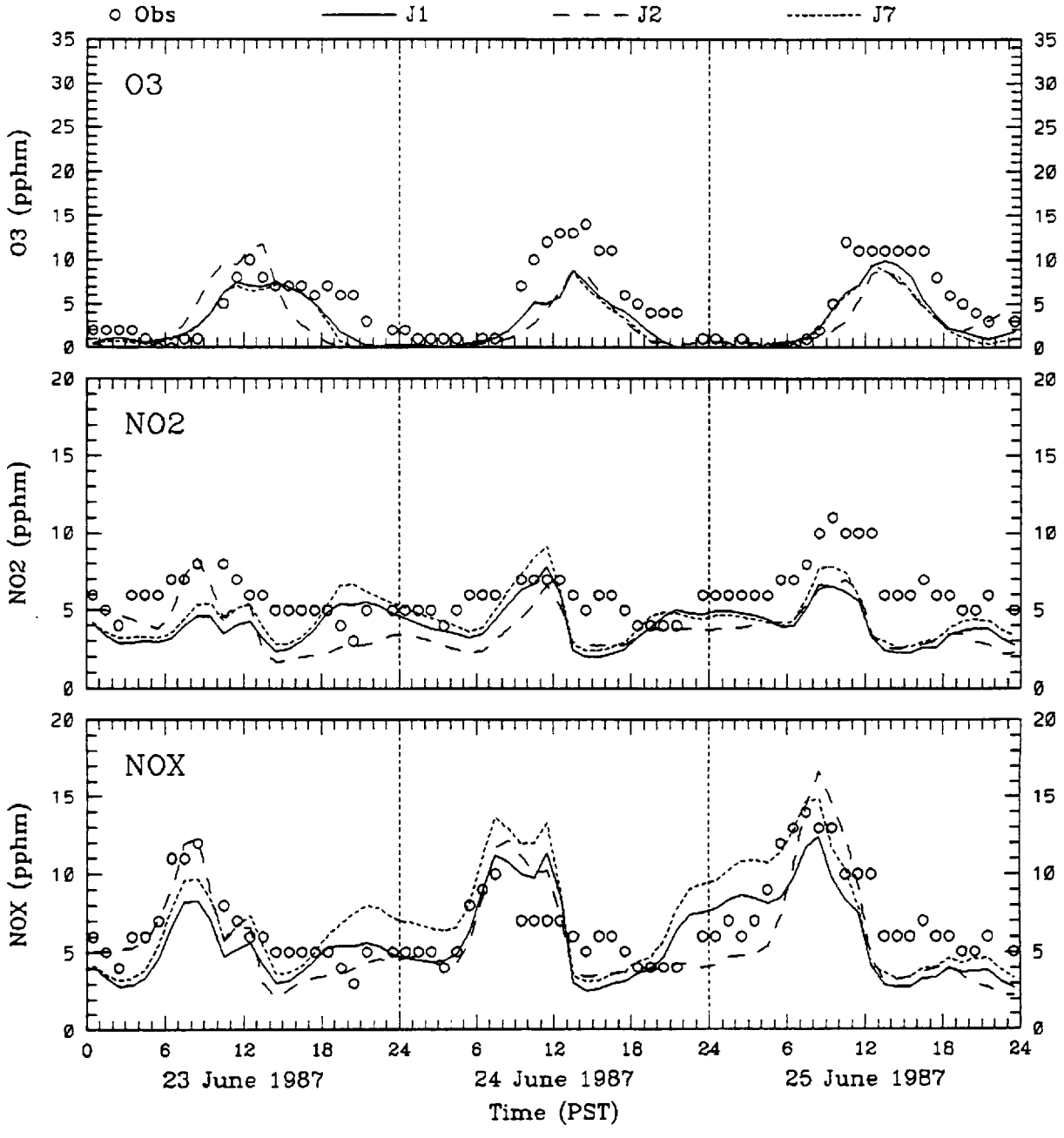




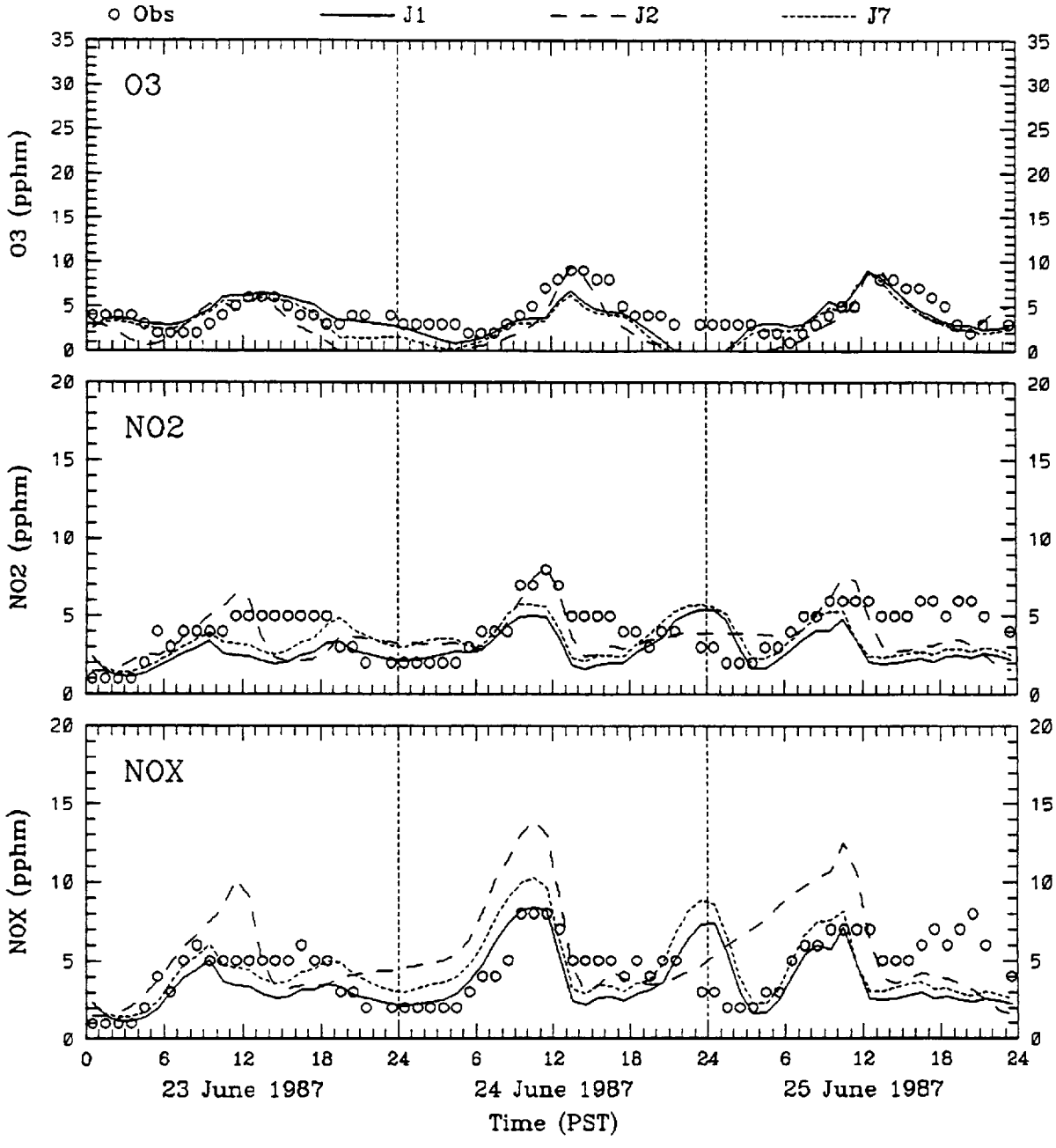
UAM Simulation Results for 23–25 June 1987
Location: LAHB Runs: J1, J2, and J7

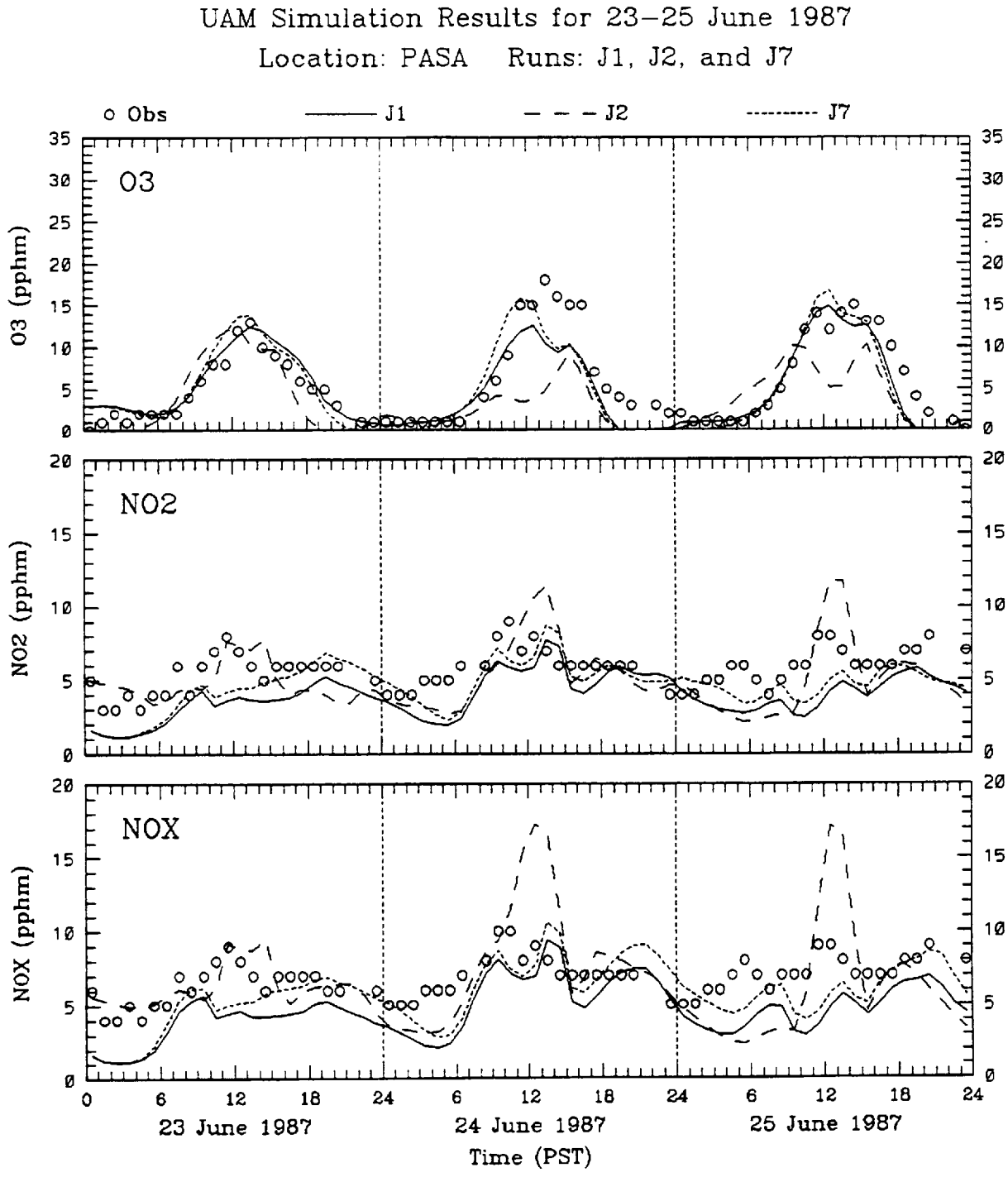


UAM Simulation Results for 23–25 June 1987
Location: CELA Runs: J1, J2, and J7

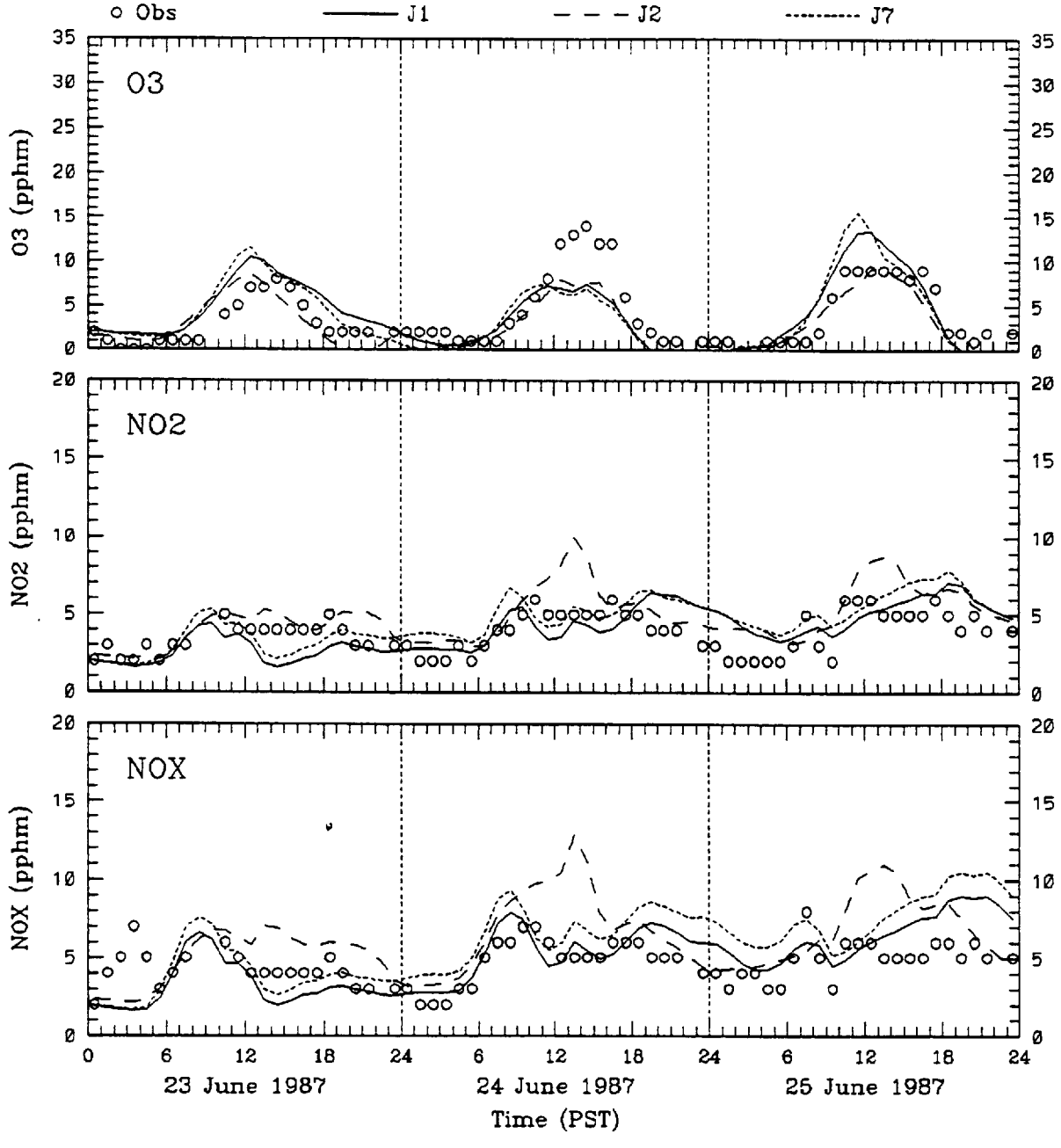


UAM Simulation Results for 23–25 June 1987
Location: LYNN Runs: J1, J2, and J7

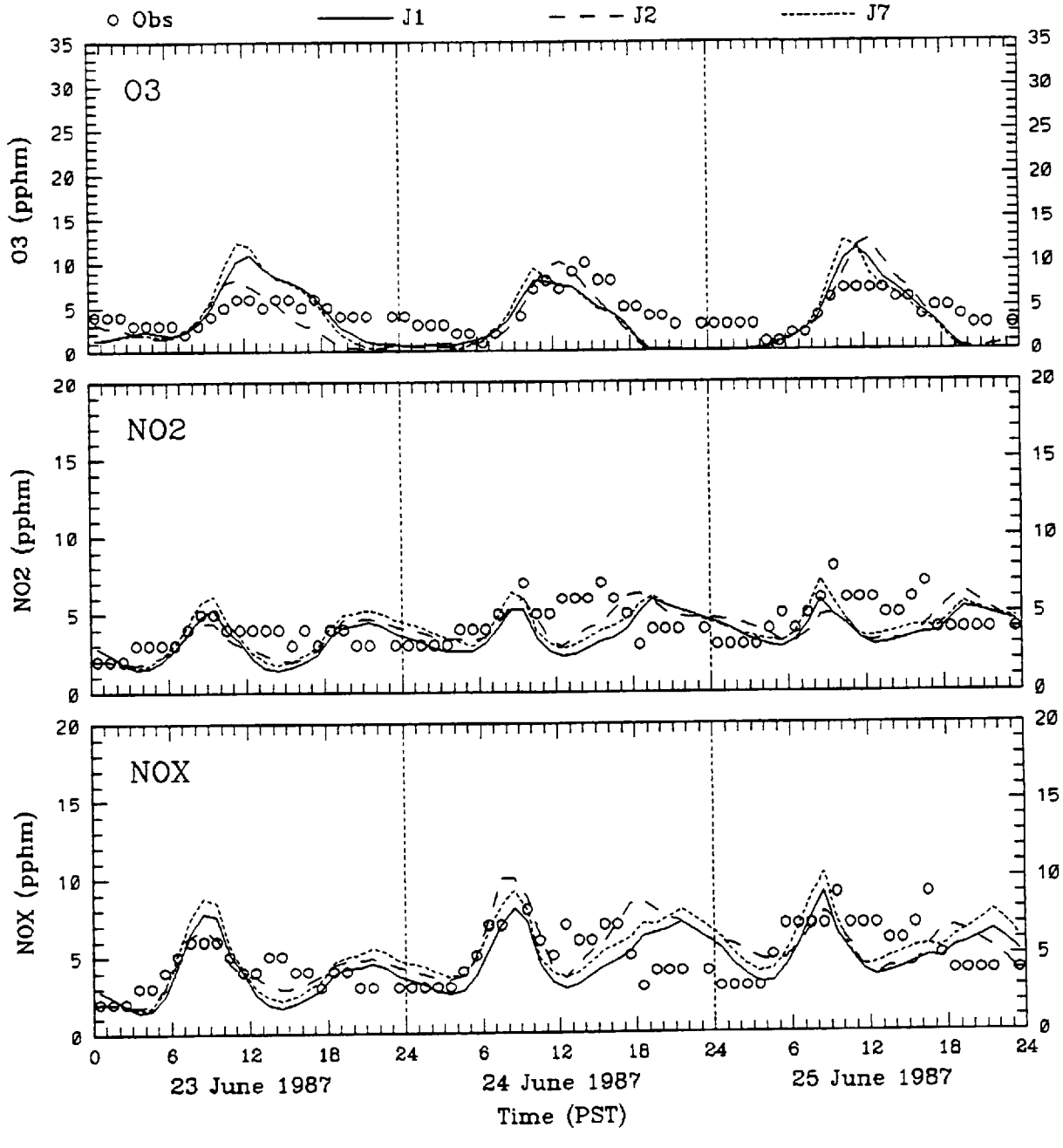


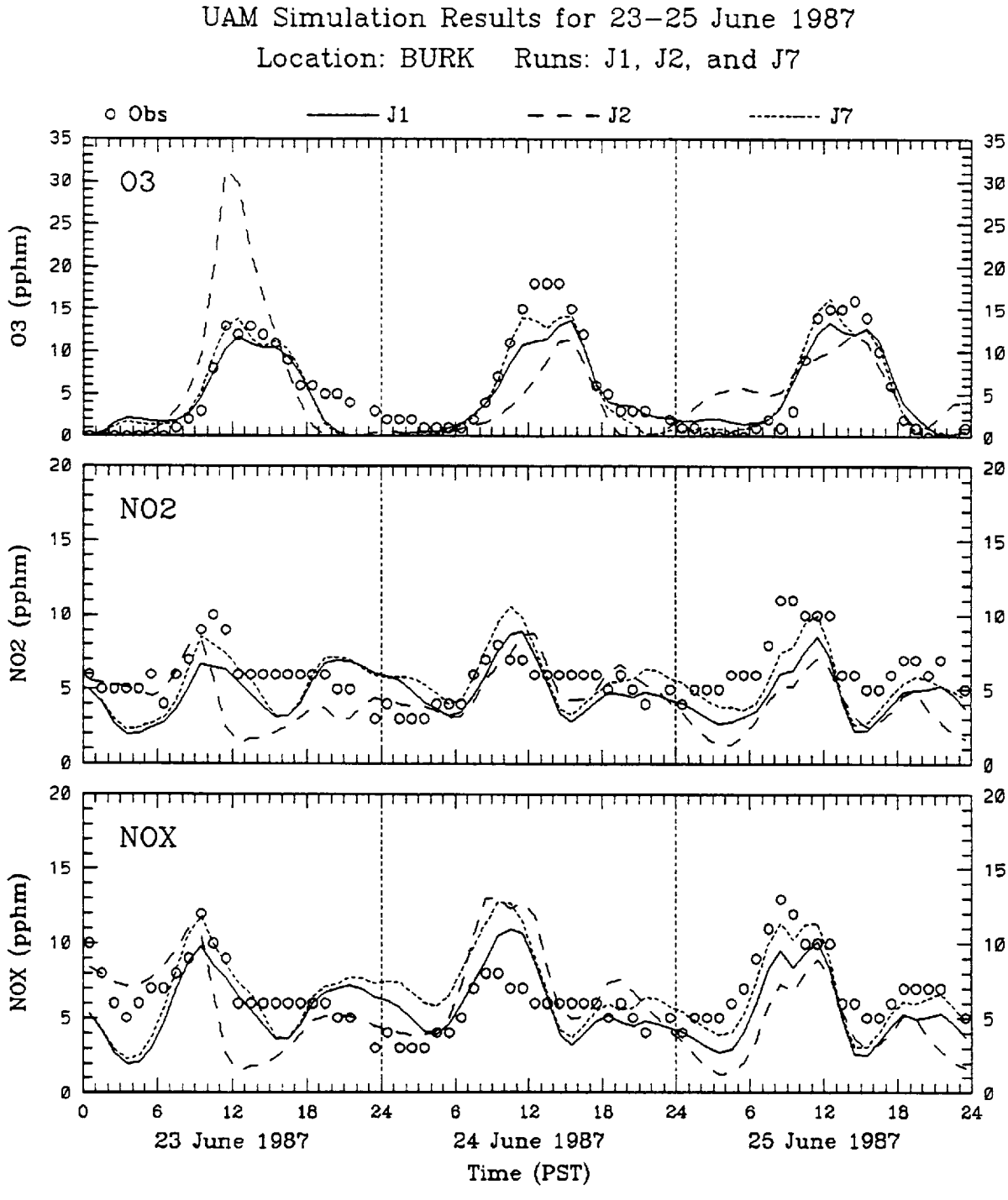


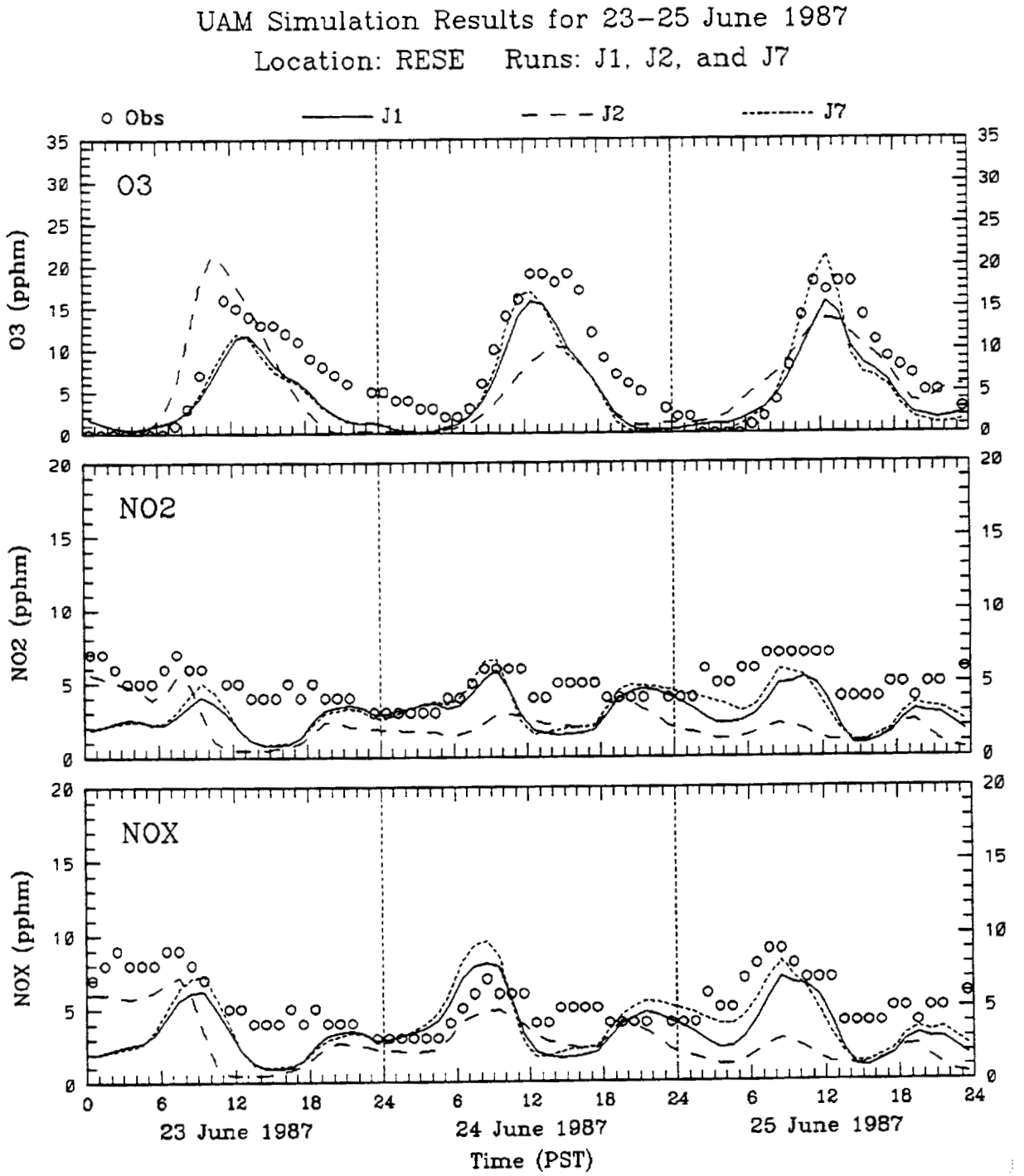
UAM Simulation Results for 23–25 June 1987
Location: PICO Runs: J1, J2, and J7



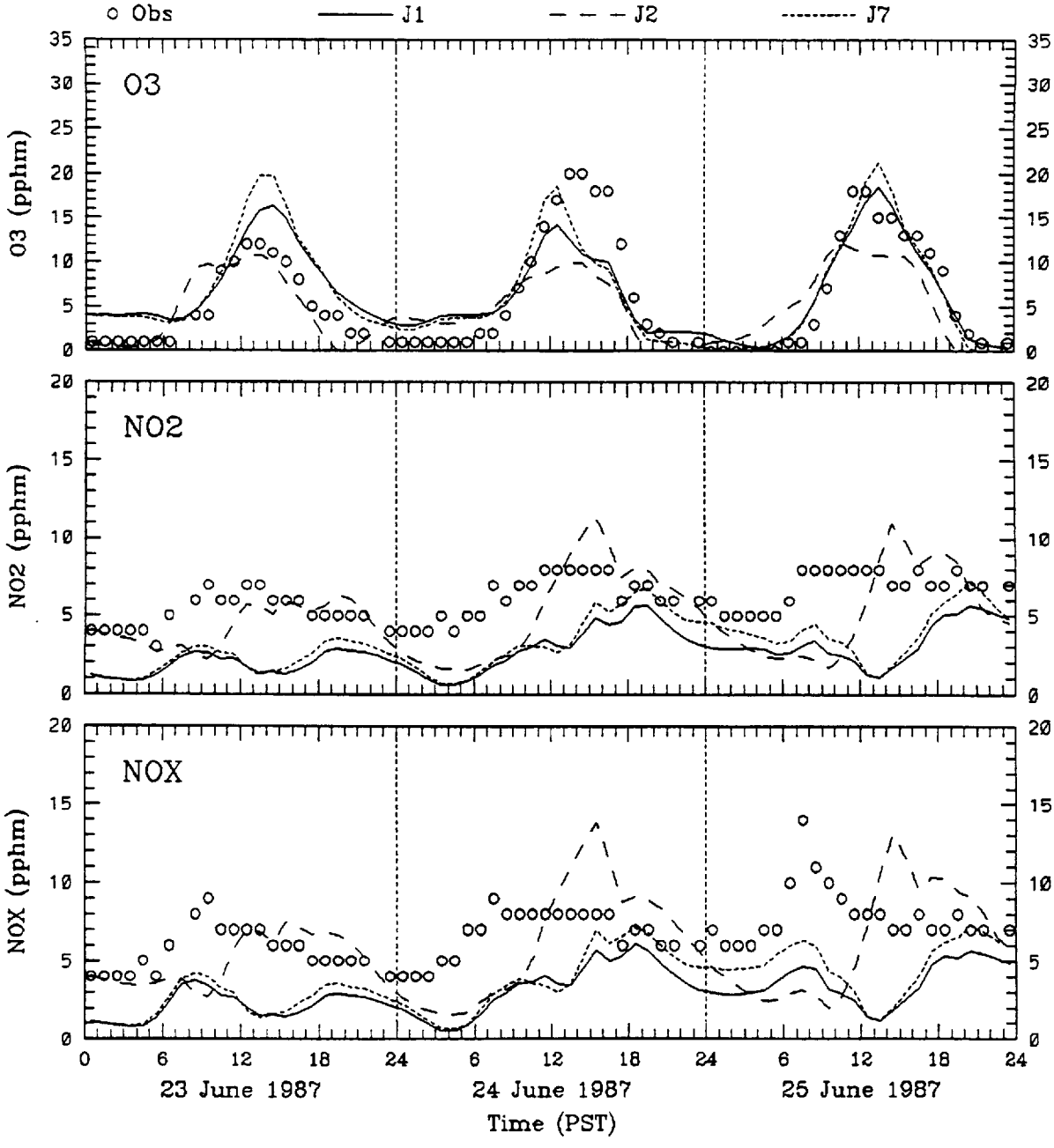
UAM Simulation Results for 23–25 June 1987
Location: WHIT Runs: J1, J2, and J7

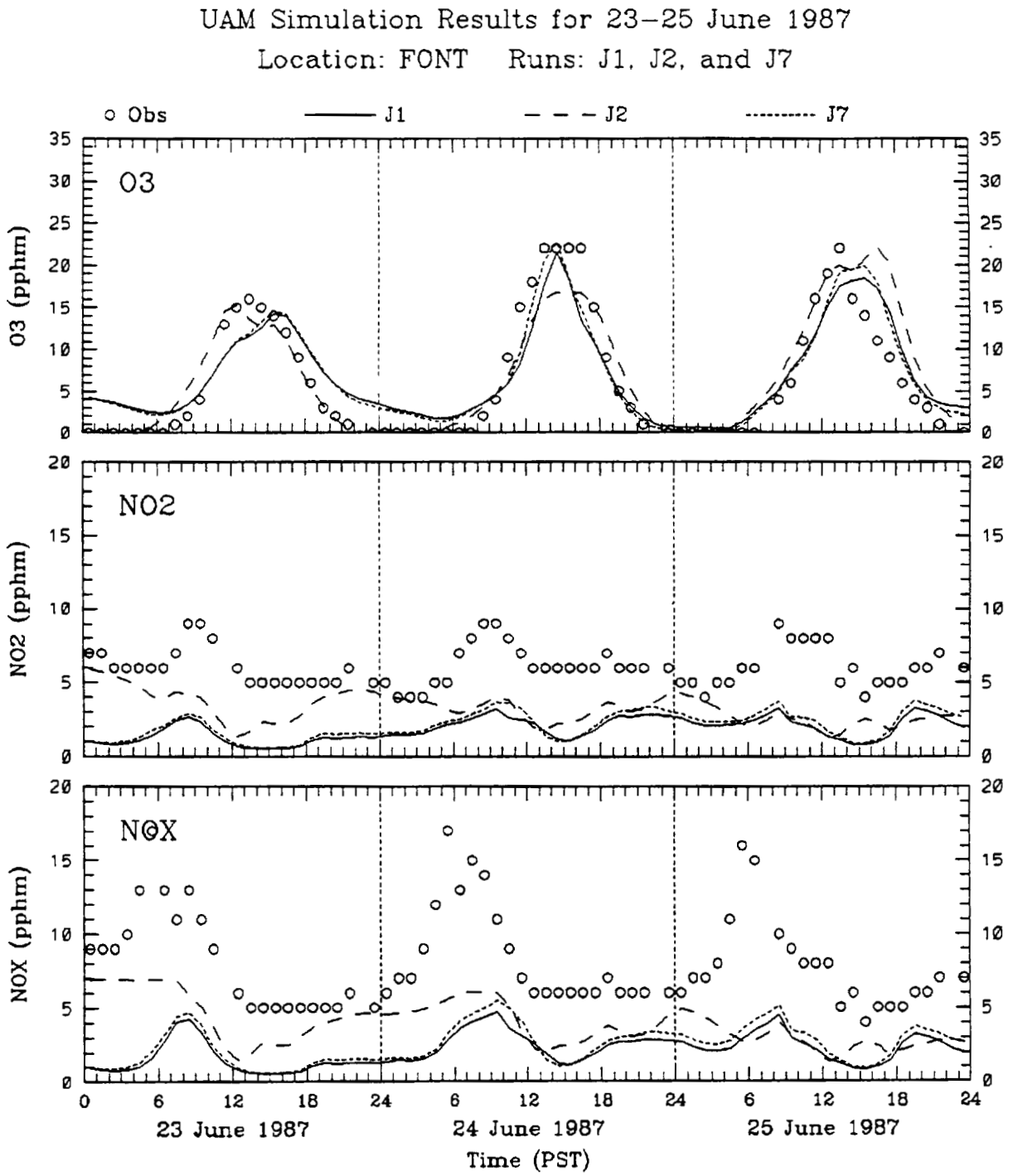




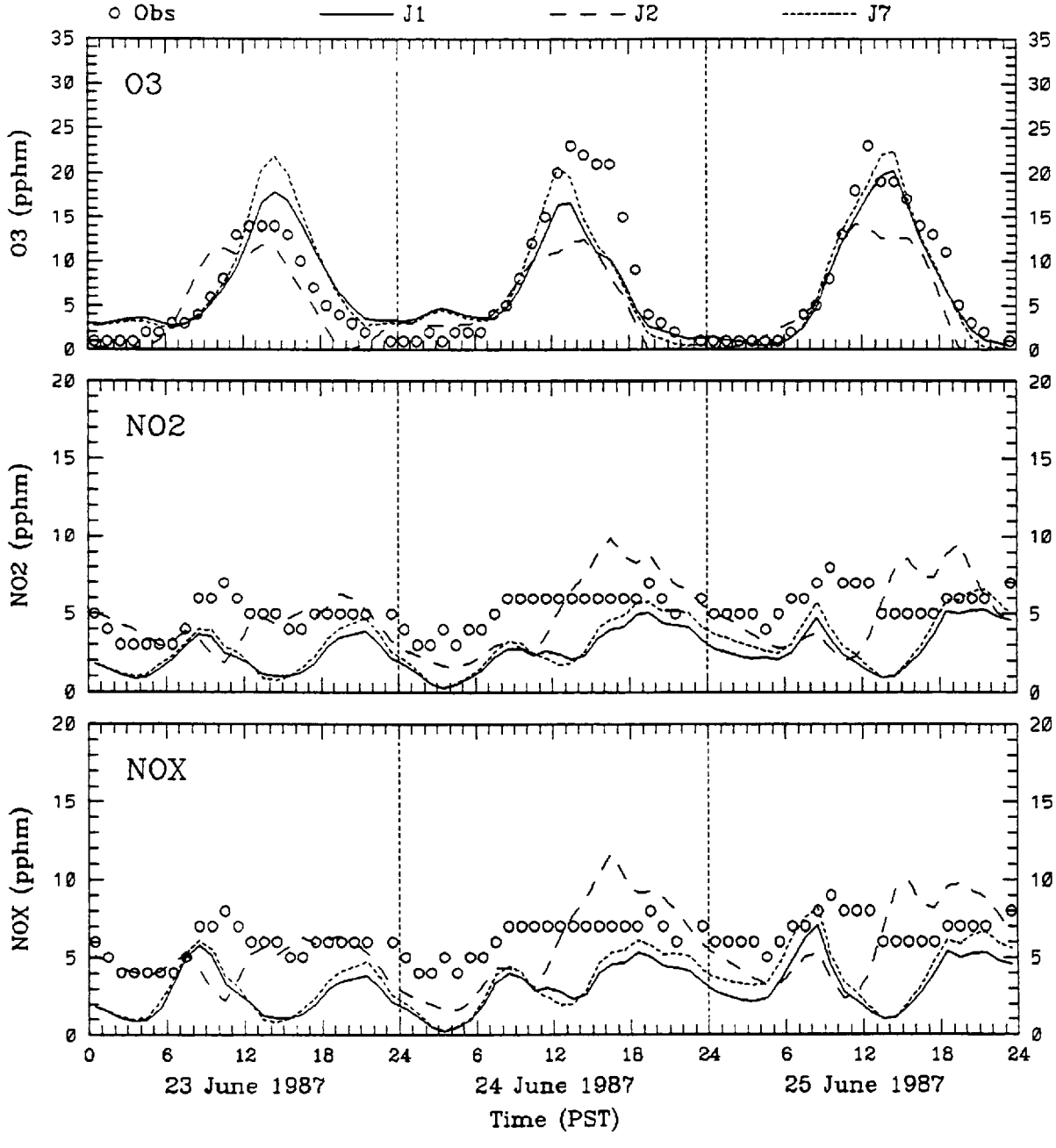


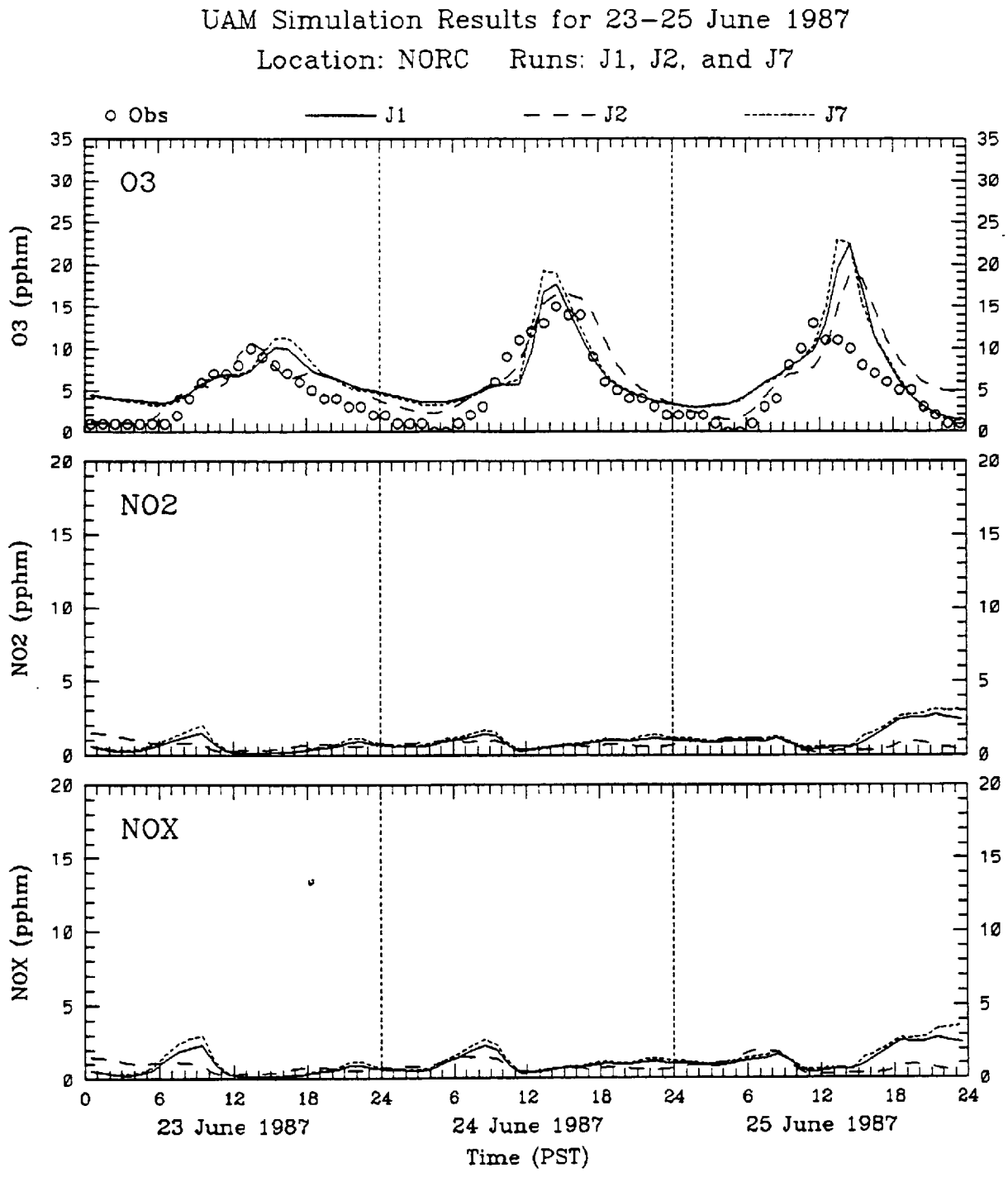
UAM Simulation Results for 23–25 June 1987
Location: AZUS Runs: J1, J2, and J7



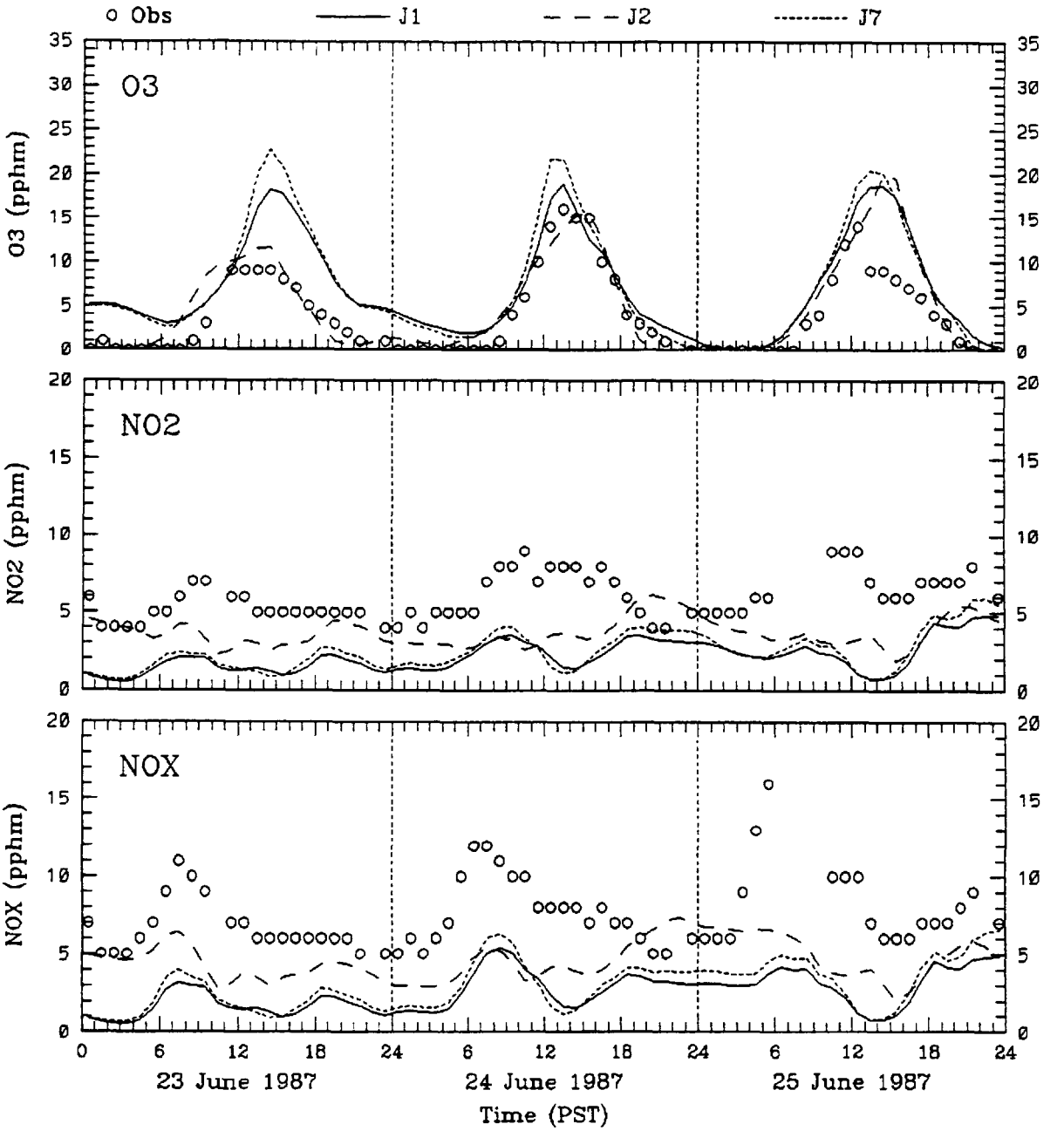


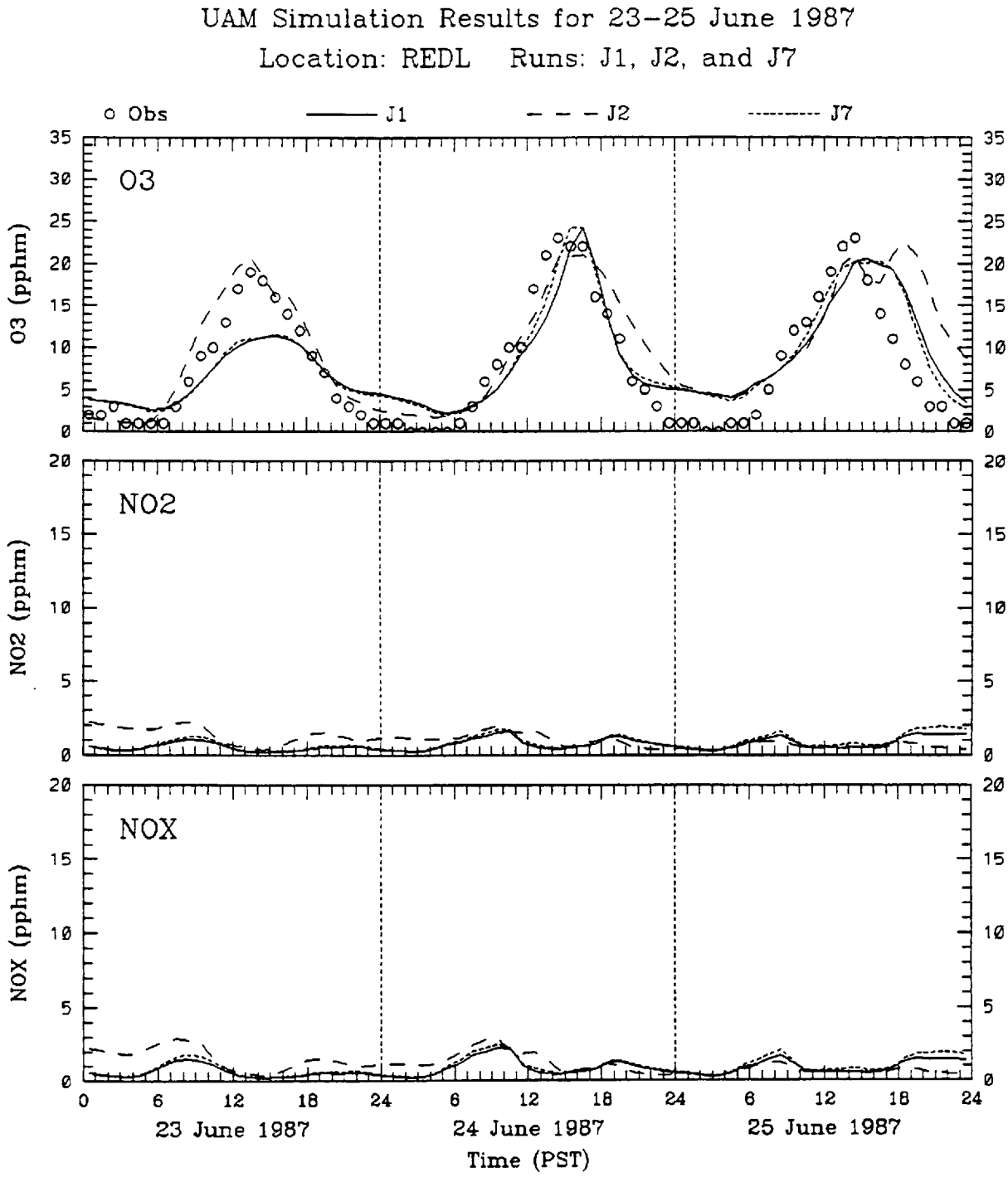
UAM Simulation Results for 23–25 June 1987
Location: GLEN Runs: J1, J2, and J7

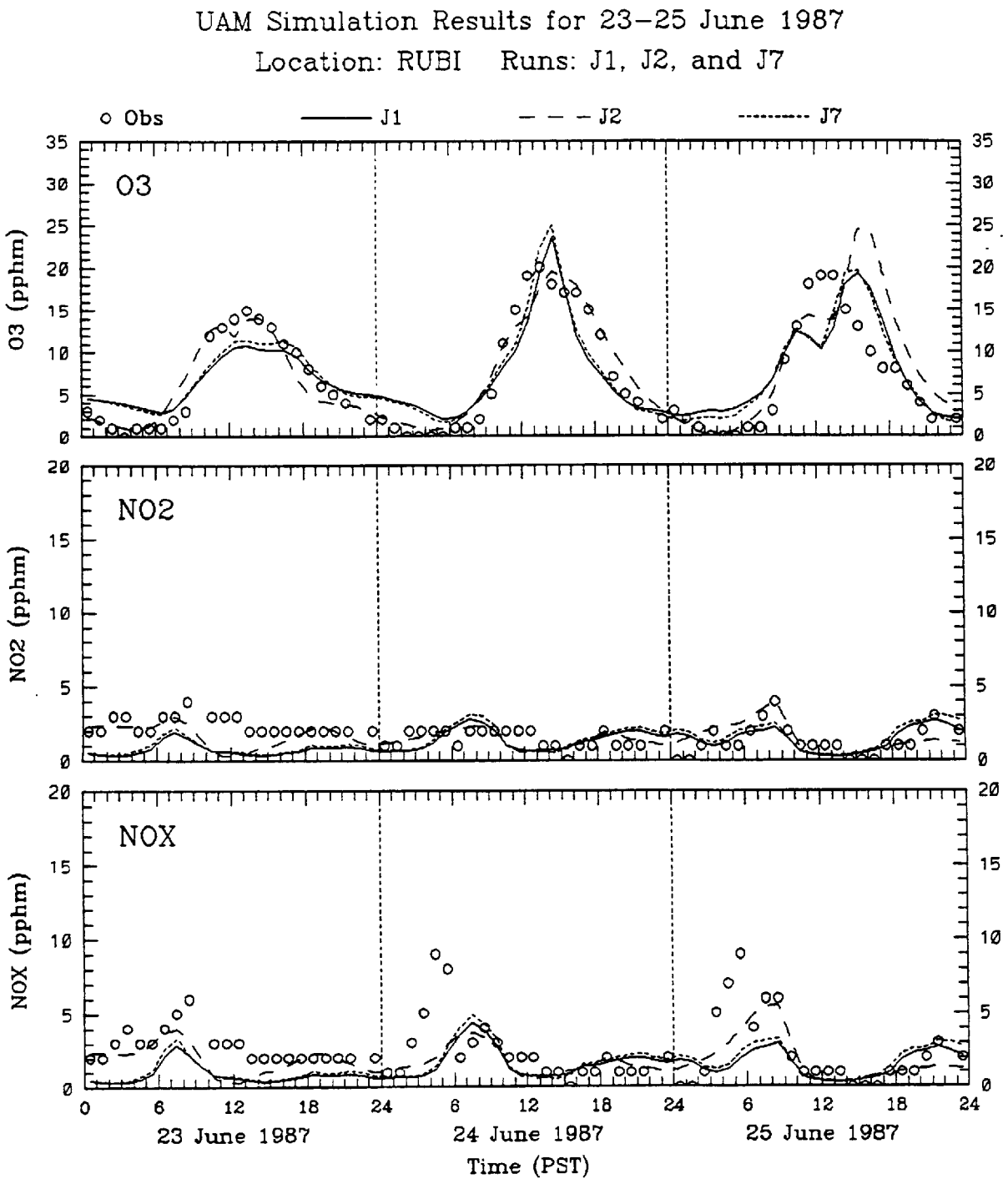


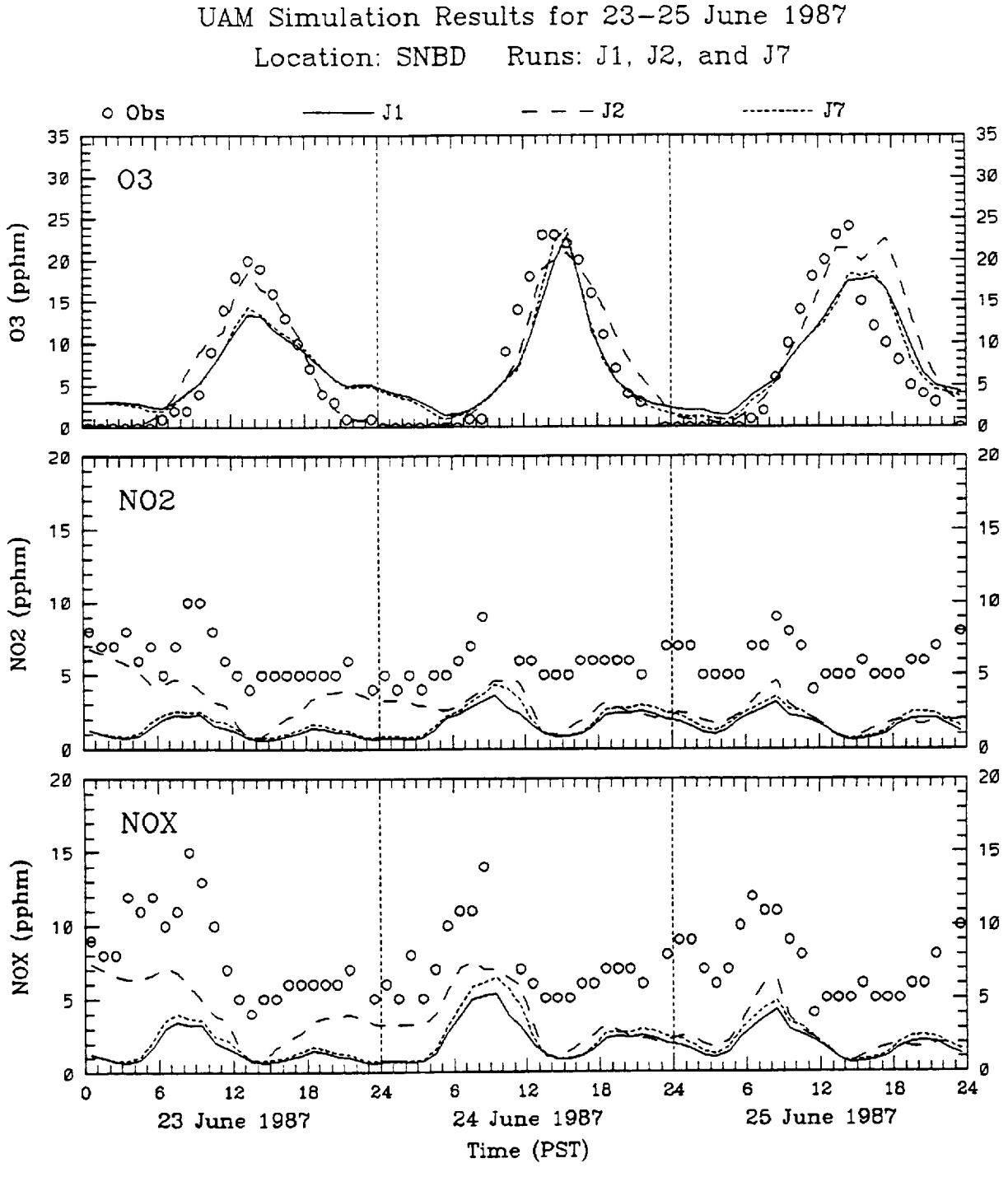


UAM Simulation Results for 23–25 June 1987
Location: POMO Runs: J1, J2, and J7

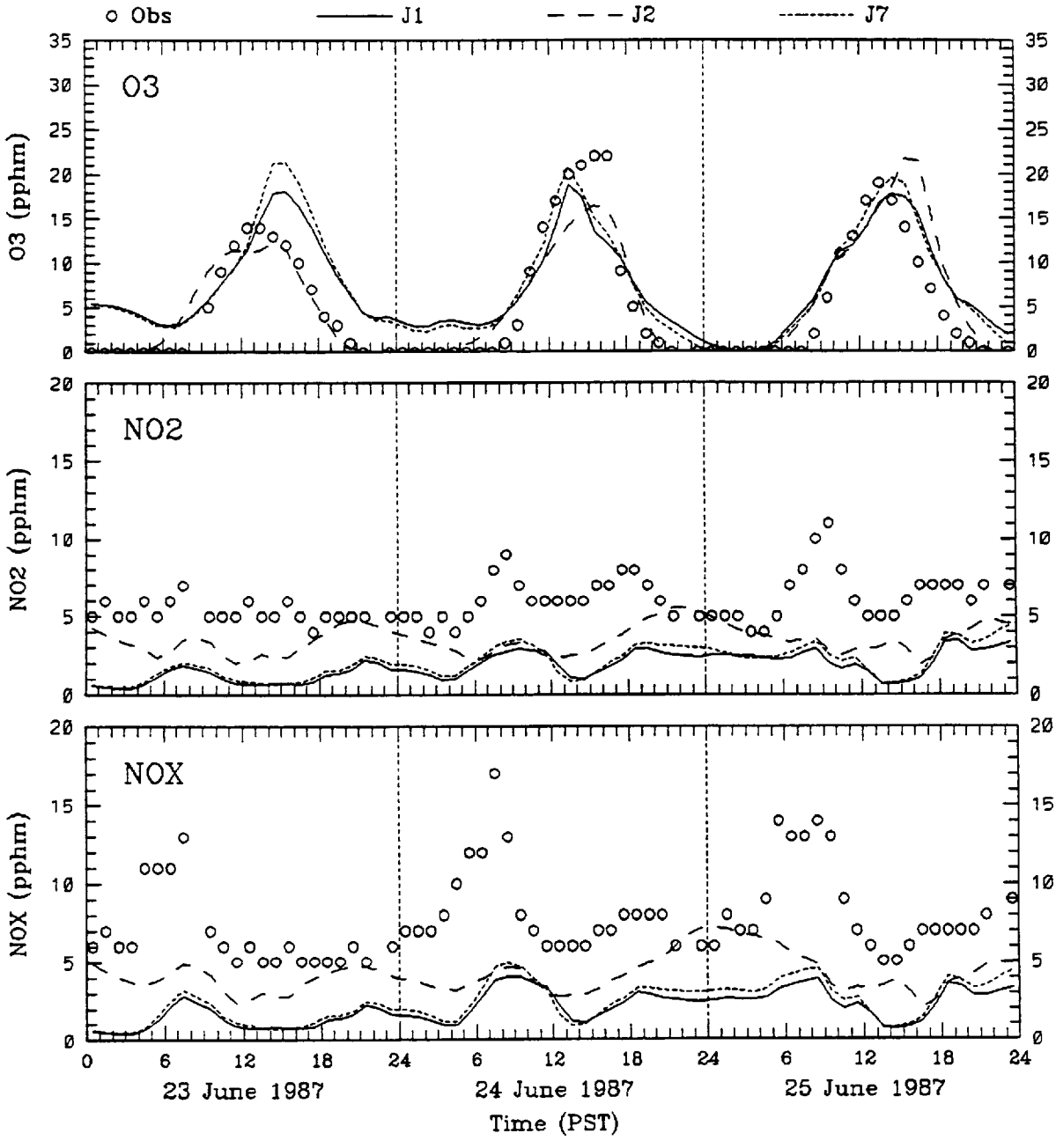


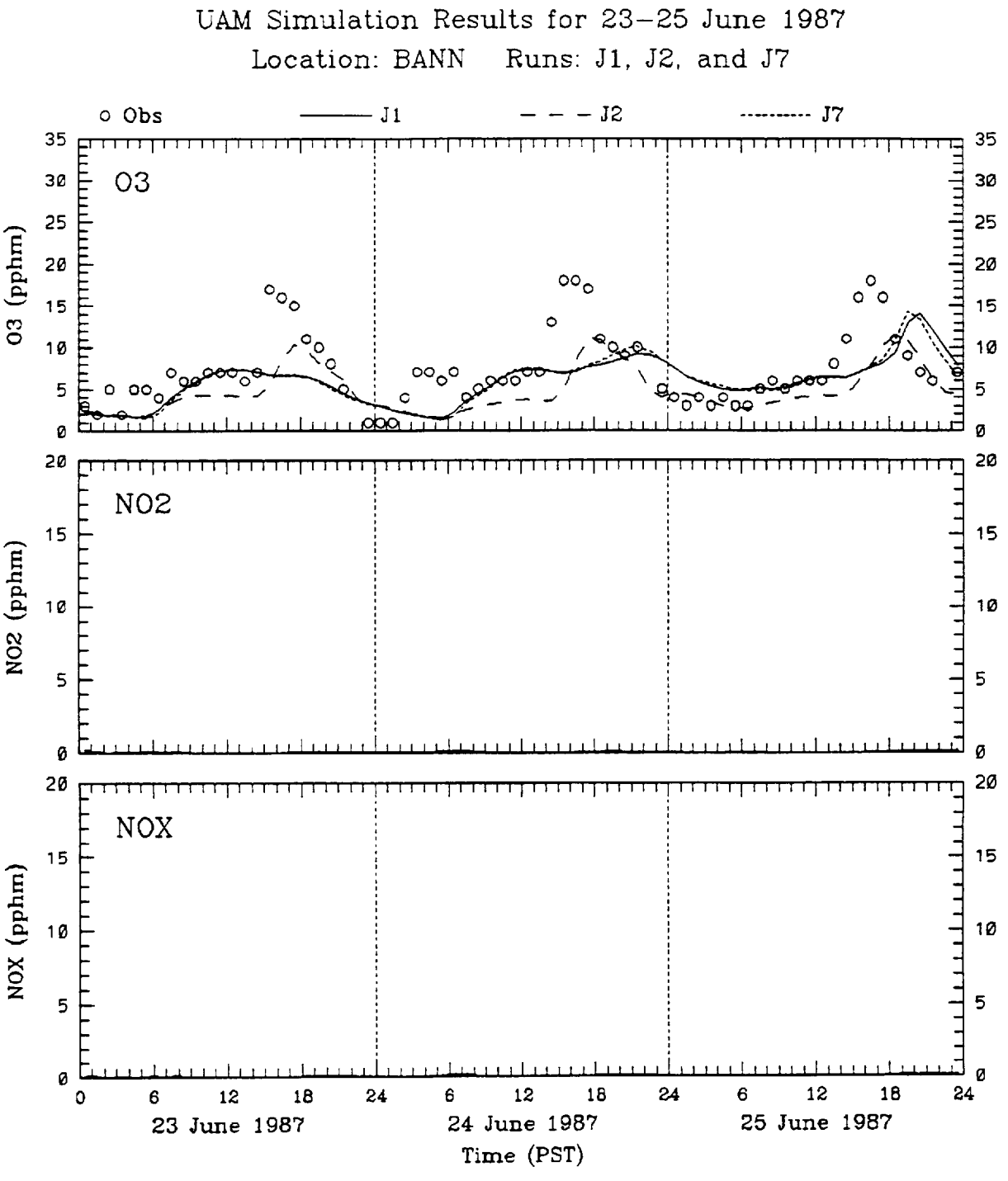




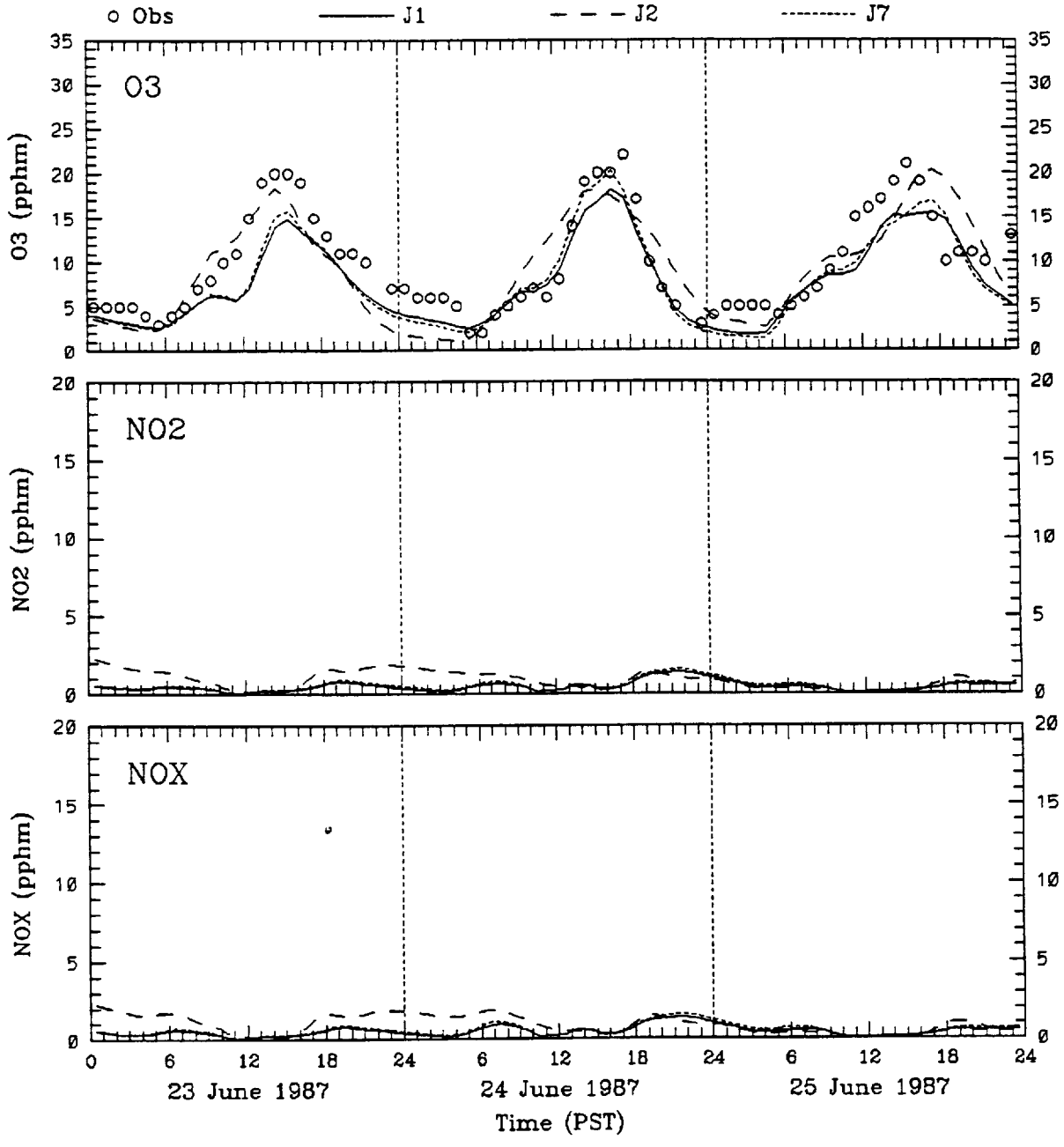


UAM Simulation Results for 23-25 June 1987
Location: UPLA Runs: J1, J2, and J7

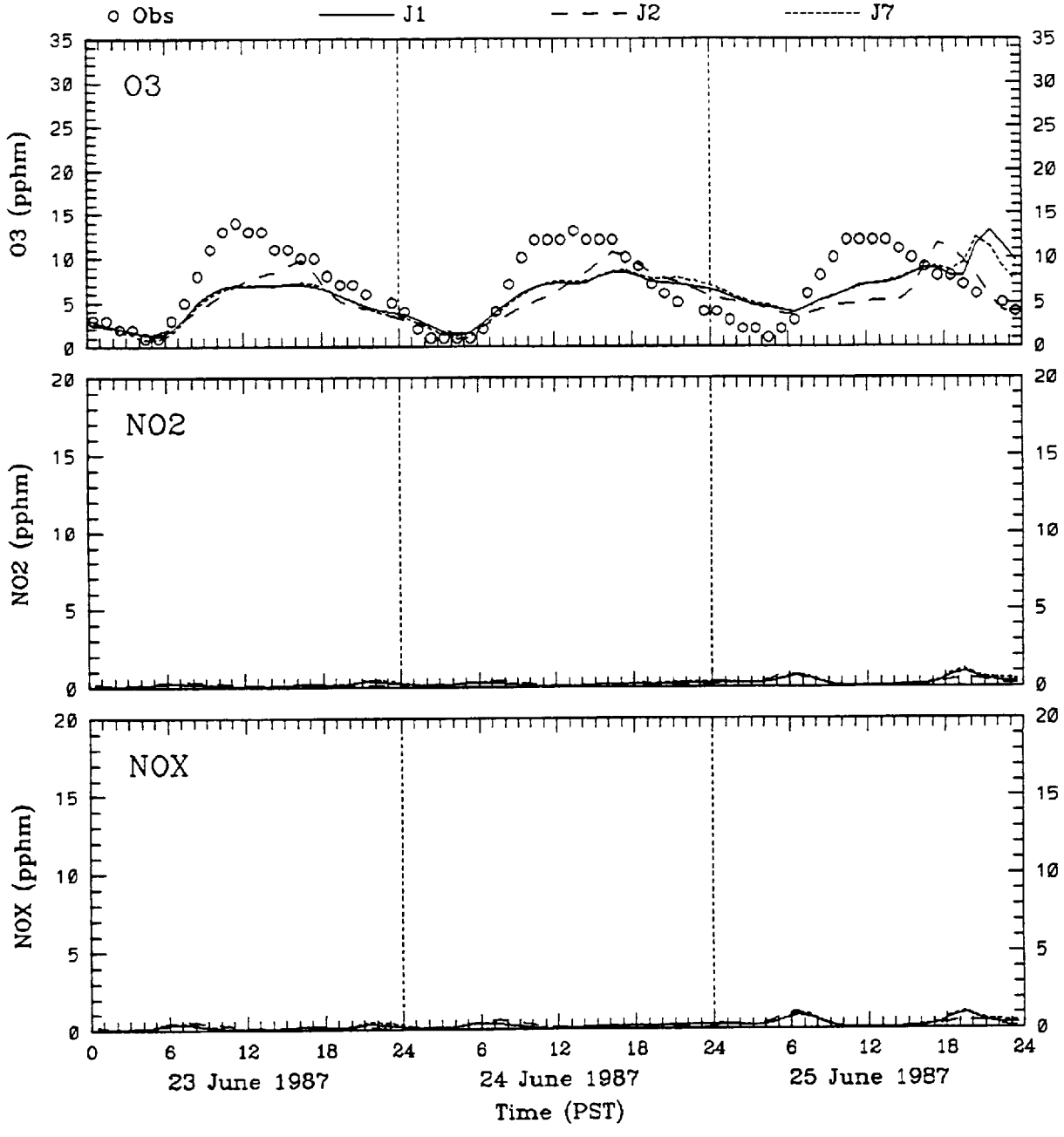




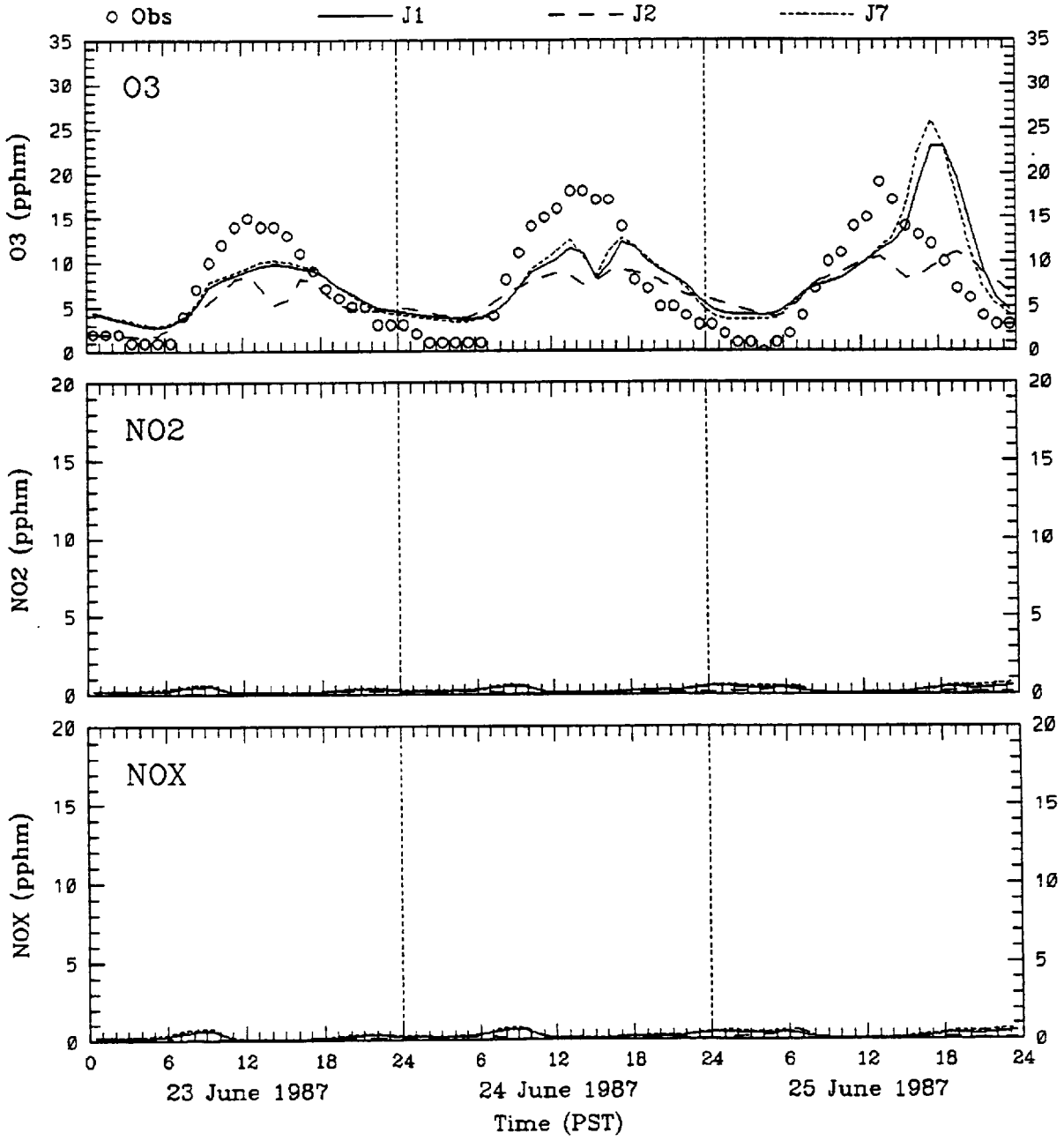
UAM Simulation Results for 23–25 June 1987
Location: CRES Runs: J1, J2, and J7

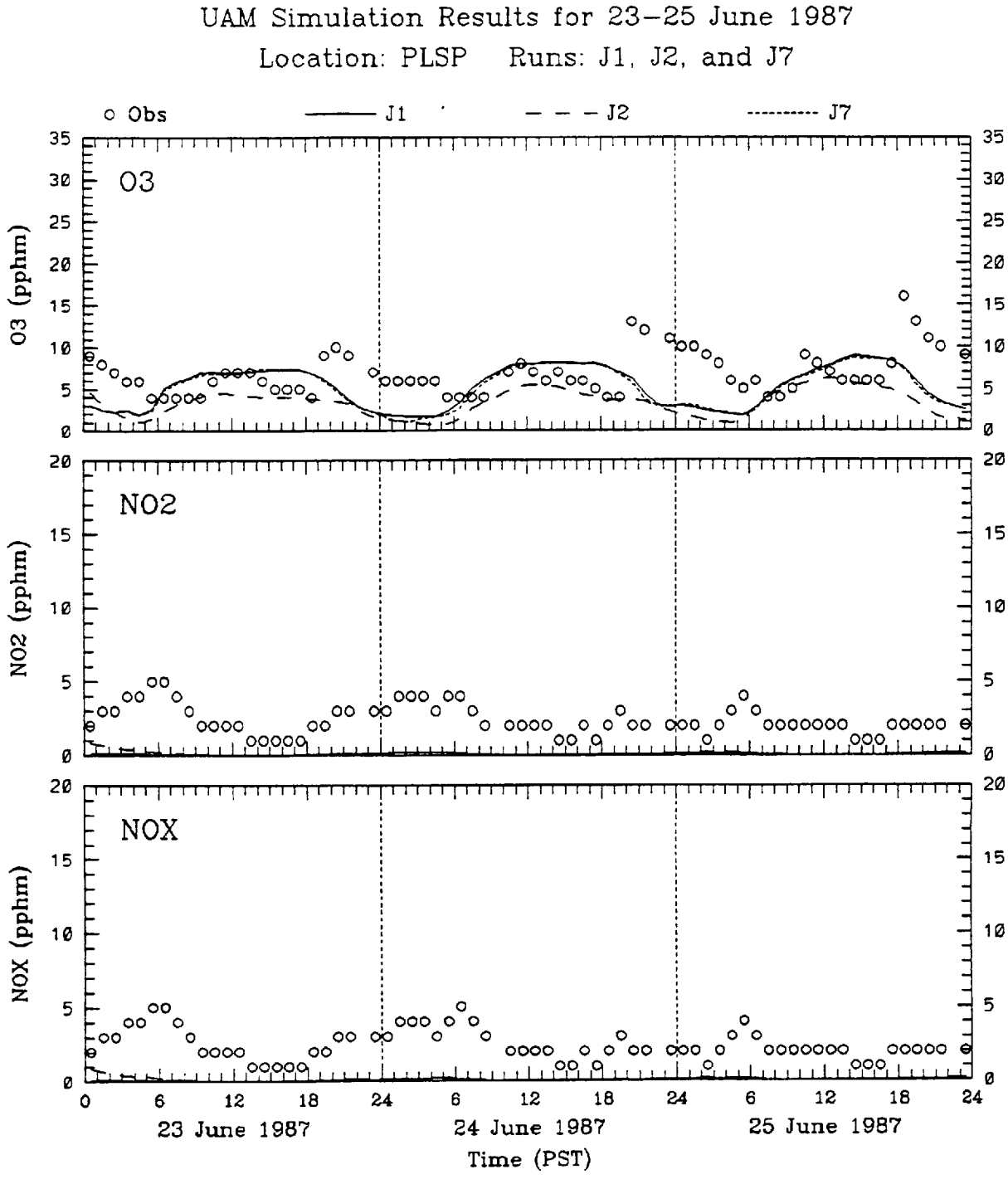


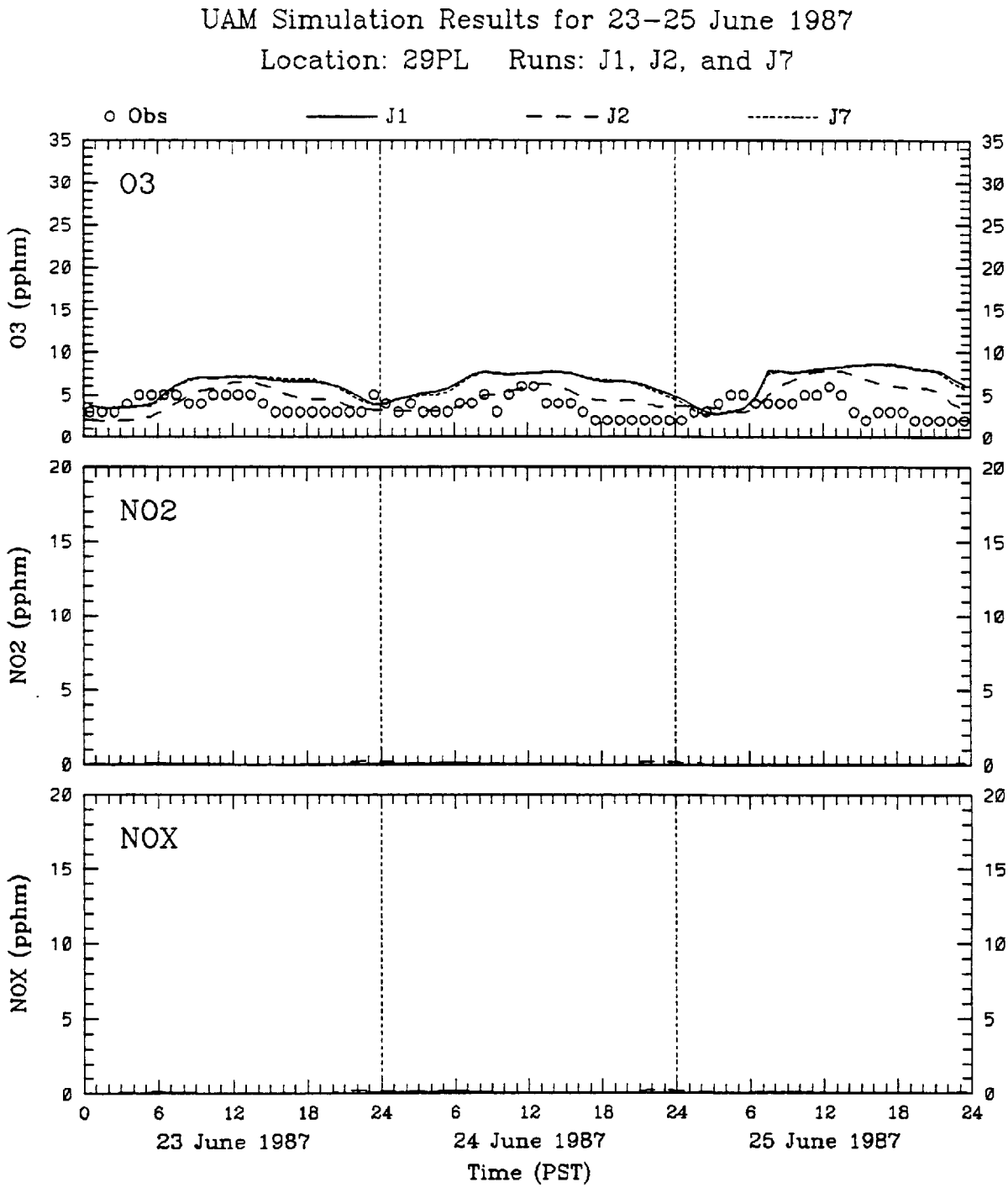
UAM Simulation Results for 23–25 June 1987
Location: HEME Runs: J1, J2, and J7

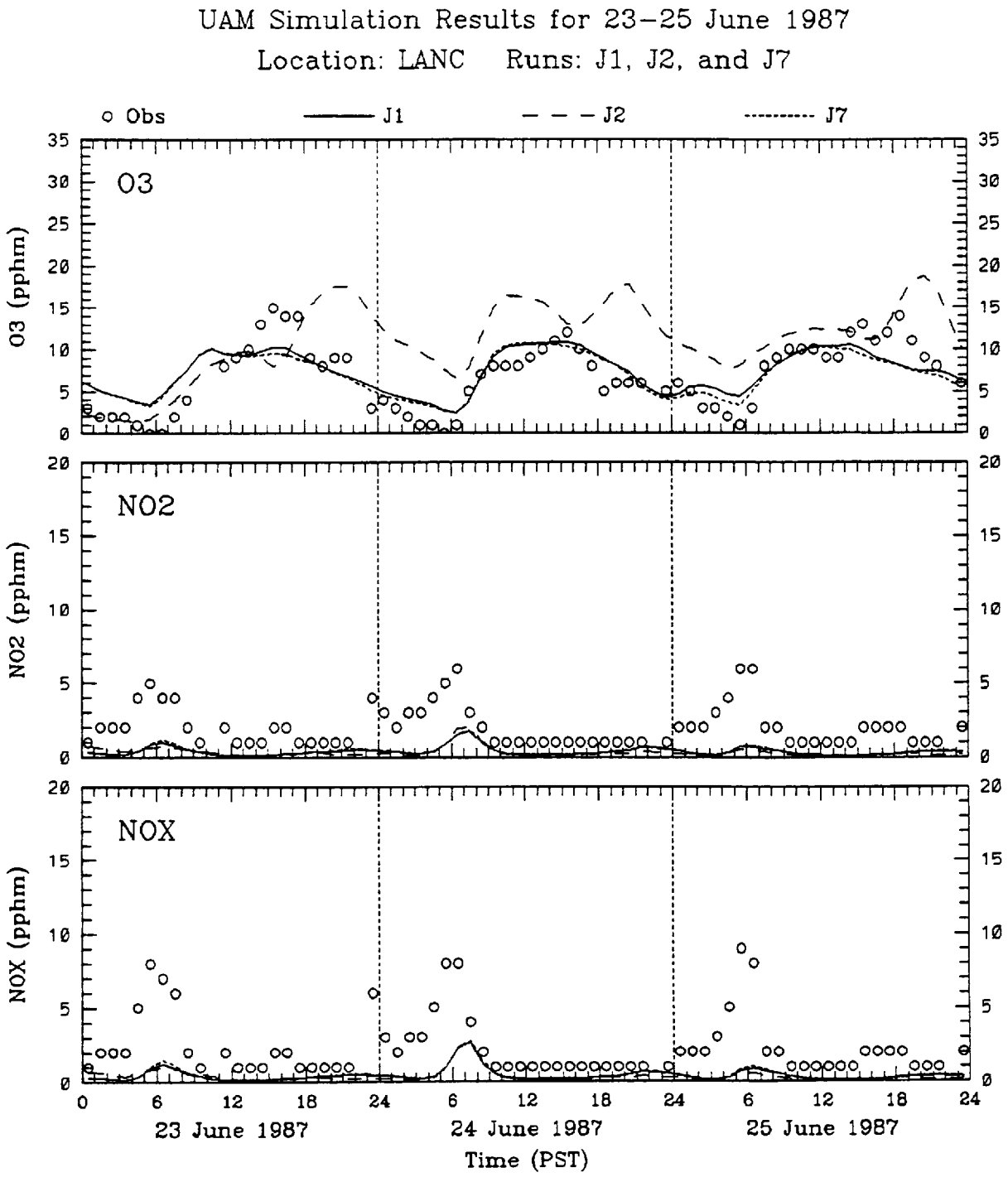


UAM Simulation Results for 23–25 June 1987
Location: PERI Runs: J1, J2, and J7

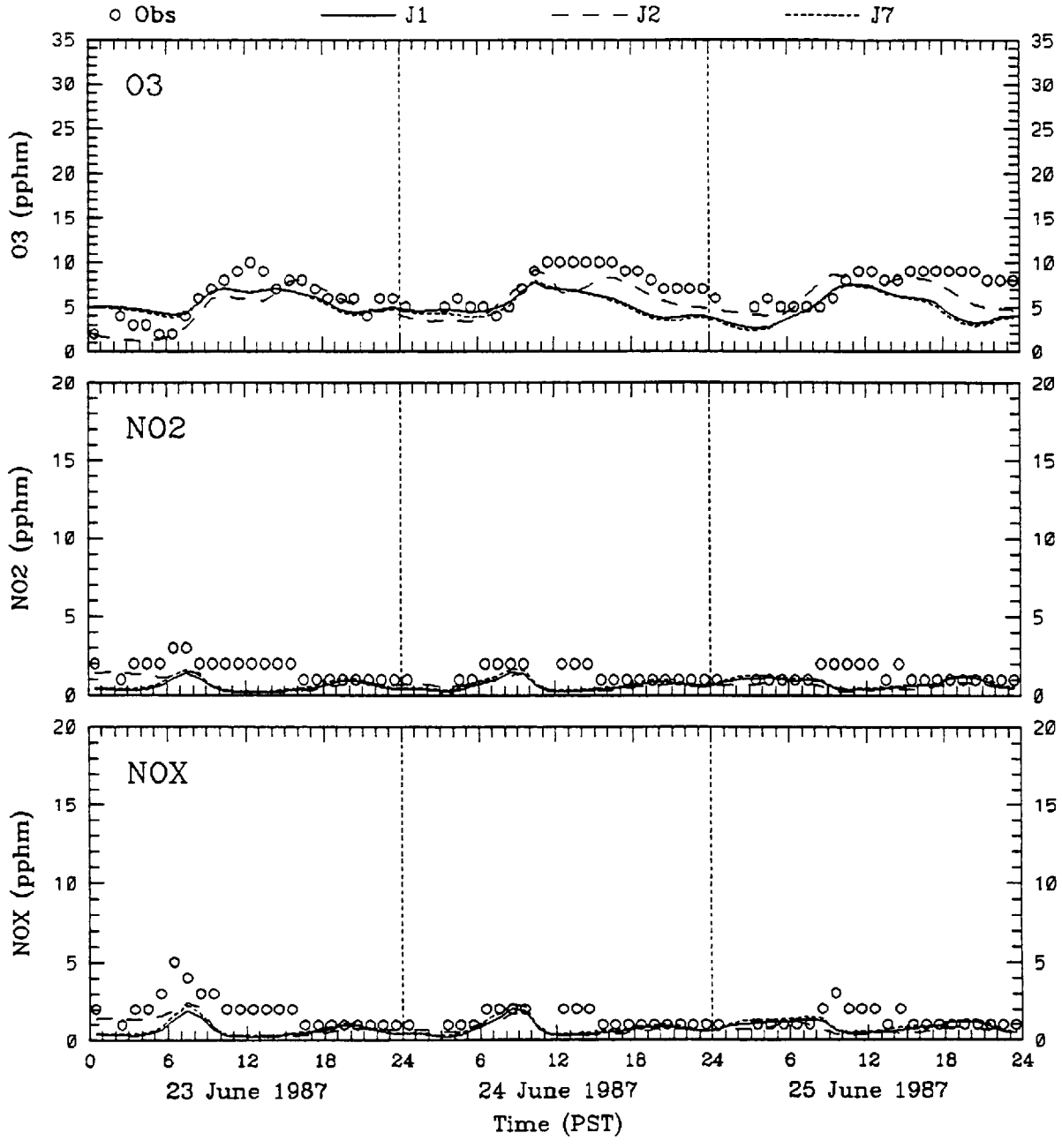


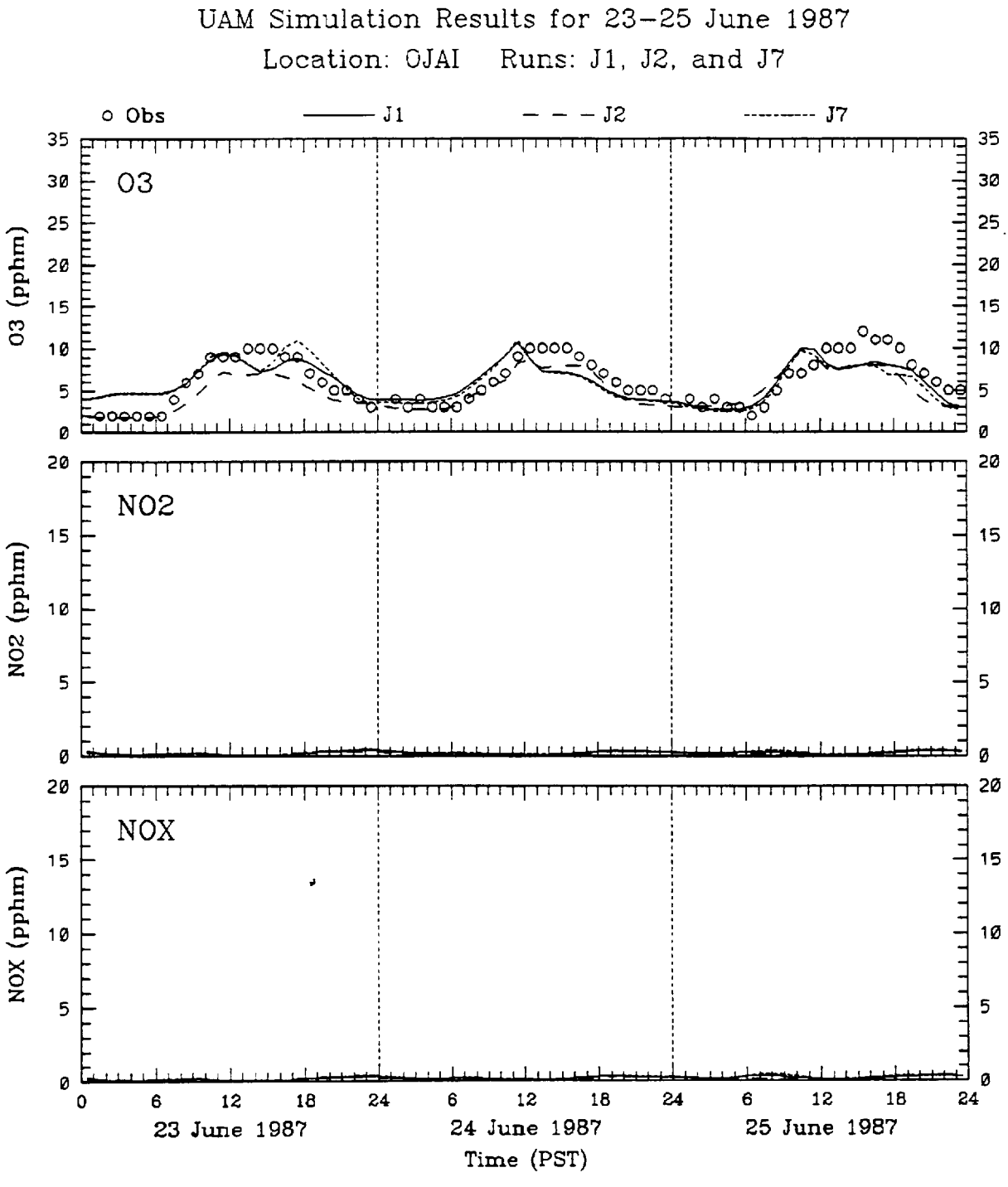




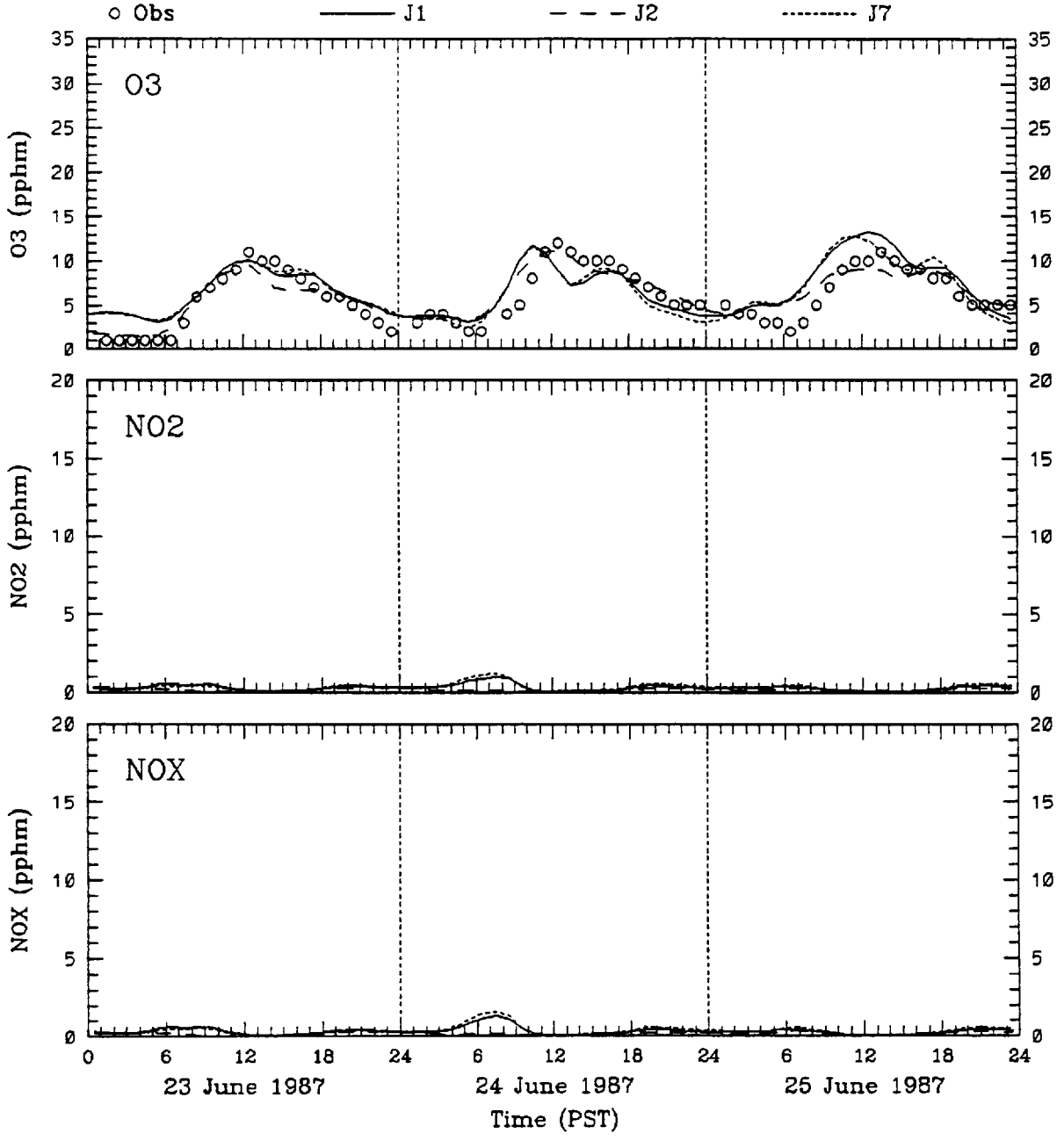


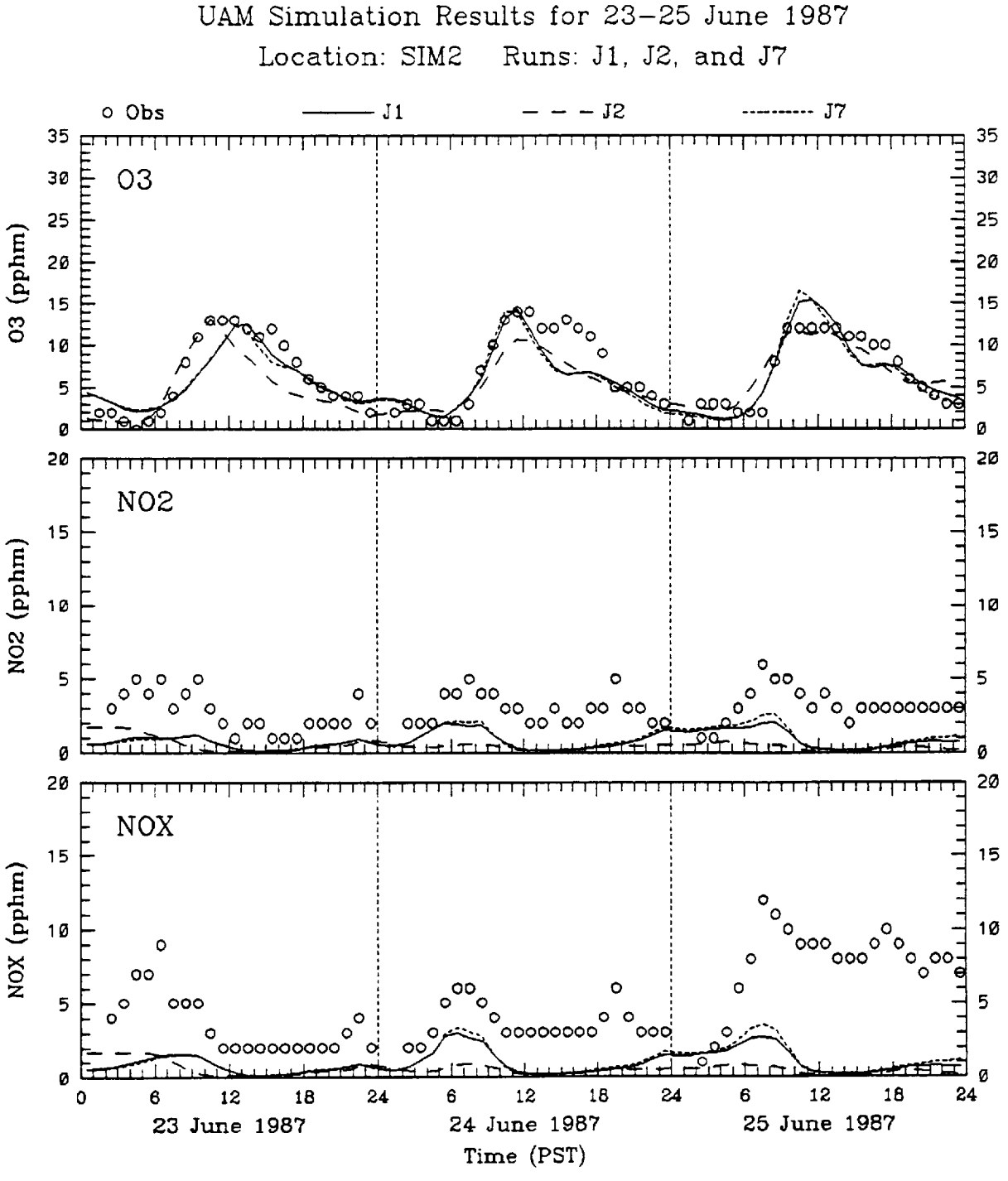
UAM Simulation Results for 23–25 June 1987
Location: ERIO Runs: J1, J2, and J7



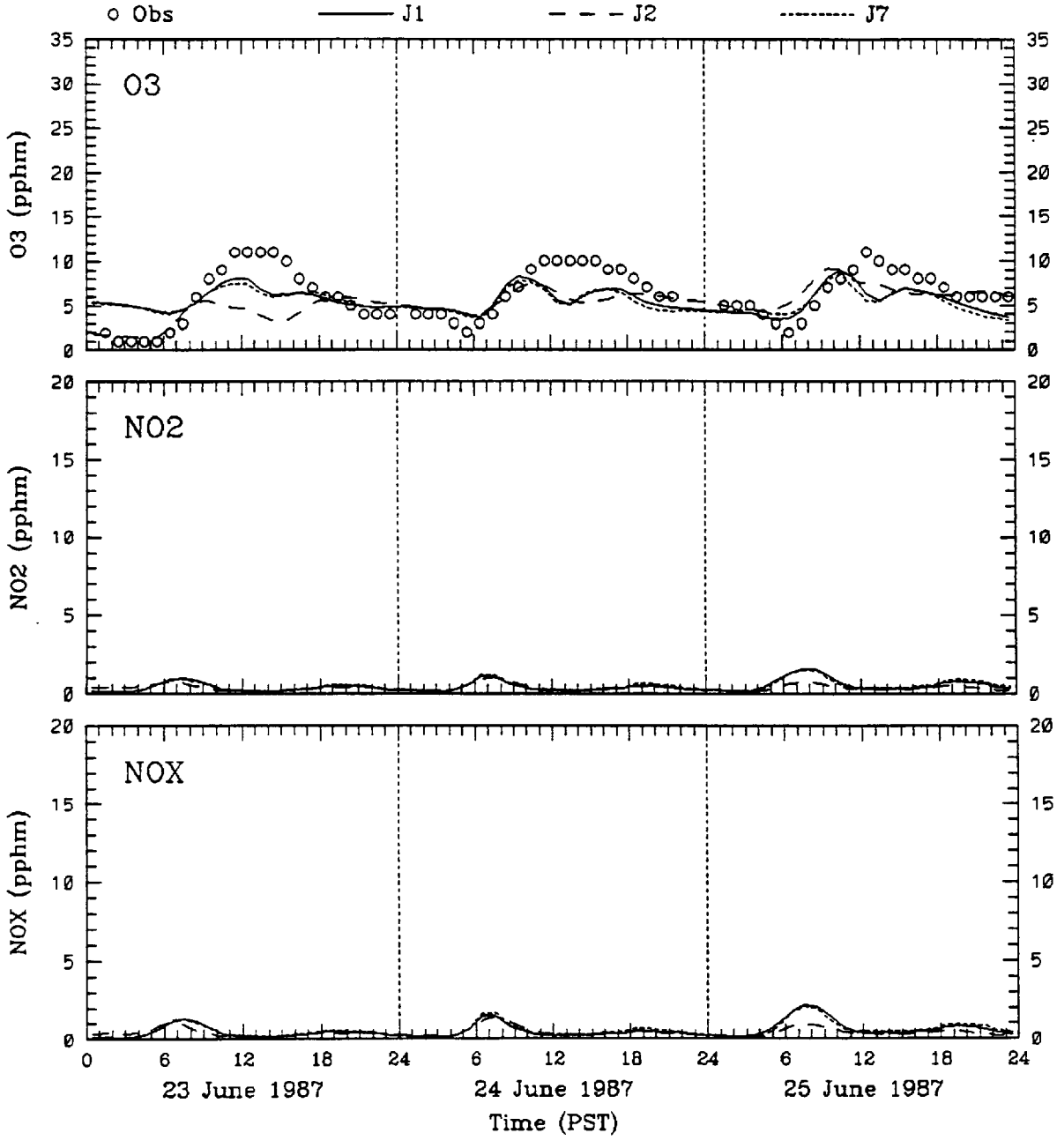


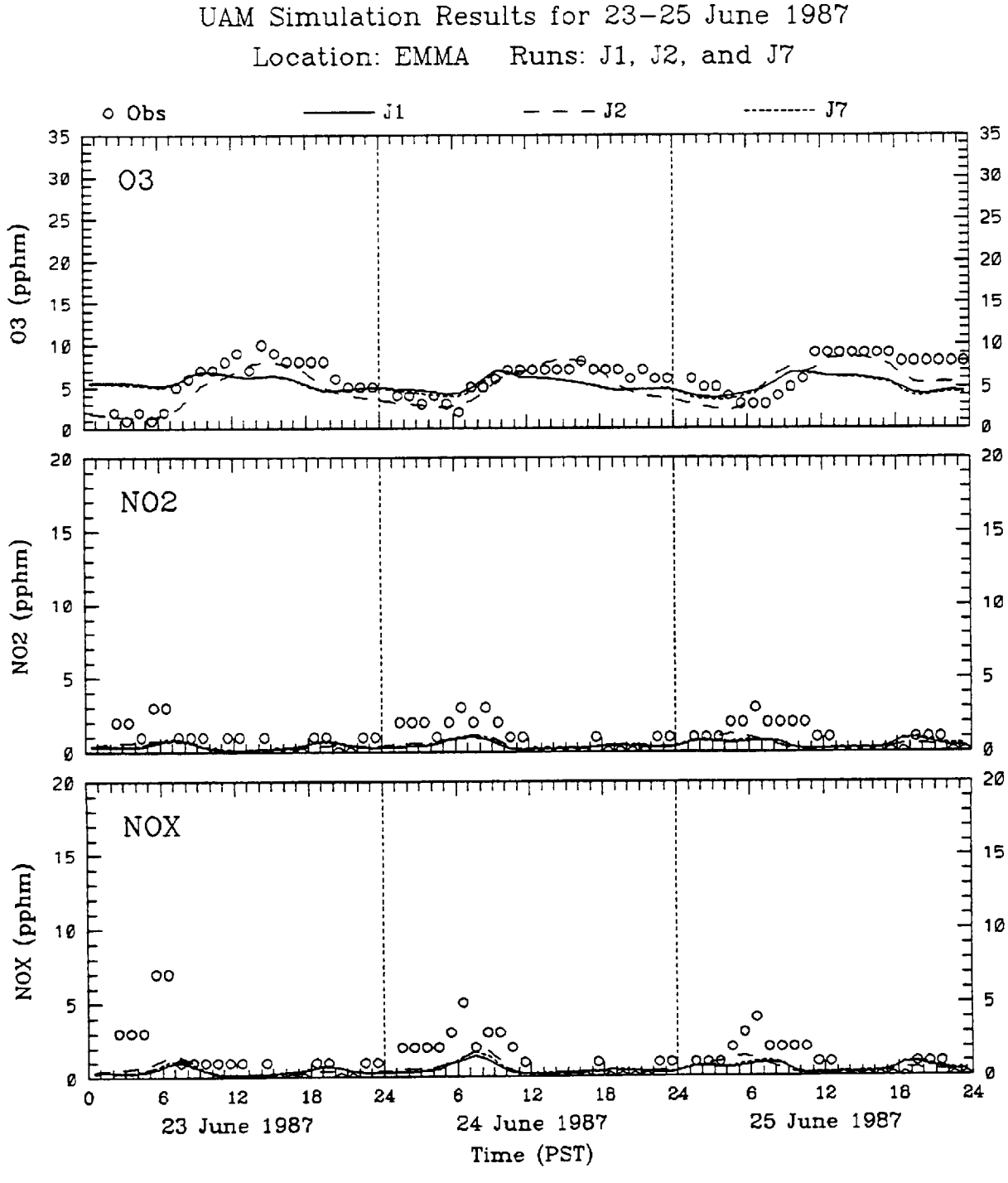
UAM Simulation Results for 23–25 June 1987
Location: PRU2 Runs: J1, J2, and J7



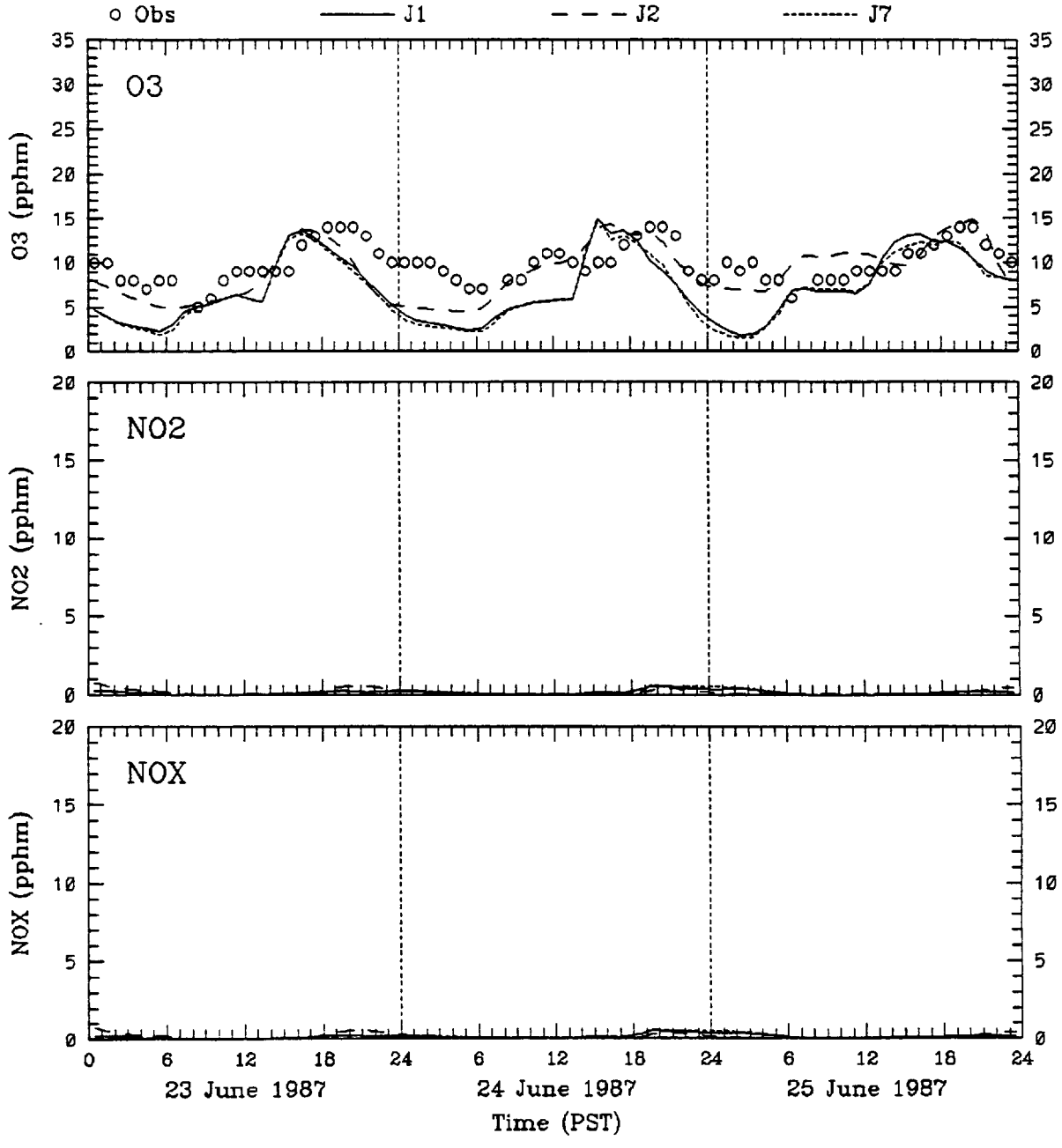


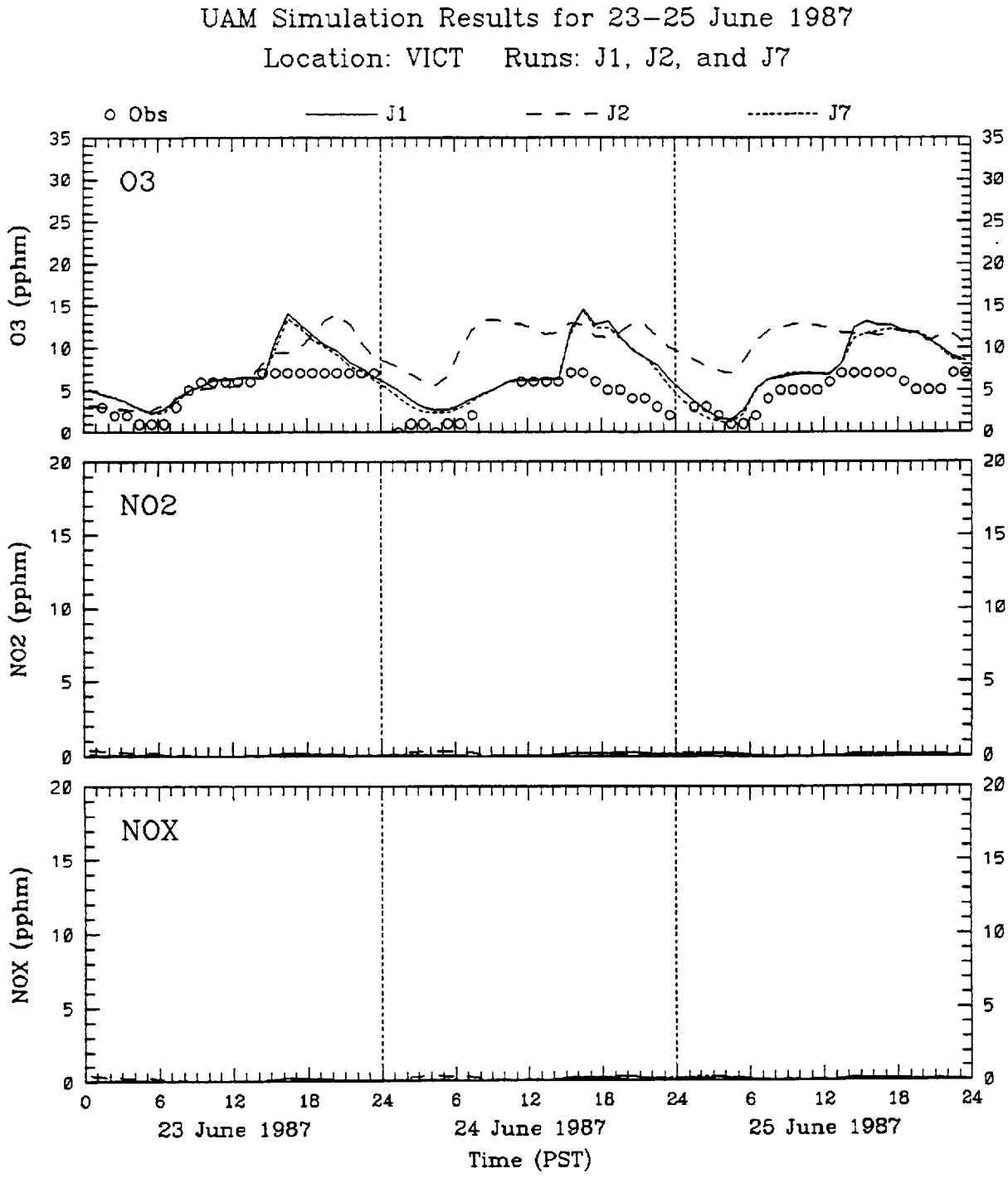
UAM Simulation Results for 23–25 June 1987
Location: OAKS Runs: J1, J2, and J7





UAM Simulation Results for 23-25 June 1987
Location: HESP Runs: J1, J2, and J7





APPENDIX D

Appendix D

VOC SIMULATION RESULTS FOR 23-25 JUNE 1987

This appendix contains time series plots showing estimated and measured concentrations for Runs J1, J2, and J7 for 23-25 June 1987. These displays illustrate the estimated and measured concentrations at air monitoring locations for various organic species simulated by the UAM. The monitoring stations are designated as follows:

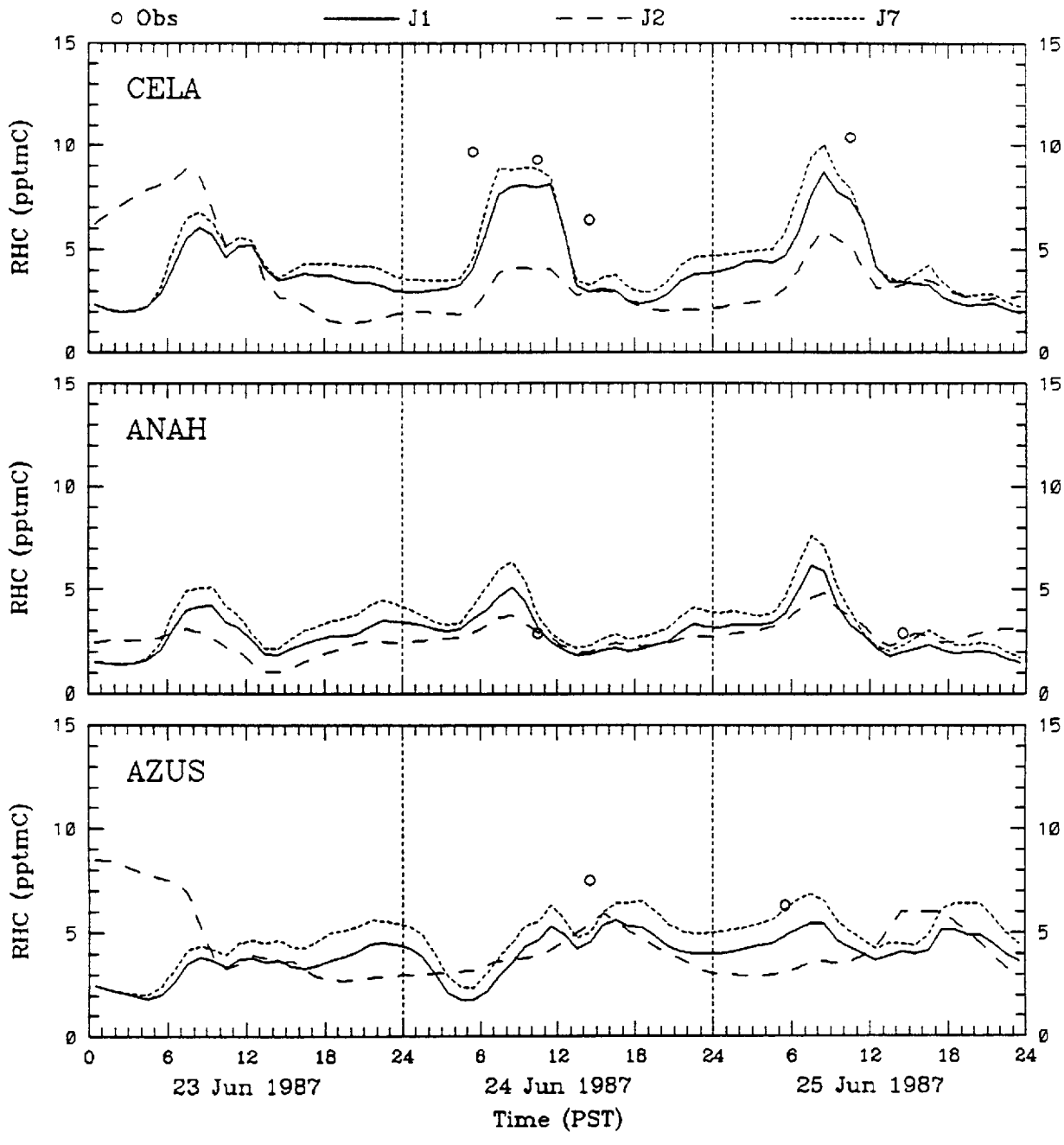
Los Angeles (CELA)
Anaheim (ANAH)
Azusa (AZUS)

Claremont College (CLAR)
Long Beach City College (LBCC)
Burbank (BURK)

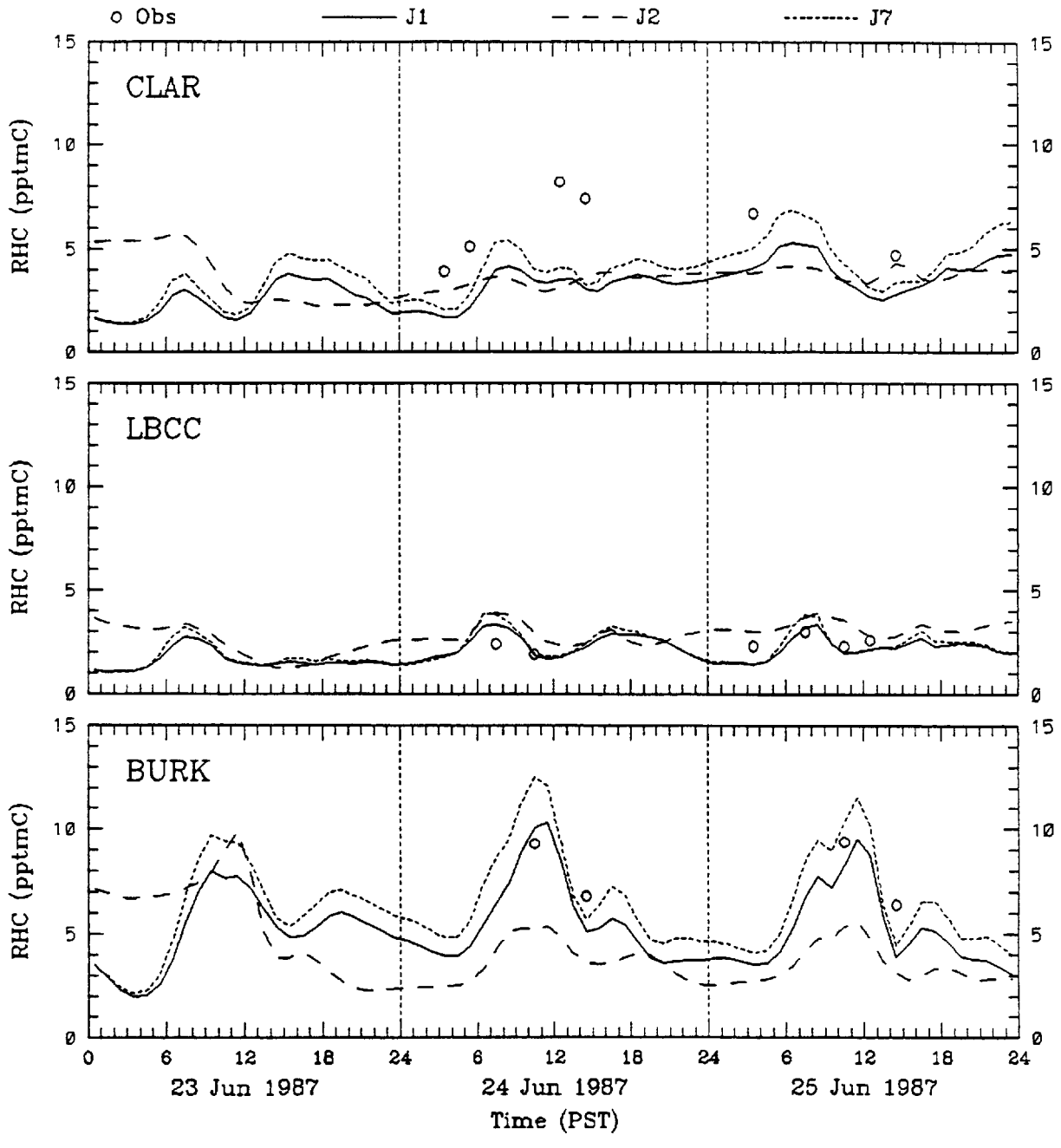
Riverside-Rubidoux (RIVR)
Hawthorn (HAWT)

Figure 2-1 in Section 2 shows the locations of these air monitoring stations.

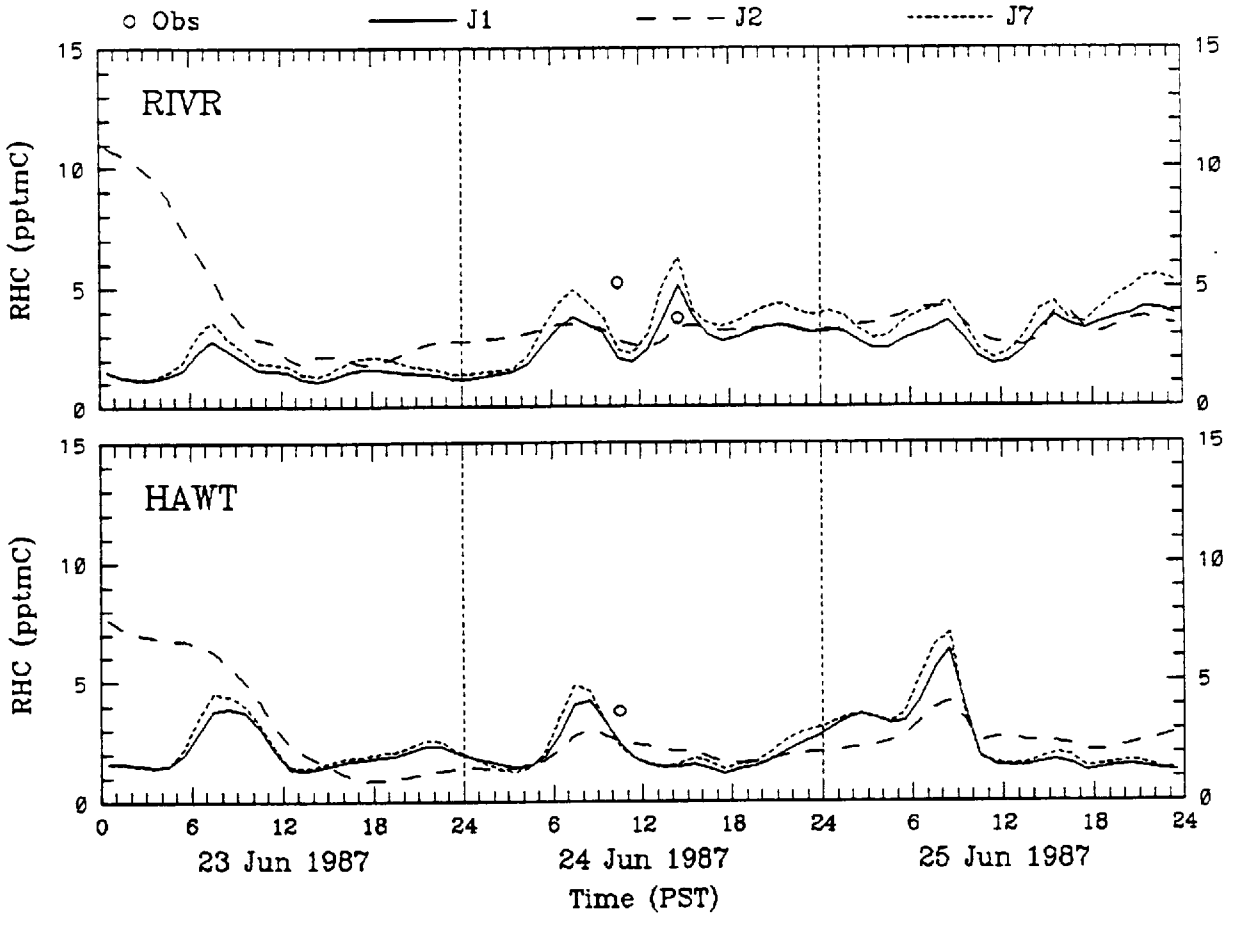
Runs J1, J2, and J7: Predicted and Observed RHC Time Series
23–25 June 1987



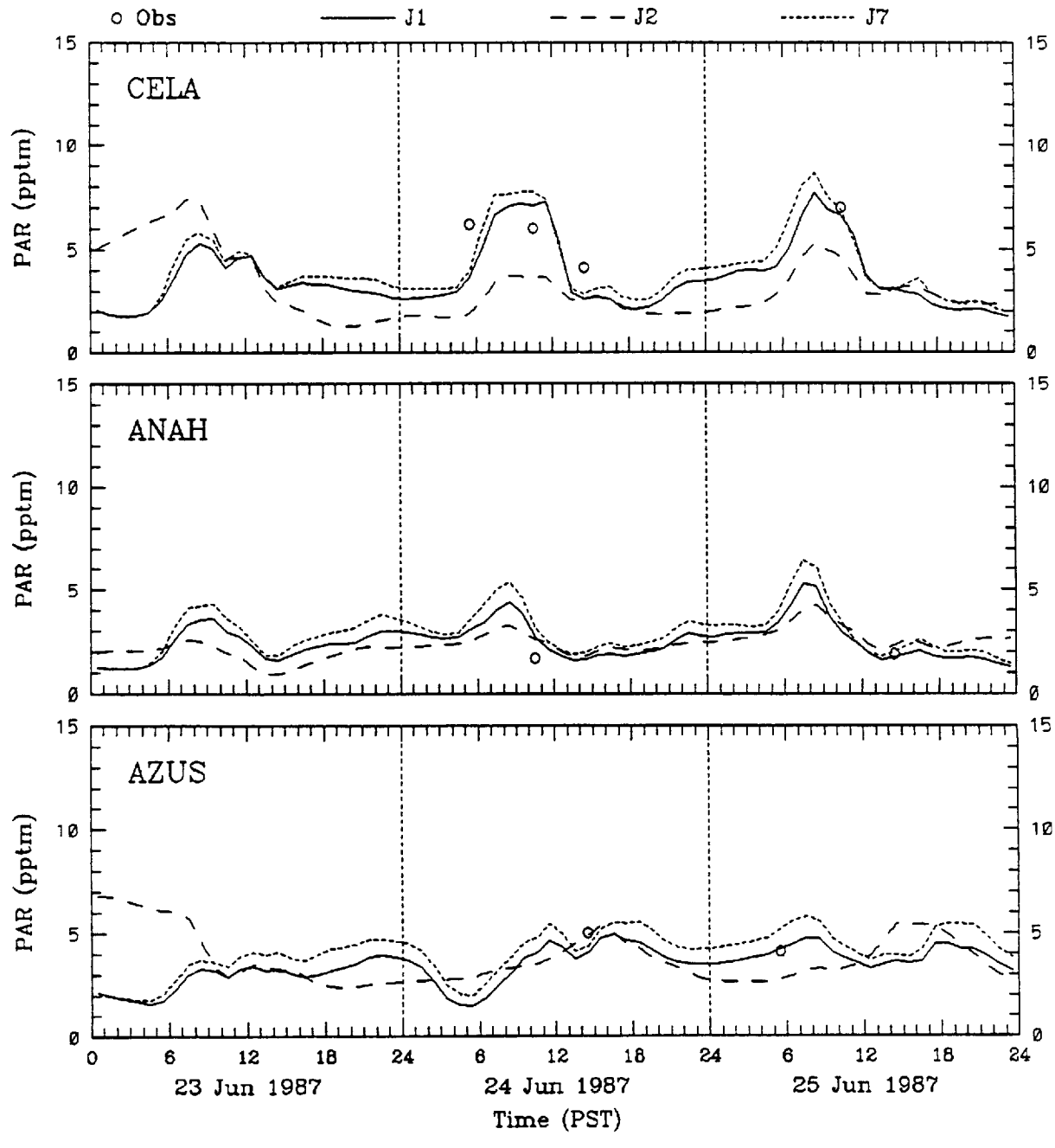
Runs J1, J2, and J7: Predicted and Observed RHC Time Series
23-25 June 1987



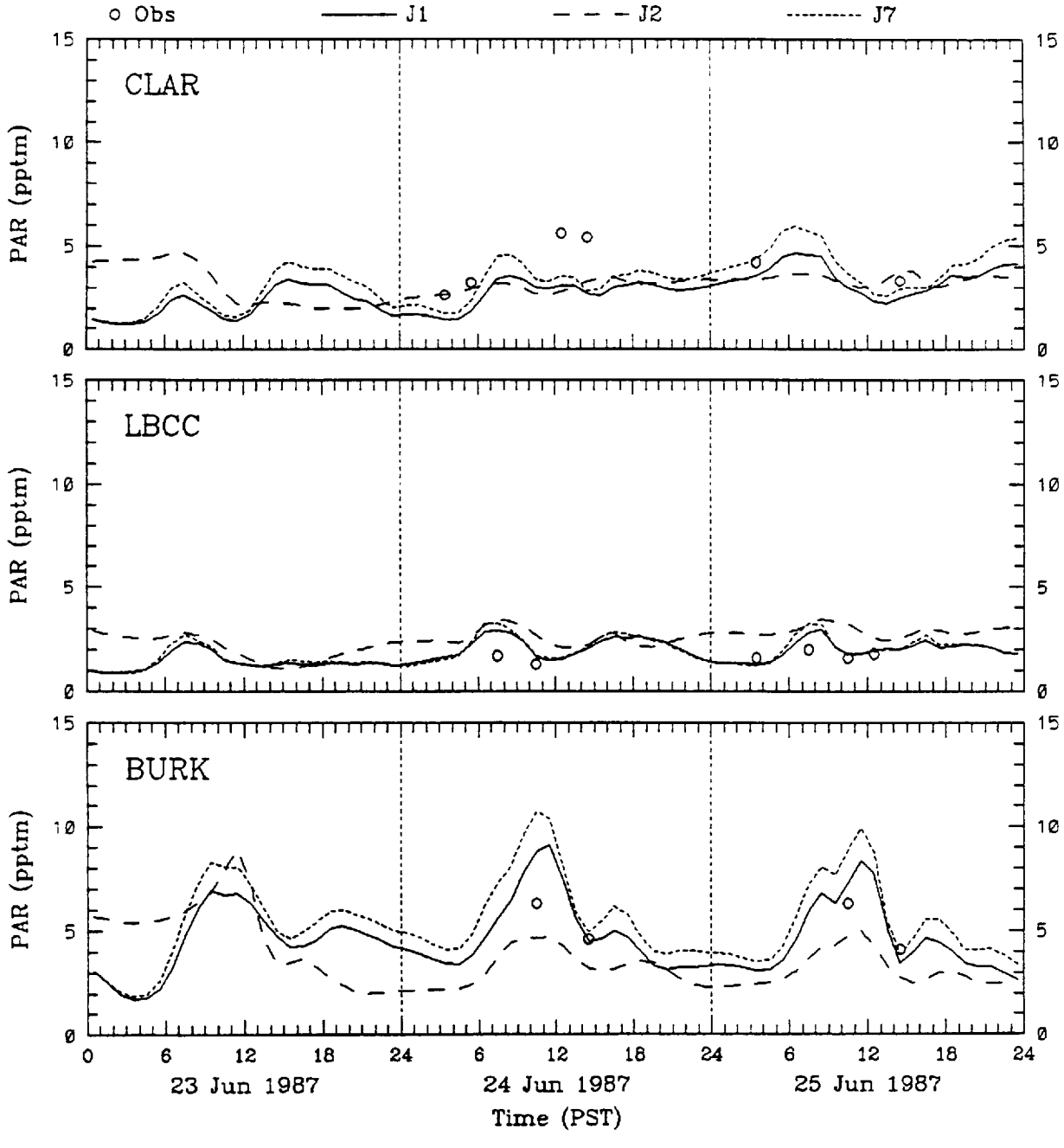
Runs J1, J2, and J7: Predicted and Observed RHC Time Series
23–25 June 1987



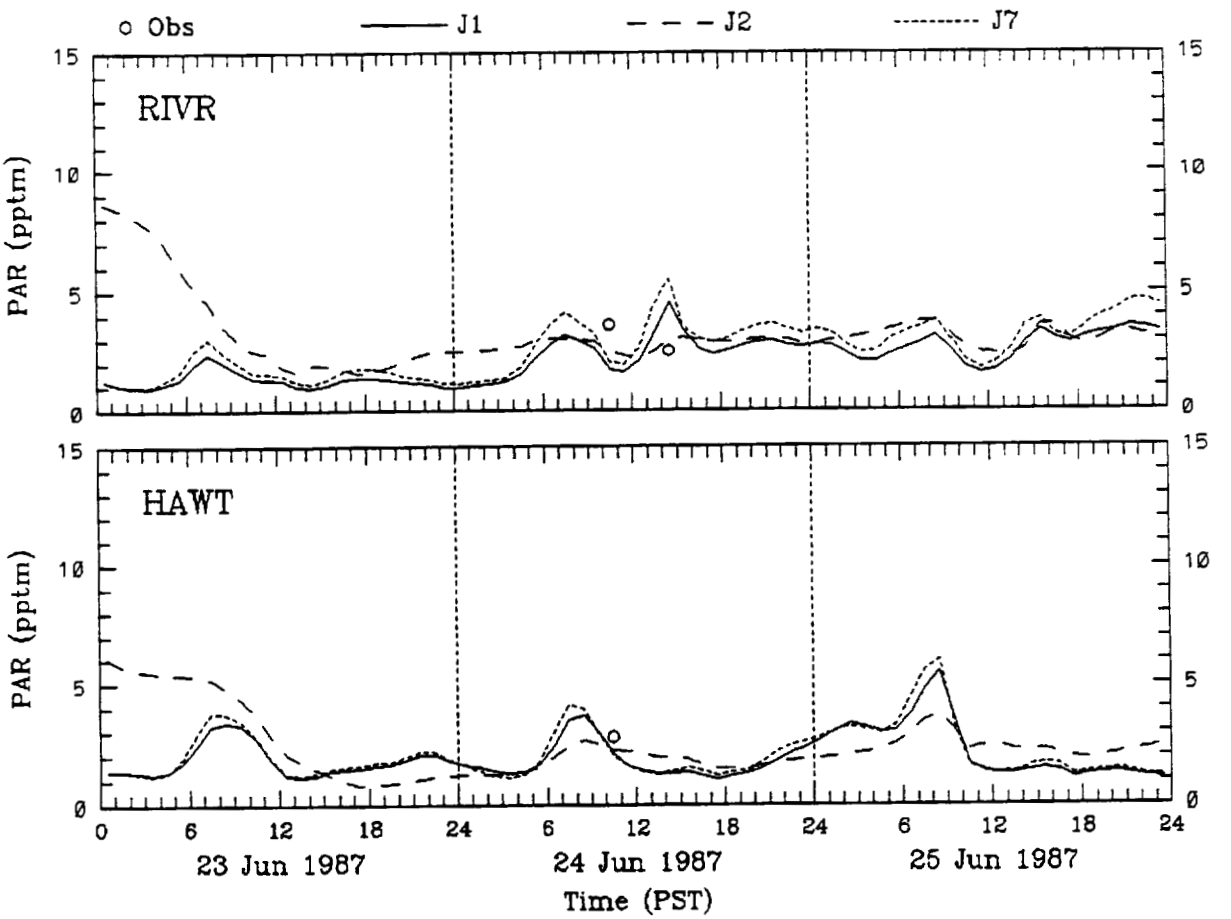
Runs J1, J2, and J7: Predicted and Observed PAR Time Series
23–25 June 1987



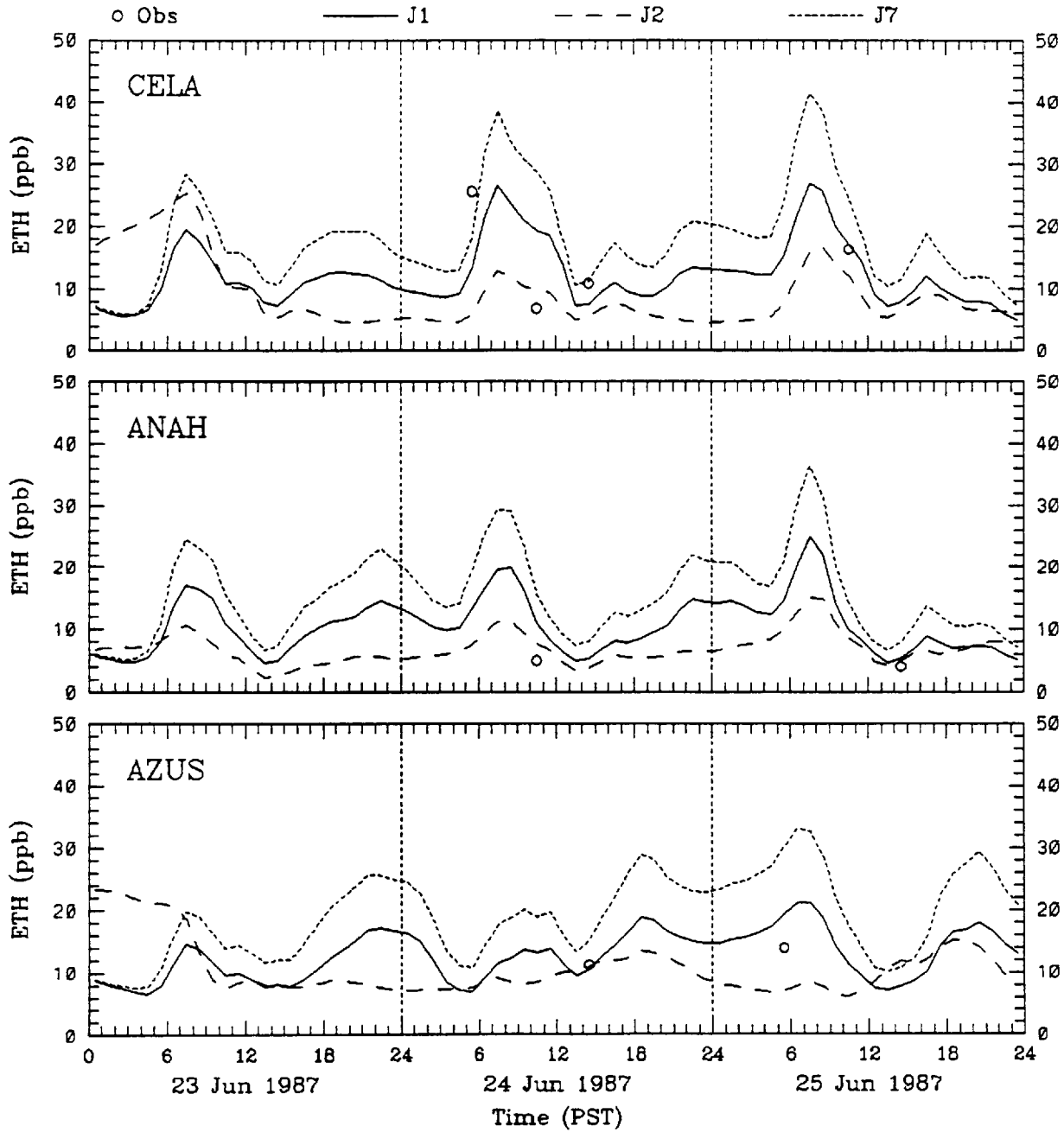
Runs J1, J2, and J7: Predicted and Observed PAR Time Series
23–25 June 1987



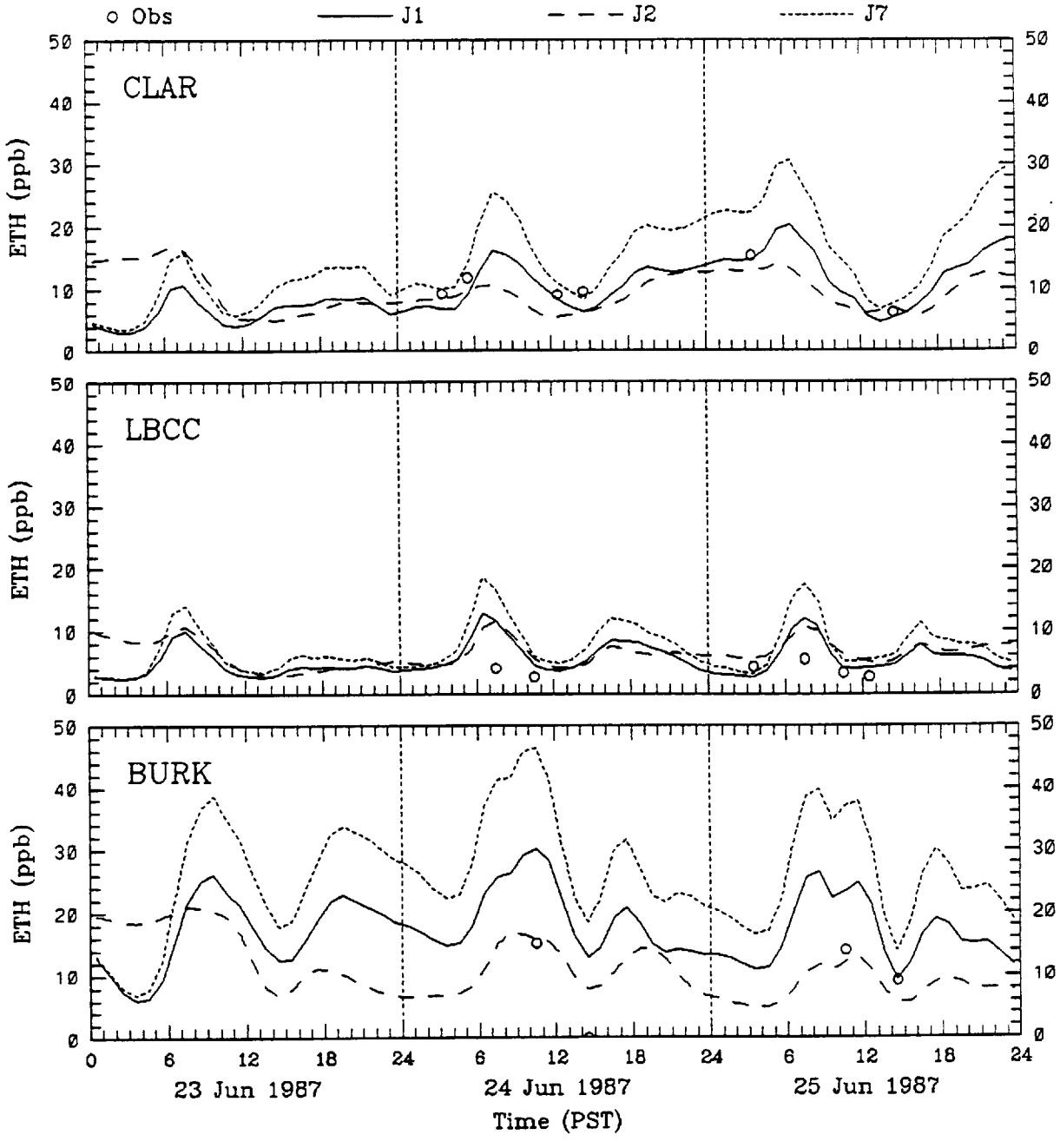
Runs J1, J2, and J7: Predicted and Observed PAR Time Series
23–25 June 1987



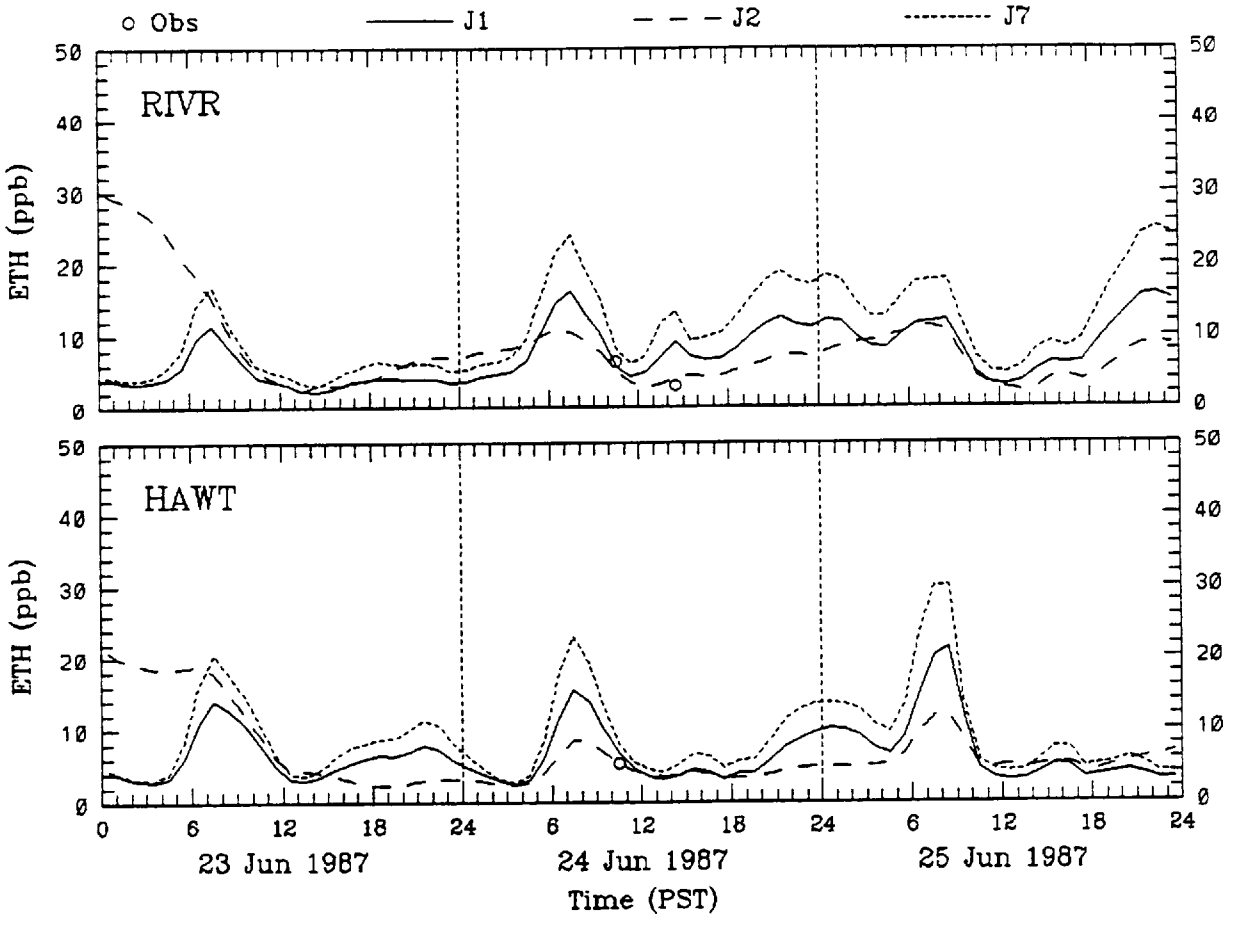
Runs J1, J2, and J7: Predicted and Observed ETH Time Series
23–25 June 1987



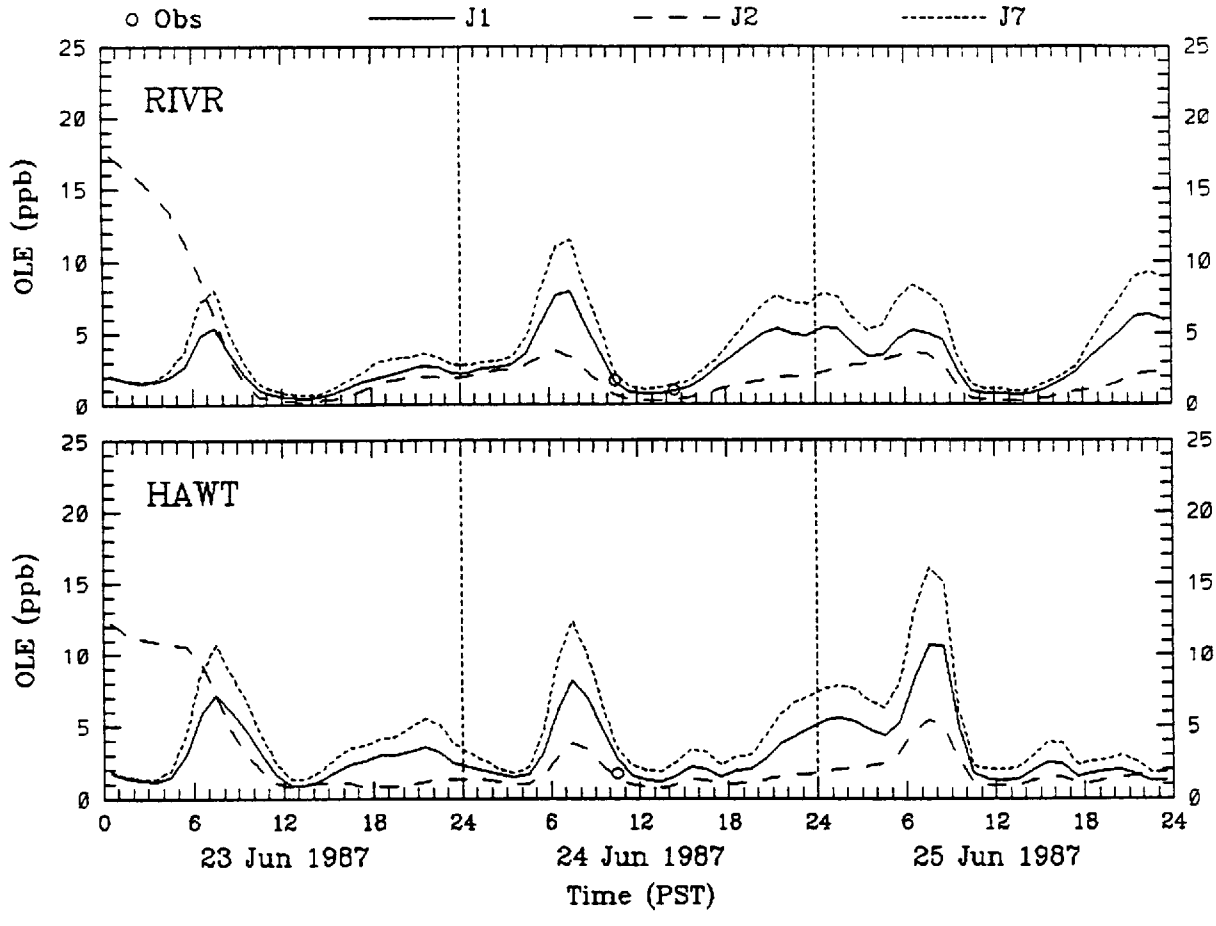
Runs J1, J2, and J7: Predicted and Observed ETH Time Series
23–25 June 1987



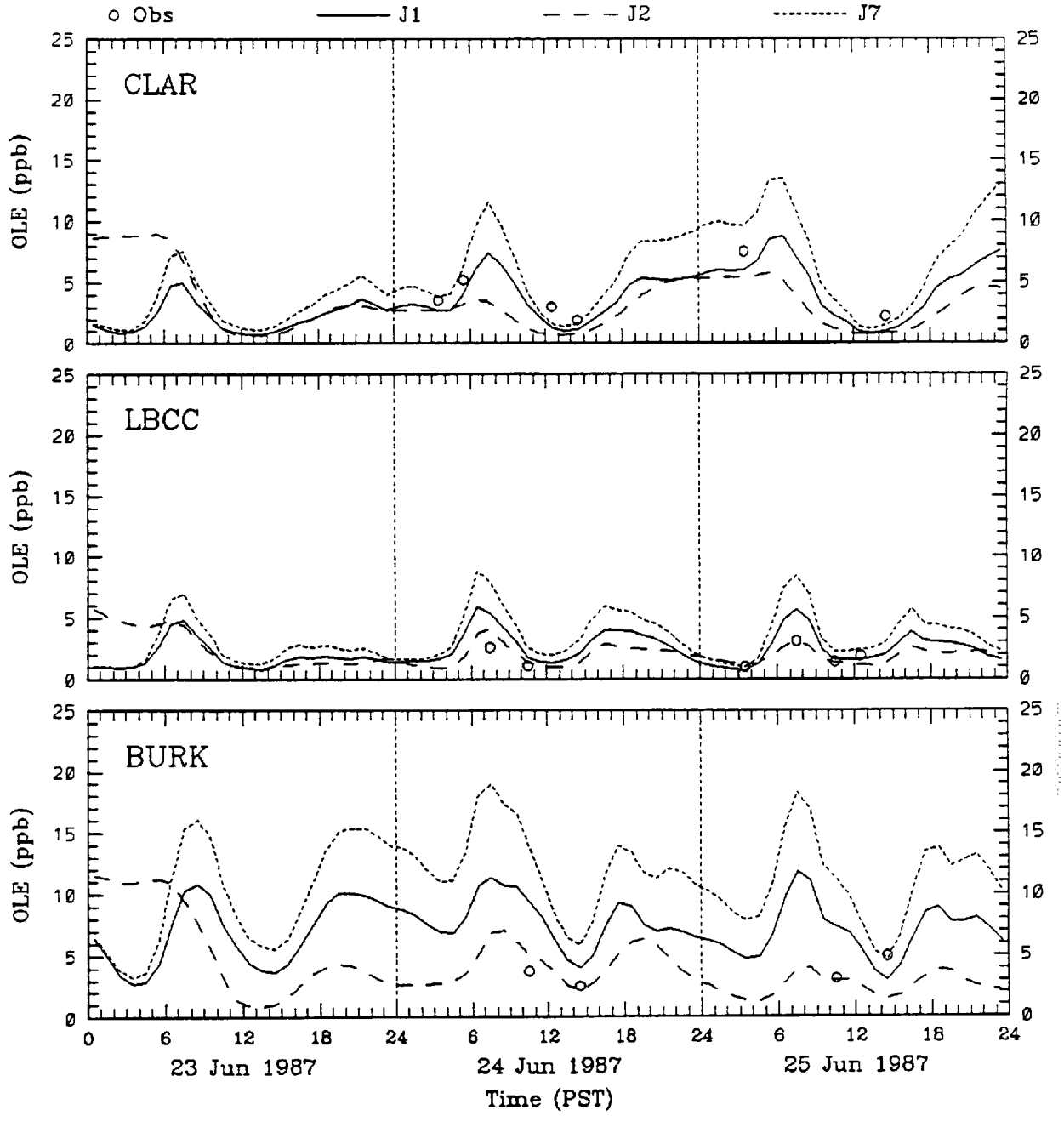
Runs J1, J2, and J7: Predicted and Observed ETH Time Series
23–25 June 1987



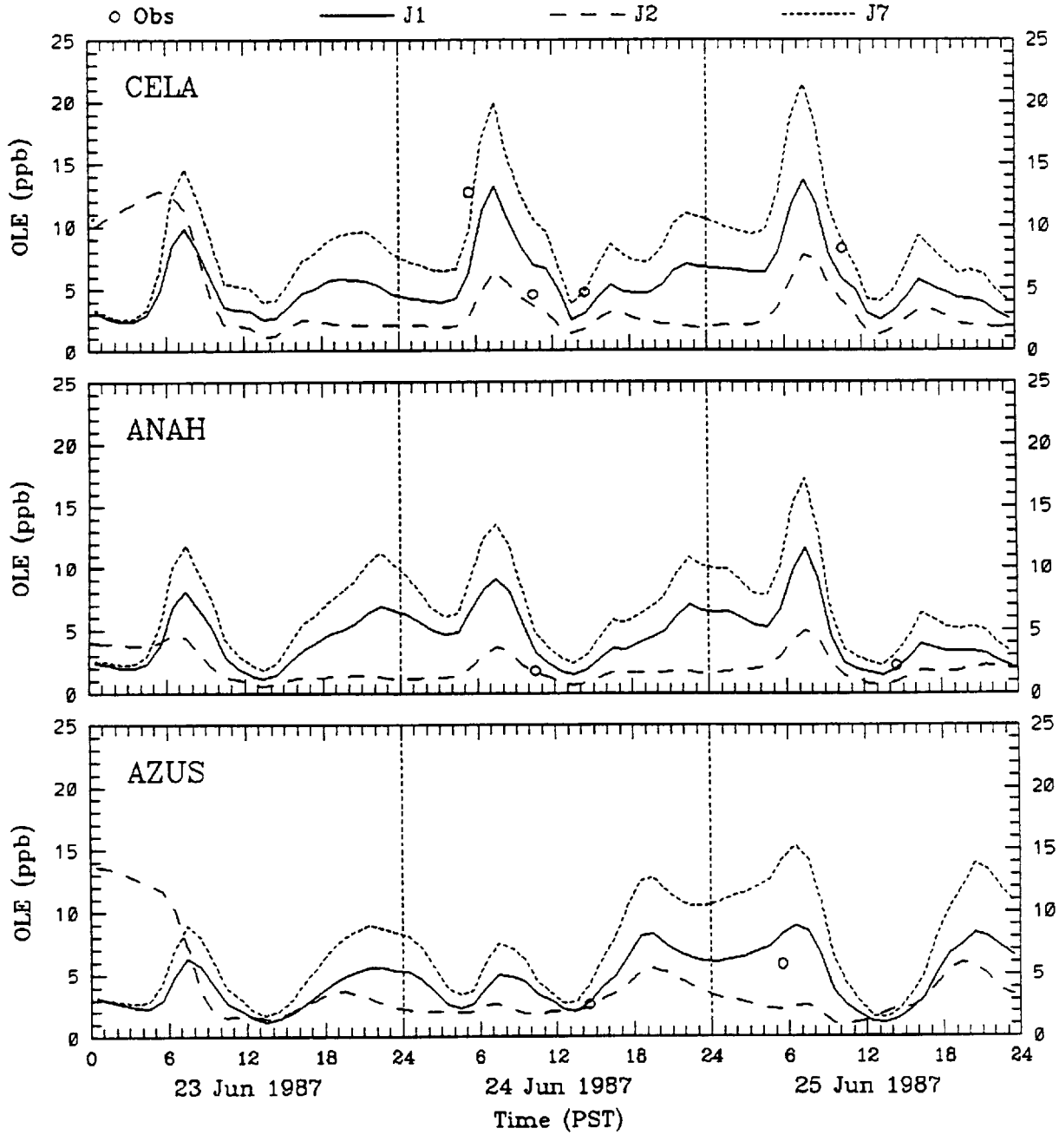
Runs J1, J2, and J7: Predicted and Observed OLE Time Series
23-25 June 1987



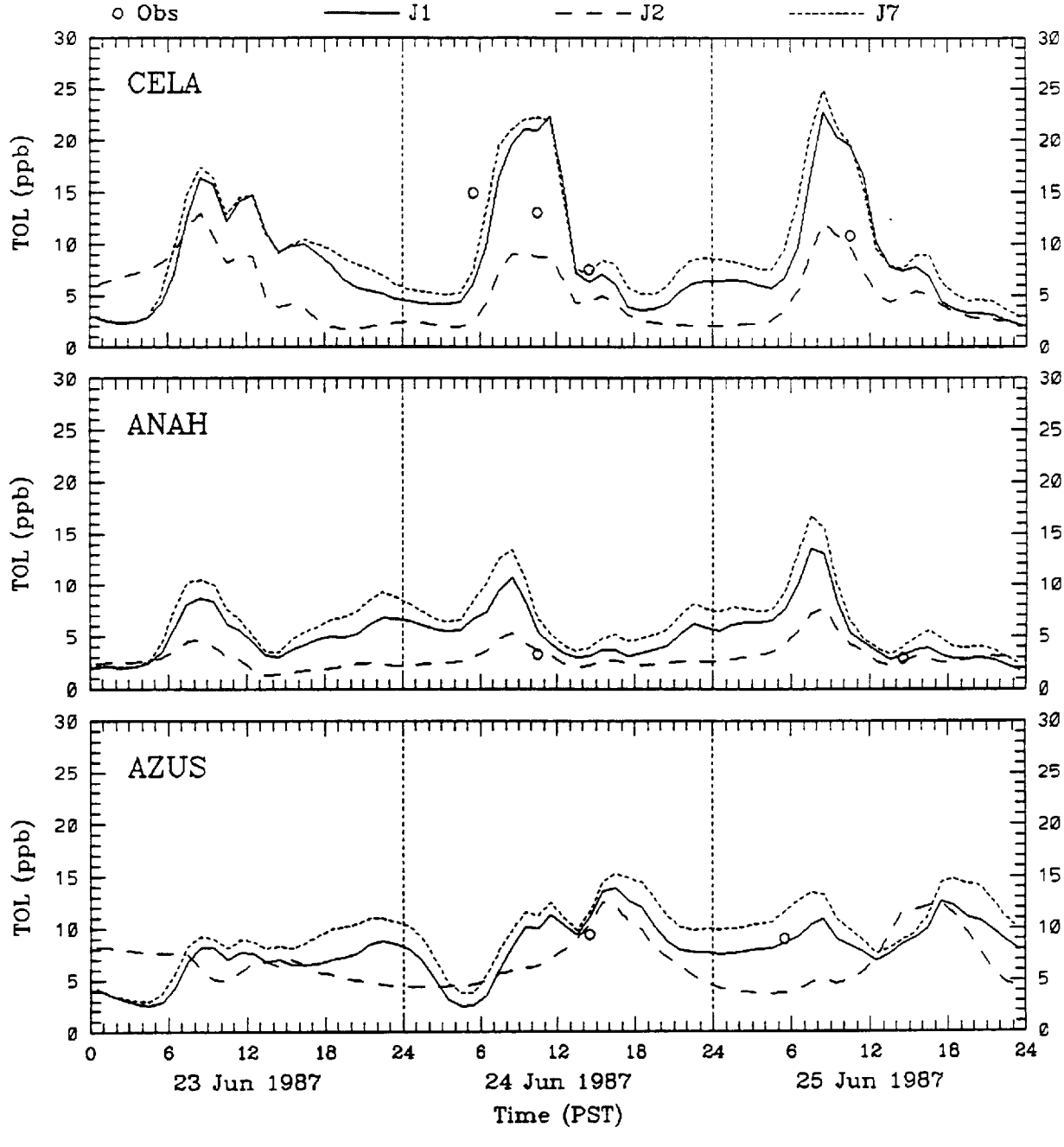
Runs J1, J2, and J7: Predicted and Observed OLE Time Series
23–25 June 1987



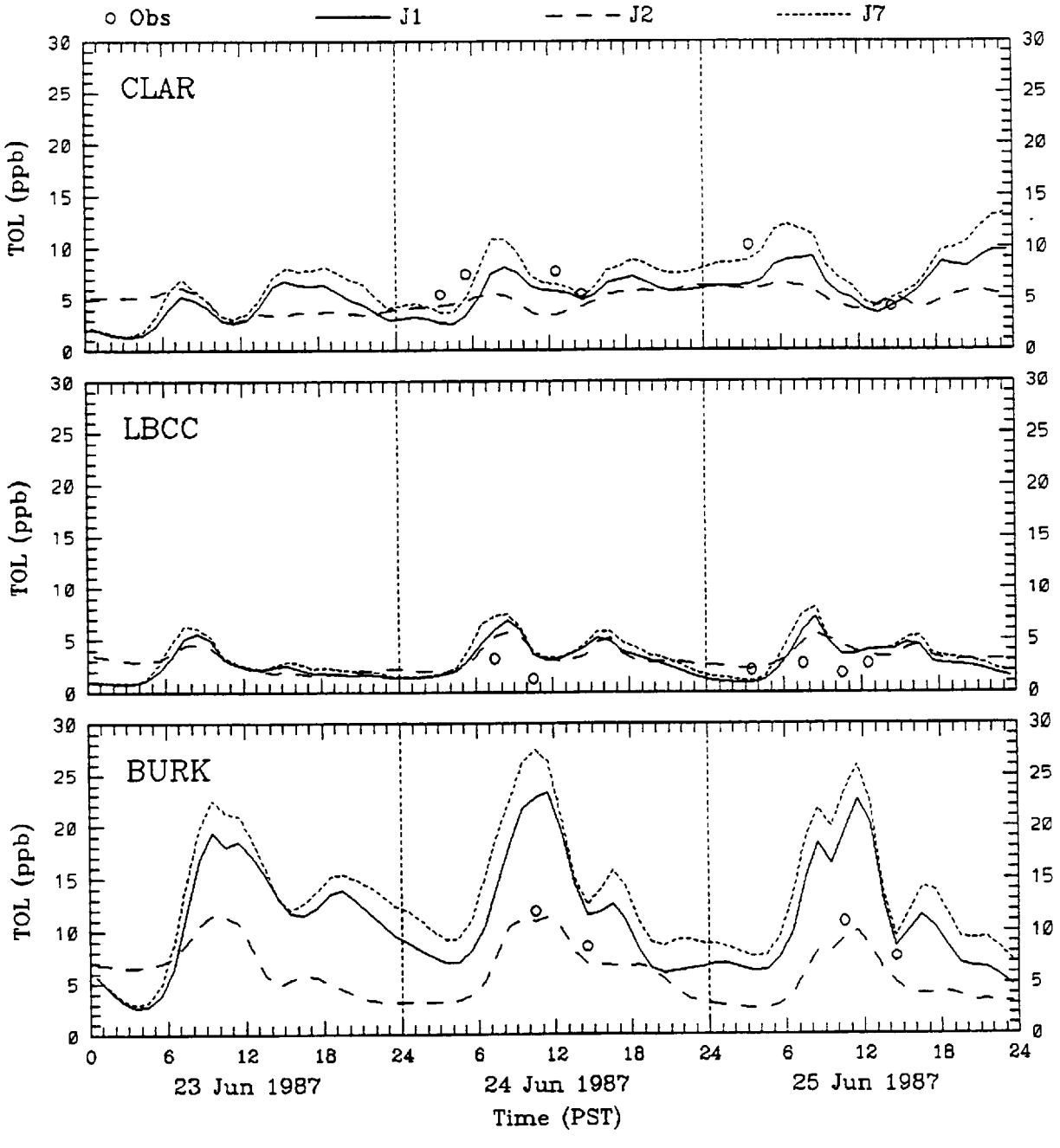
Runs J1, J2, and J7: Predicted and Observed OLE Time Series
23–25 June 1987



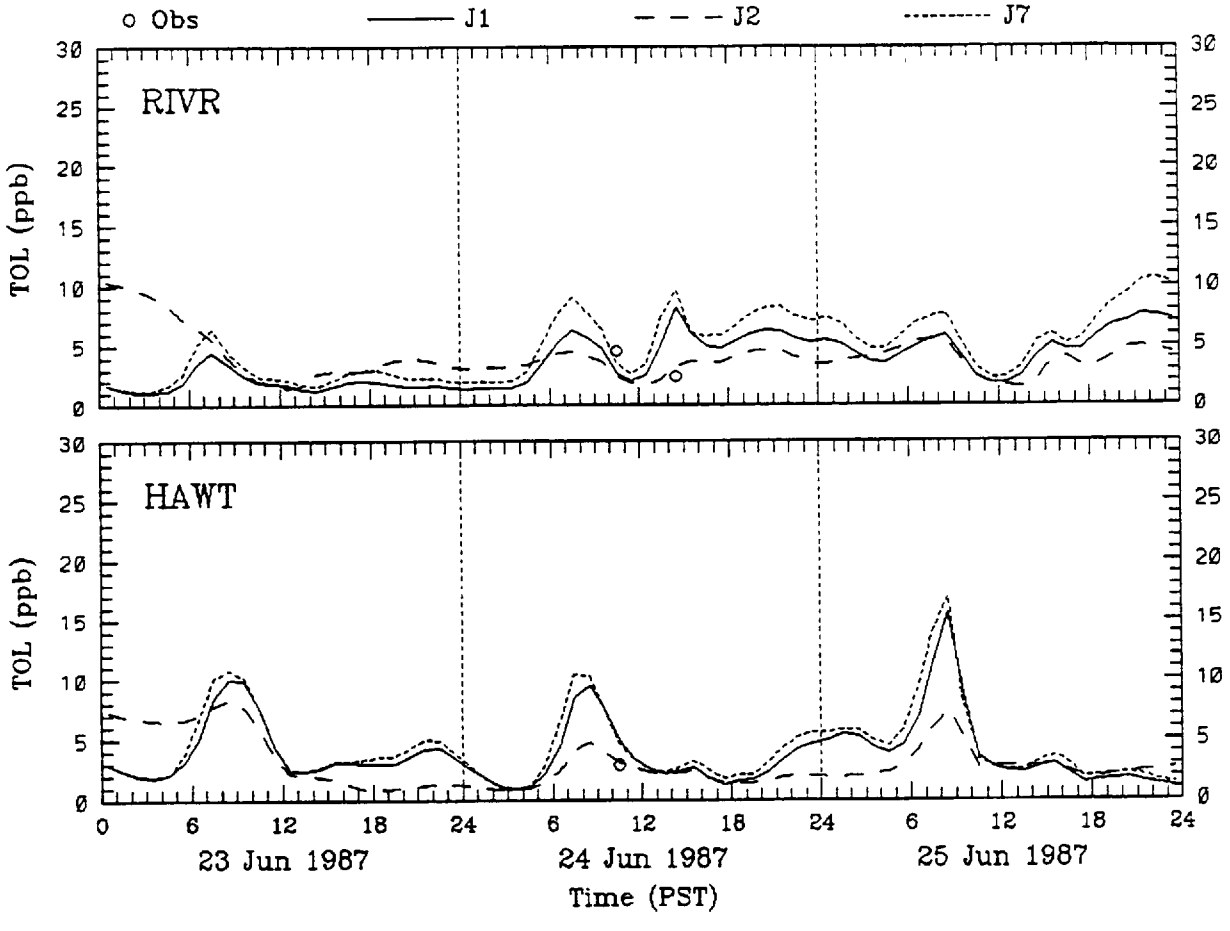
Runs J1, J2, and J7: Predicted and Observed TOL Time Series
23–25 June 1987



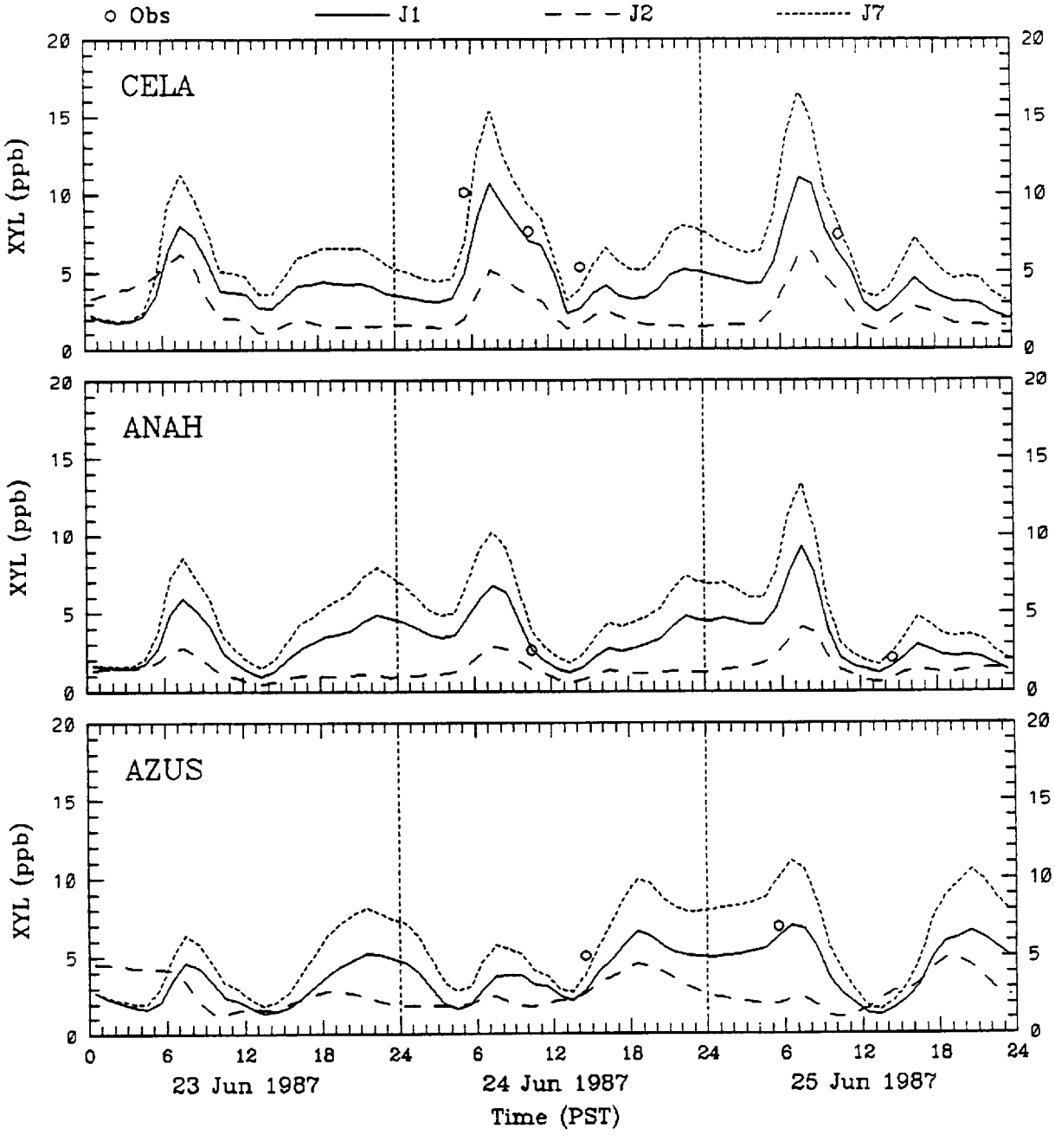
Runs J1, J2, and J7: Predicted and Observed TOL Time Series
23–25 June 1987



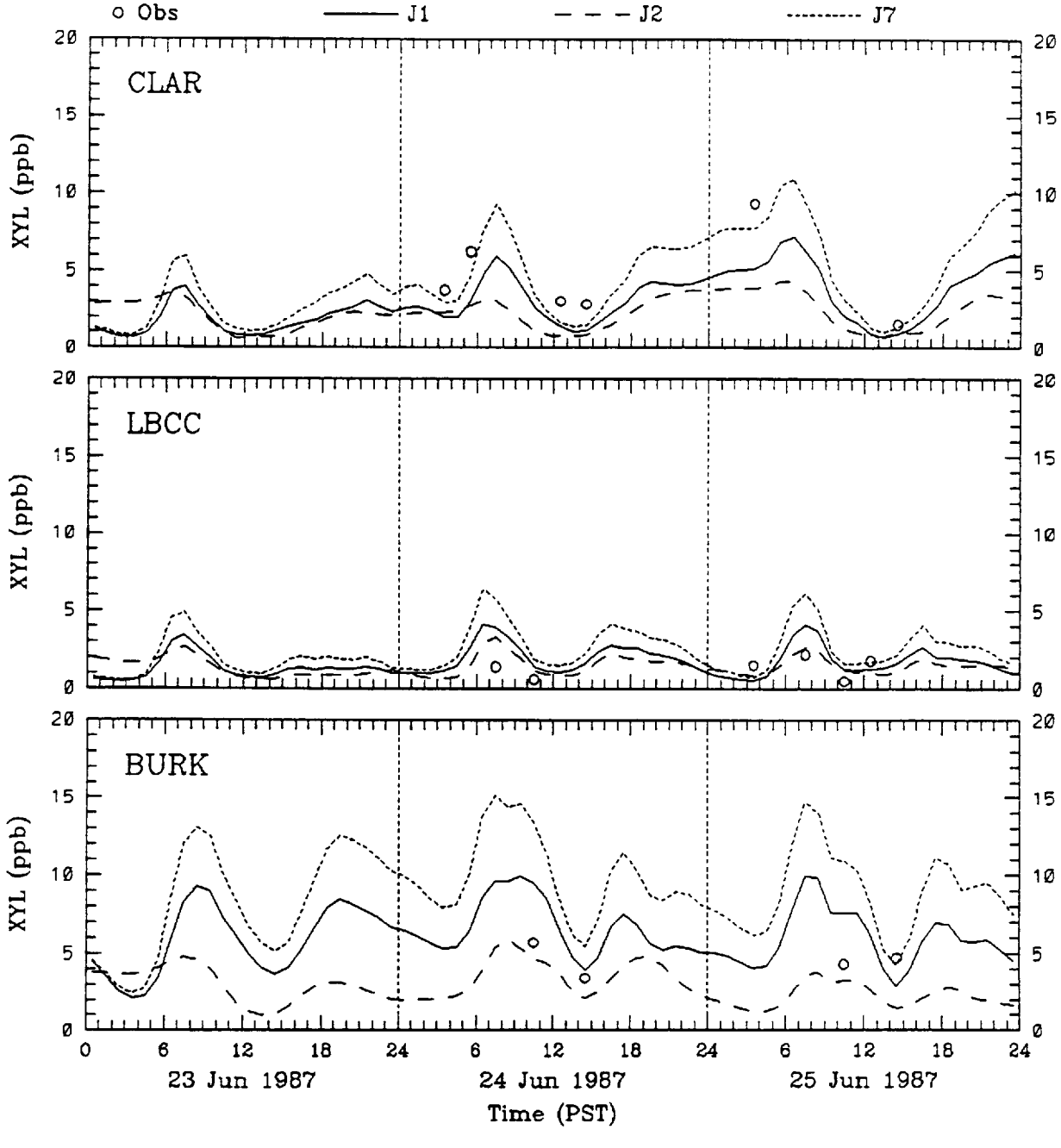
Runs J1, J2, and J7: Predicted and Observed TOL Time Series
23–25 June 1987



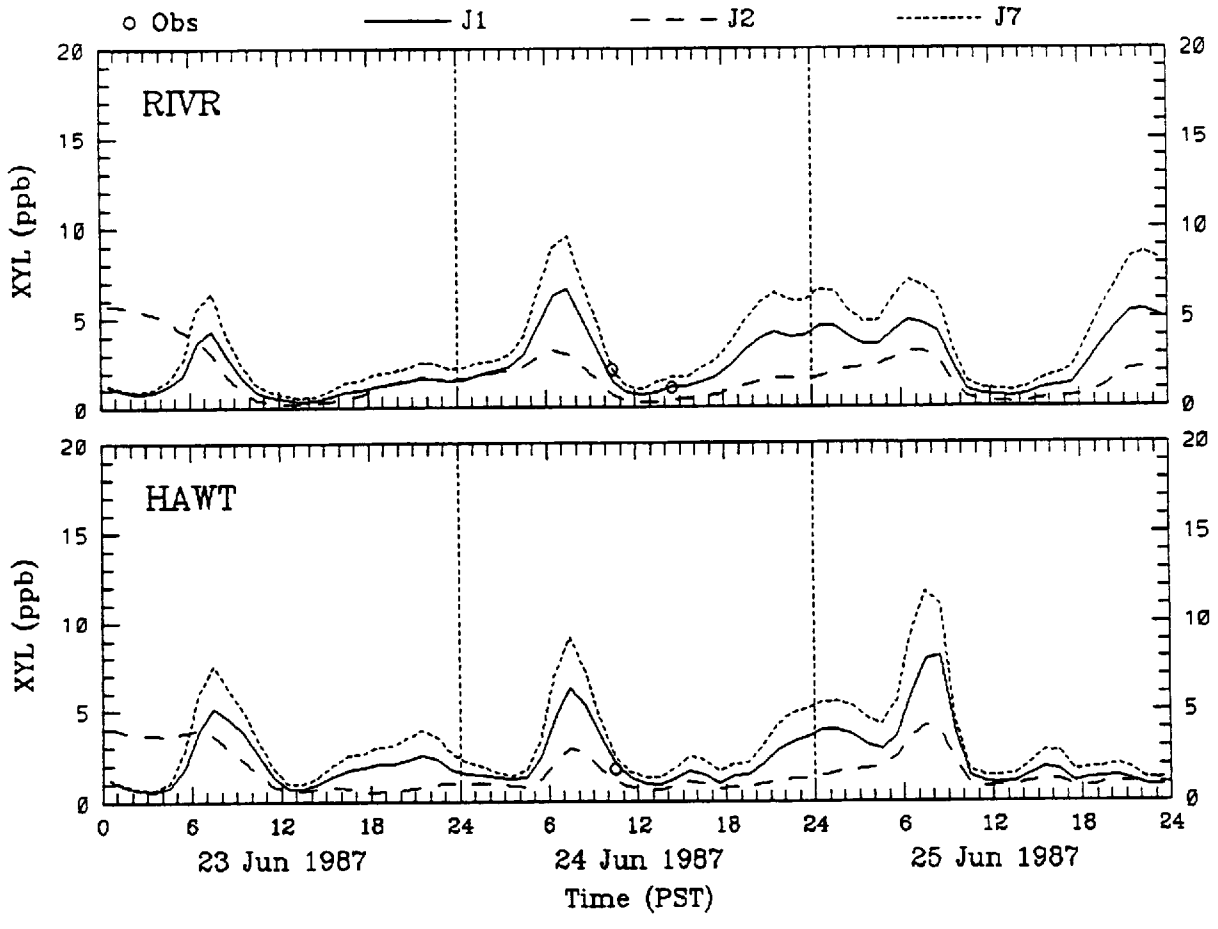
Runs J1, J2, and J7: Predicted and Observed XYL Time Series
23–25 June 1987



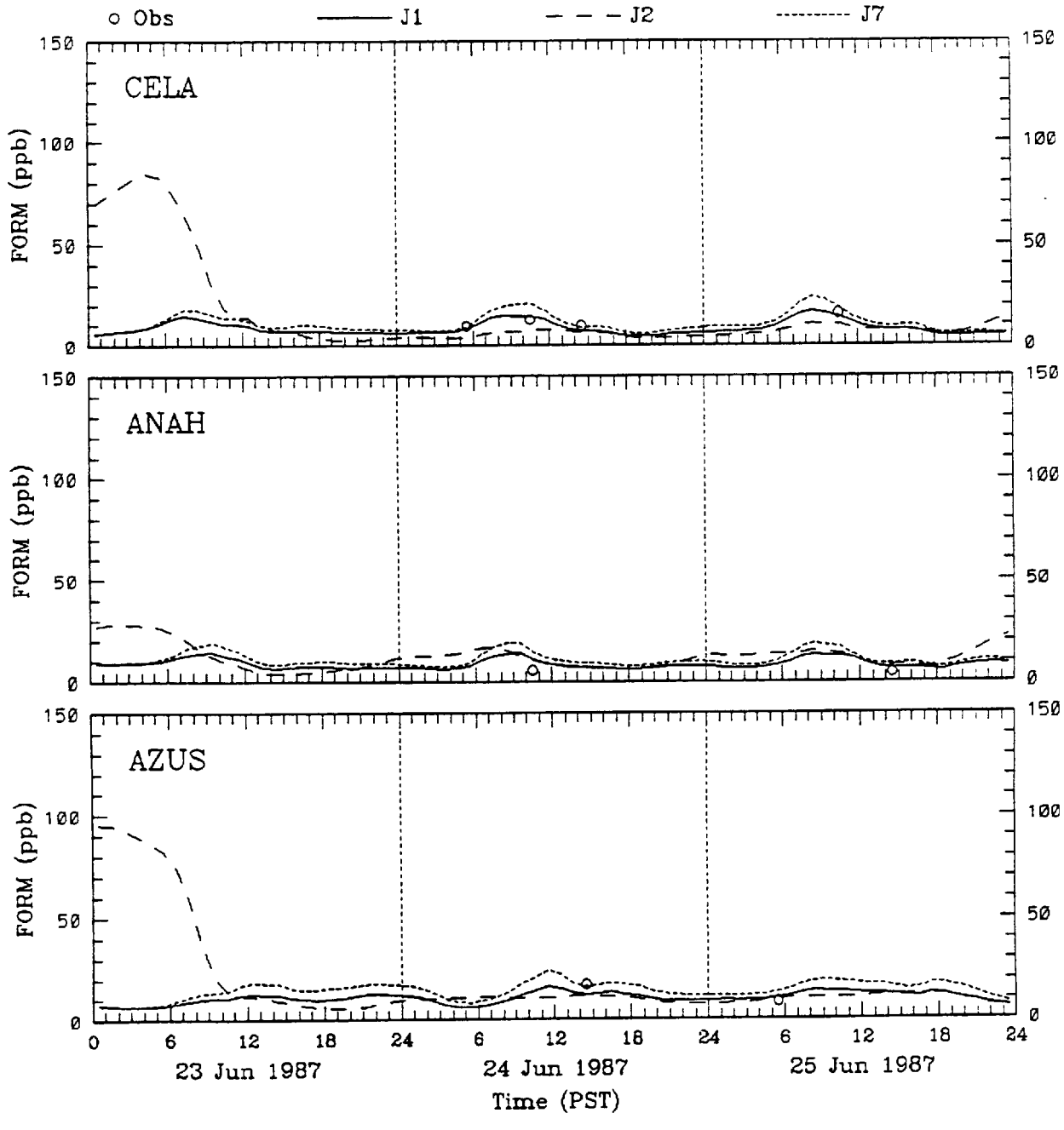
Runs J1, J2, and J7: Predicted and Observed XYL Time Series
23–25 June 1987



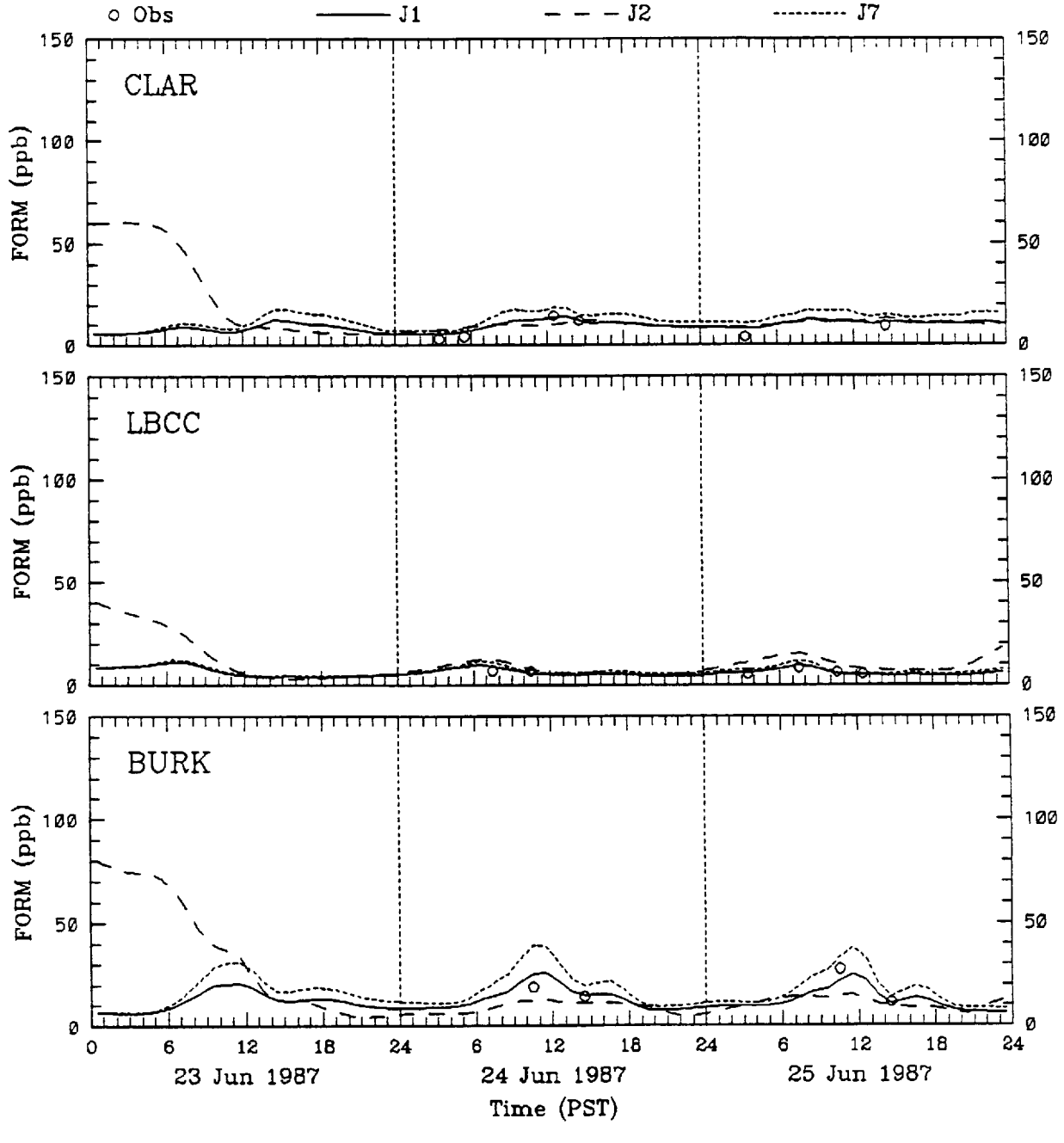
Runs J1, J2, and J7: Predicted and Observed XYL Time Series
23-25 June 1987



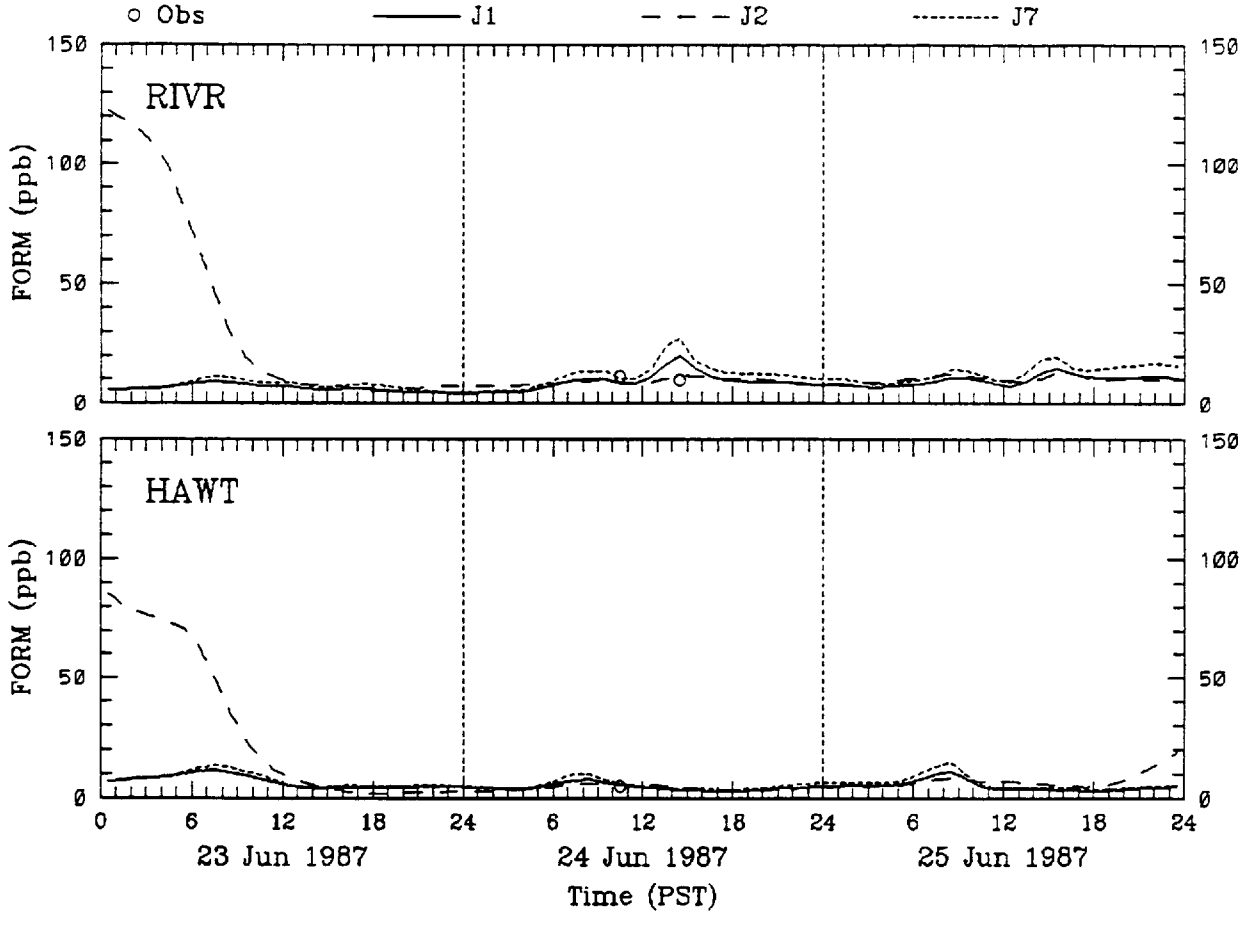
Runs J1, J2, and J7: Predicted and Observed FORM Time Series
23–25 June 1987



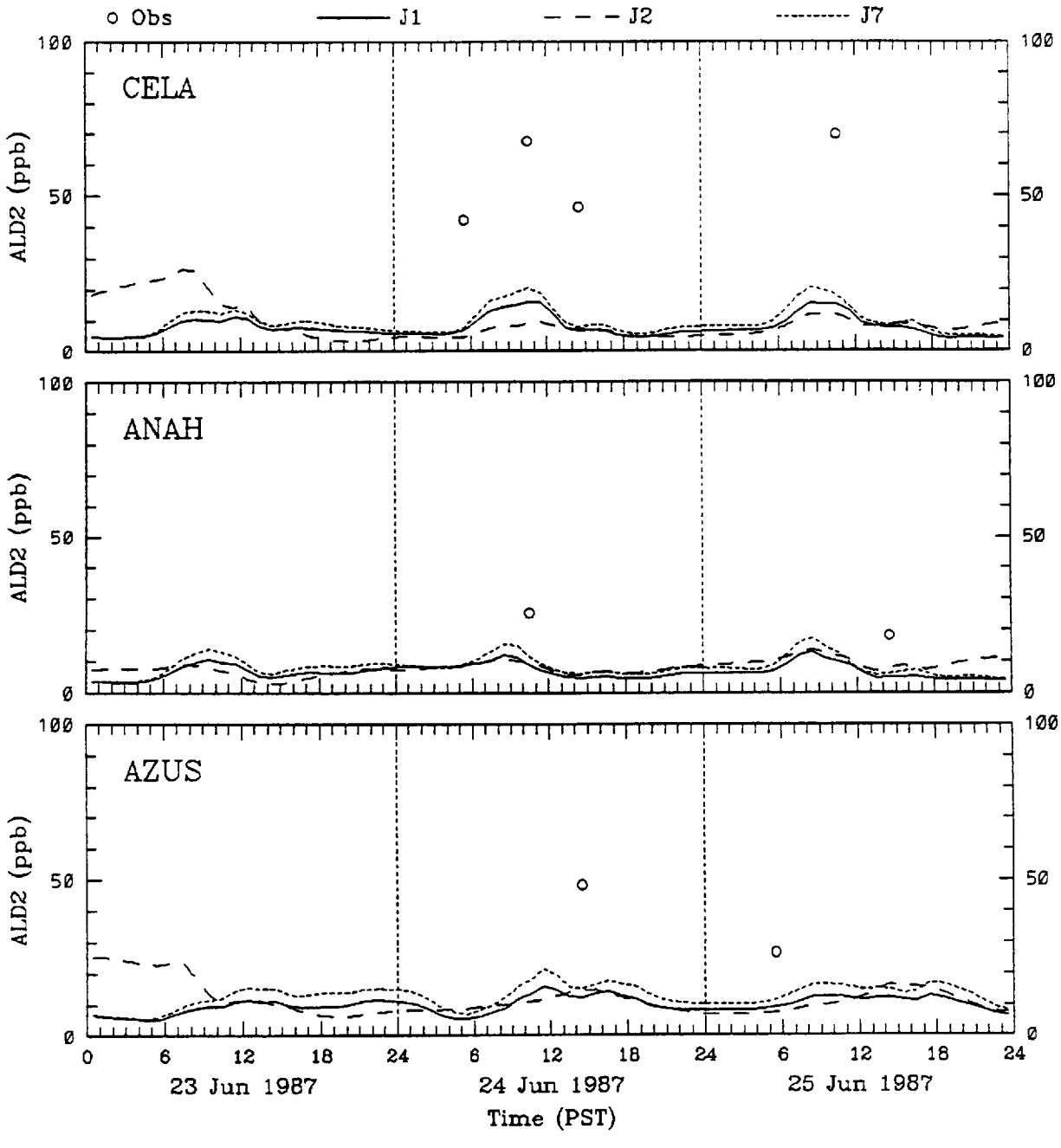
Runs J1, J2, and J7: Predicted and Observed FORM Time Series
23–25 June 1987



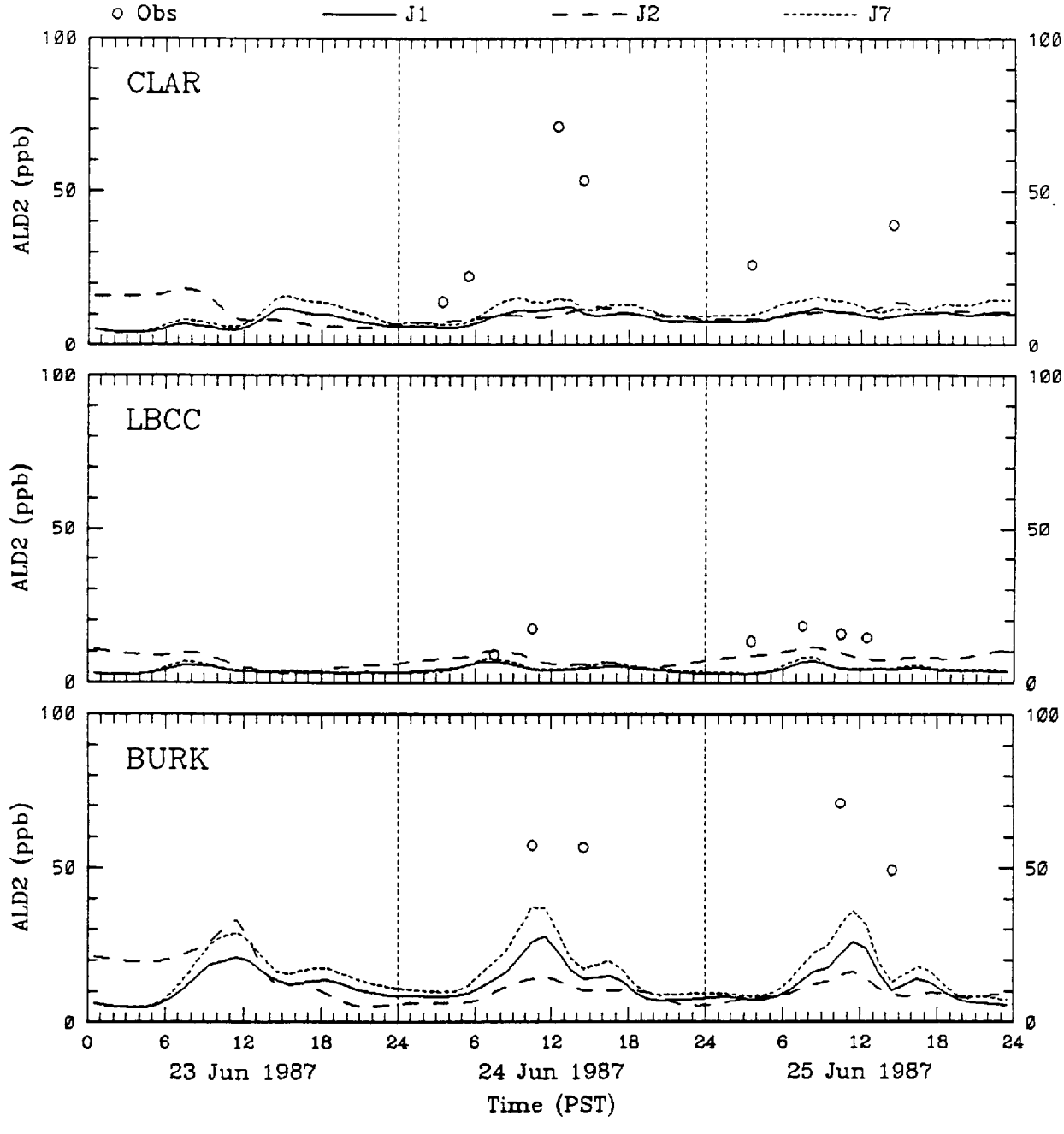
Runs J1, J2, and J7: Predicted and Observed FORM Time Series
23–25 June 1987



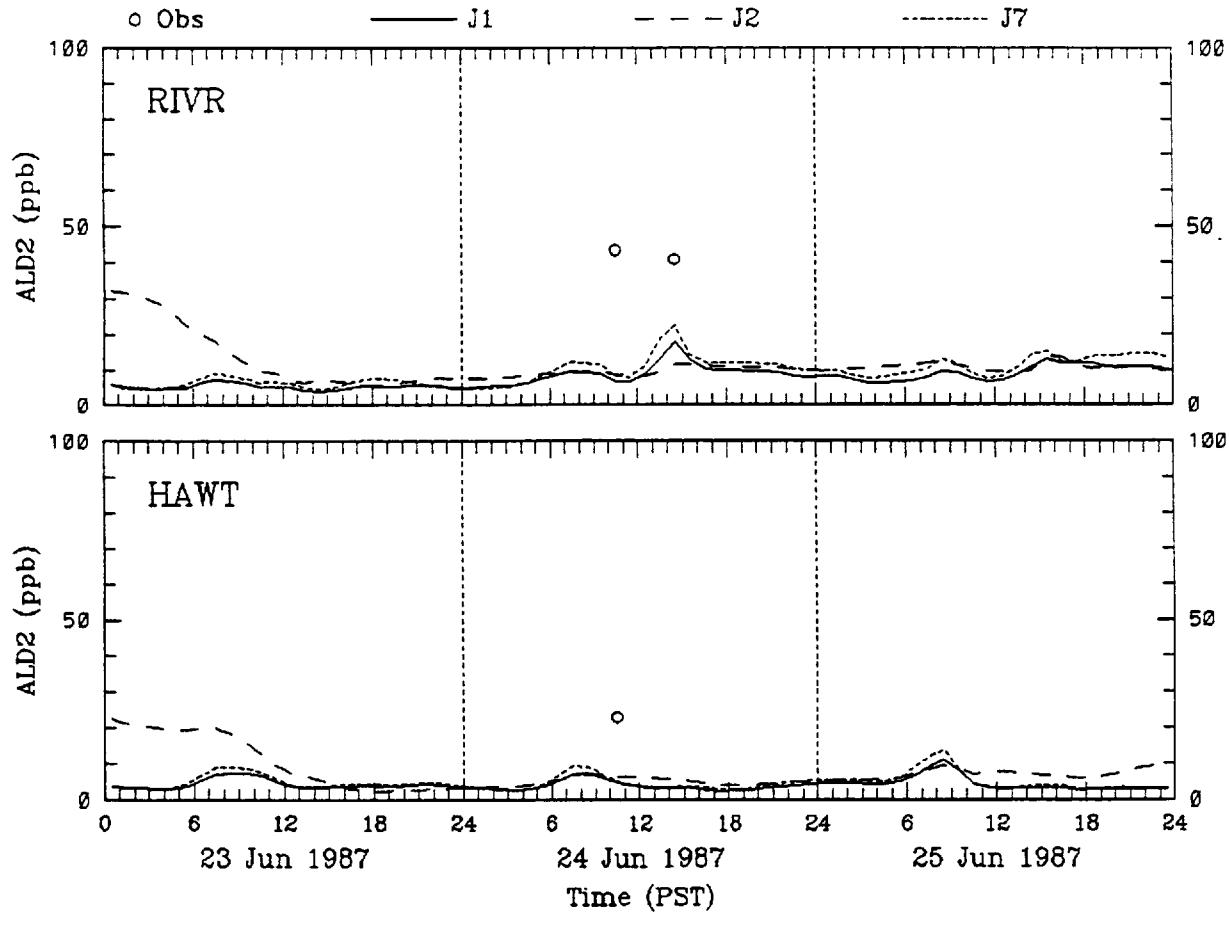
Runs J1, J2, and J7: Predicted and Observed ALD2 Time Series
23–25 June 1987



Runs J1, J2, and J7: Predicted and Observed ALD2 Time Series
23–25 June 1987



Runs J1, J2, and J7: Predicted and Observed ALD2 Time Series
23–25 June 1987



APPENDIX E

Appendix E

O_3, NO_2, AND NO_x SIMULATION RESULTS FOR 26-28 AUGUST 1987

This appendix contains time series plots showing estimated and measured concentrations for Runs A4 and A5 for 26-28 August 1987. Each display illustrates the estimated and measured concentrations for O_3, NO_2, and NO_x at an air monitoring station. The figures are organized by subregion as indicated below:

- Region A--Coastal Region

  Anaheim (ANAH)
  Costa Mesa (COST)
  El Toro (TORO)
  Long Beach (LGBH)
  Long Beach City College (LBCC)
  Los Alamitos (LSAL)
  West Los Angeles (WSLA)

- Region B--Central Basin

  La Habra (LAHB)
  Los Angeles (CELA)
  Lynnwood (LYNN)
  Pasadena (PASA)
  Pico Rivera (PICO)
  Whittier (WHIT)

- Region C--San Fernando Valley

  Burbank (BURK)
  Reseda (RESE)

- Region D--Eastern Region

  Azusa (AZUS)
  Fontana (FONT)
  Glendora (GLEN)
  Norco (NORC)
  Pomona (POMA)

Redlands (REDL)
Riverside-Rubidoux (RIVR)
Rubidoux (RUBI)
San Bernardino (SNBD)
Upland (UPLA)

- Region E--Basin Rim

  Banning (BANN)
  Crestline (CRES)
  Hemet (HEME)
  Perris (PERI)

- Region F--Far Eastern Region

  Palm Springs (PLSP)
  29 Palms (29PL)

- Region G--Lancaster

  Lancaster (LANC)

- Region H--Ventura County

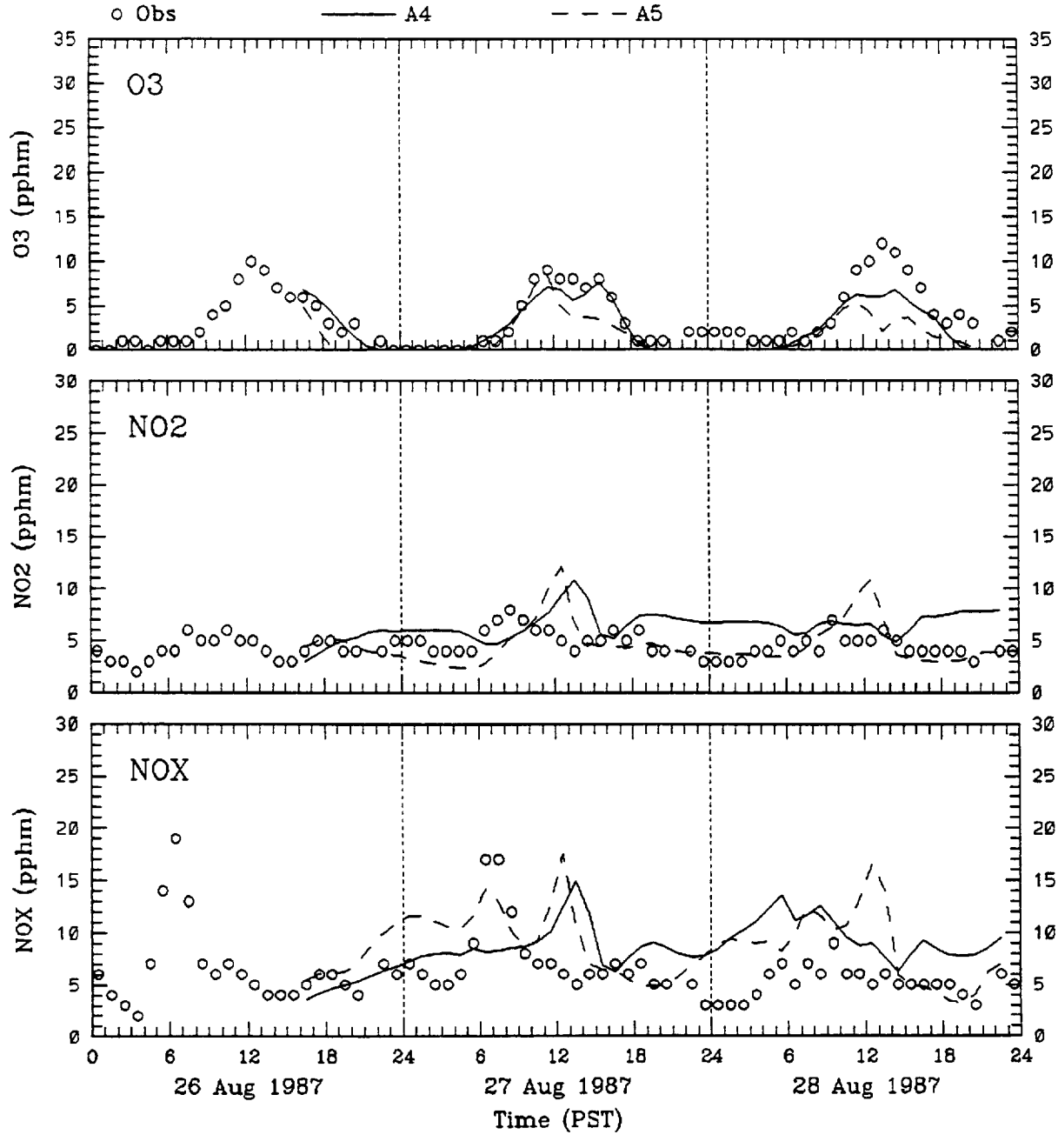
  El Rio-Rio Mesa H.S. (ERIO)
  Ojai (OJAI)
  Piru-2SW (PRU2)
  Simi Valley-Cochran (SIM2)
  Thousand Oaks-Windsor (OAKS)
  Ventura-Emma Wood (EMMA)

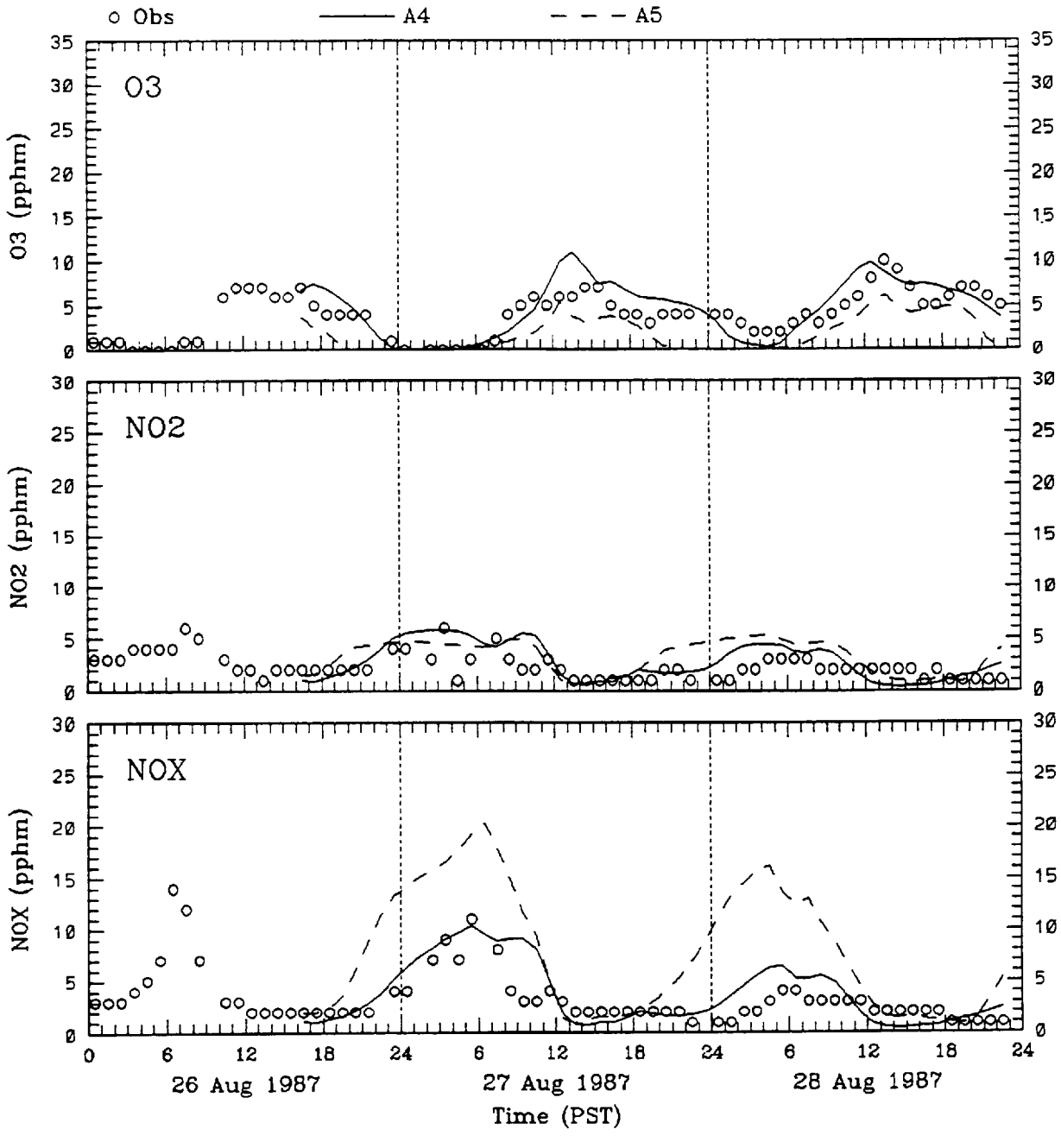
- Region I--Victorville and Hesperia

  Hesperia (HESP)
  Victorville (VICT)

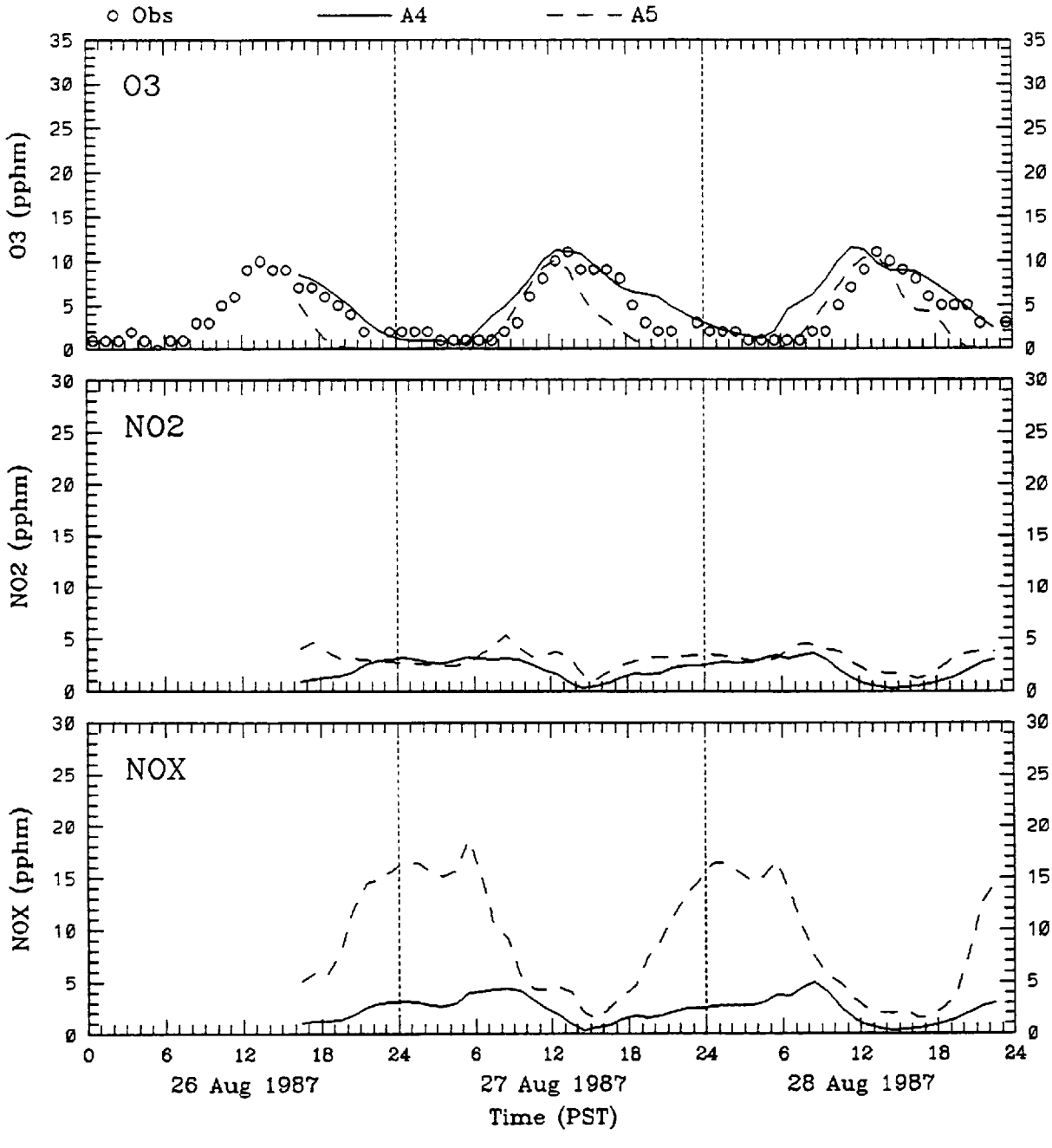
Figure 2-1 in Section 2 shows the locations of these air monitoring stations.

UAM Simulation Results for 26-28 August 1987
Location: ANAH Runs: A4 and A5

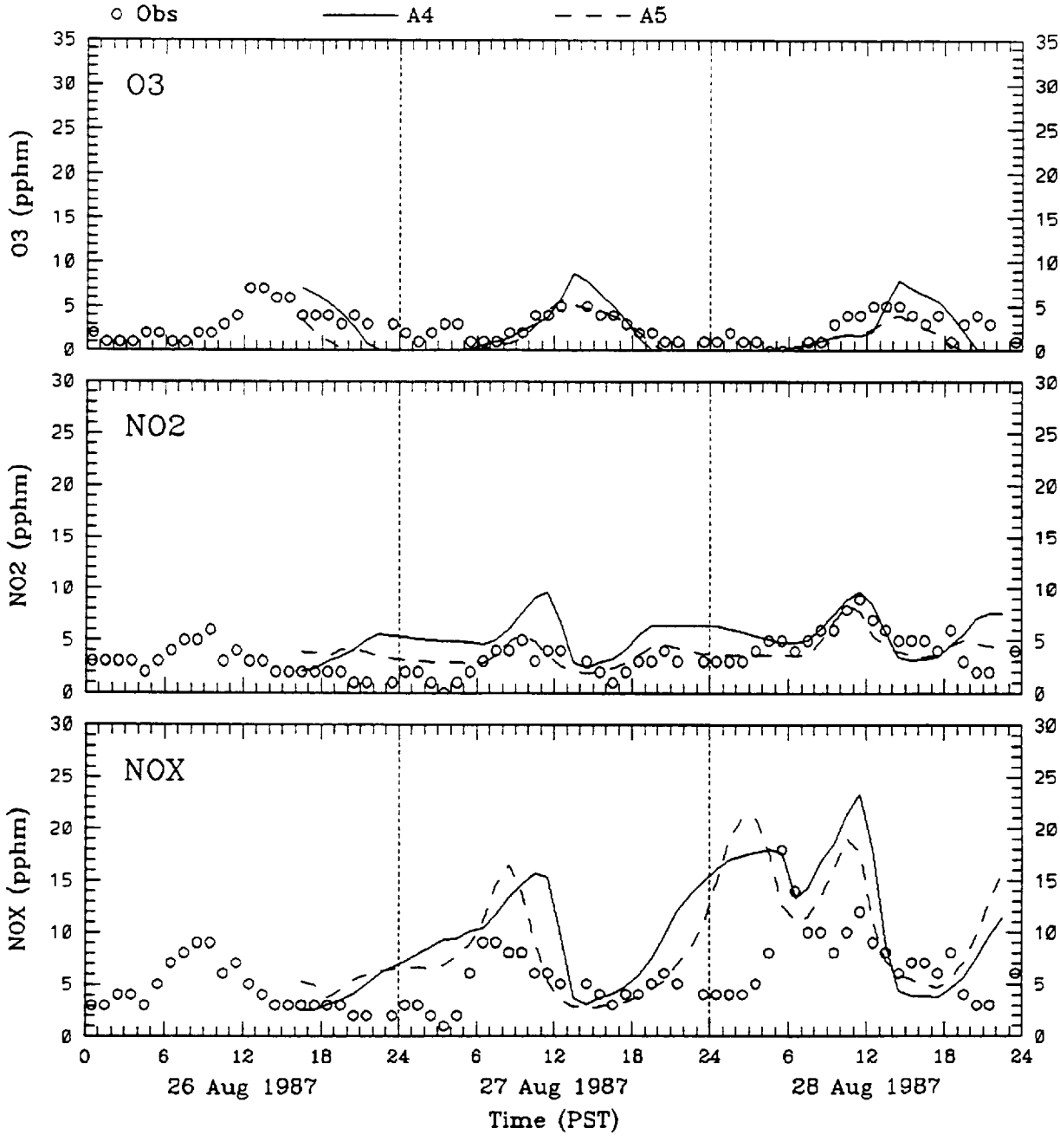




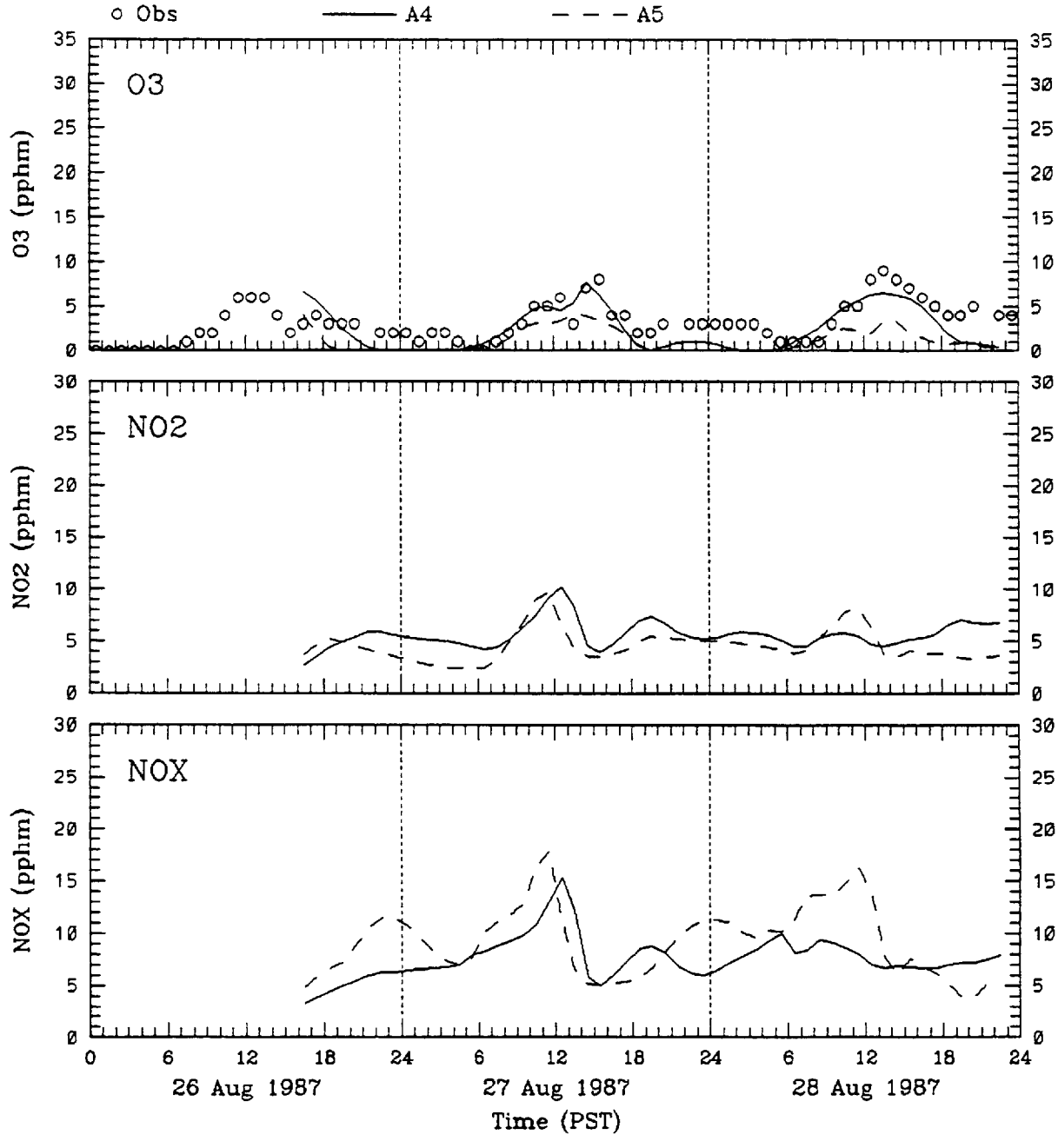
UAM Simulation Results for 26–28 August 1987
Location: TORO Runs: A4 and A5



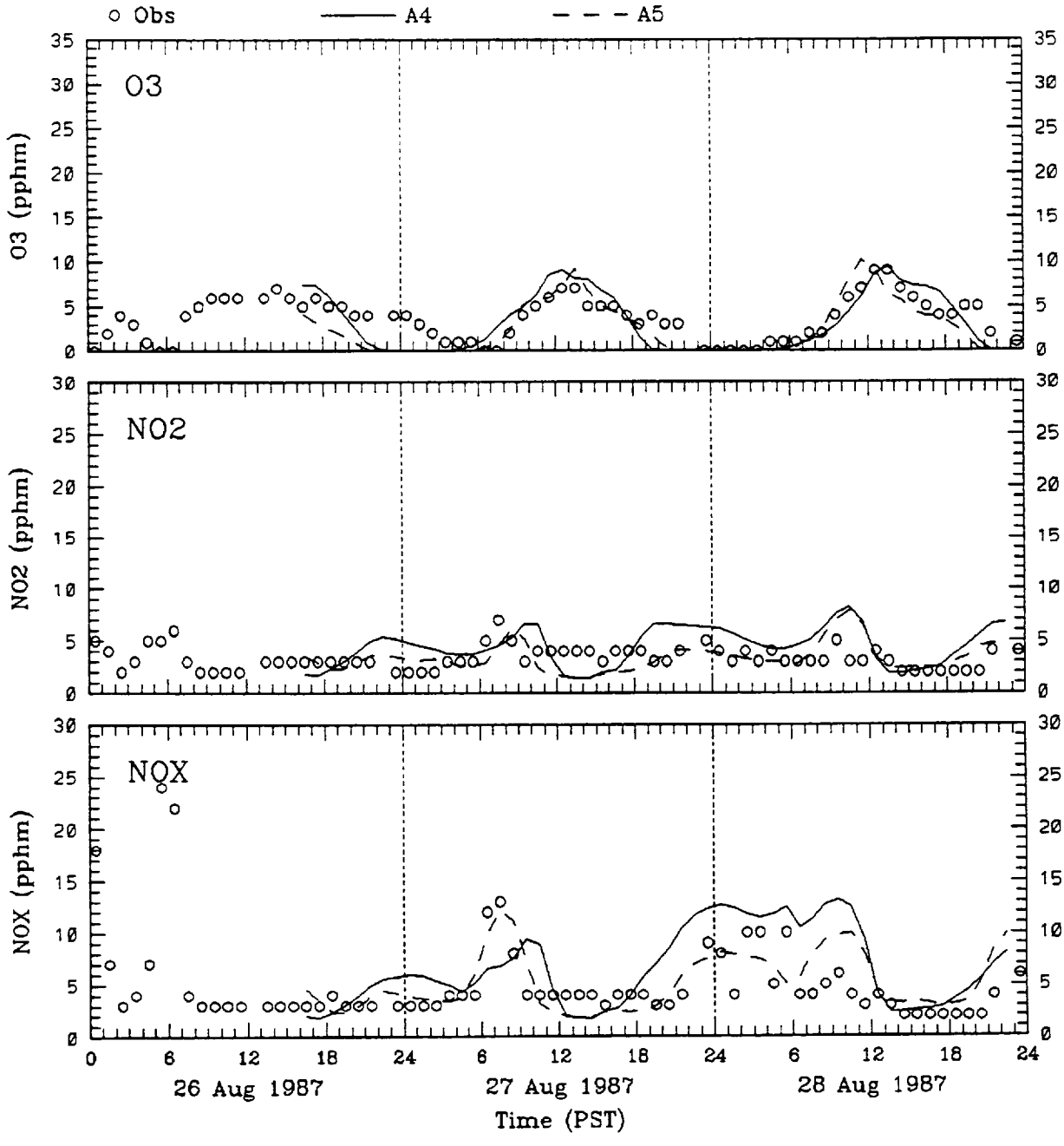
UAM Simulation Results for 26-28 August 1987
Location: LGBH Runs: A4 and A5

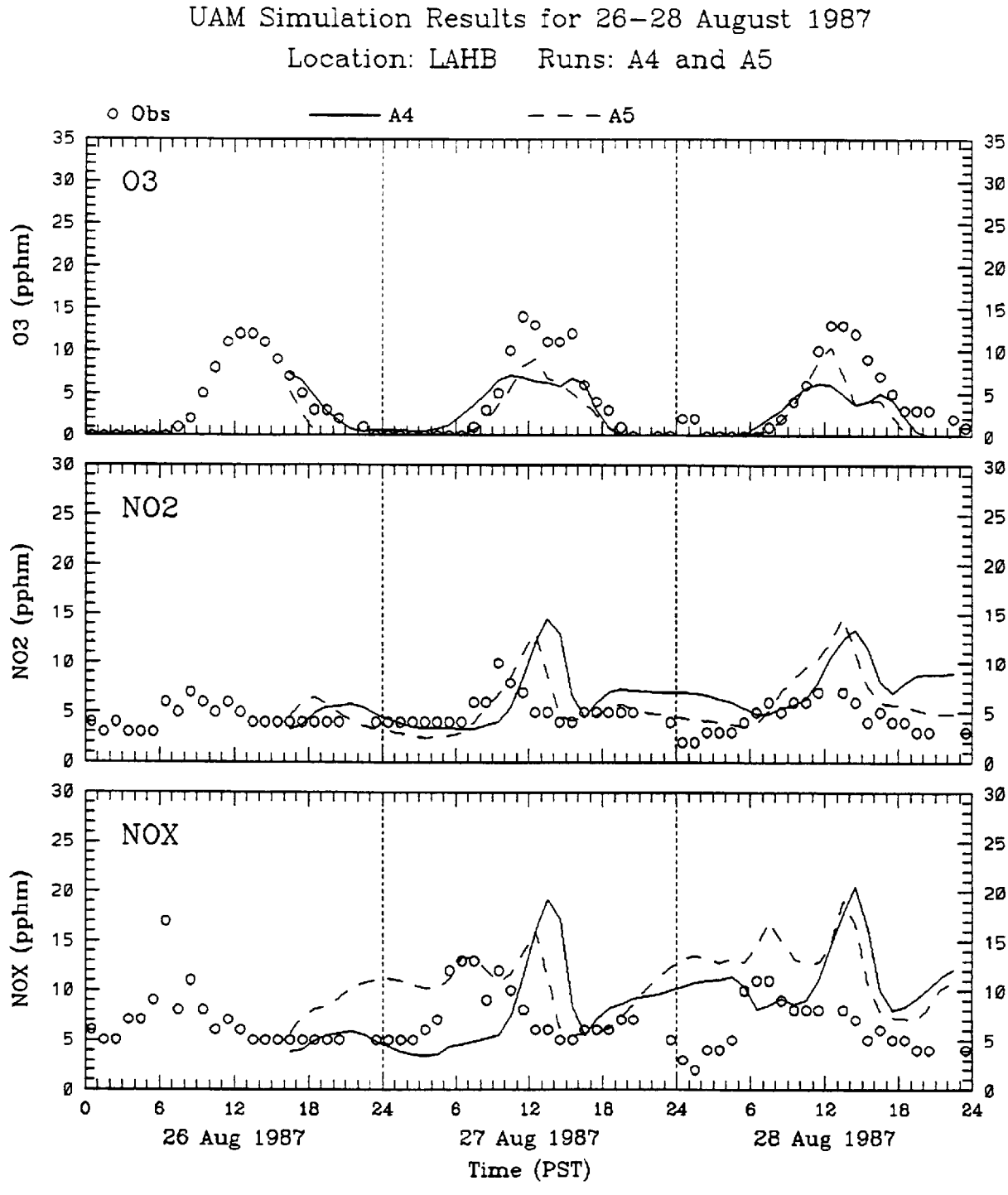


UAM Simulation Results for 26-28 August 1987
Location: LSAL Runs: A4 and A5

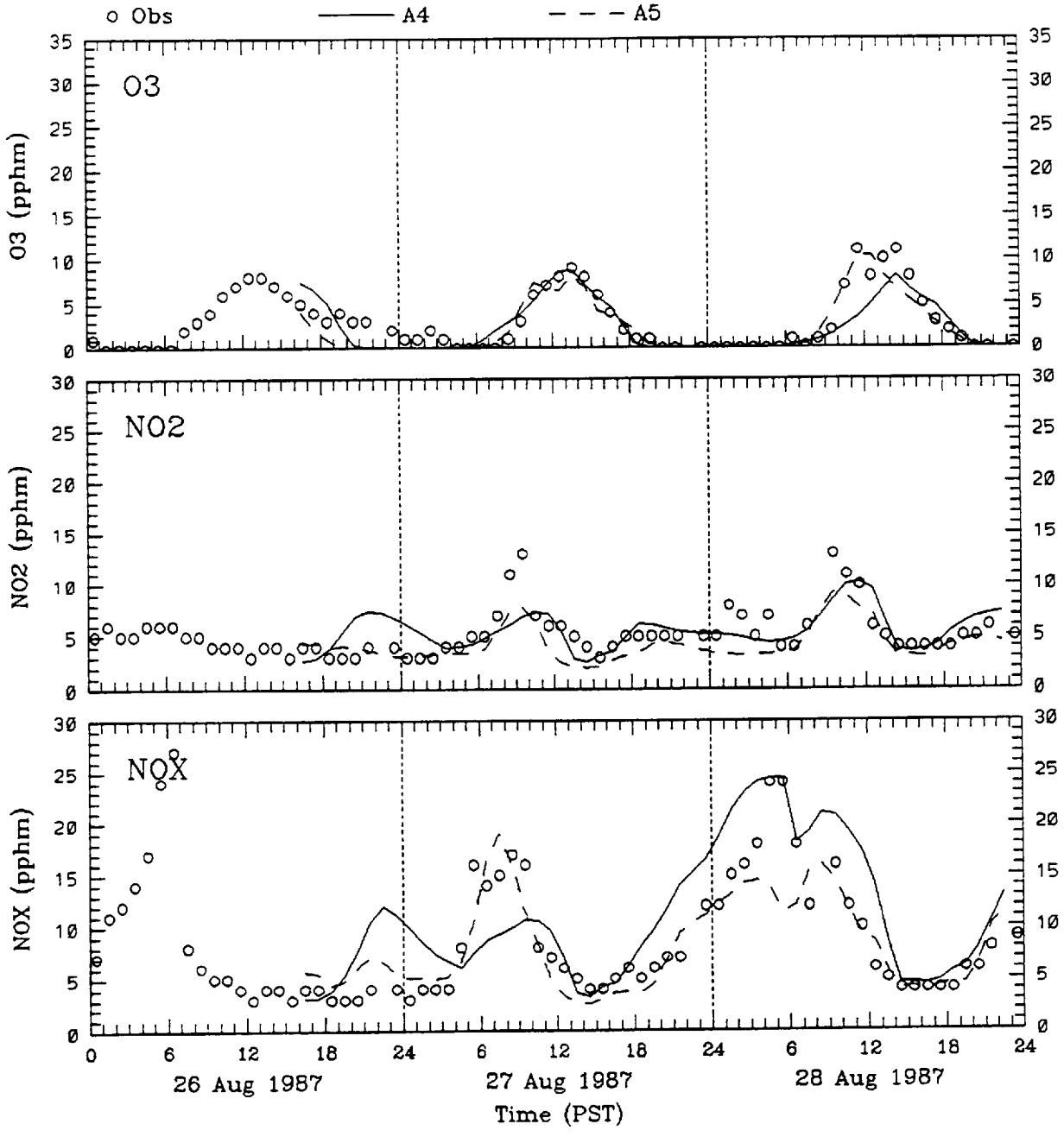


UAM Simulation Results for 26–28 August 1987
Location: WSLA Runs: A4 and A5

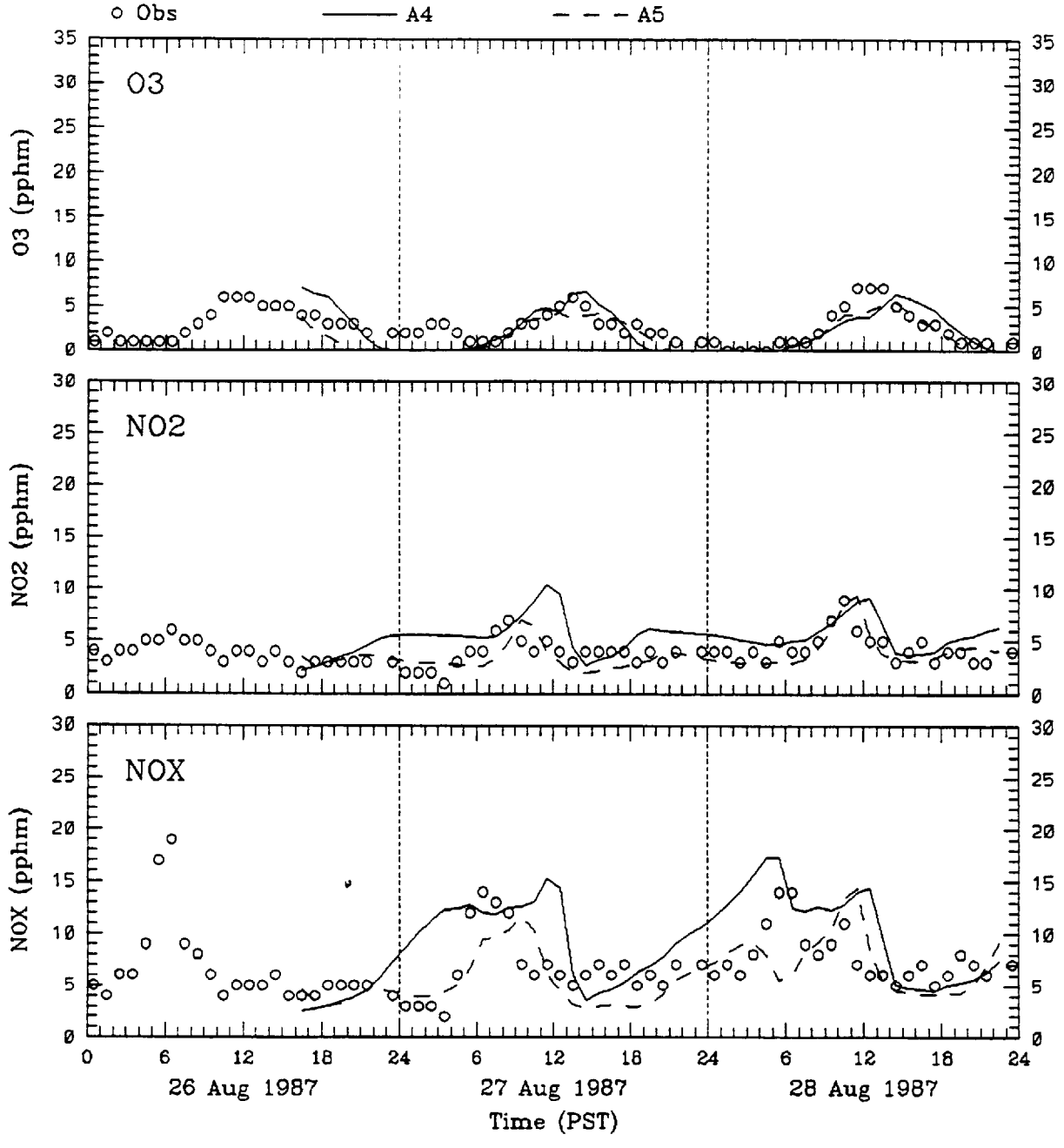




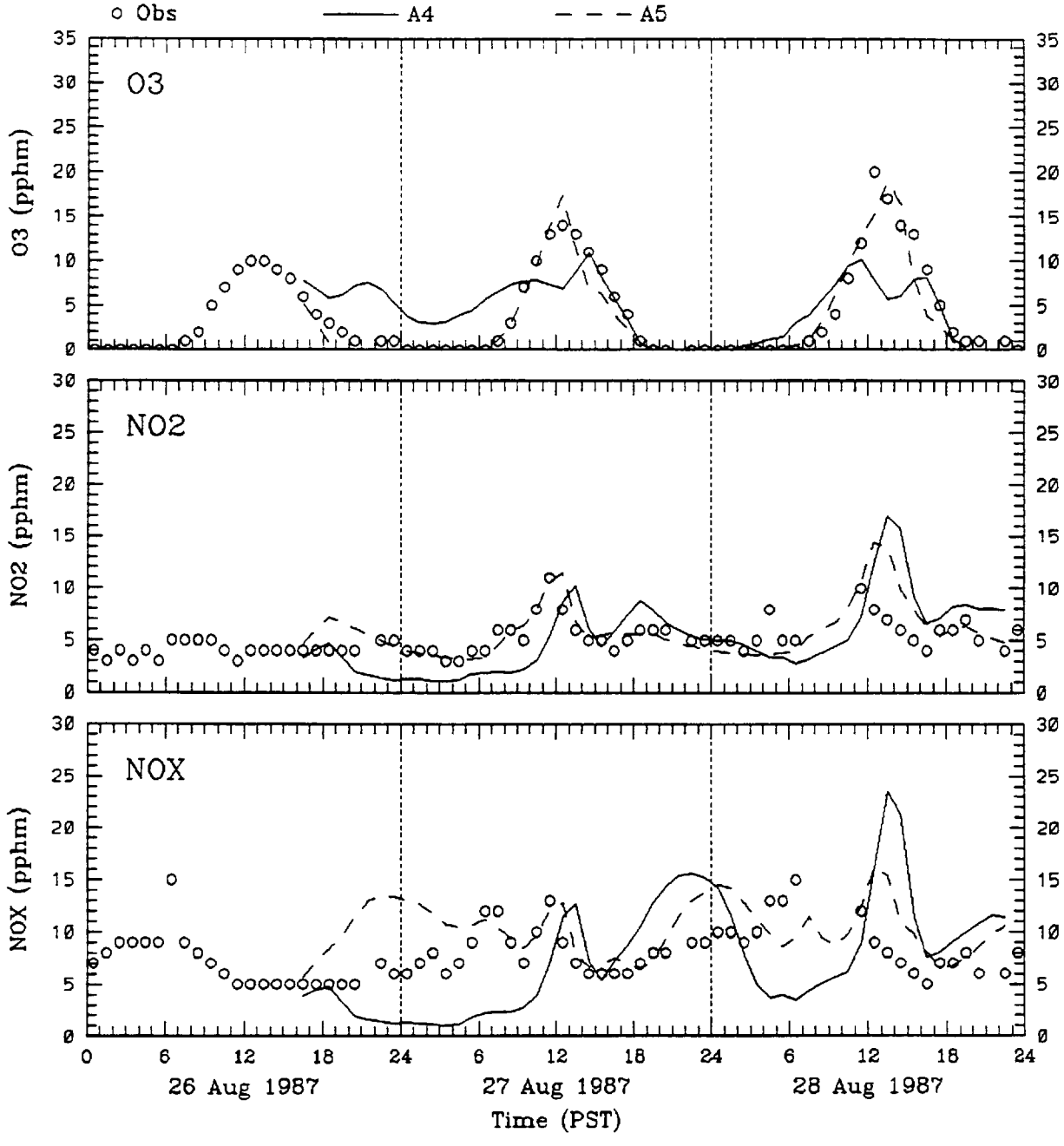
UAM Simulation Results for 26-28 August 1987
Location: CELA Runs: A4 and A5

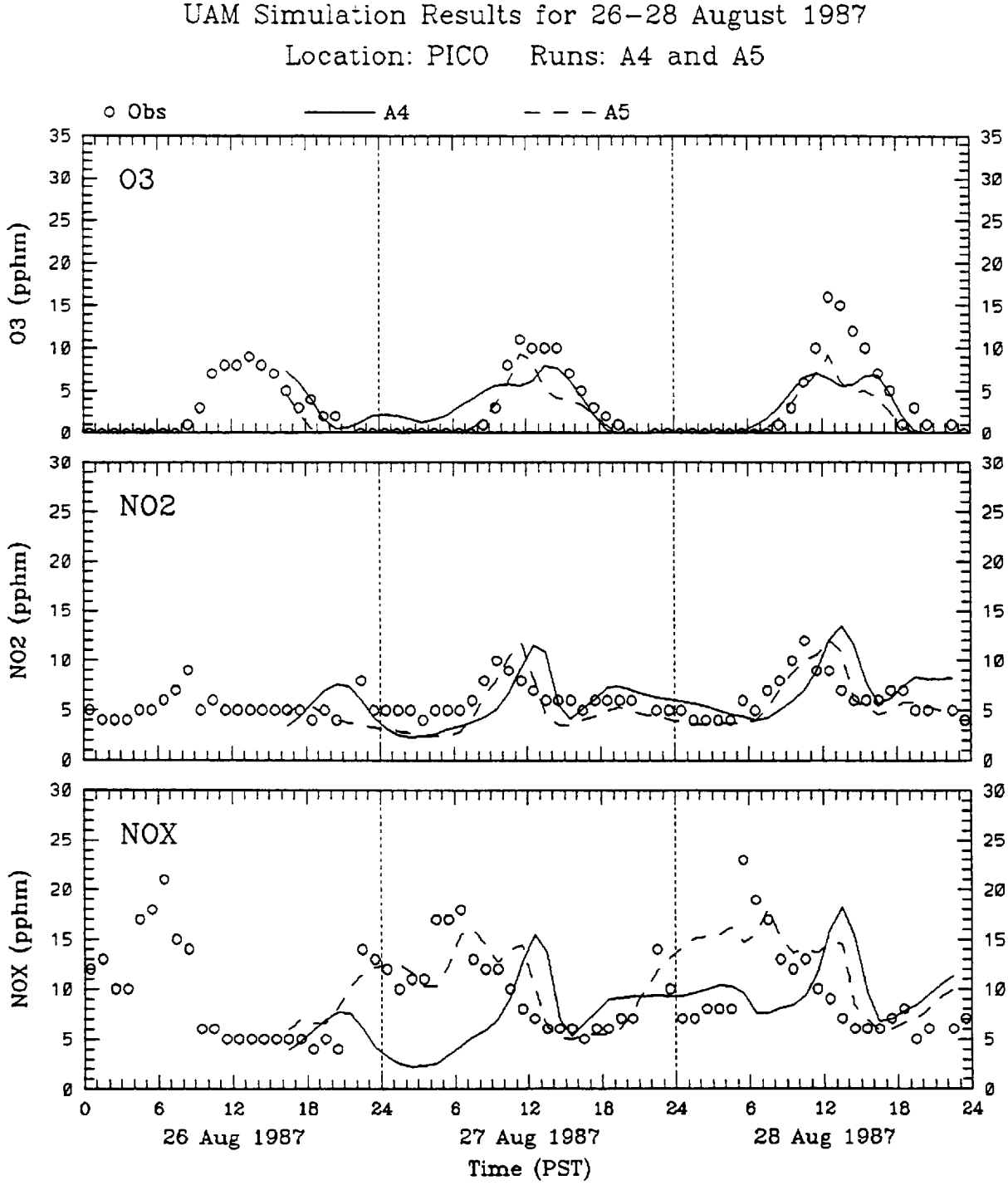


UAM Simulation Results for 26–28 August 1987
Location: LYNN Runs: A4 and A5

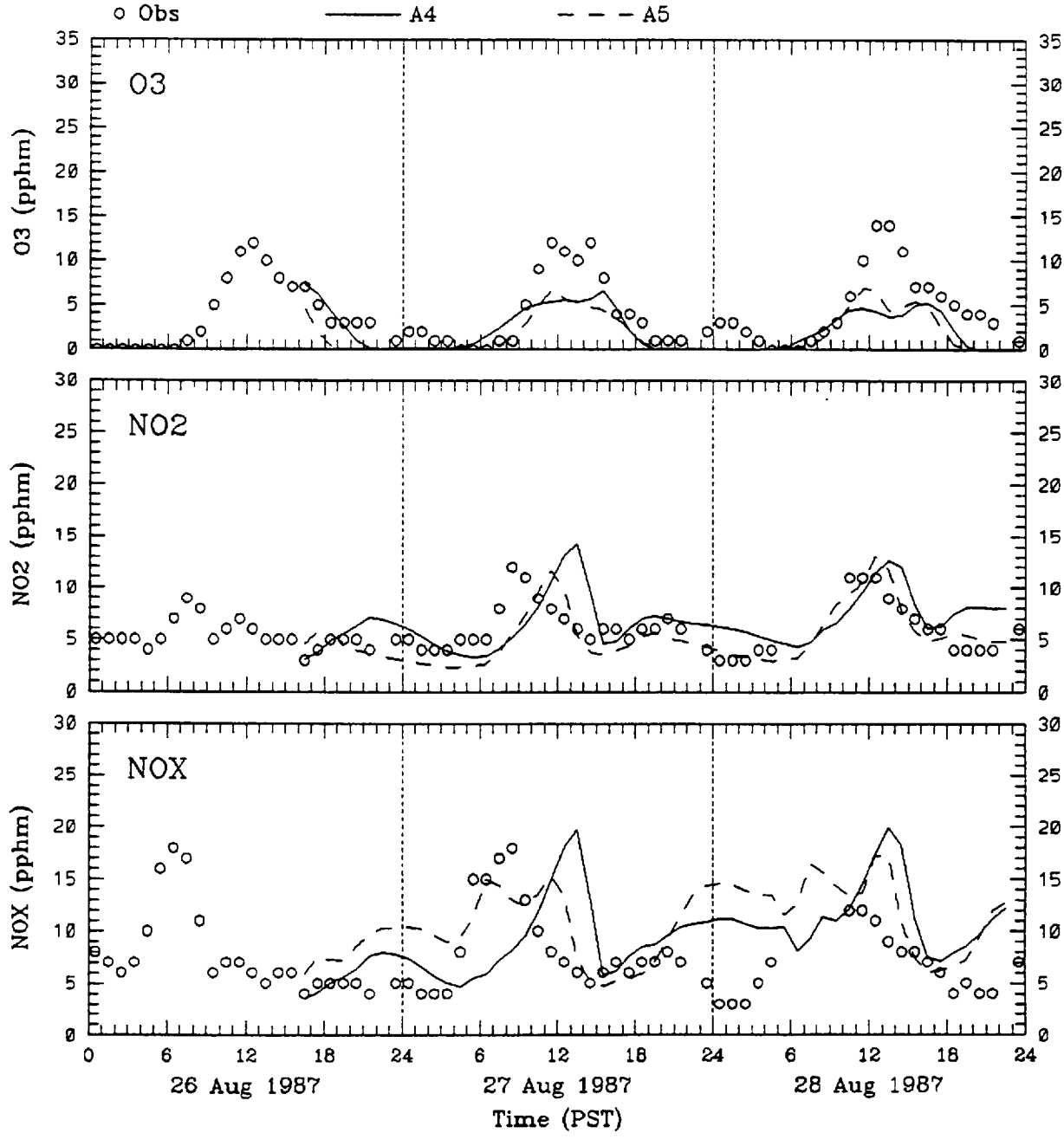


UAM Simulation Results for 26-28 August 1987
Location: PASA Runs: A4 and A5

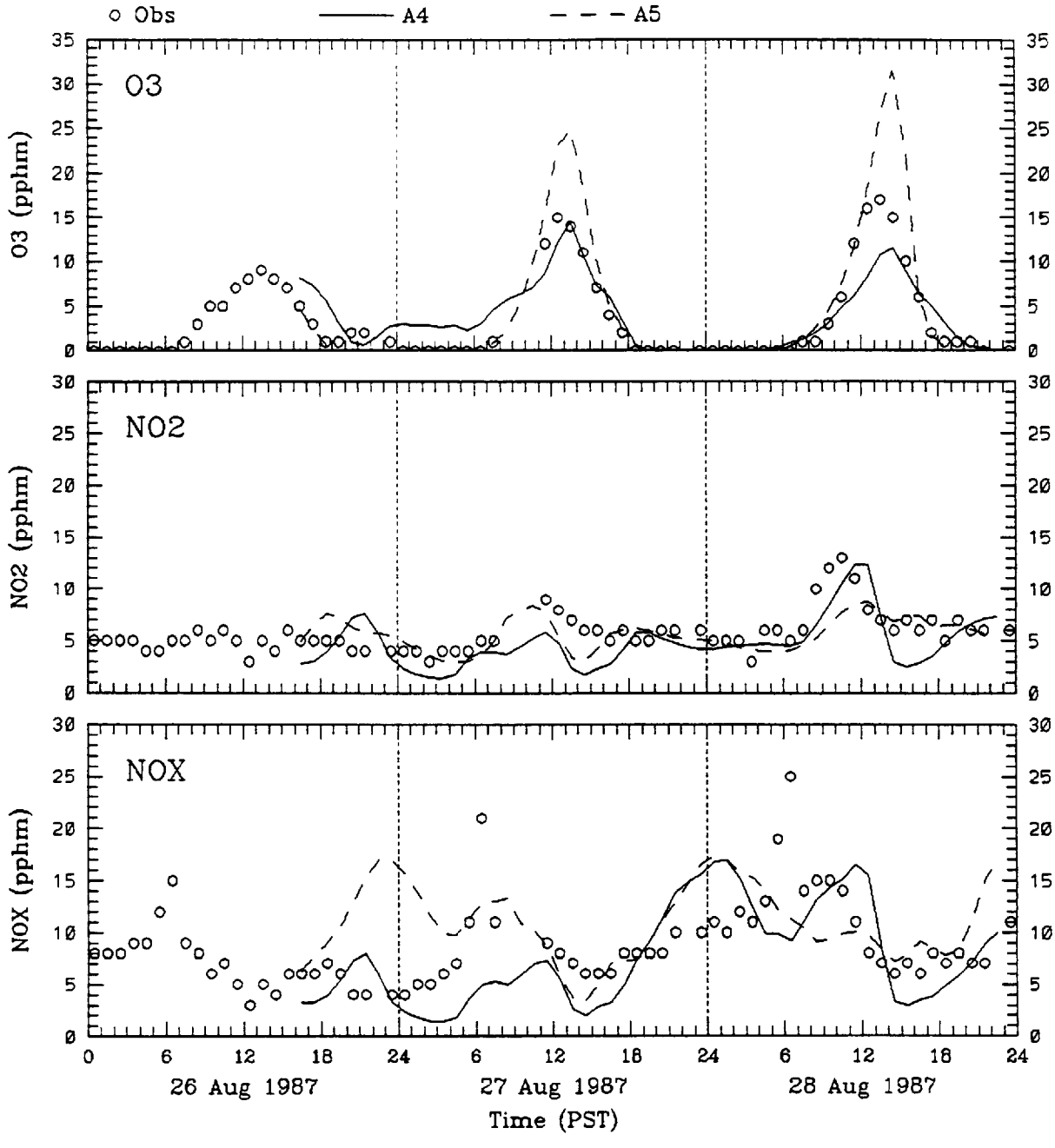


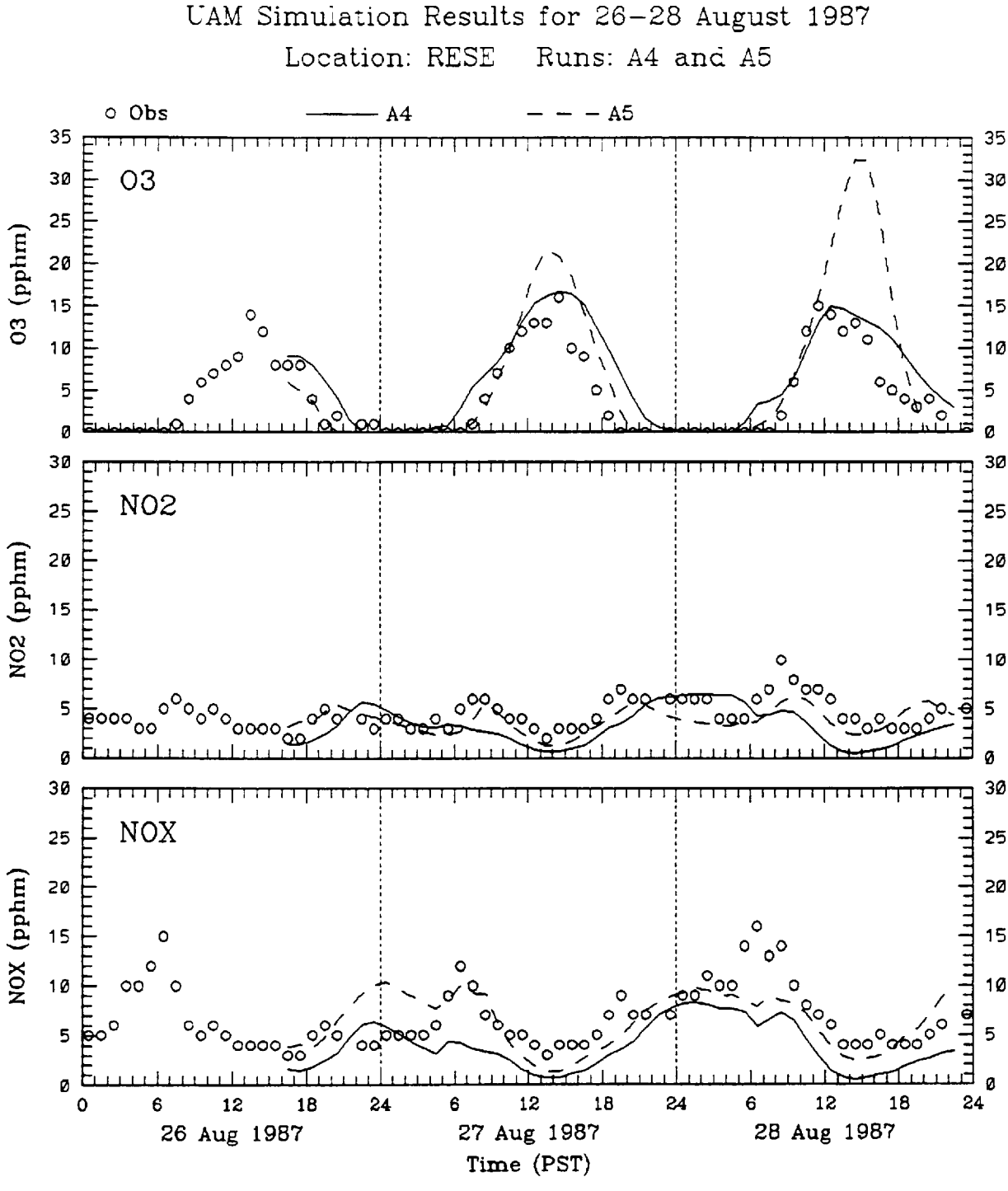


UAM Simulation Results for 26-28 August 1987
Location: WHIT Runs: A4 and A5

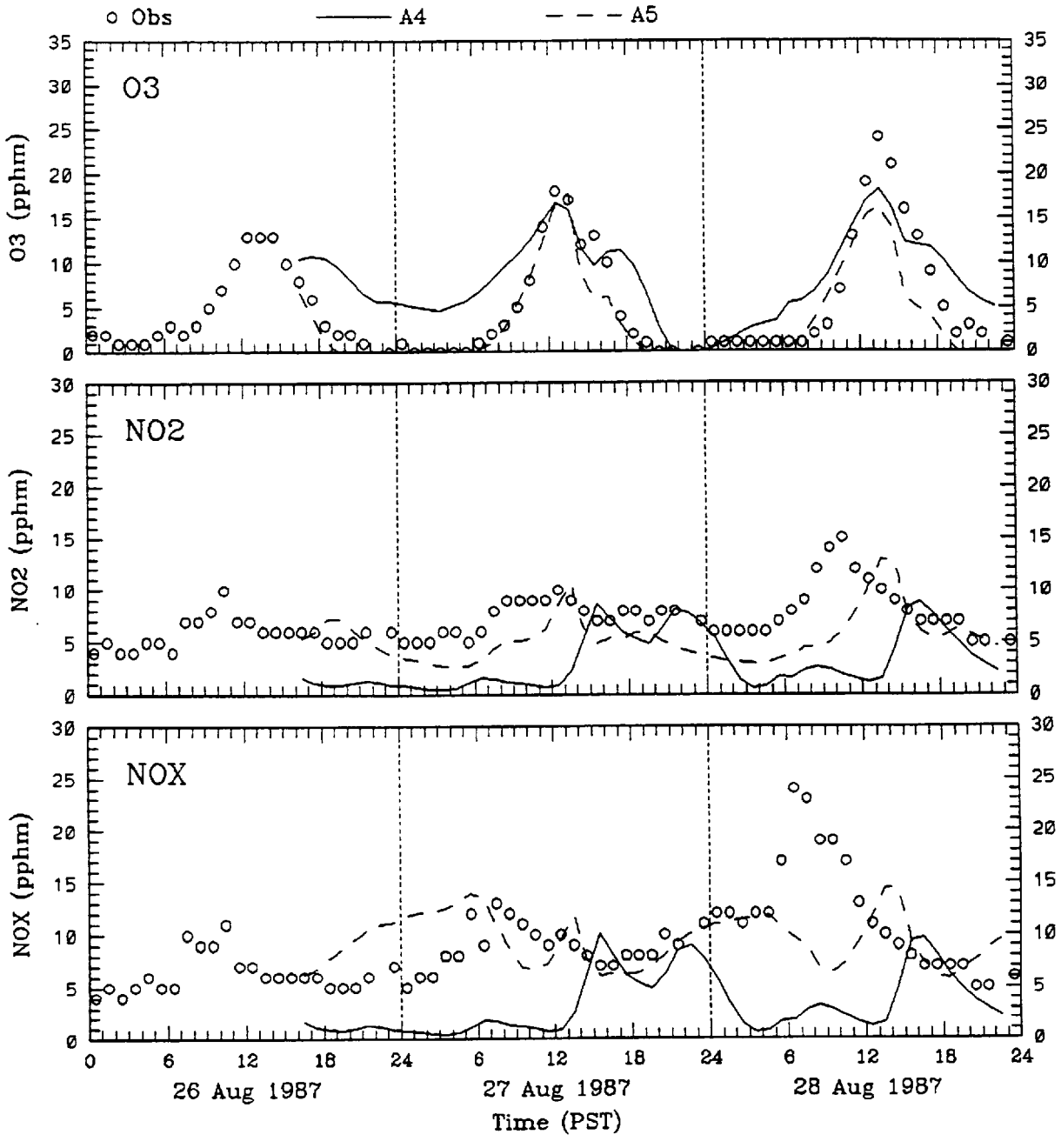


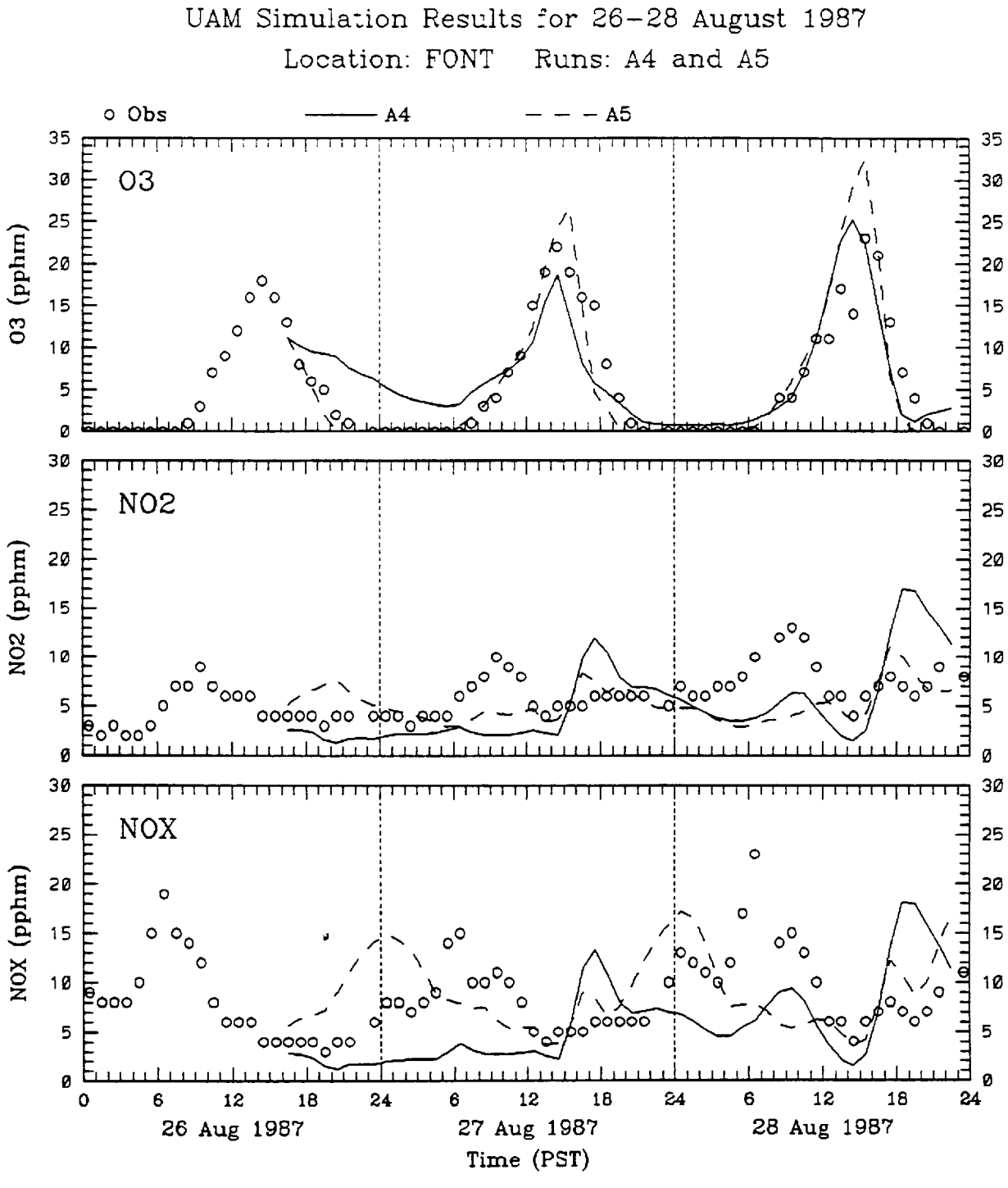
UAM Simulation Results for 26–28 August 1987
Location: BURK Runs: A4 and A5



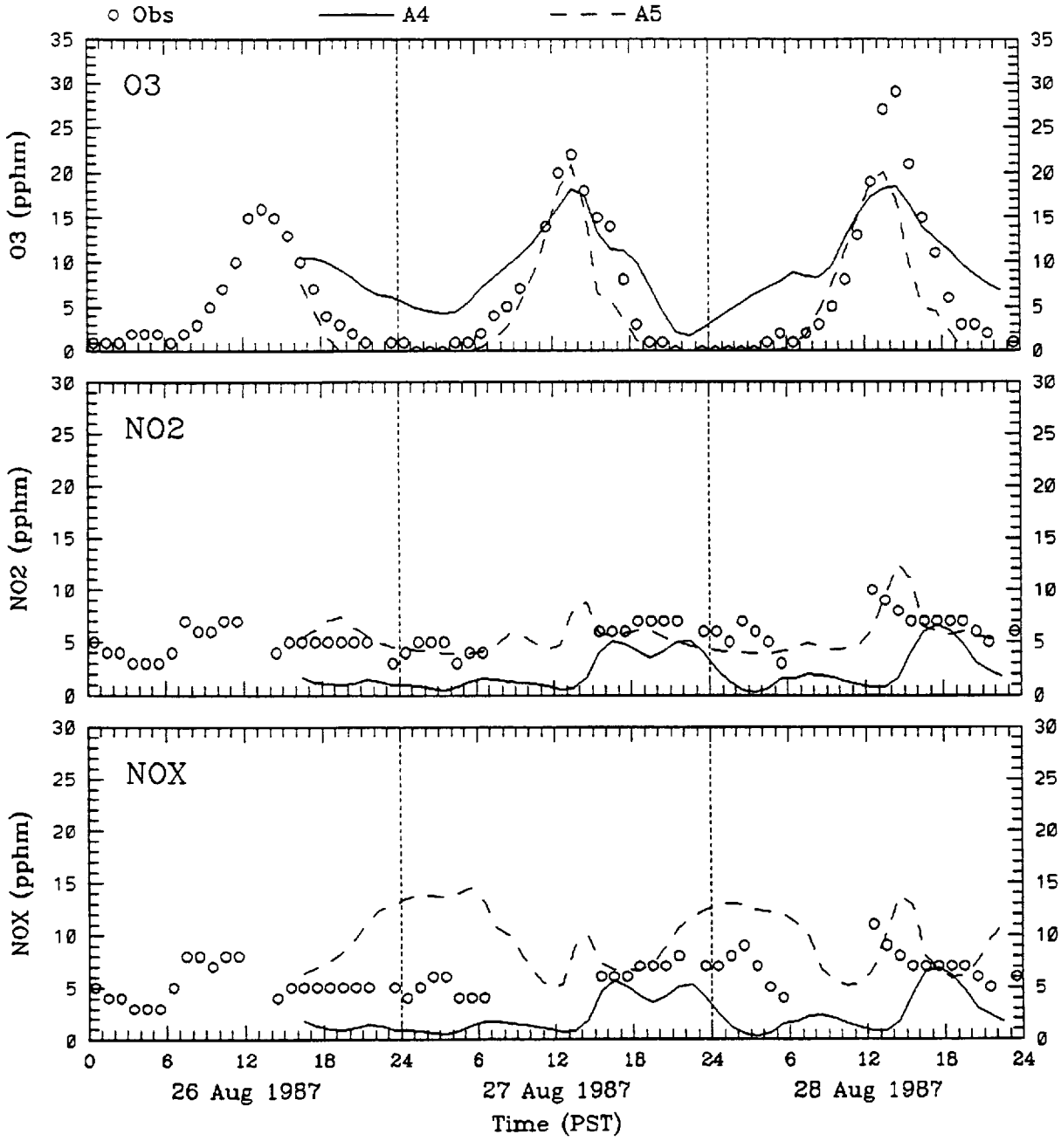


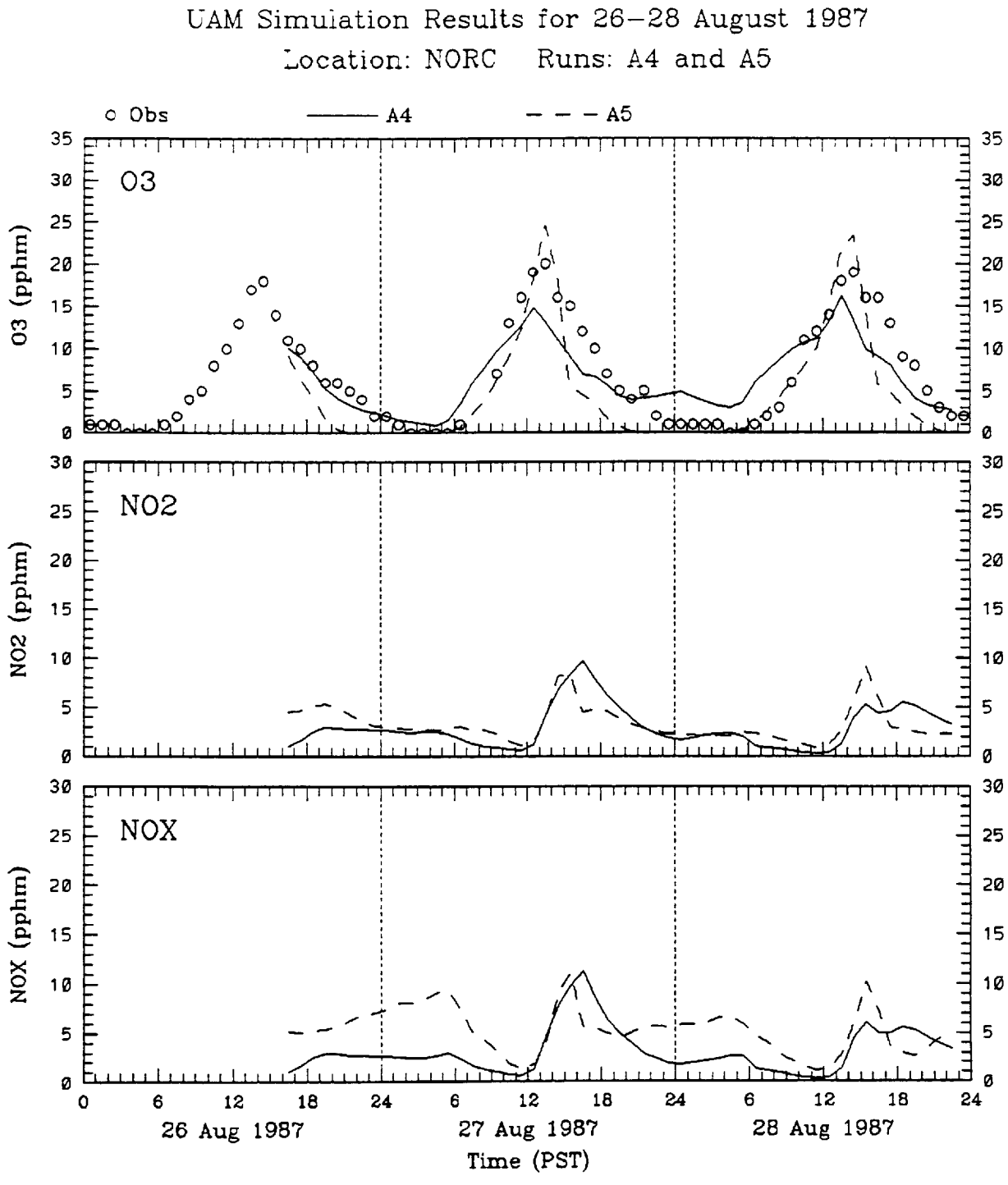
UAM Simulation Results for 26-28 August 1987
Location: AZUS Runs: A4 and A5



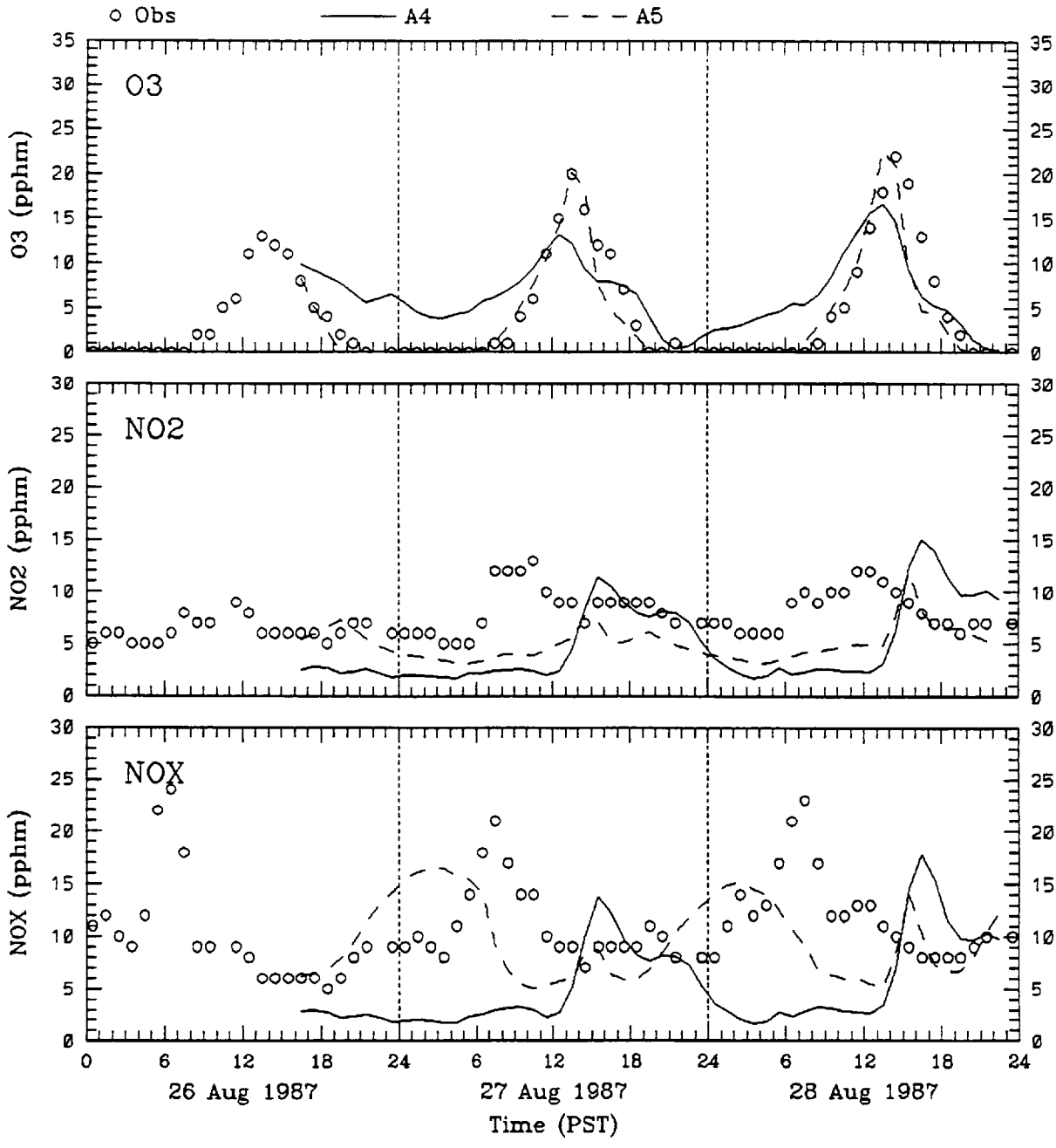


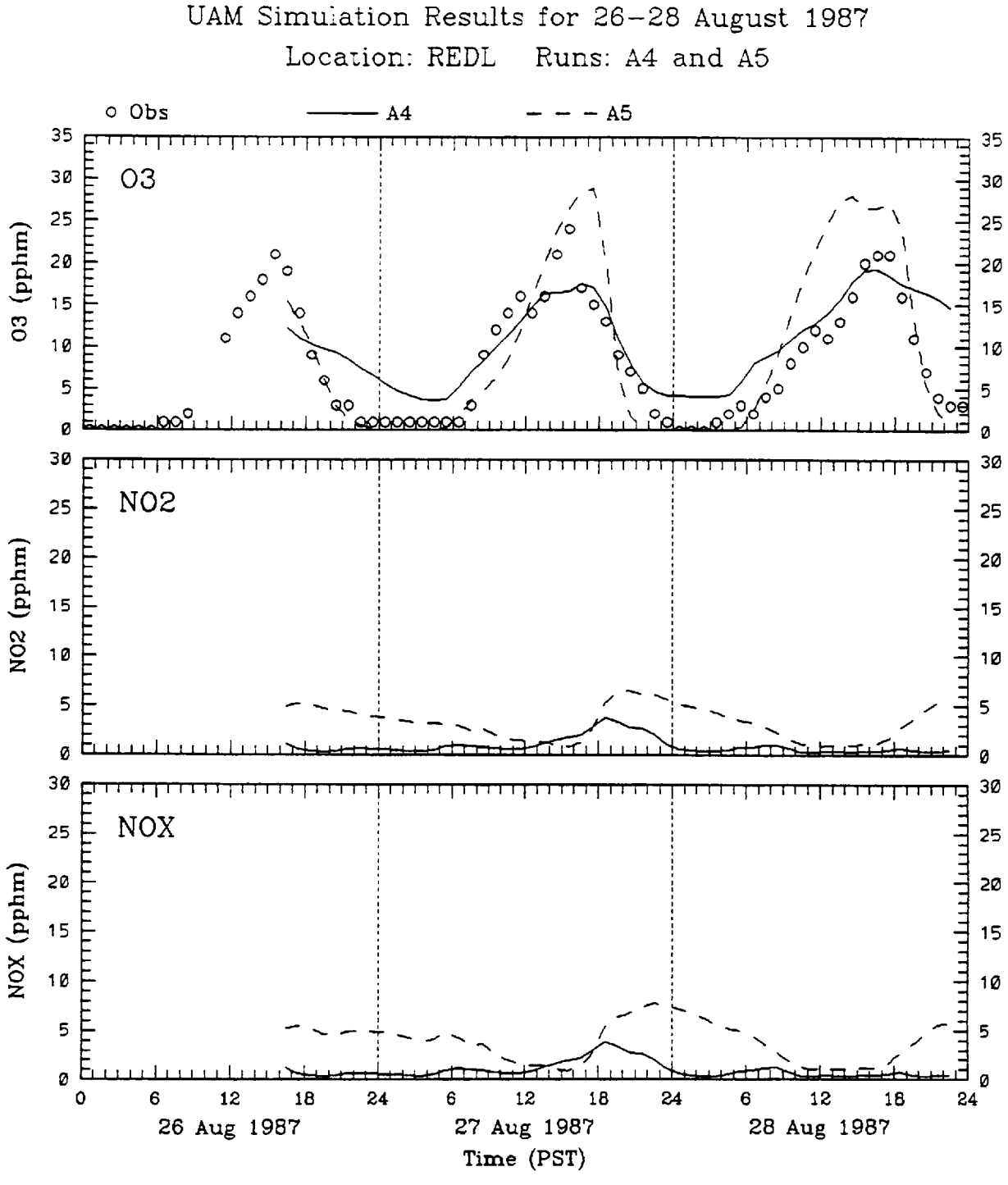
UAM Simulation Results for 26–28 August 1987
Location: GLEN Runs: A4 and A5



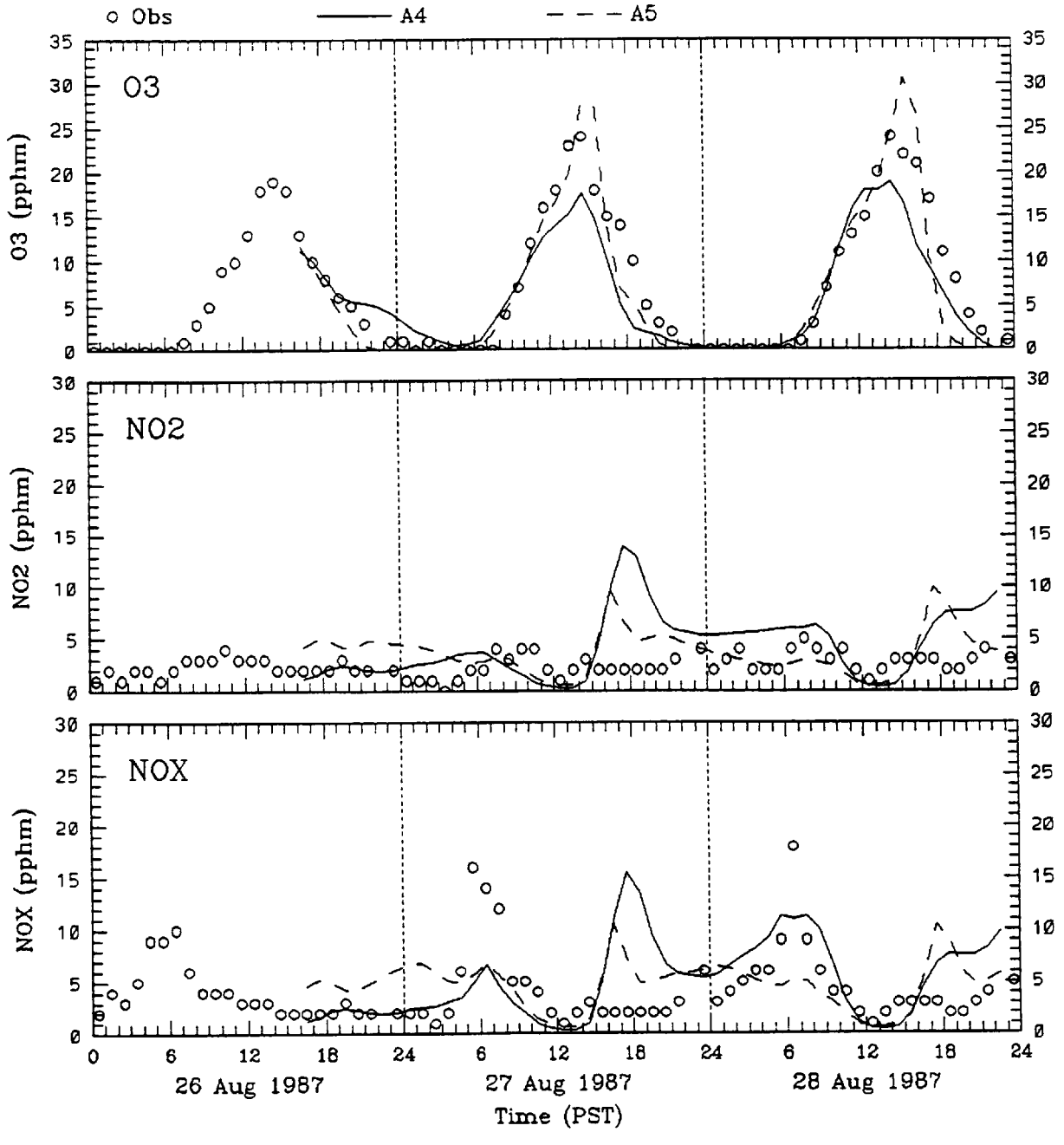


UAM Simulation Results for 26-28 August 1987
Location: POMO Runs: A4 and A5

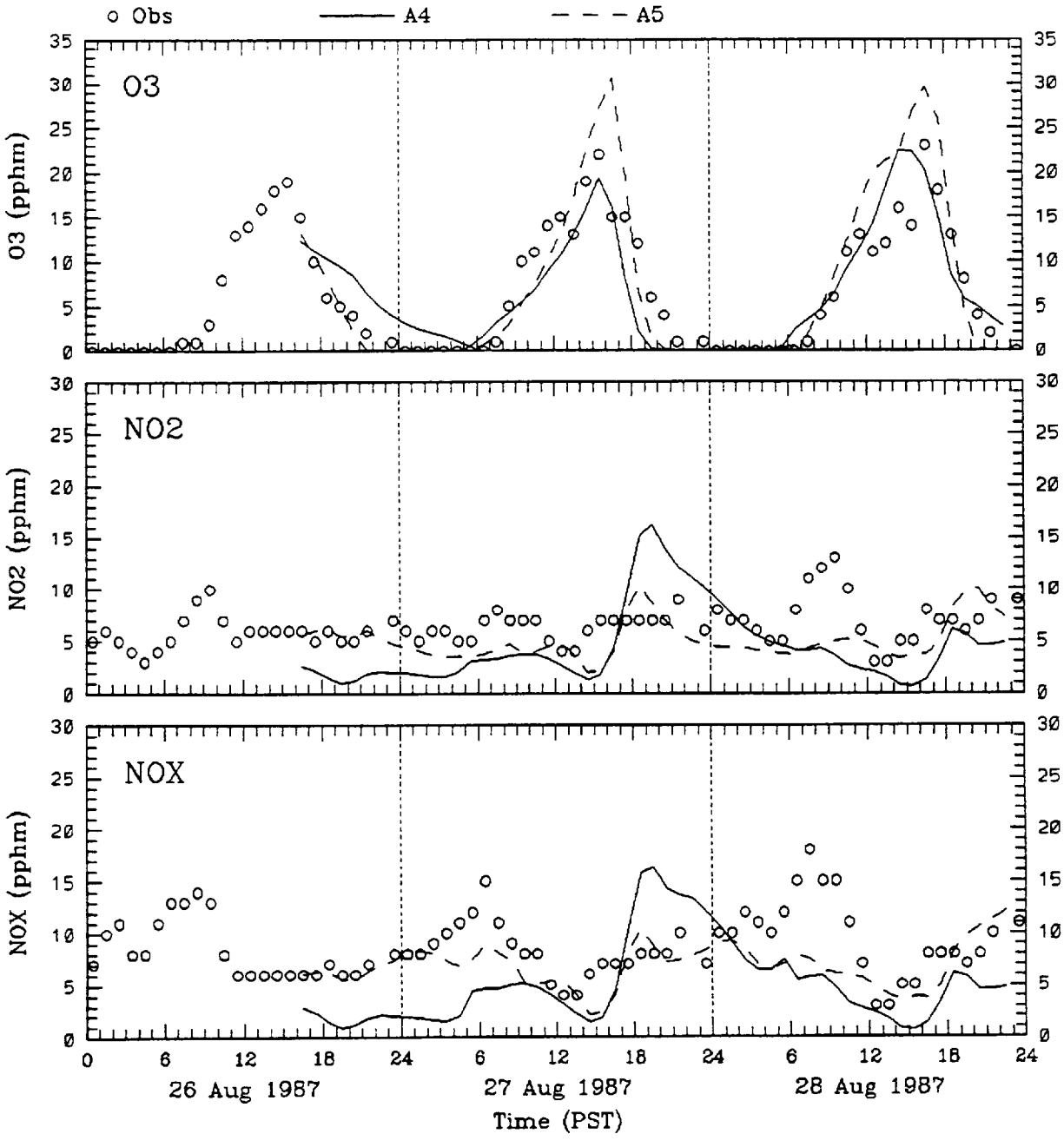




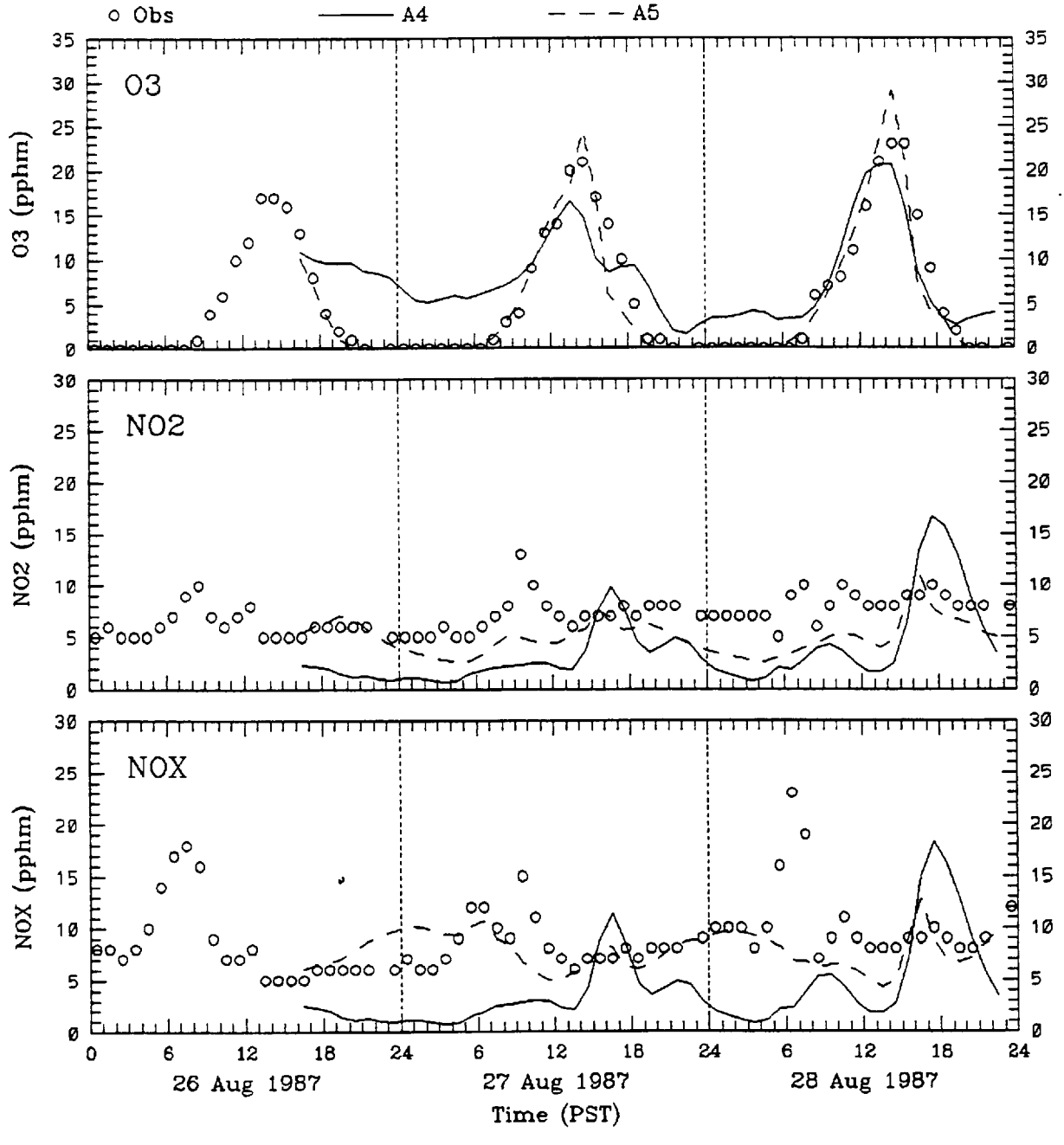
UAM Simulation Results for 26–28 August 1987
Location: RUBI Runs: A4 and A5

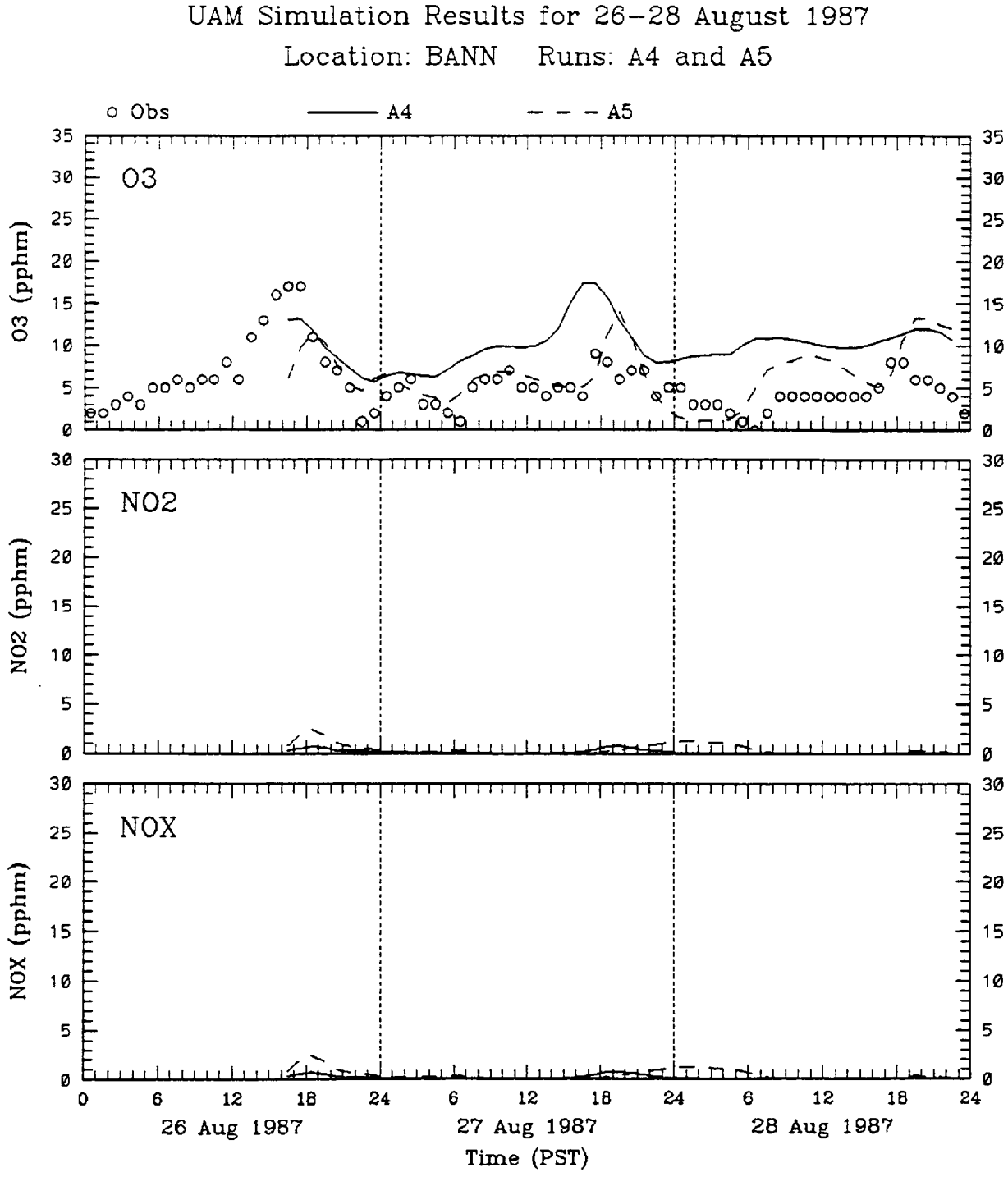


UAM Simulation Results for 26-28 August 1987
Location: SNBD Runs: A4 and A5

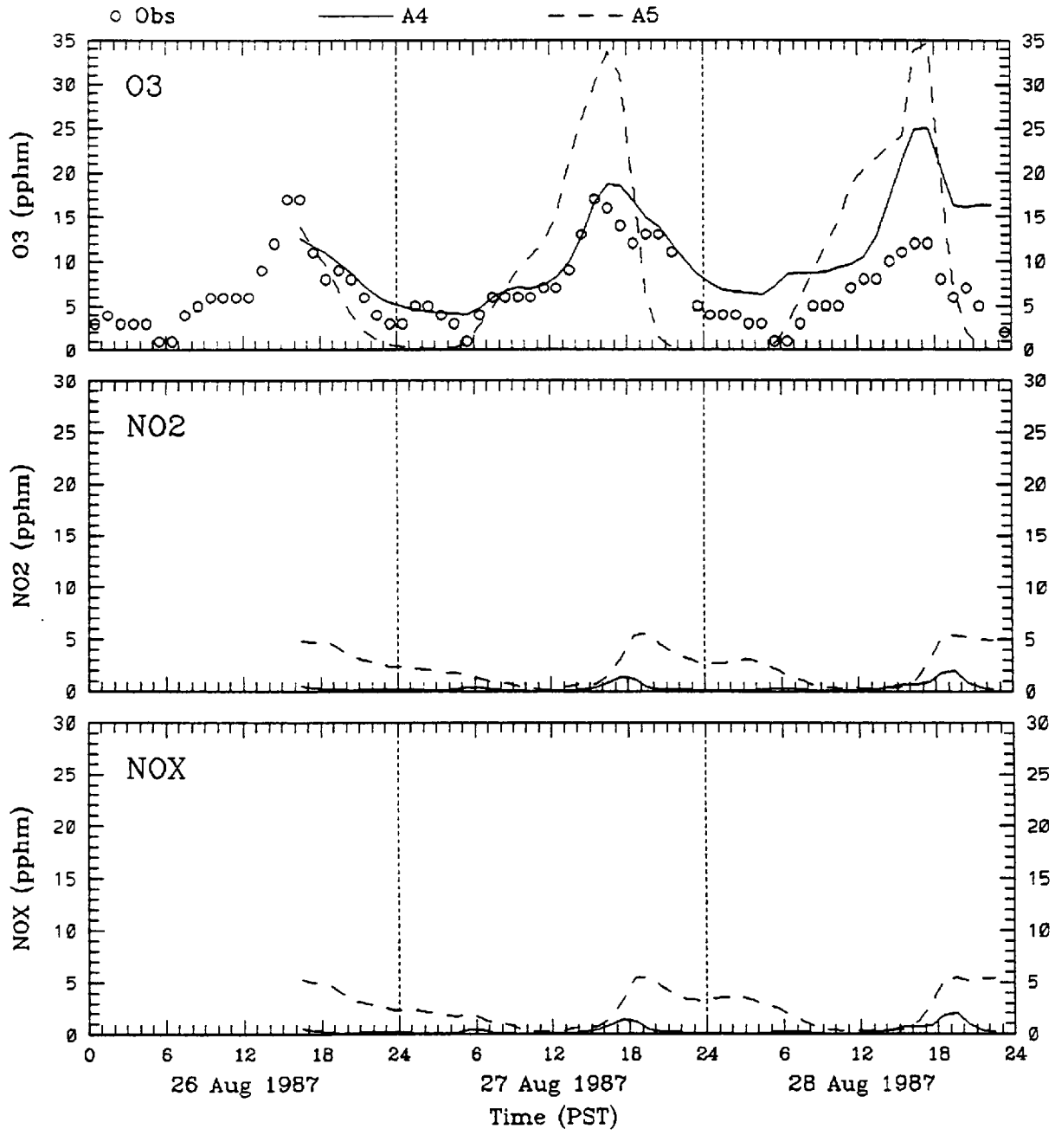


UAM Simulation Results for 26-28 August 1987
Location: UPLA Runs: A4 and A5

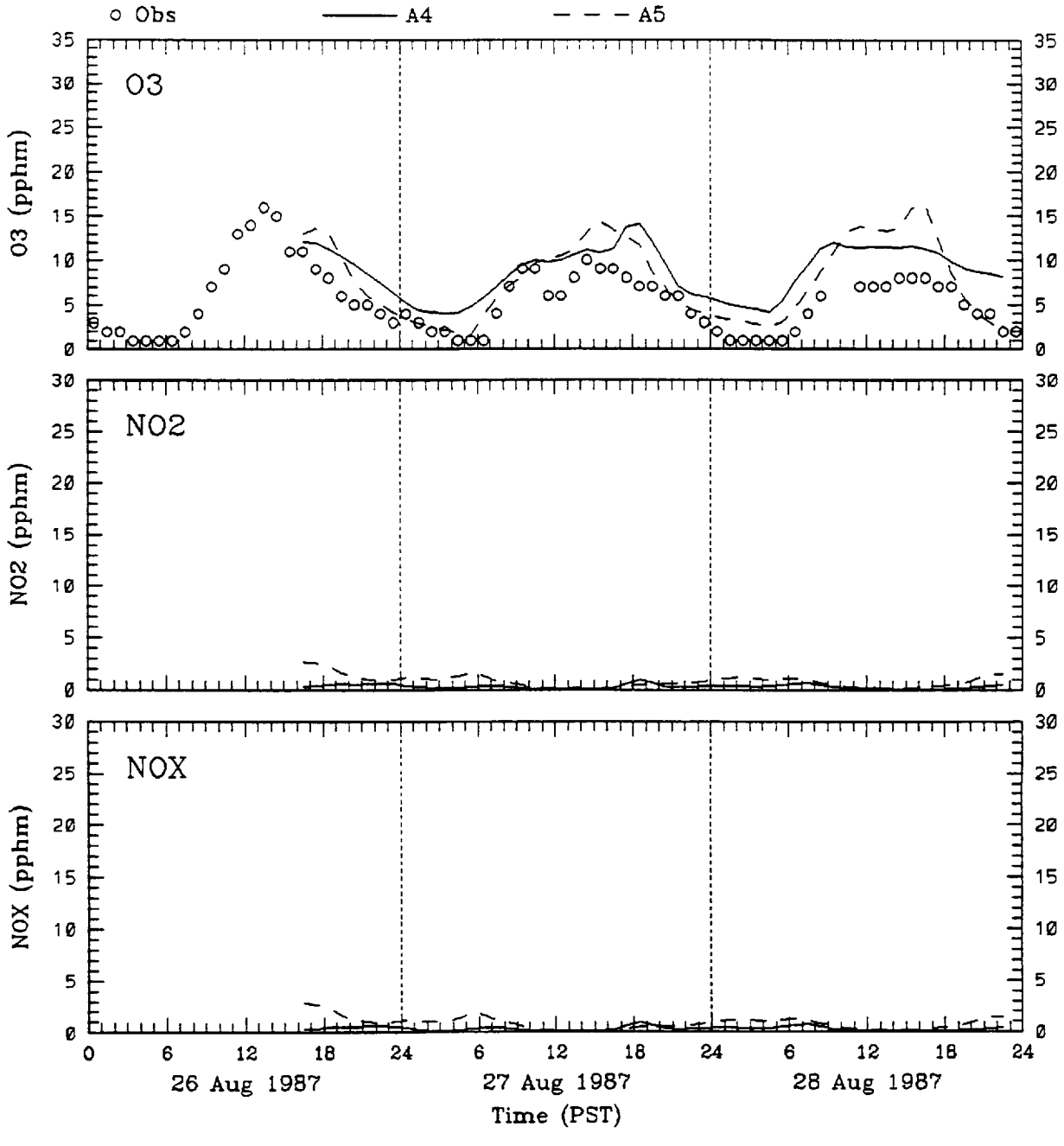




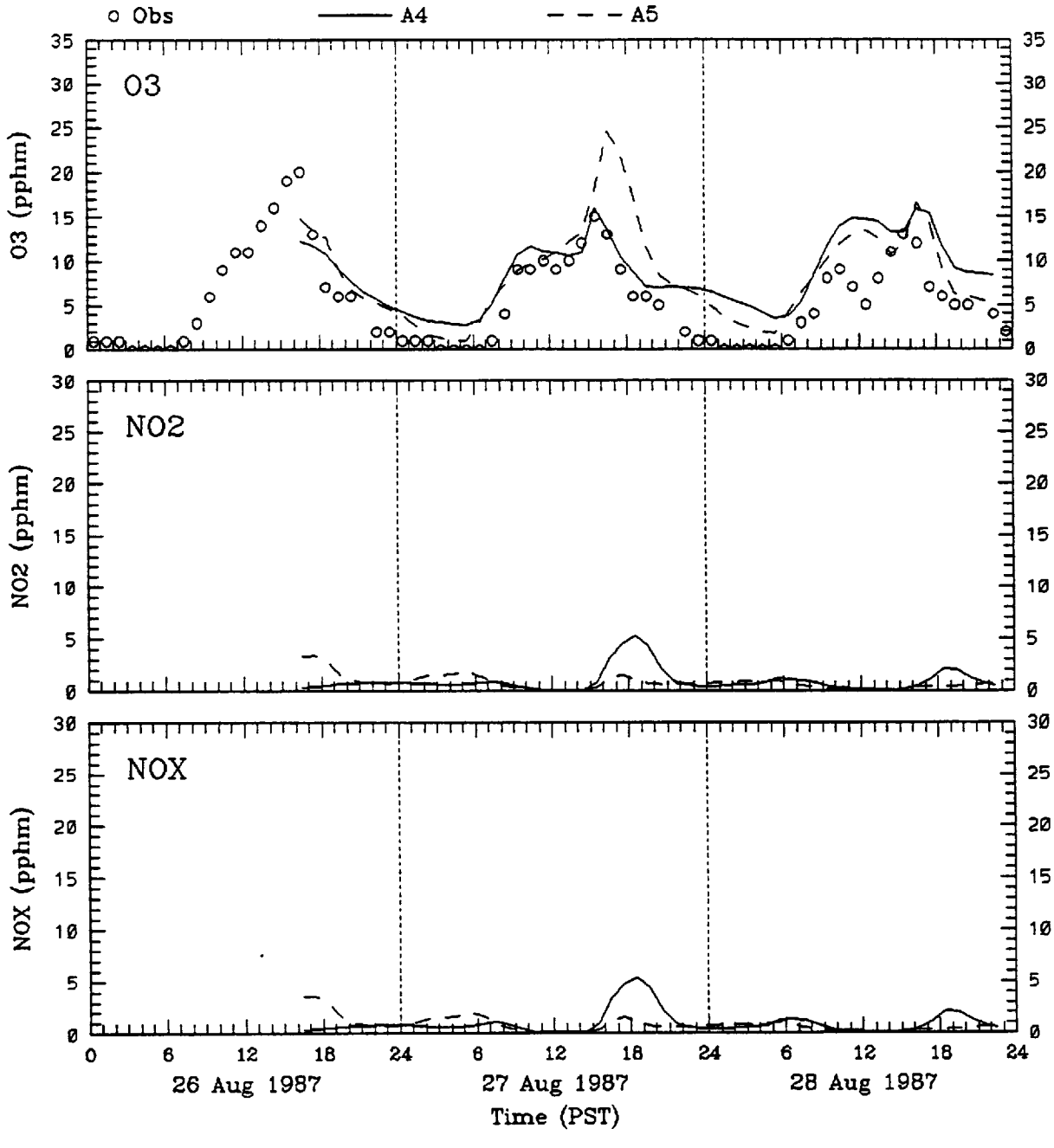
UAM Simulation Results for 26–28 August 1987
Location: CRES Runs: A4 and A5

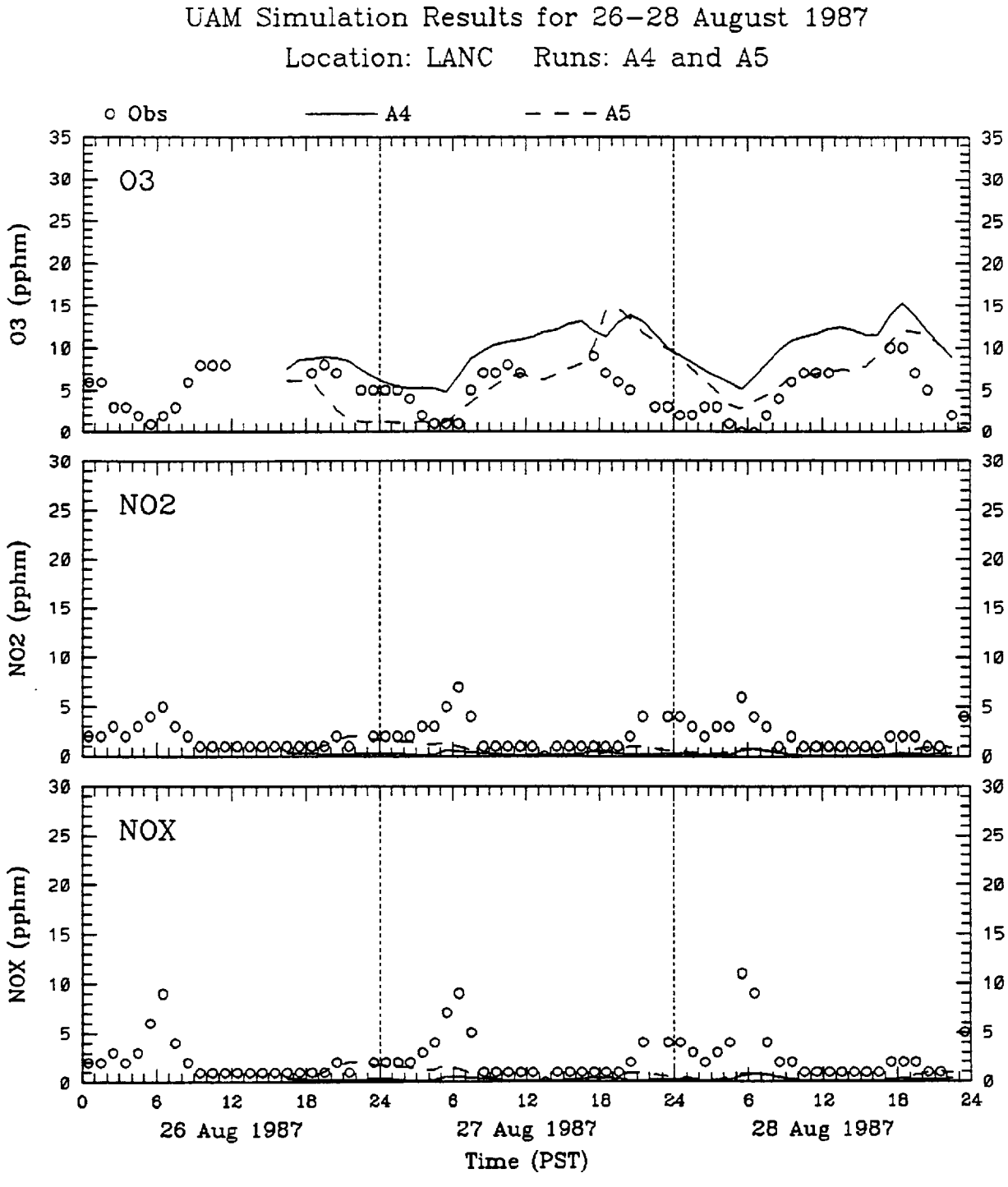


UAM Simulation Results for 26–28 August 1987
Location: HEME Runs: A4 and A5

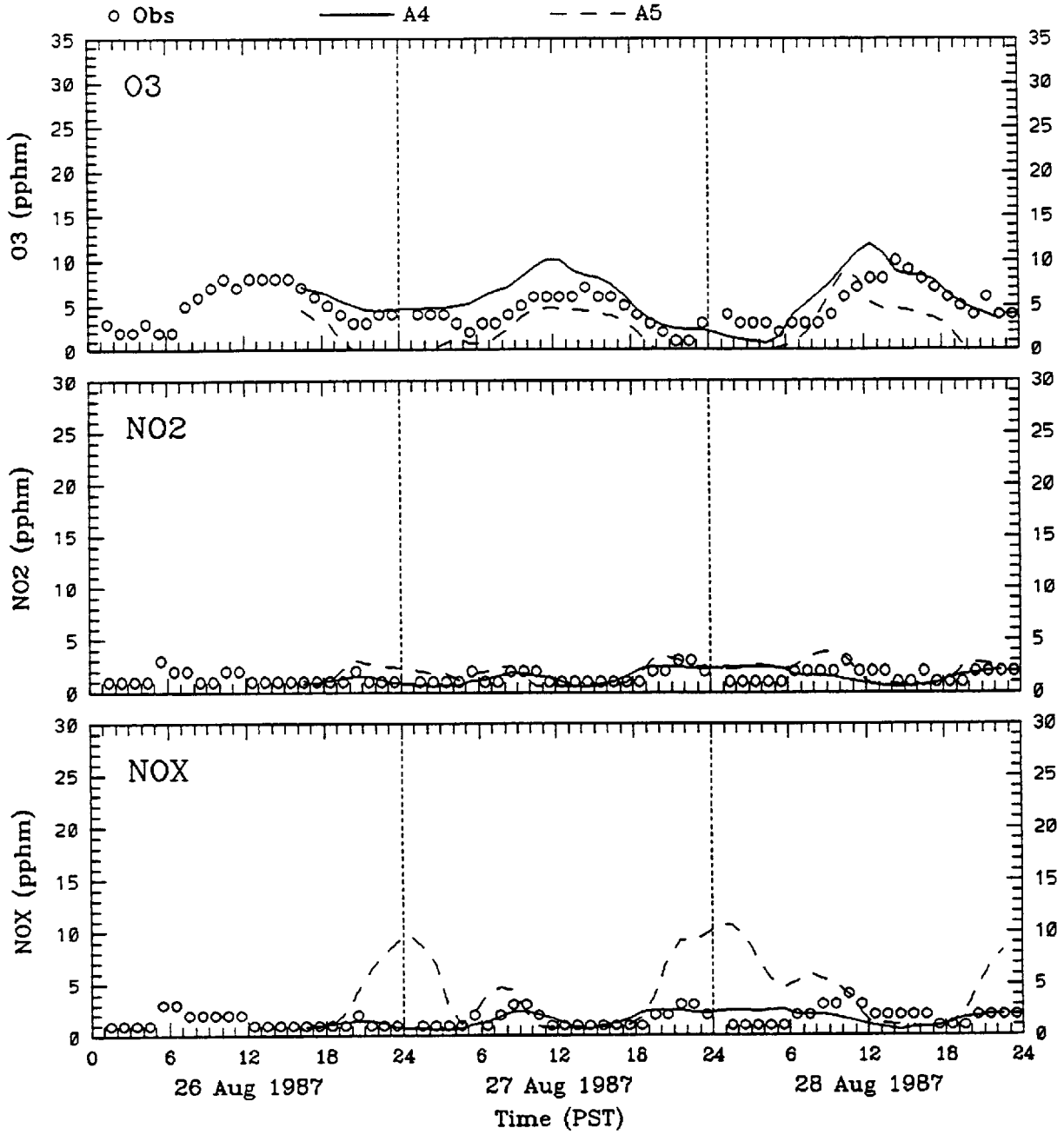


UAM Simulation Results for 26–28 August 1987
Location: PERI Runs: A4 and A5

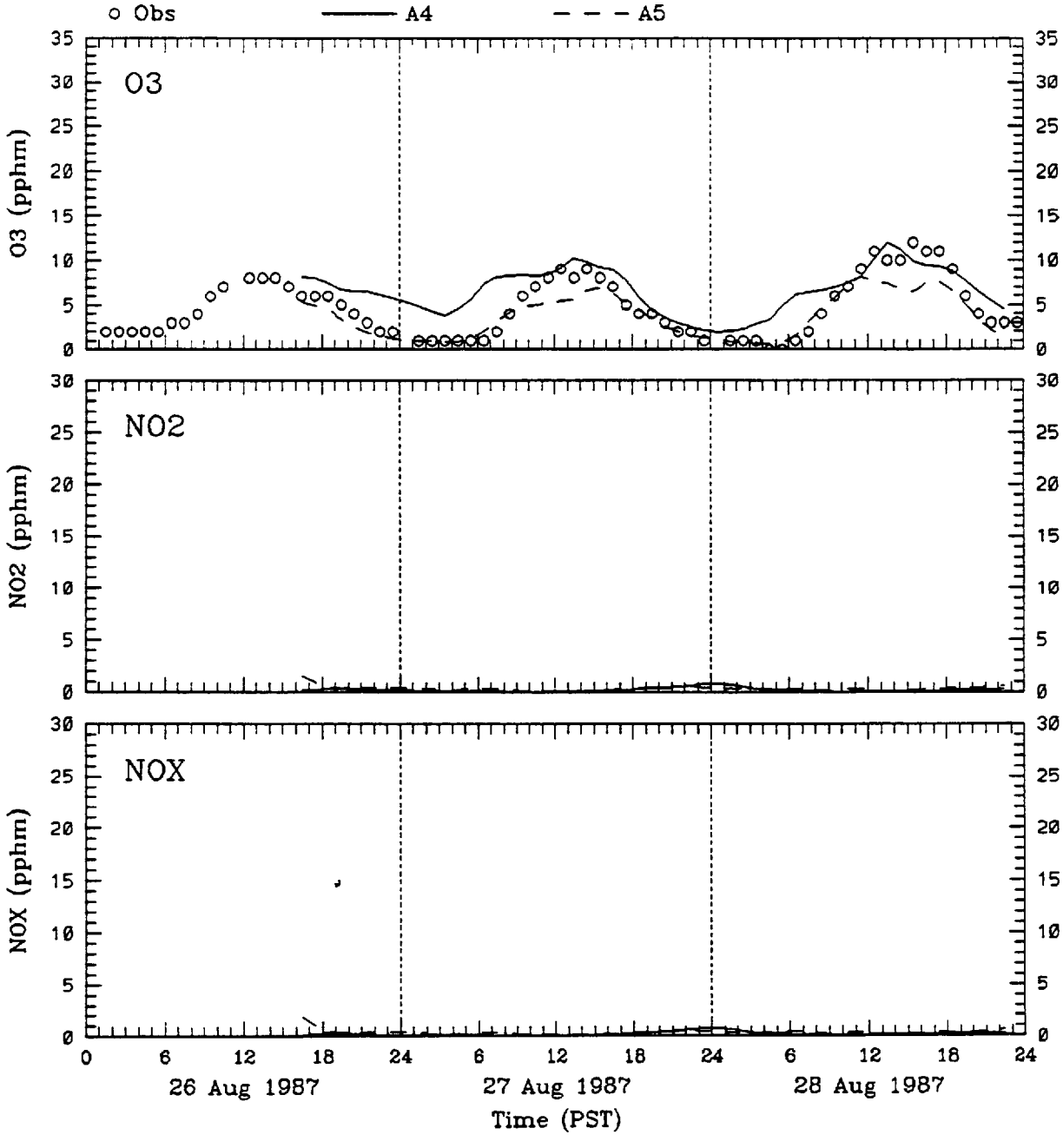




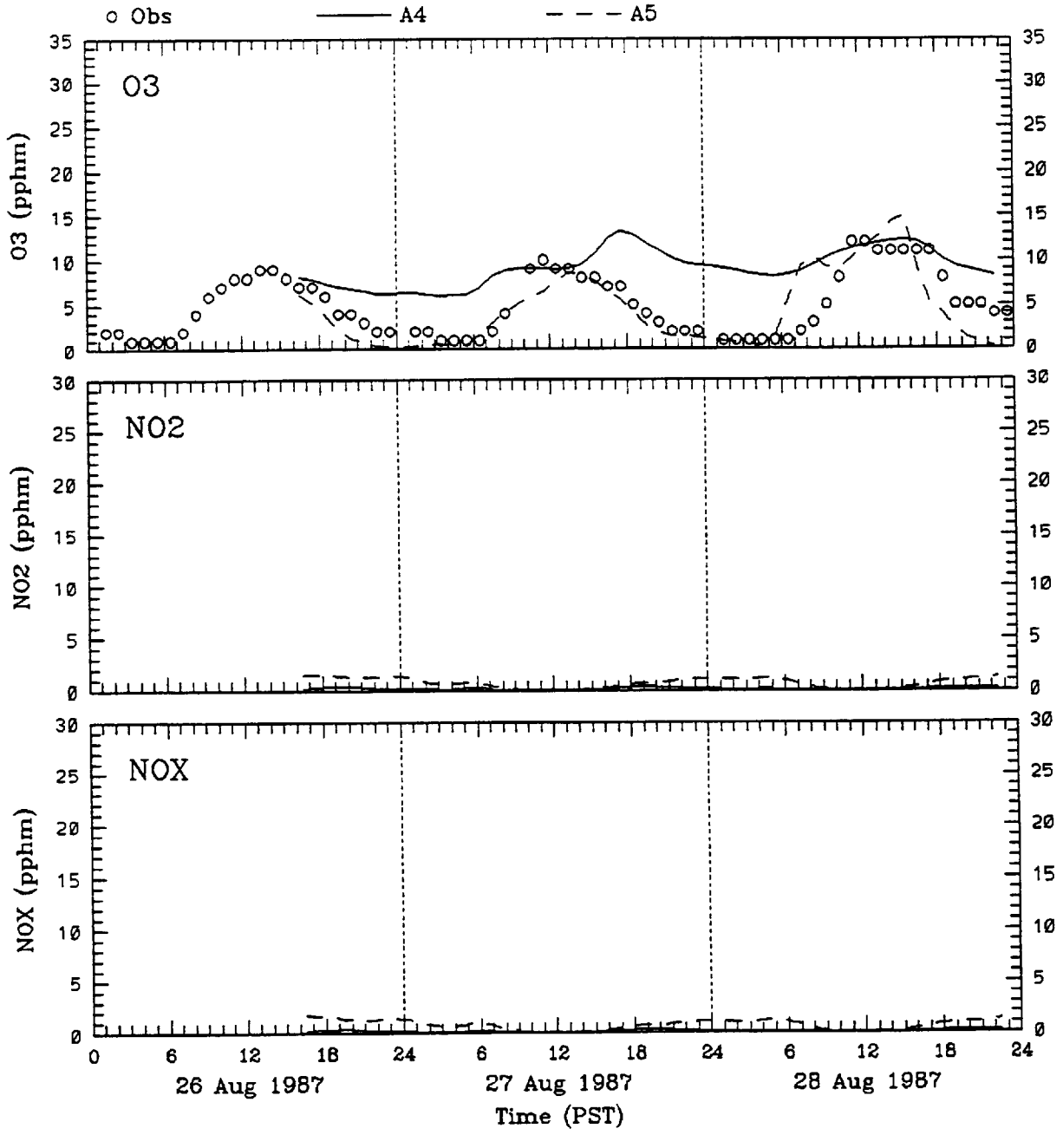
UAM Simulation Results for 26-28 August 1987
Location: ERIO Runs: A4 and A5

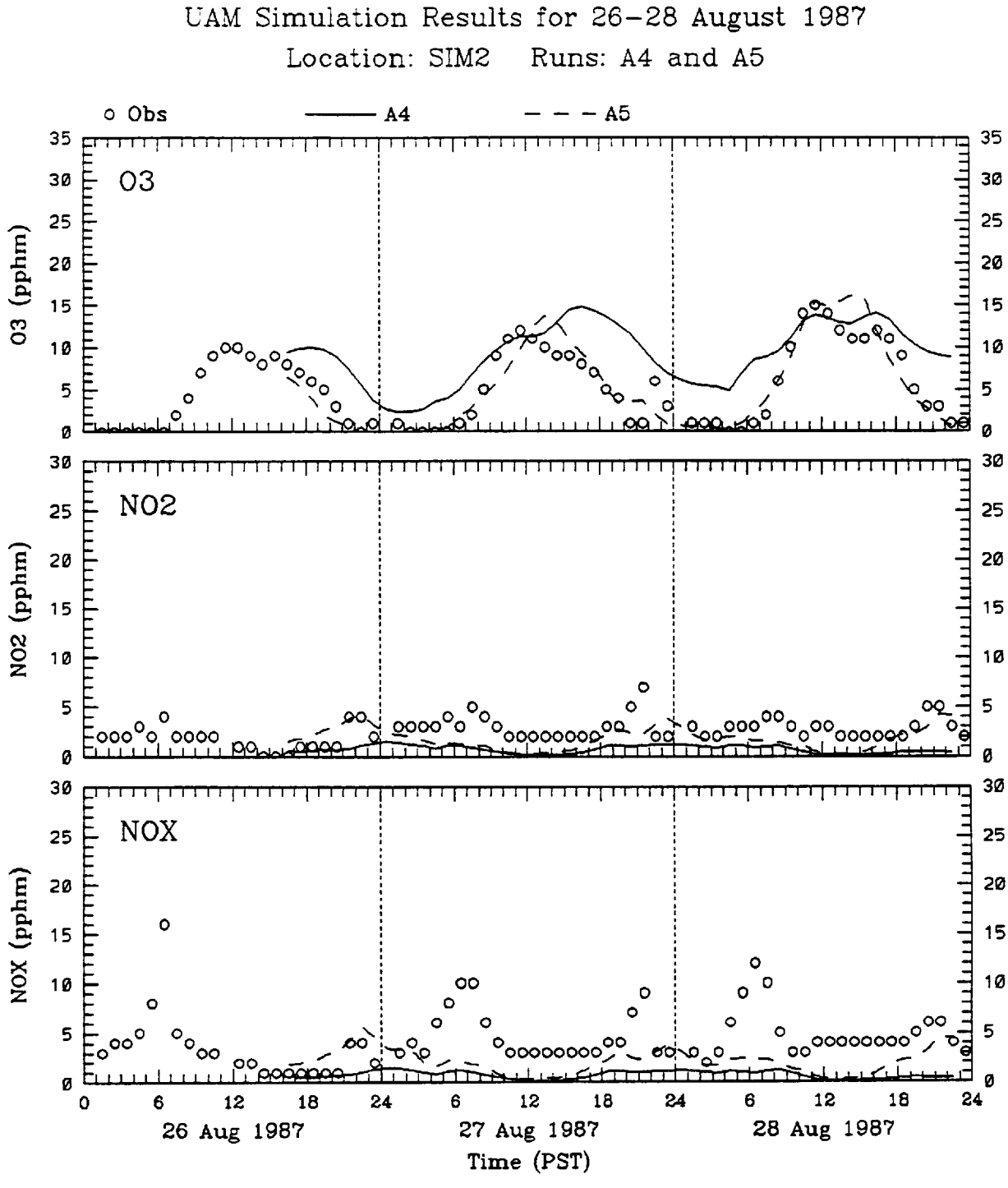


UAM Simulation Results for 26-28 August 1987
Location: OJAI Runs: A4 and A5

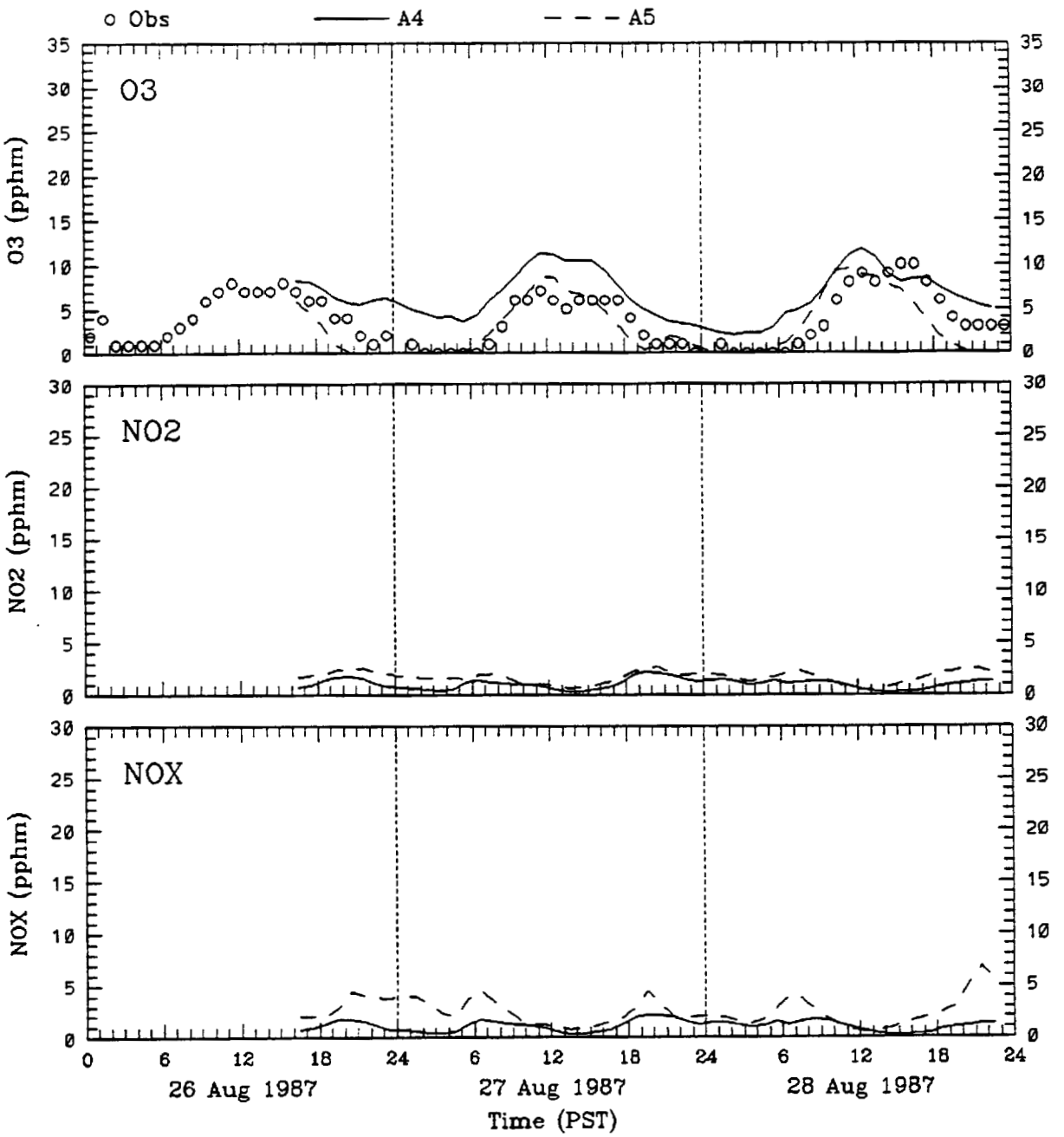


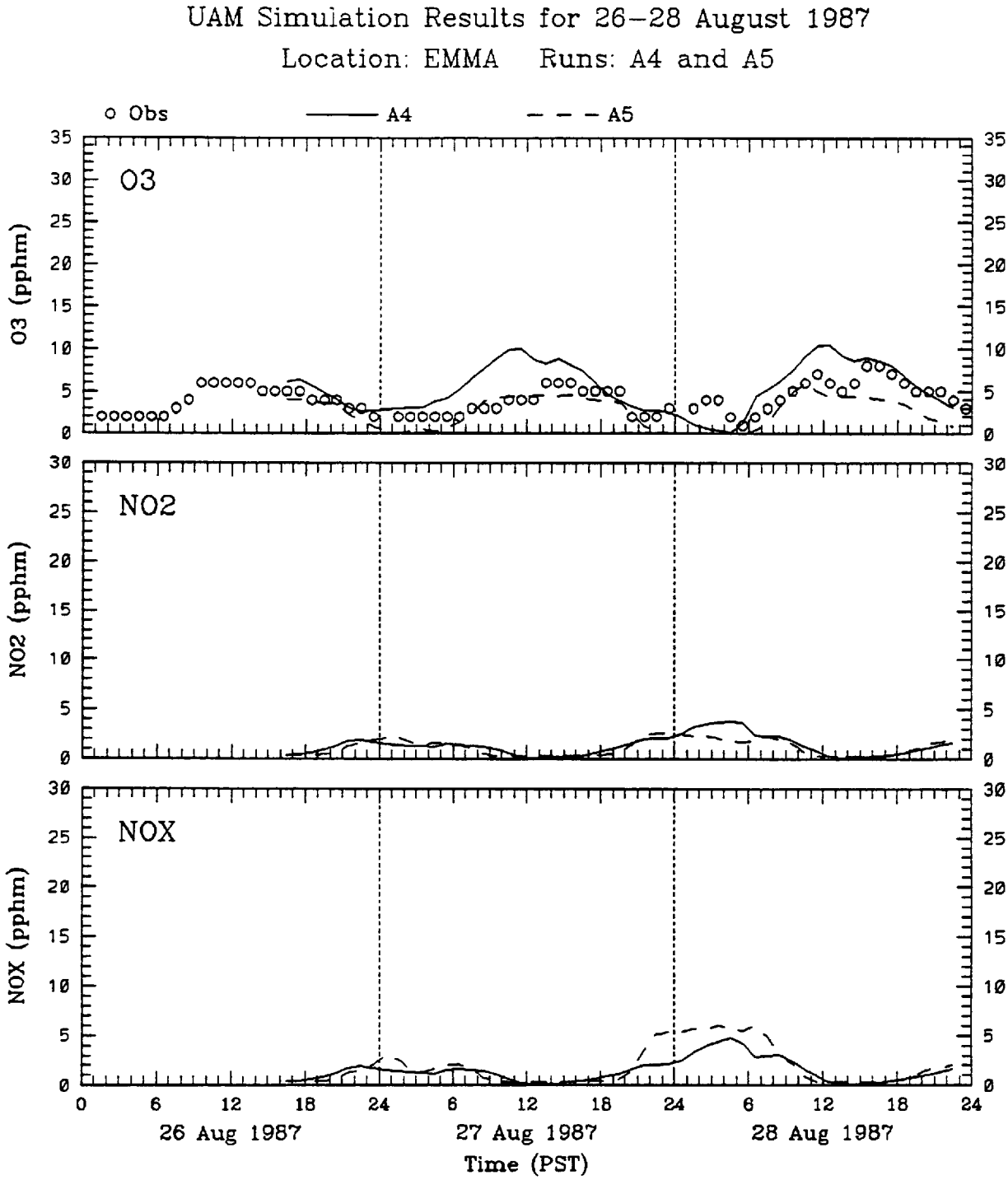
UAM Simulation Results for 26–28 August 1987
Location: PRU2 Runs: A4 and A5



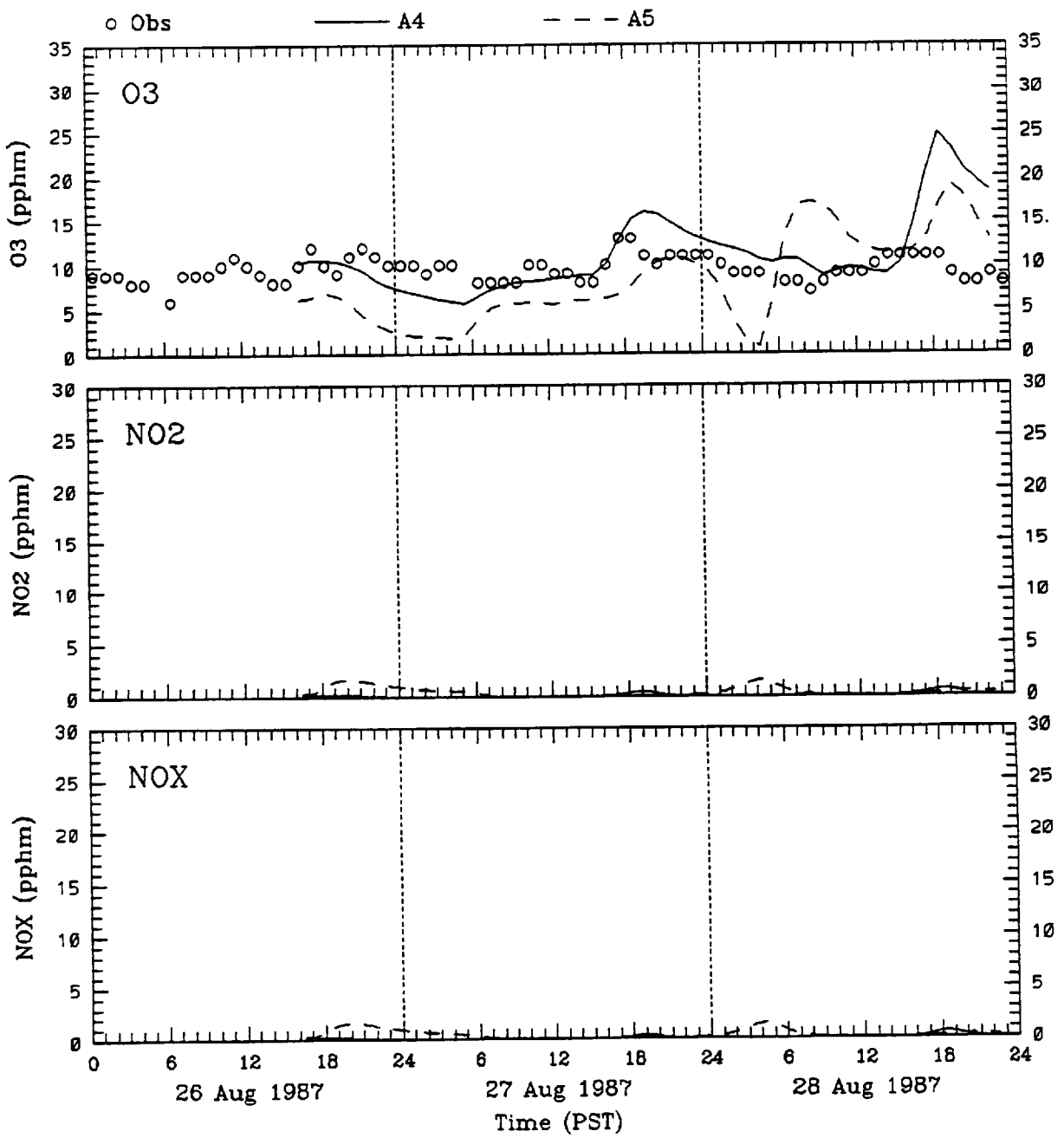


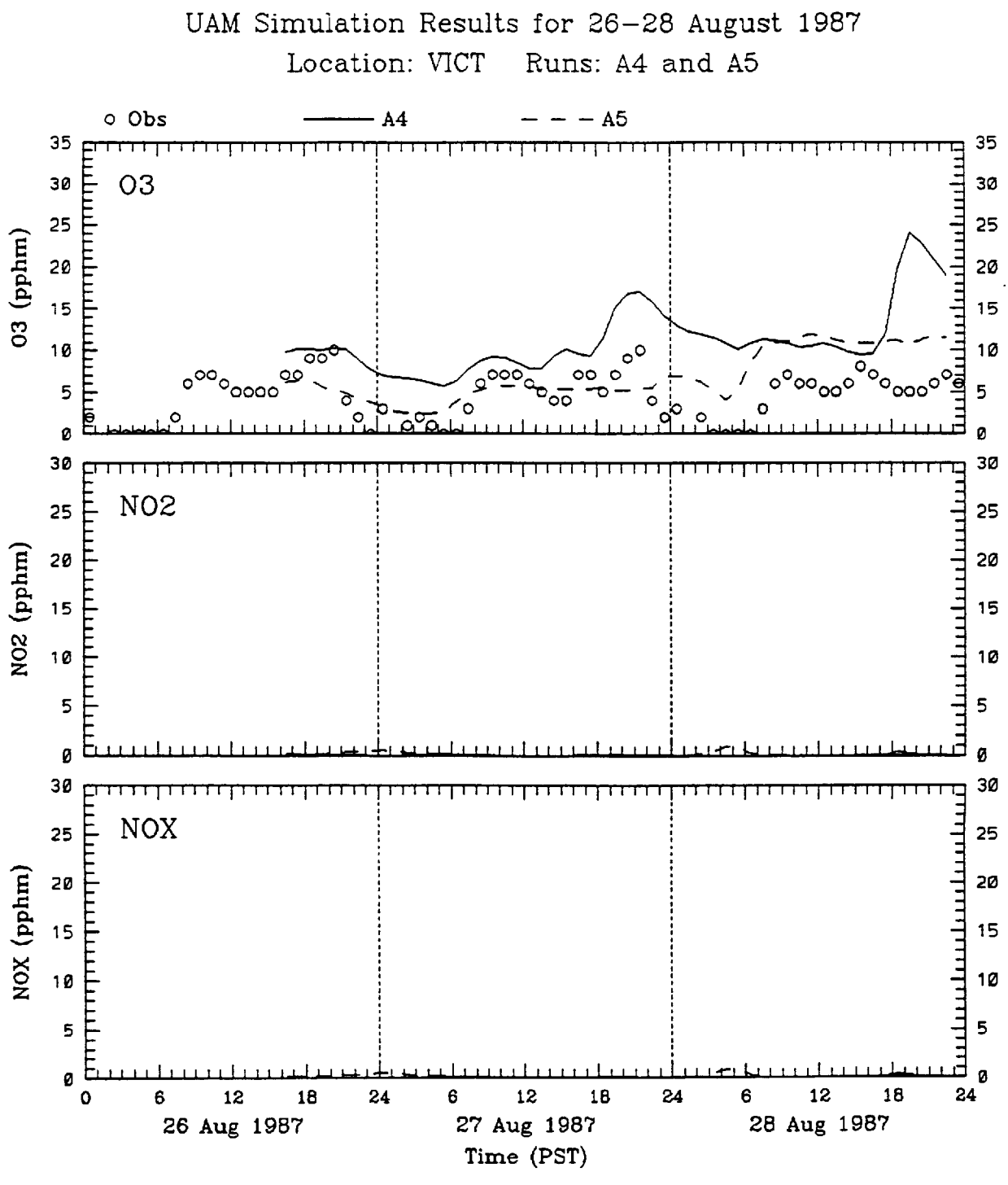
UAM Simulation Results for 26–28 August 1987
Location: OAKS Runs: A4 and A5





UAM Simulation Results for 26-28 August 1987
Location: HESP Runs: A4 and A5





APPENDIX F

Appendix F

VOC SIMULATION RESULTS FOR 26-28 AUGUST 1987

This appendix contains time series plots showing estimated and measured concentrations for Runs A4 and A5 for 26-28 August 1987. These displays illustrate the estimated and measured concentrations at air monitoring locations for various organic species simulated by the UAM. The monitoring stations are designated as follows:

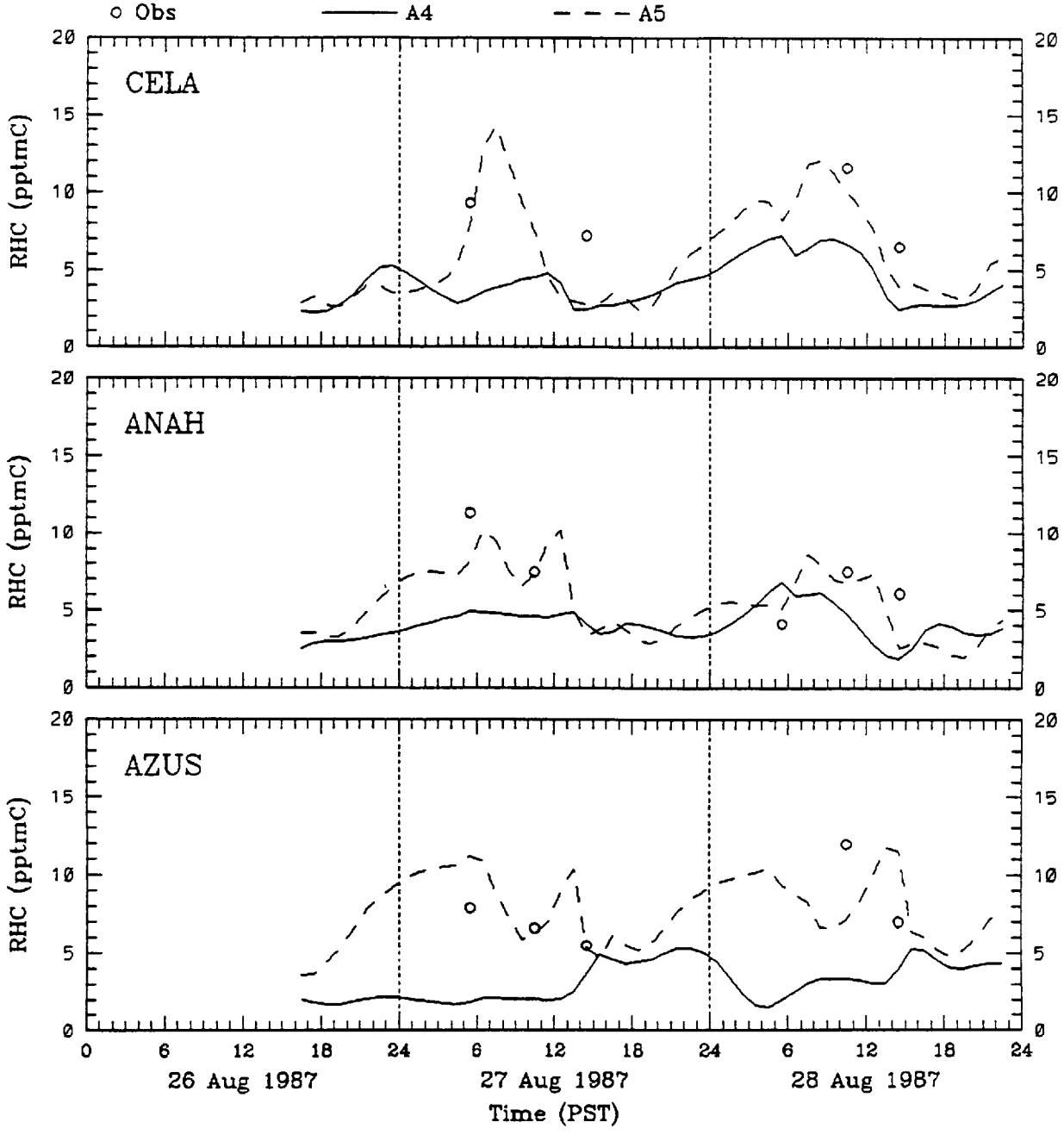
Los Angeles (CELA)
Anaheim (ANAH)
Azusa (AZUS)

Claremont College (CLAR)
Long Beach City College (LBCC)
Burbank (BURK)

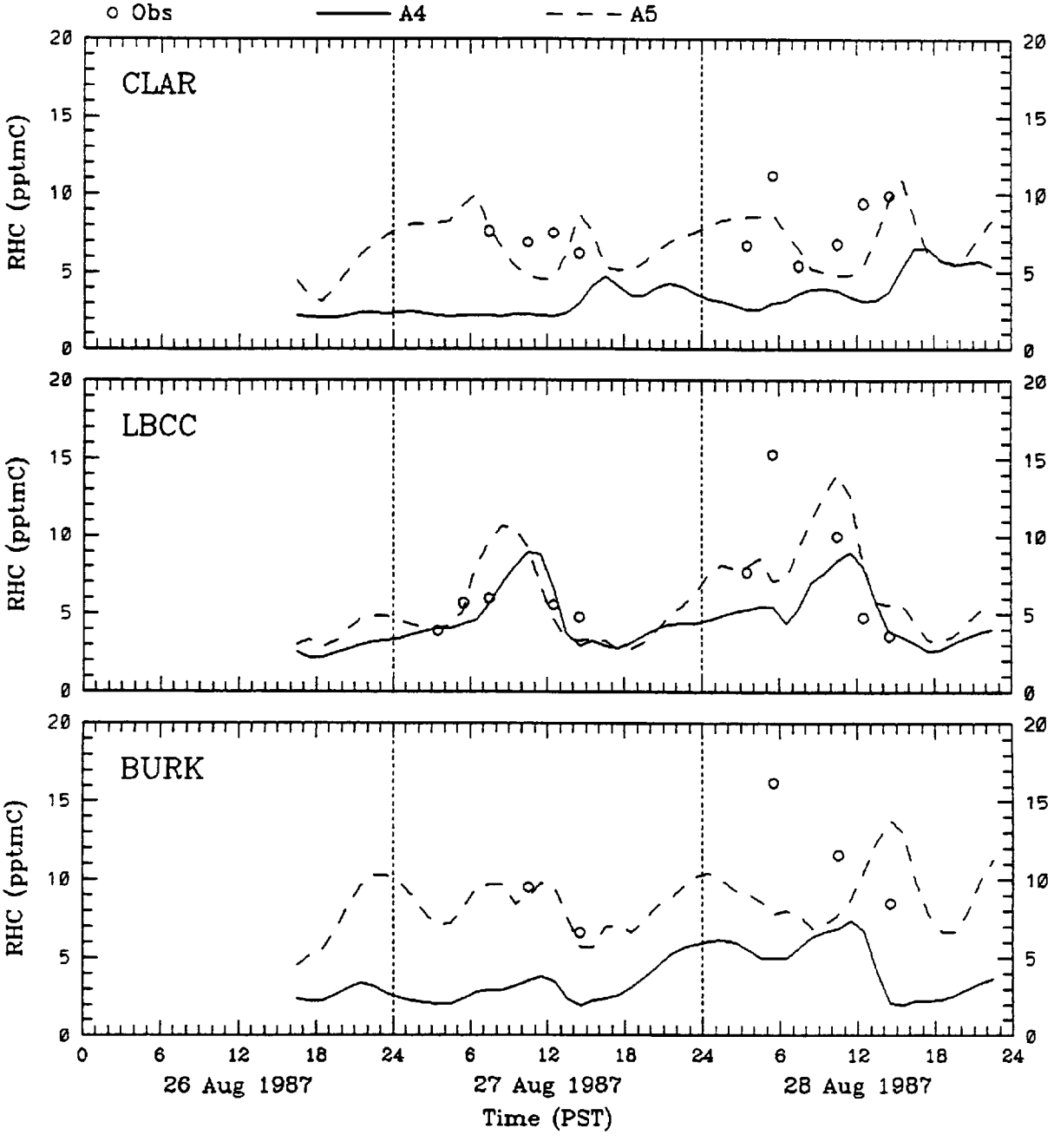
Riverside-Rubidoux (RIVR)
Hawthorn (HAWT)

Figure 2-1 in Section 2 shows the locations of these air monitoring stations.

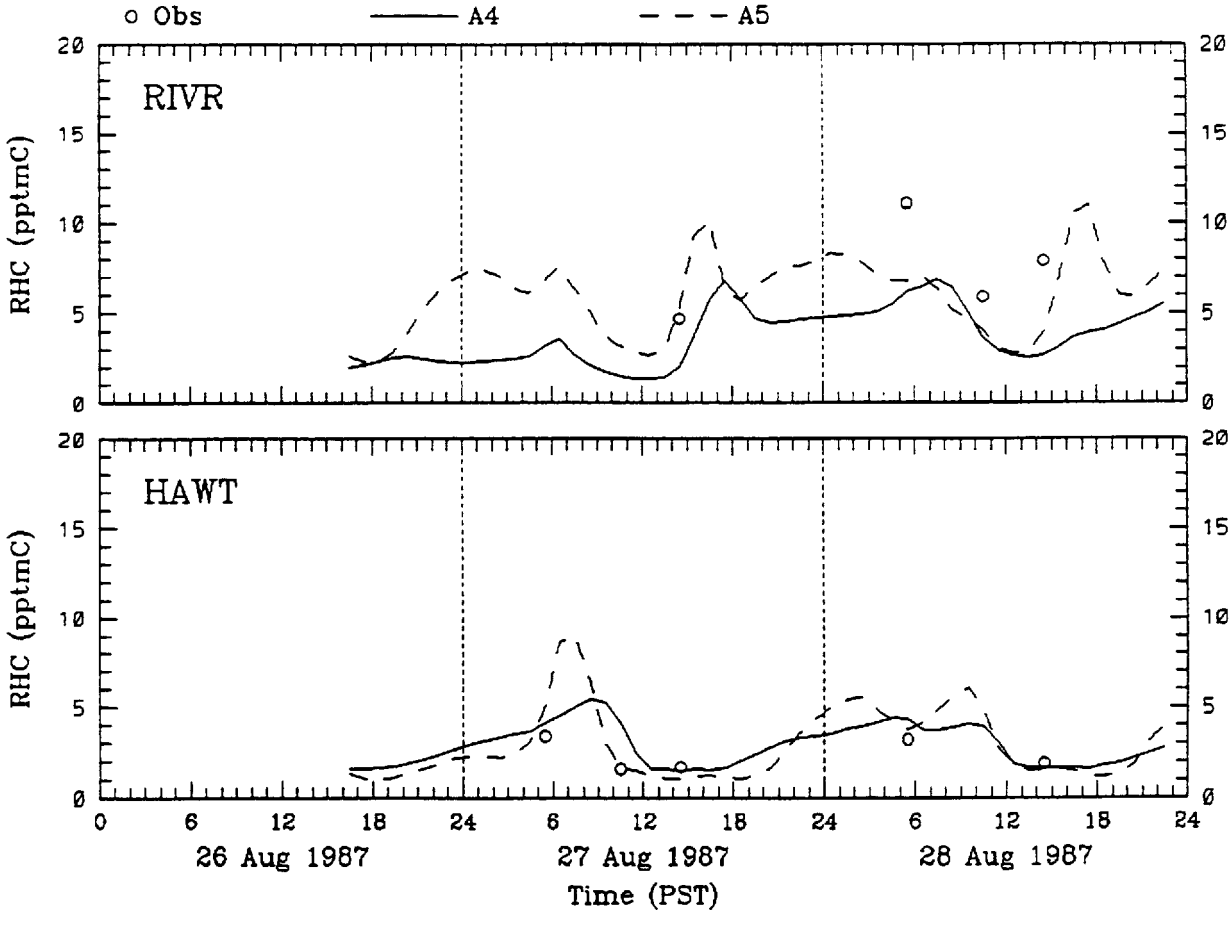
Runs A4 and A5: Predicted and Observed RHC Time Series
26–28 August 1987



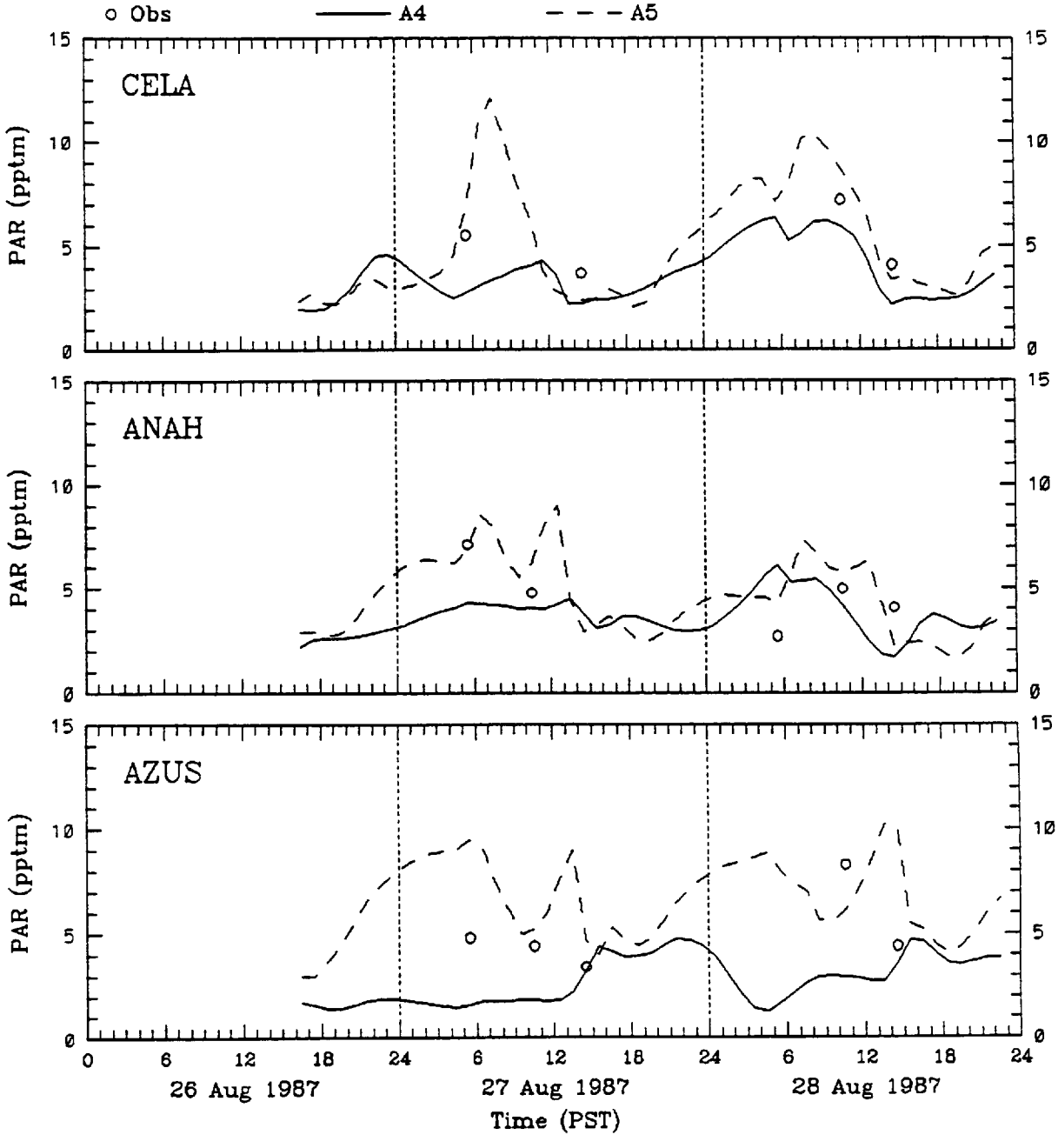
Runs A4 and A5: Predicted and Observed RHC Time Series
26–28 August 1987



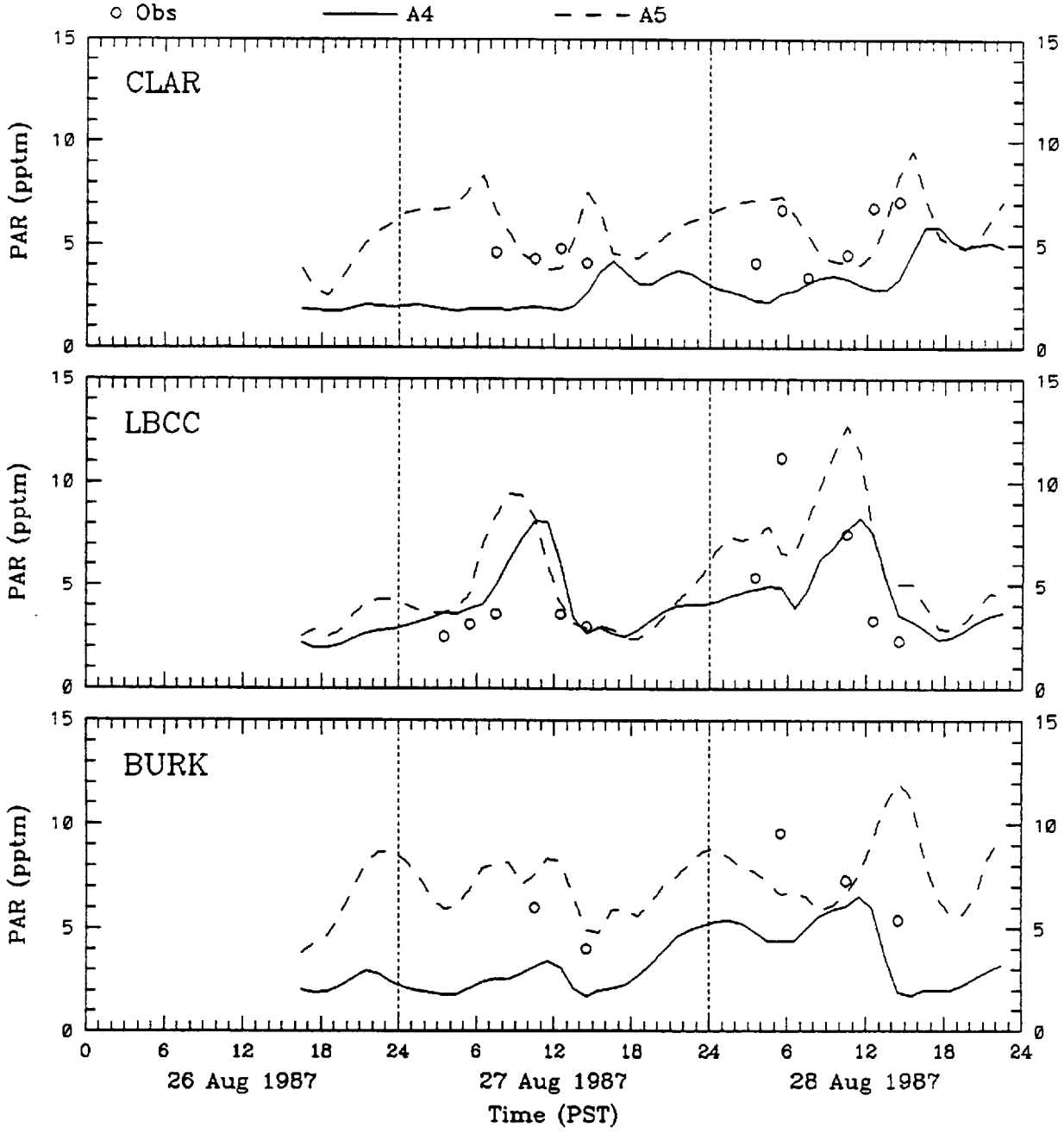
Runs A4 and A5: Predicted and Observed RHC Time Series
26–28 August 1987



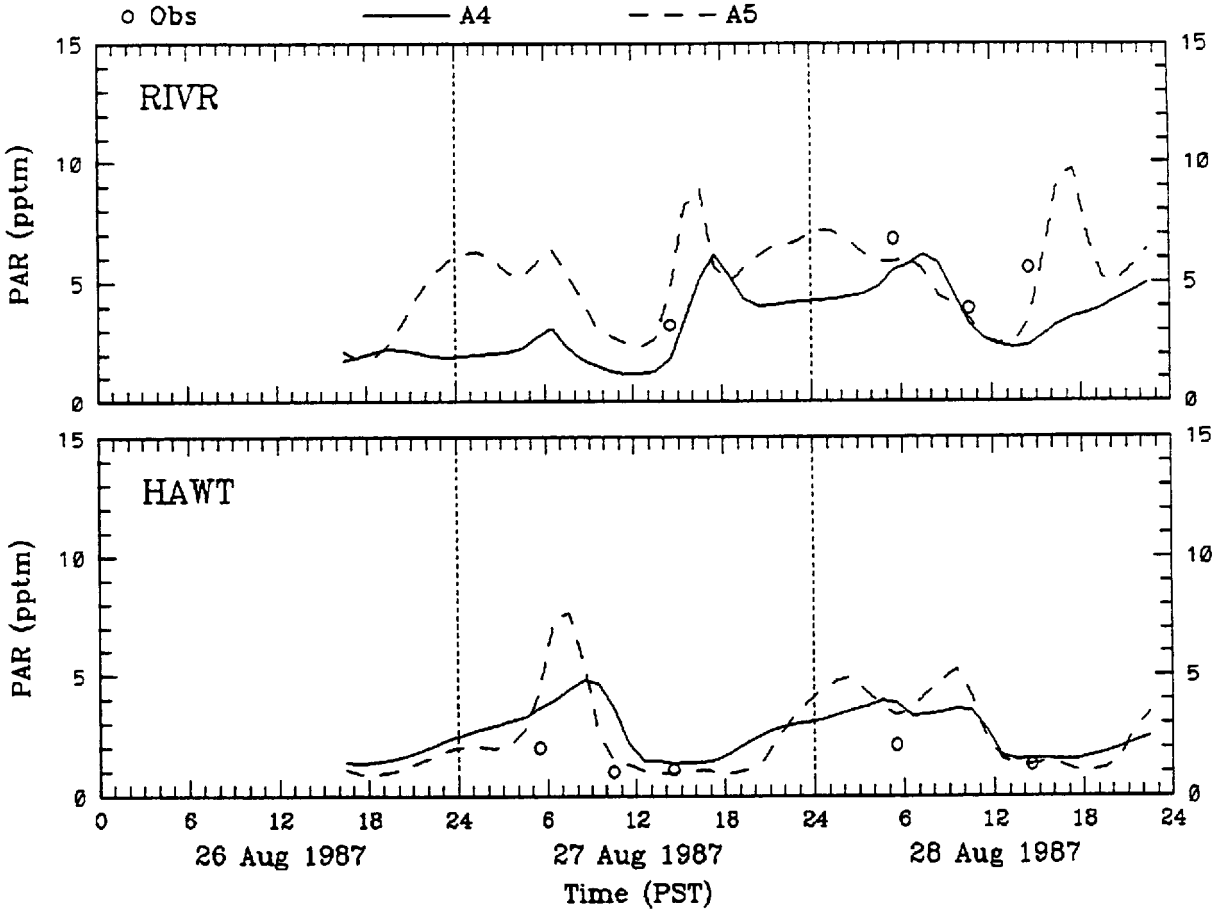
Runs A4 and A5: Predicted and Observed PAR Time Series
26–28 August 1987



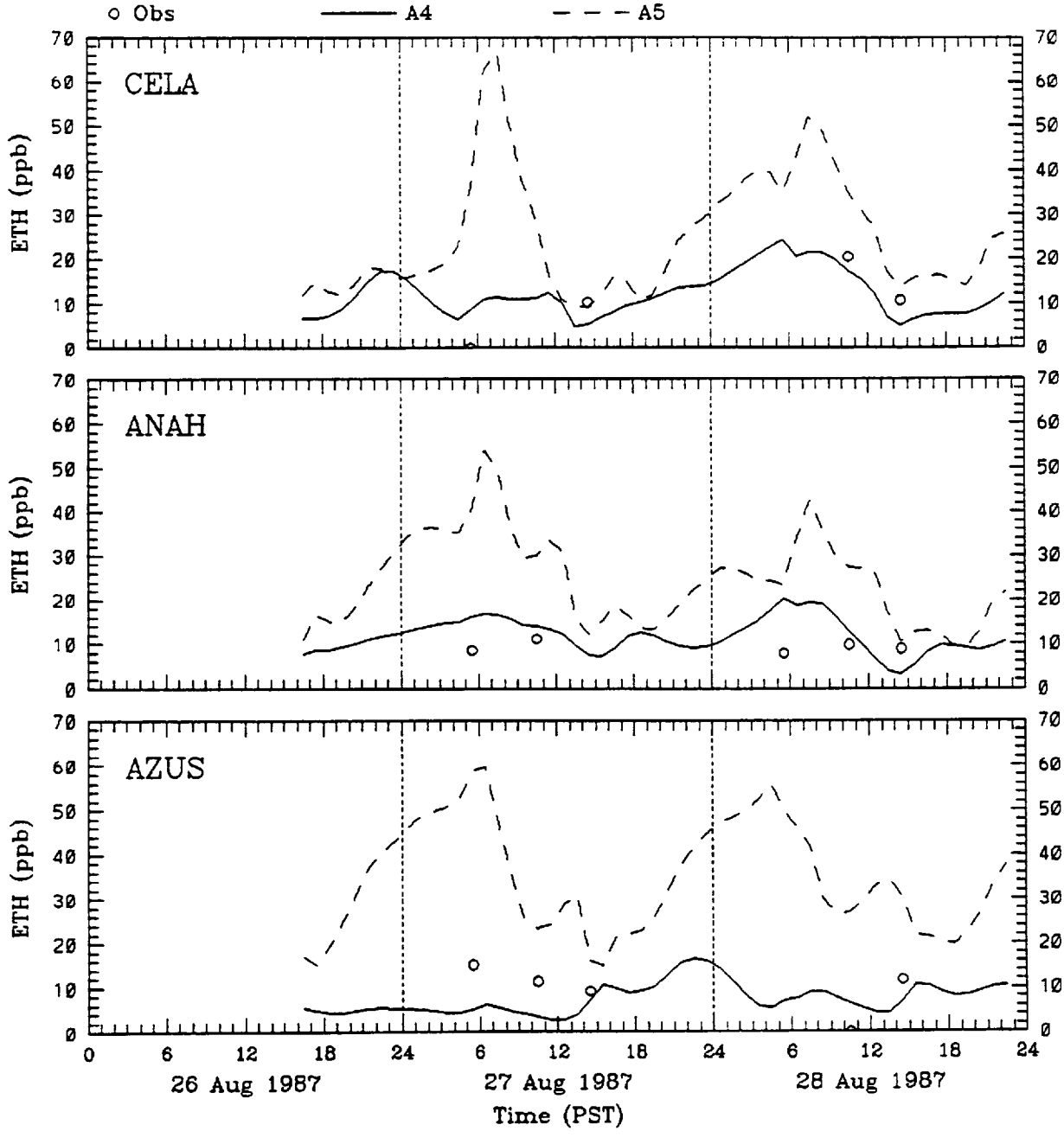
Runs A4 and A5: Predicted and Observed PAR Time Series
26–28 August 1987



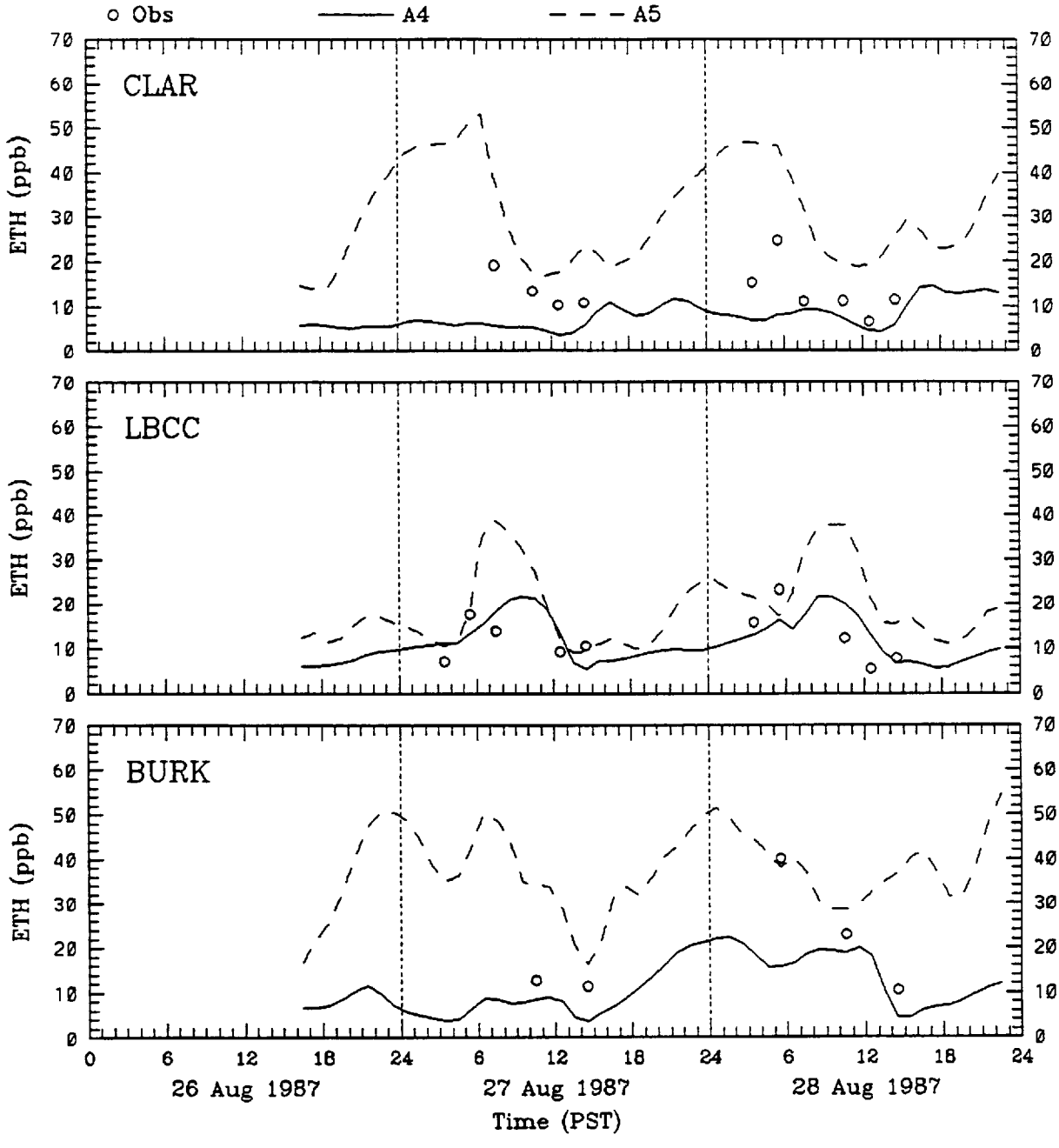
Runs A4 and A5: Predicted and Observed PAR Time Series
26-28 August 1987



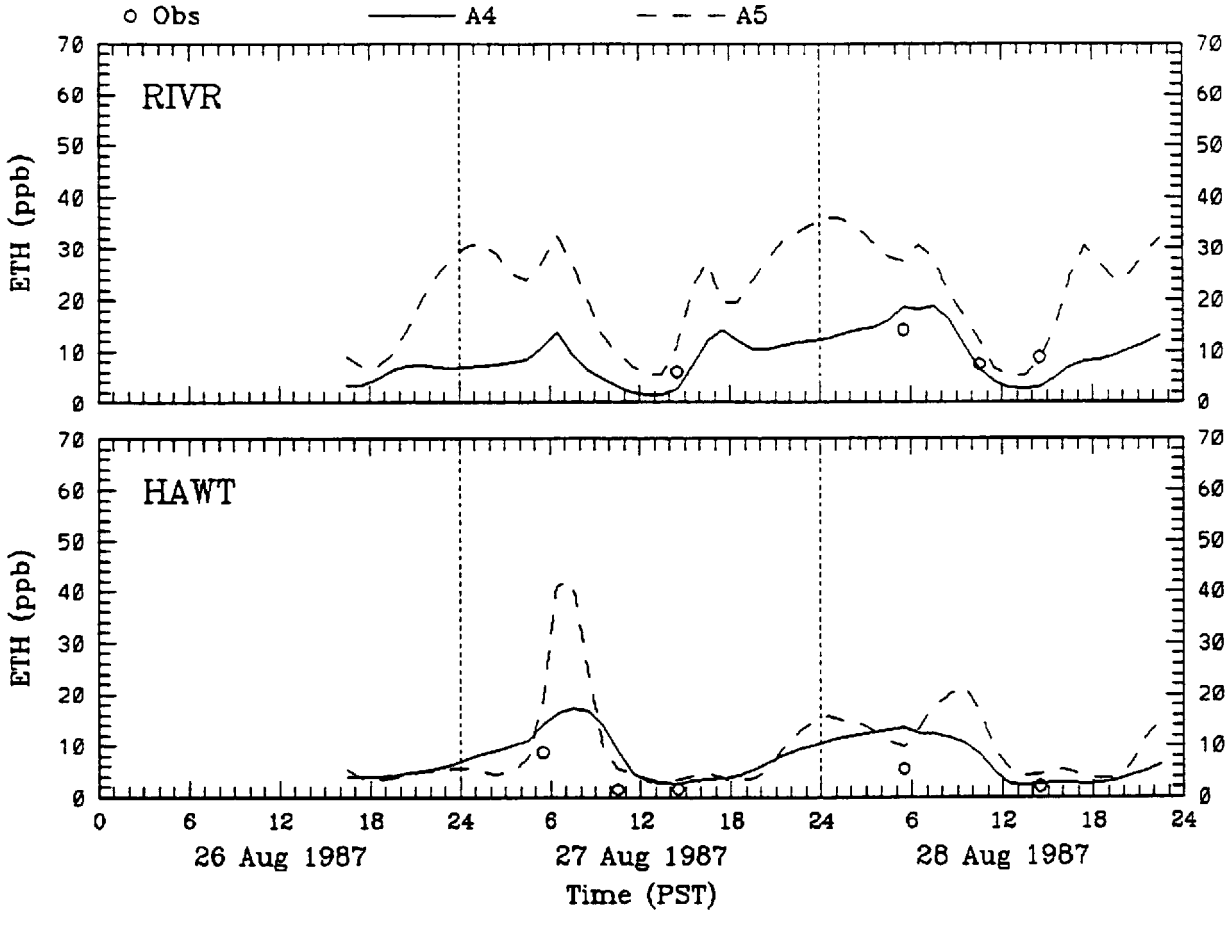
Runs A4 and A5: Predicted and Observed ETH Time Series
26-28 August 1987



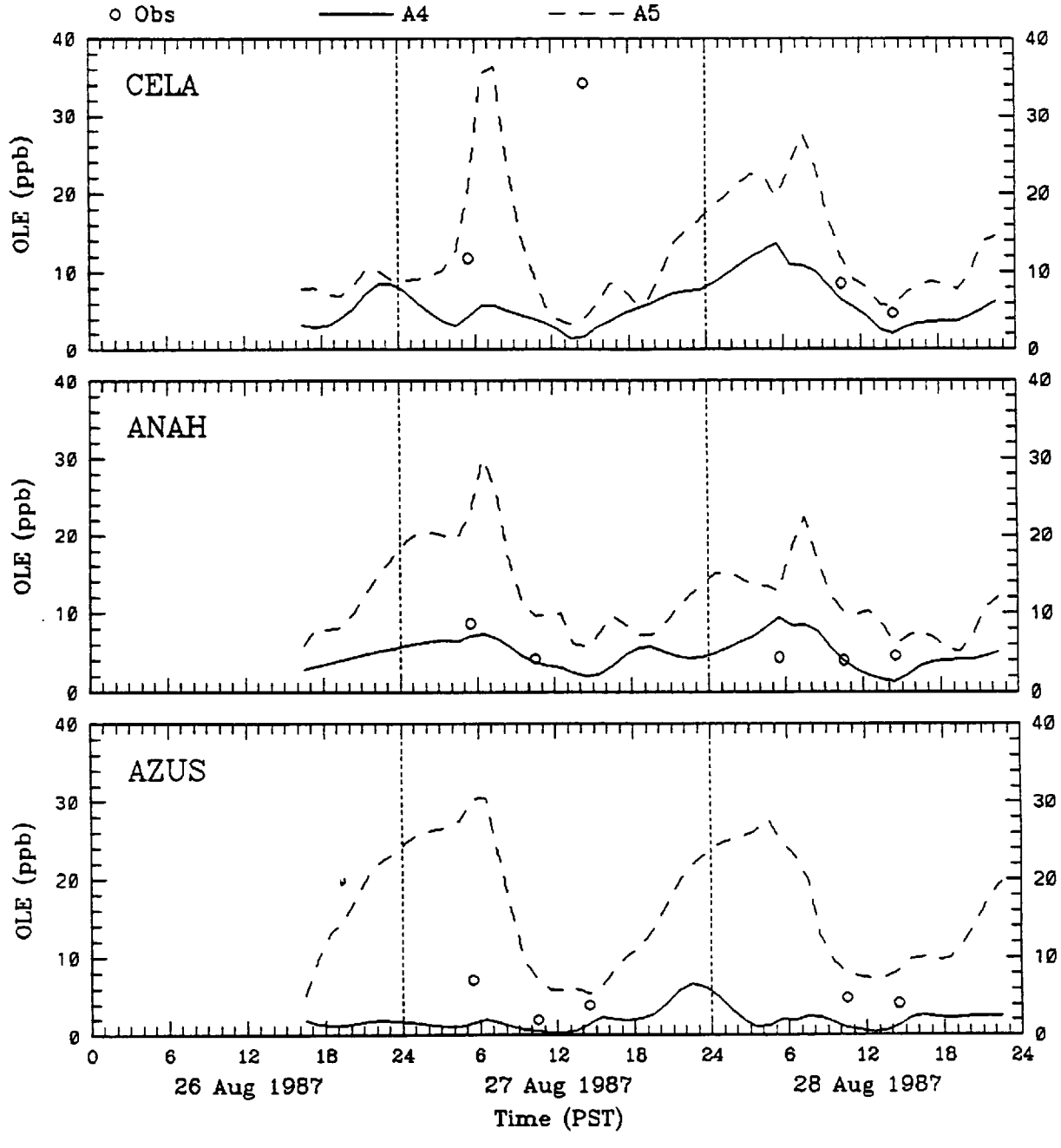
Runs A4 and A5: Predicted and Observed ETH Time Series
26–28 August 1987



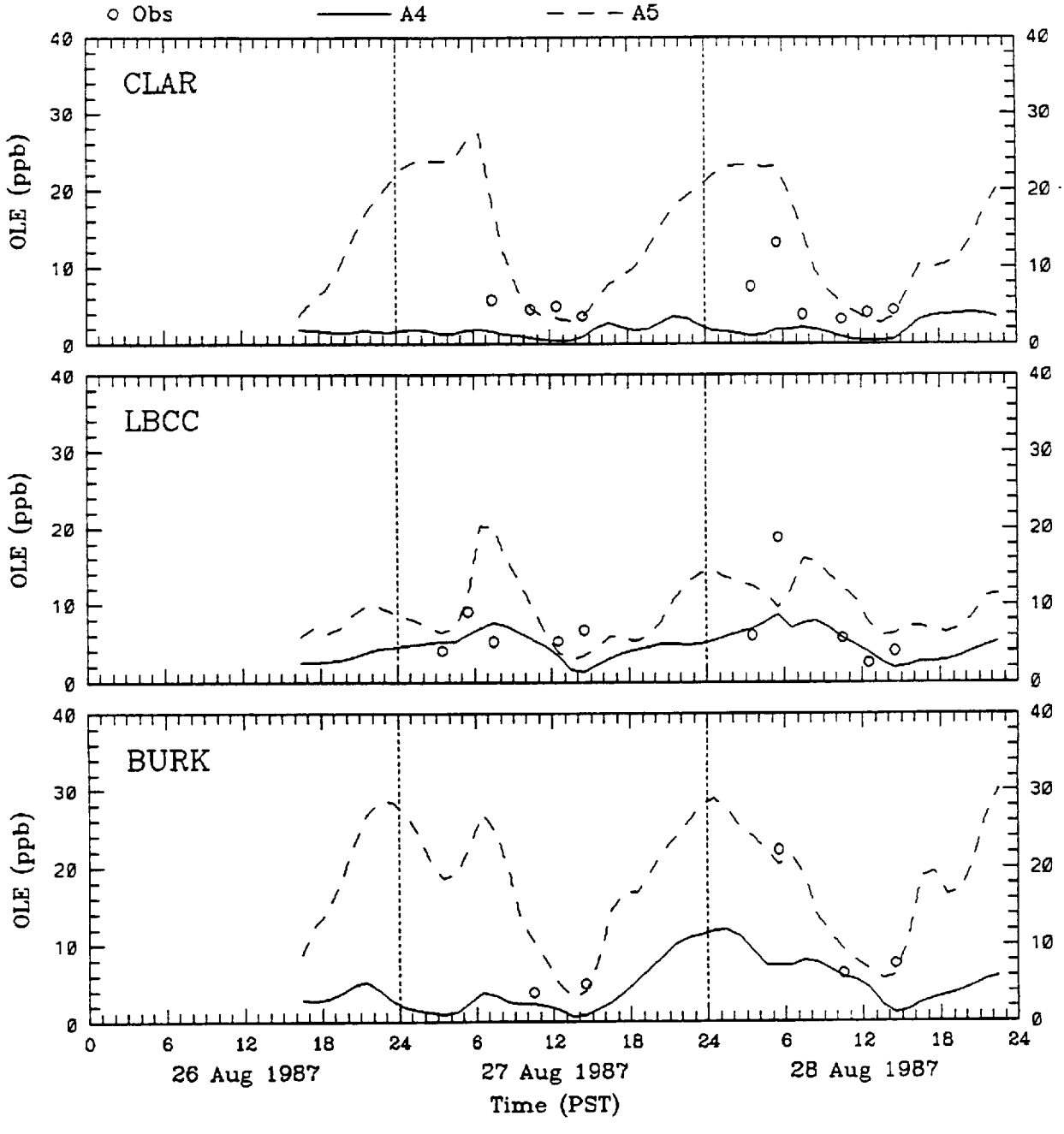
Runs A4 and A5: Predicted and Observed ETH Time Series
26–28 August 1987



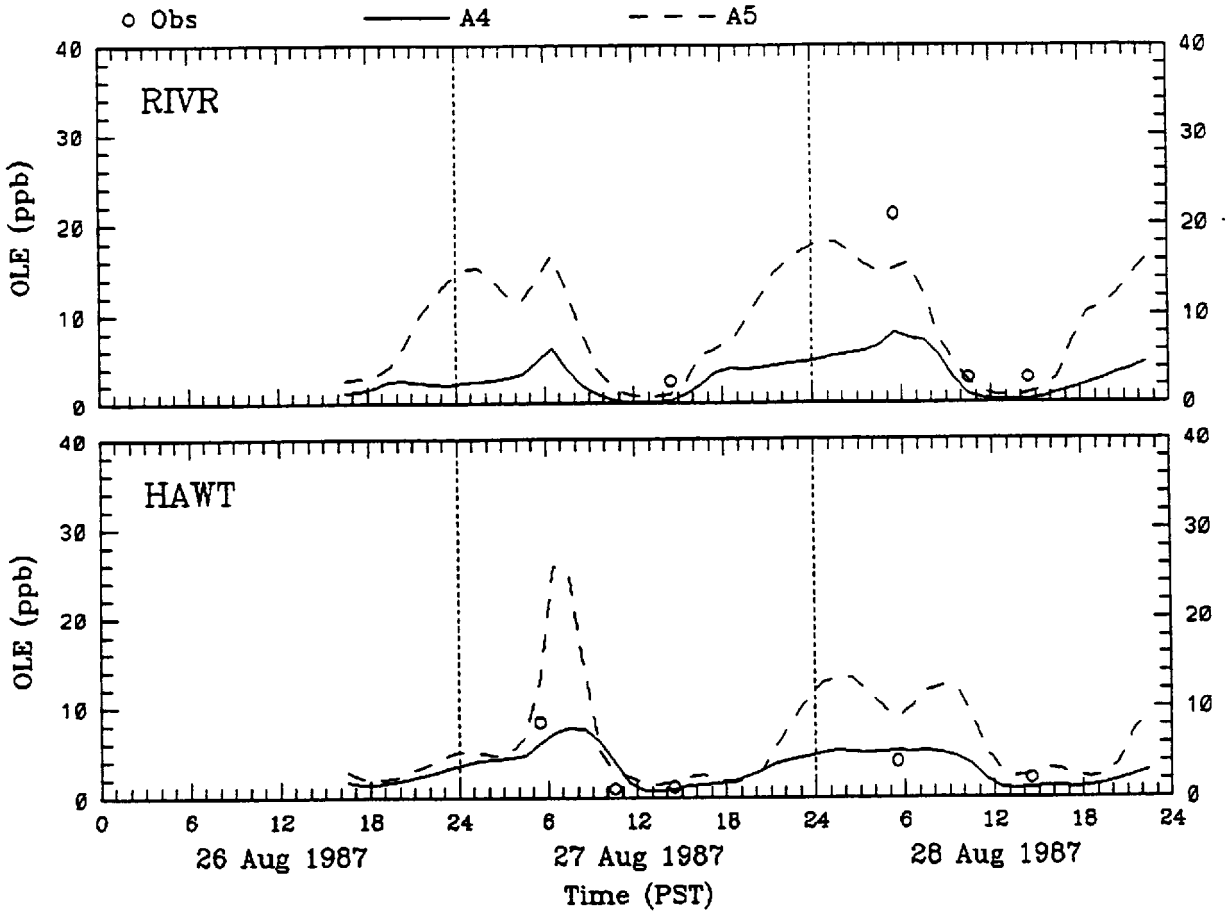
Runs A4 and A5: Predicted and Observed OLE Time Series
26–28 August 1987



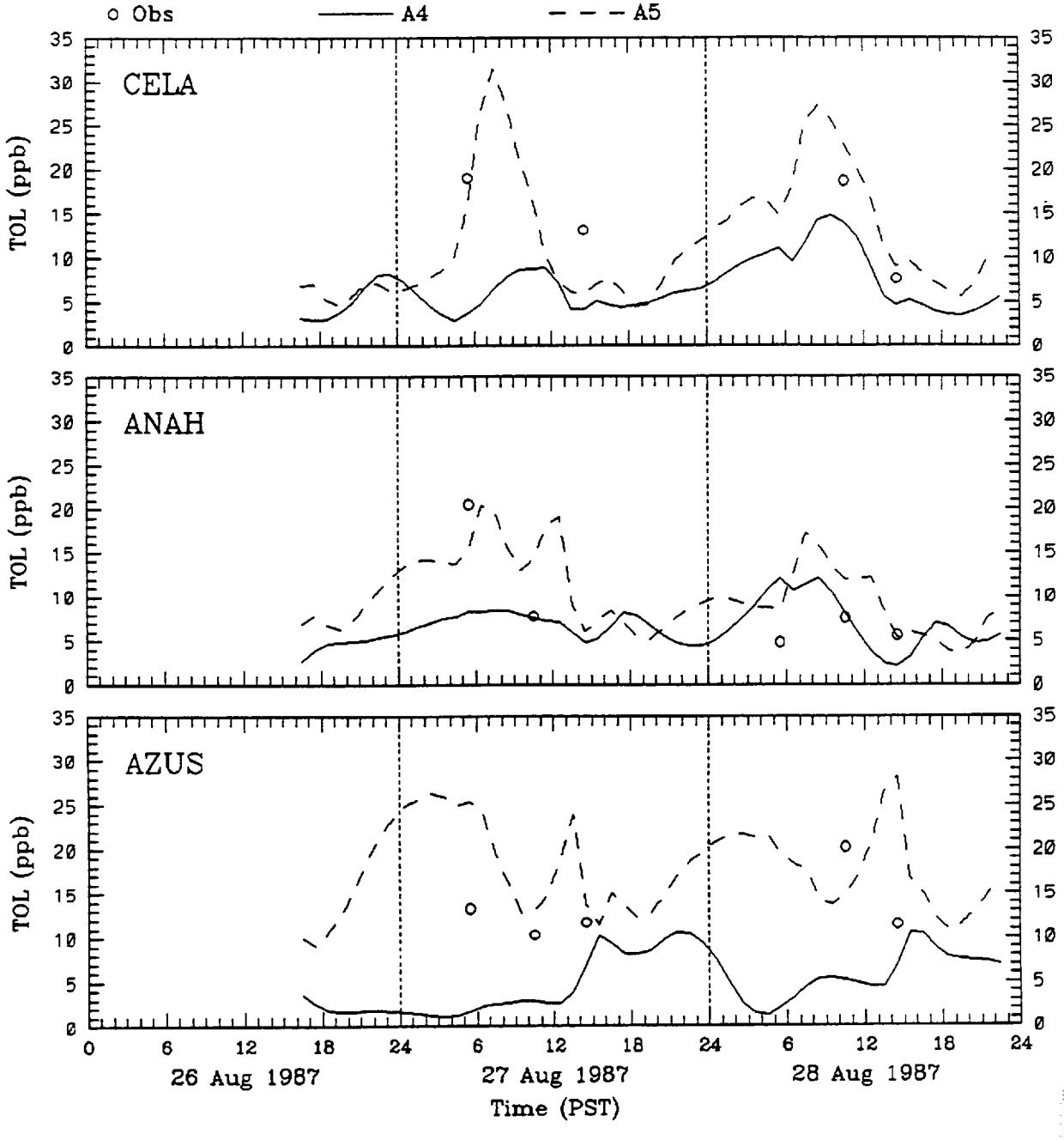
Runs A4 and A5: Predicted and Observed OLE Time Series
26–28 August 1987



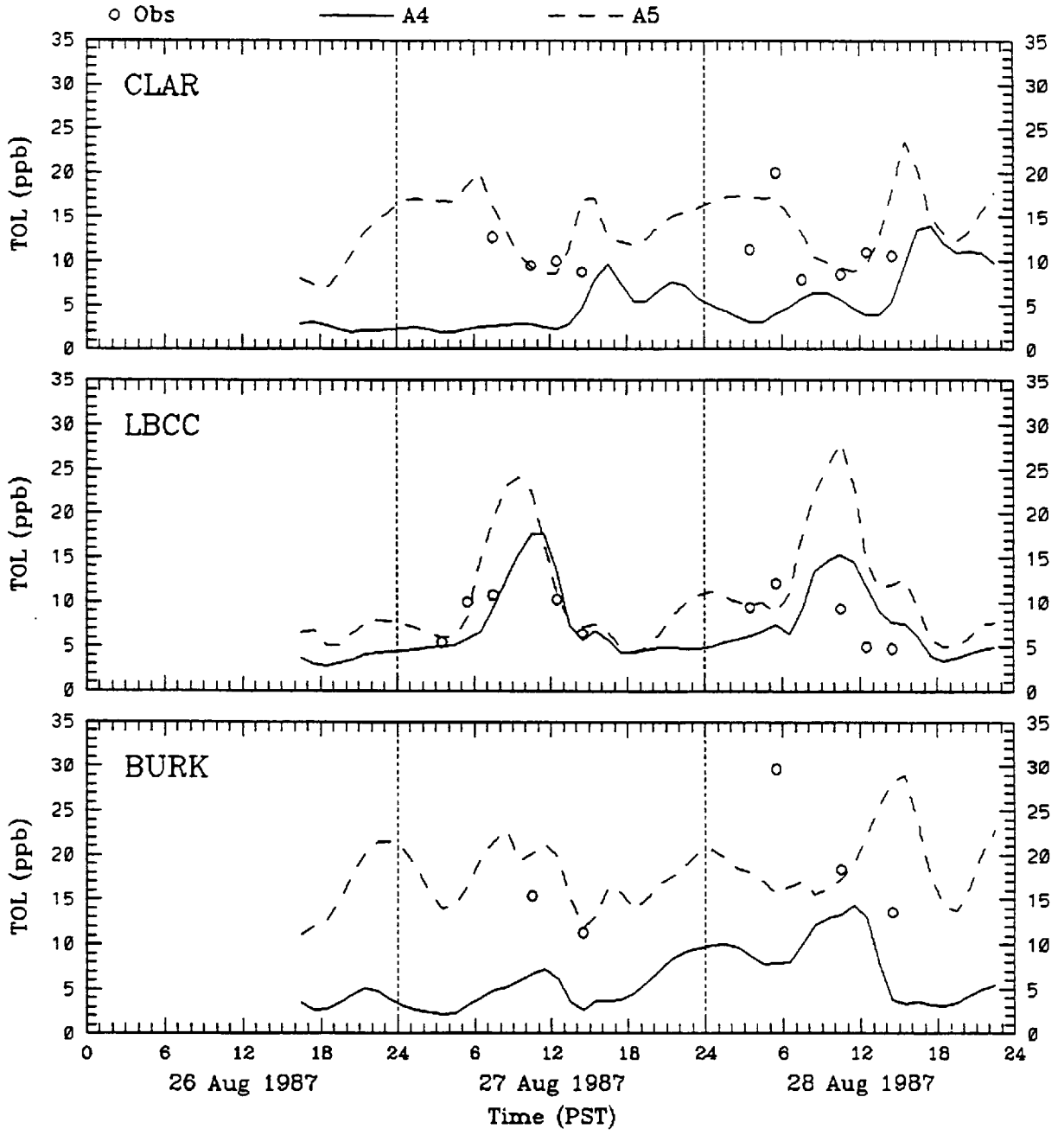
Runs A4 and A5: Predicted and Observed OLE Time Series
26-28 August 1987



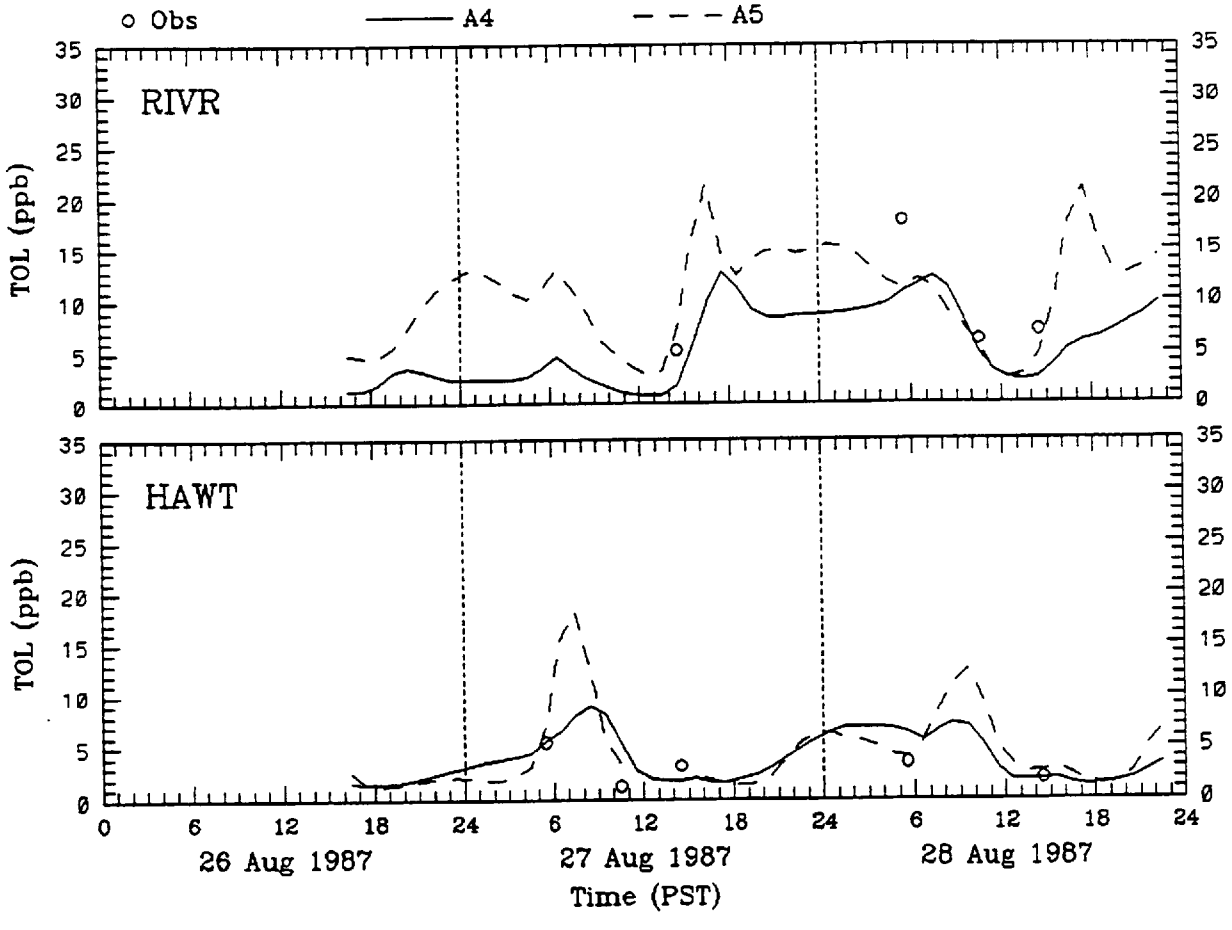
Runs A4 and A5: Predicted and Observed TOL Time Series
26–28 August 1987



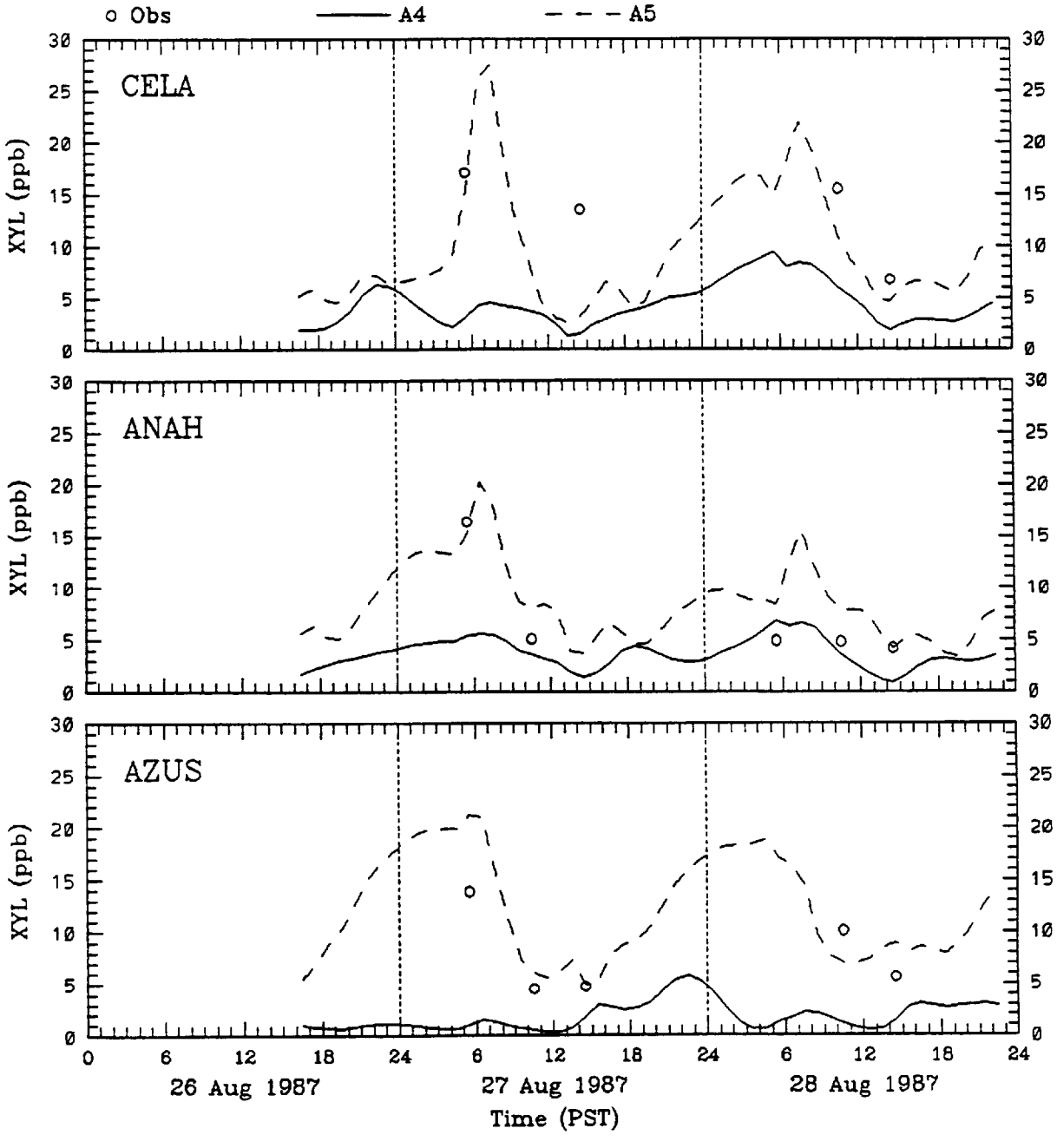
Runs A4 and A5: Predicted and Observed TOL Time Series
26–28 August 1987



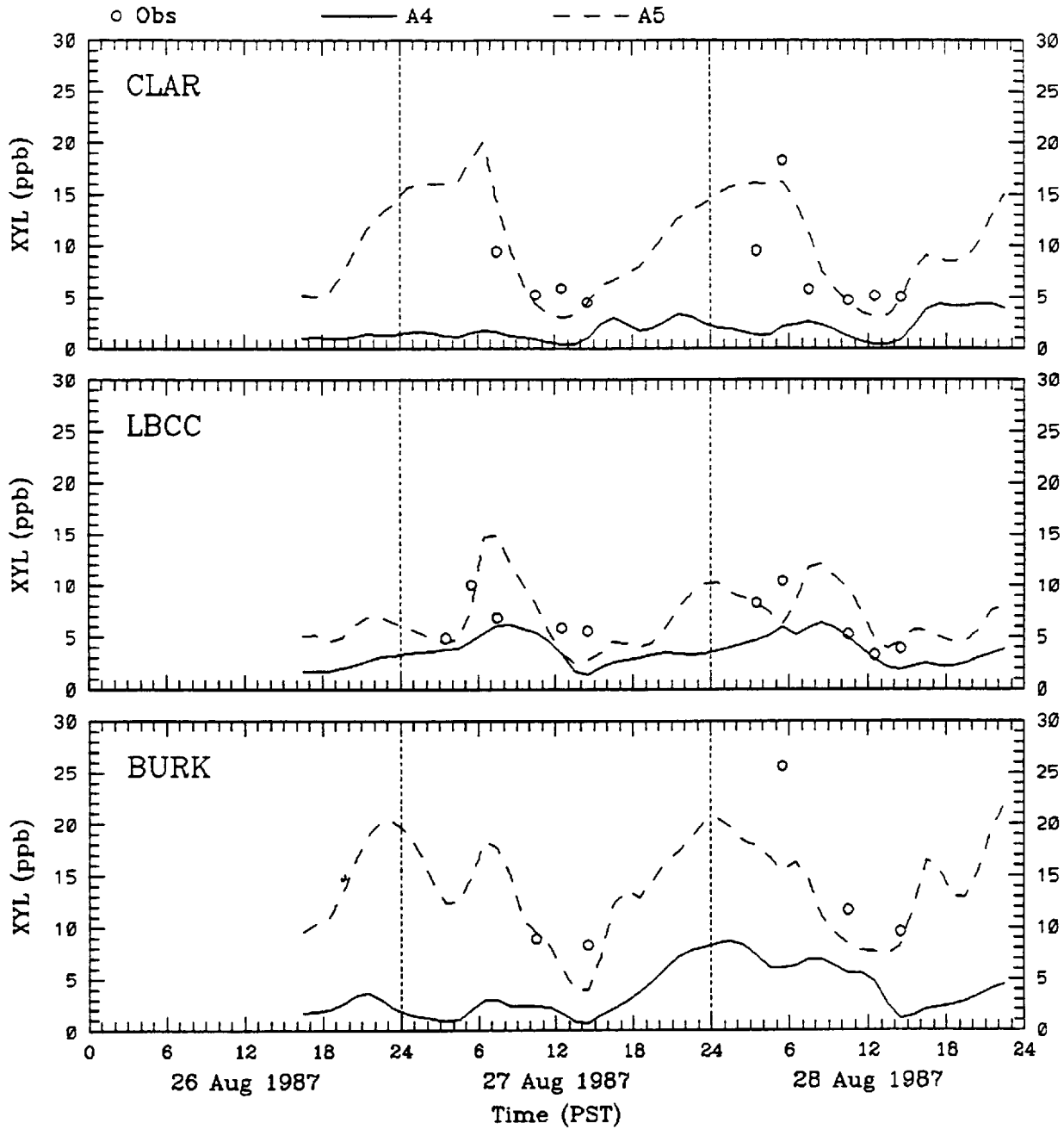
Runs A4 and A5: Predicted and Observed TOL Time Series
26–28 August 1987



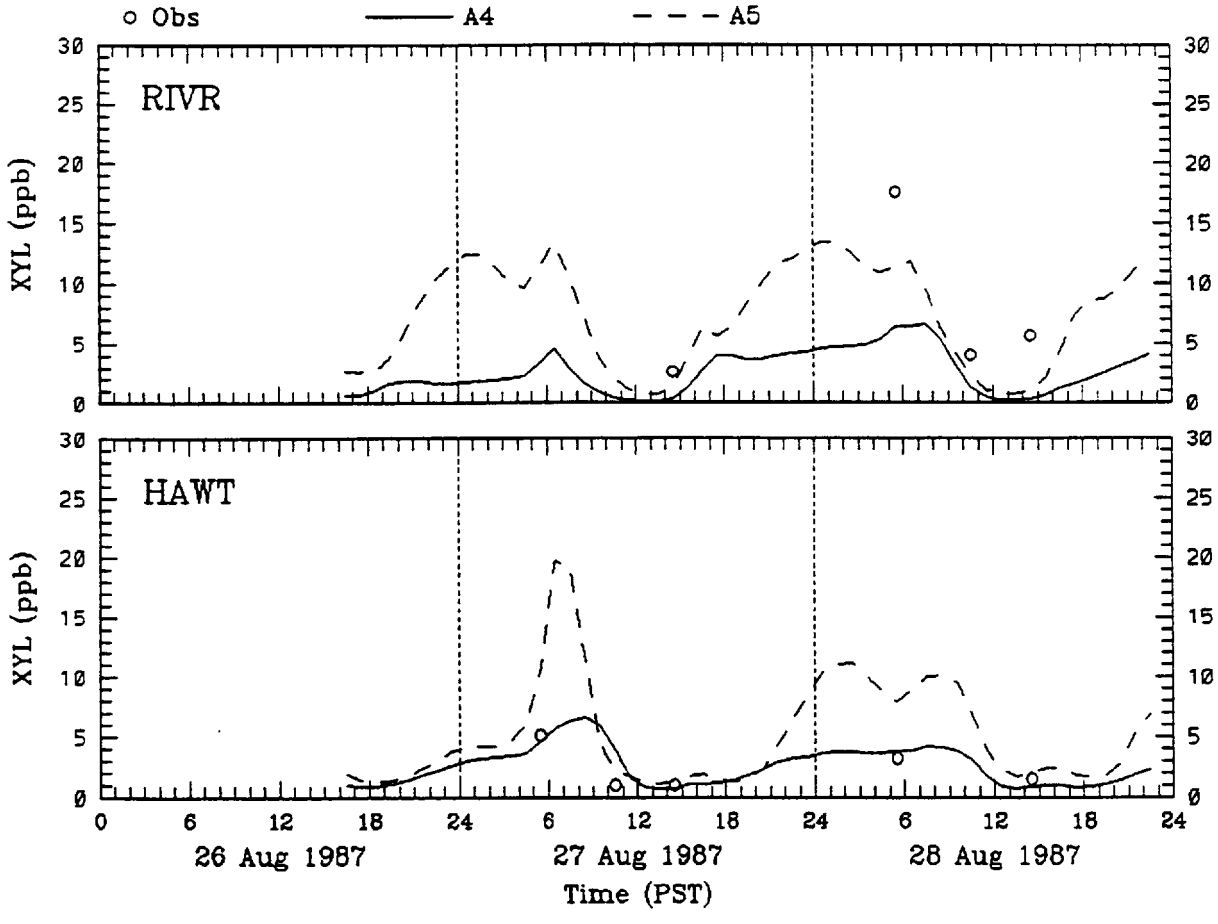
Runs A4 and A5: Predicted and Observed XYL Time Series
26–28 August 1987



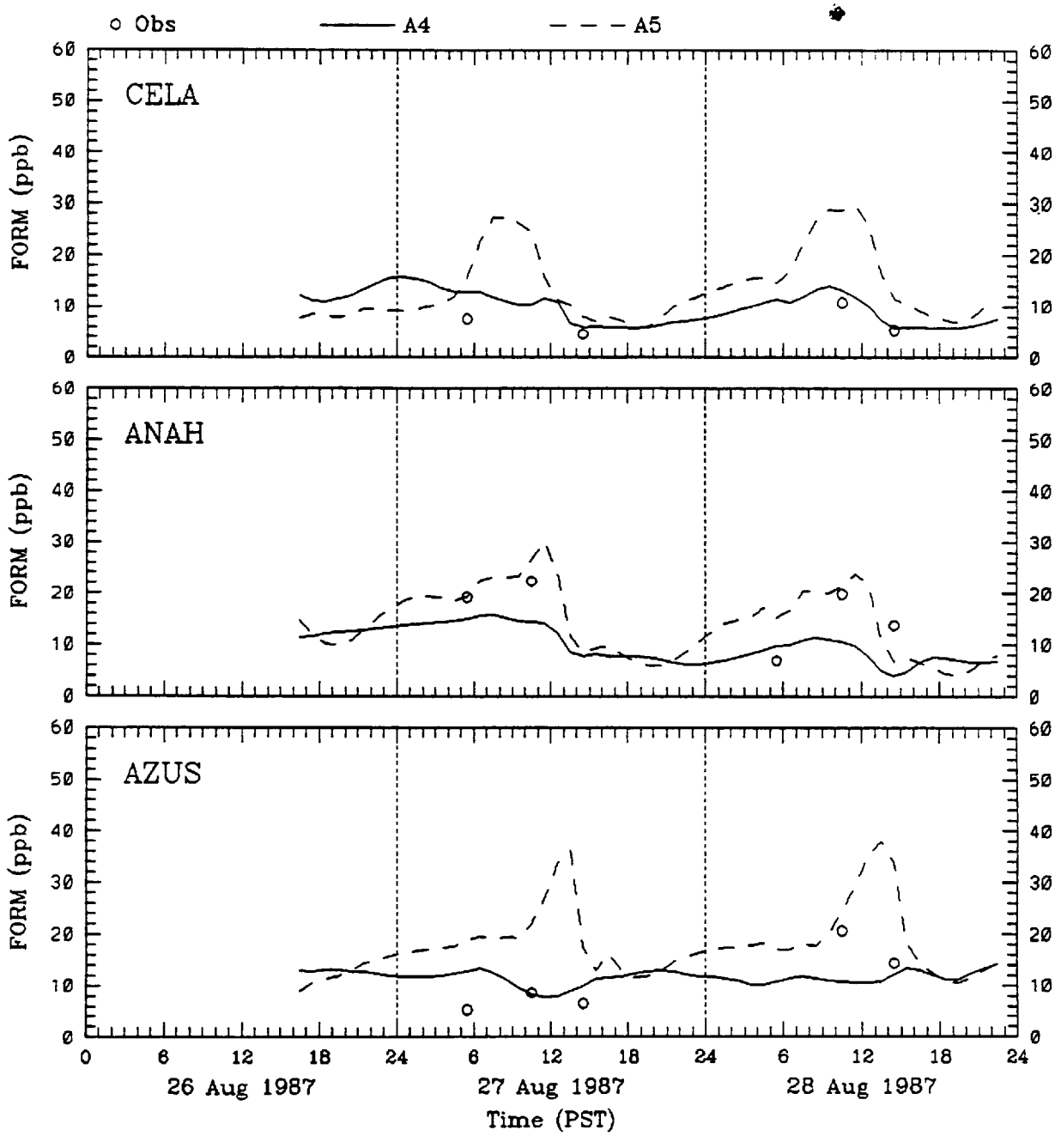
Runs A4 and A5: Predicted and Observed XYL Time Series
26–28 August 1987



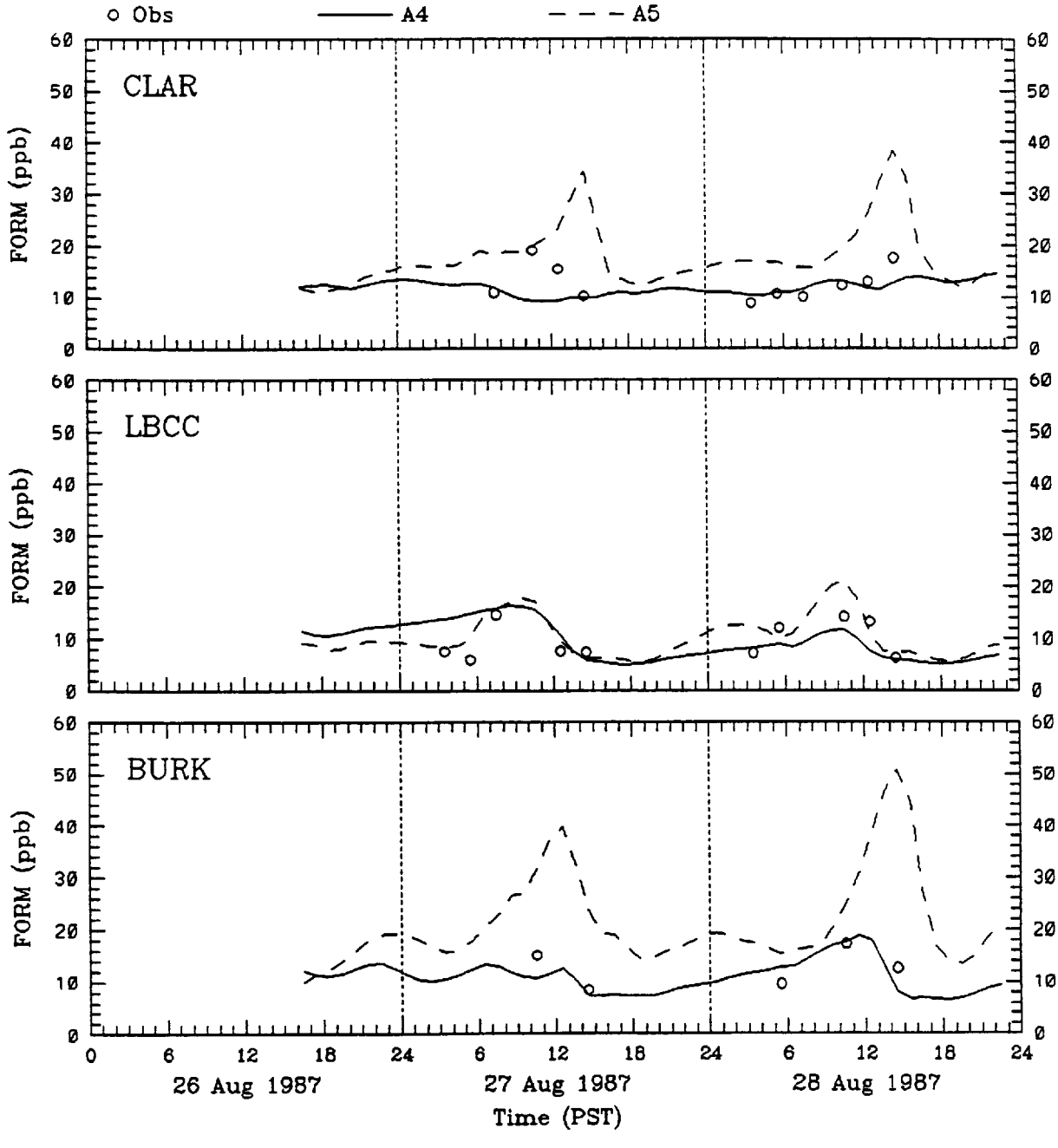
Runs A4 and A5: Predicted and Observed XYL Time Series
26–28 August 1987



Runs A4 and A5: Predicted and Observed FORM Time Series
26–28 August 1987



Runs A4 and A5: Predicted and Observed FORM Time Series
26-28 August 1987



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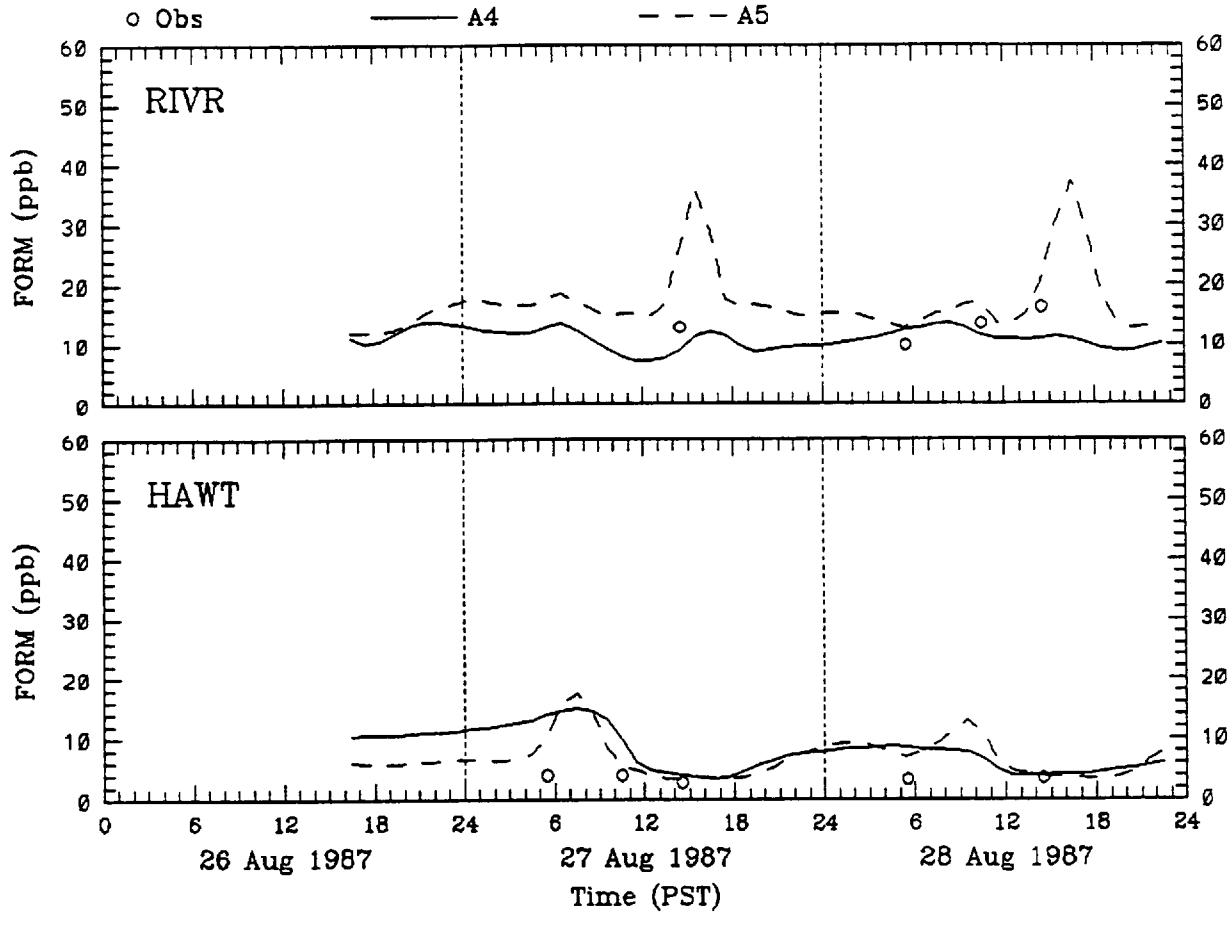
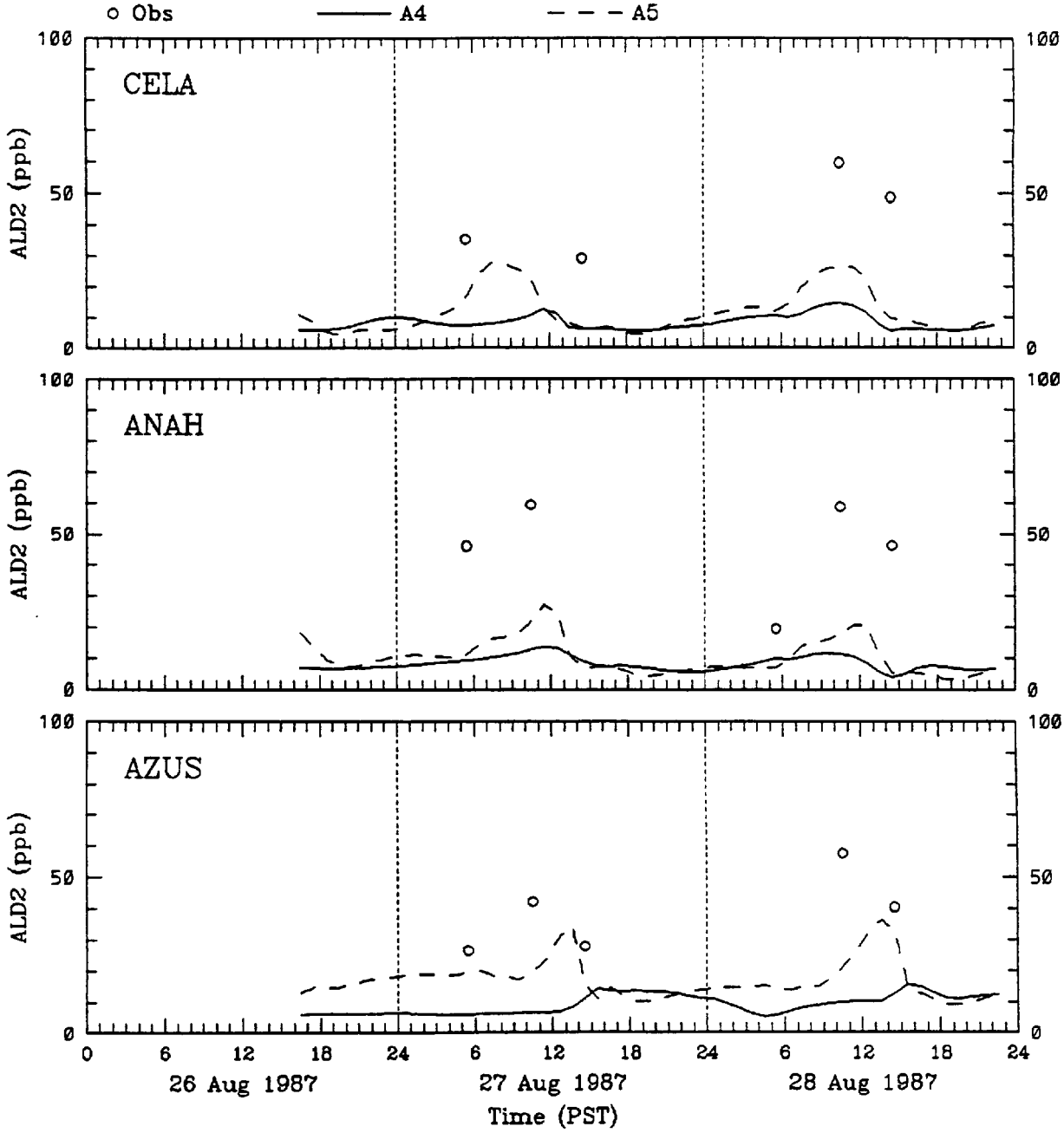
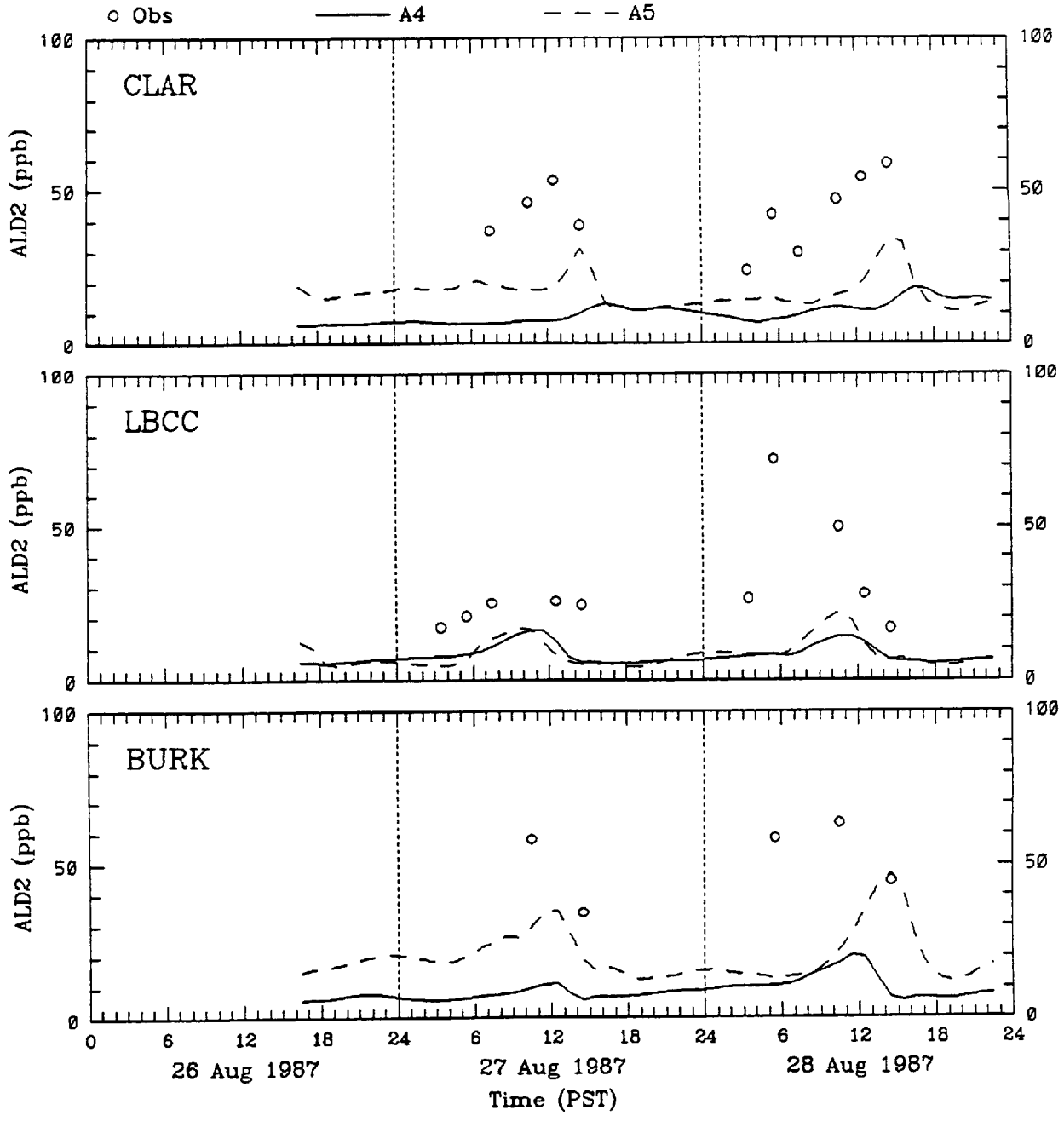
26–28 August 1987



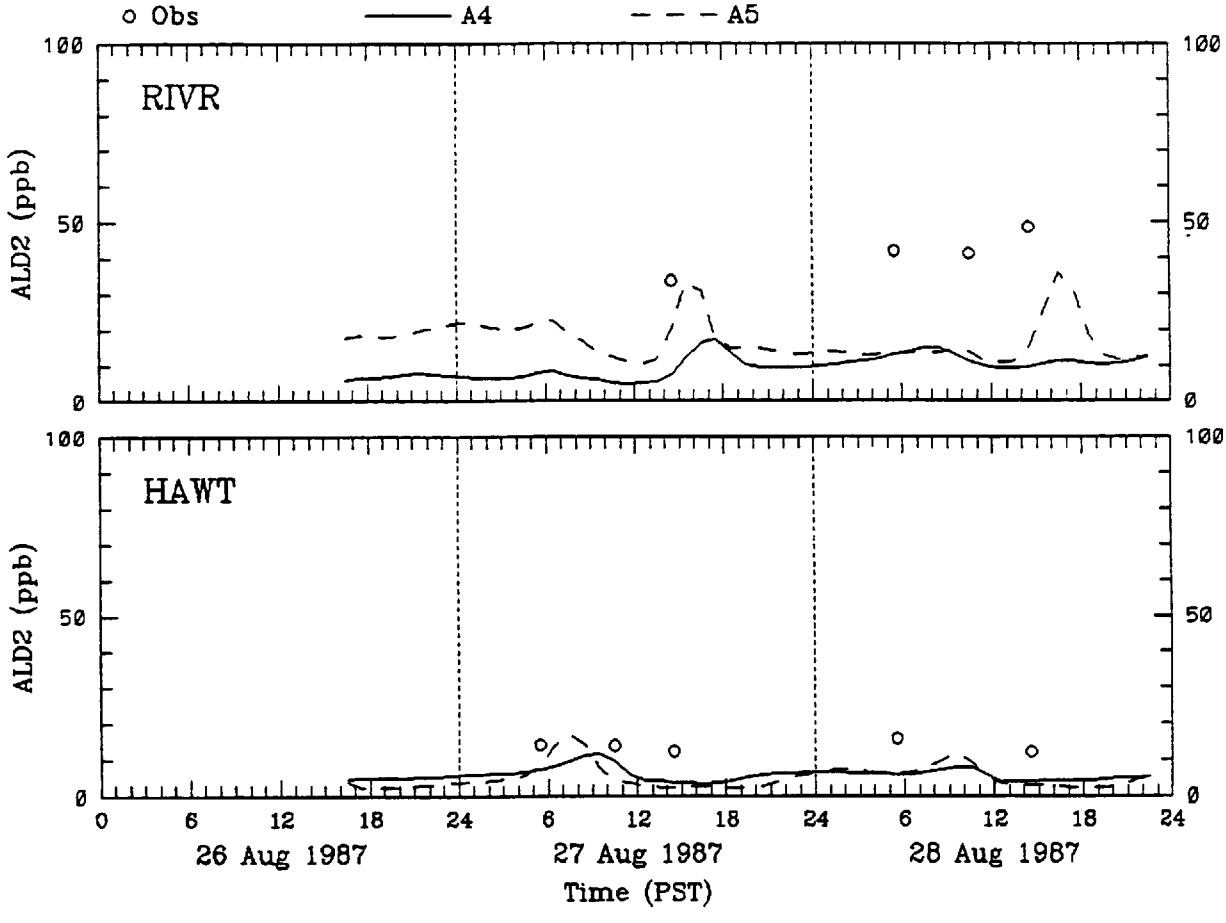
Runs A4 and A5: Predicted and Observed ALD2 Time Series
26–28 August 1987



Runs A4 and A5: Predicted and Observed ALD2 Time Series
26–28 August 1987



Runs A4 and A5: Predicted and Observed ALD2 Time Series
26–28 August 1987



APPENDIX G

Appendix G

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.

SURFACE CONCENTRATION ASSESSMENTS

Model evaluation procedures identified in the protocol were based on those recommended by Tesche *et al.* (1990). Both statistical and graphical comparisons of calculated and measured O_3 and precursor concentrations were performed. Particular attention was given to assessing model performance on the second and third days of the episode period since these were the days when the highest O_3 concentrations were observed and since simulation results on the first day may be subject to uncertainties in the specification of initial concentration inputs. Numerical measures employed to characterize model performance were developed using the Model Performance Evaluation, Analysis, and Plotting (MAPS) software developed by Alpine Geophysics. Specific measures included:

- peak estimation accuracy (paired in time and space)--the discrepancy between the magnitude of the measured peak one-hour concentration and the calculated concentration at the same time and location

$$A_{ts} = \frac{c_e(\hat{x},\hat{t}) - c_o(\hat{x},\hat{t})}{c_o(\hat{x},\hat{t})} \times 100$$

where the subscript e refers to the estimated concentration, the subscript o to the observed

concentration, and the hat, ^, to the location or time of the maximum observation.

- peak estimation accuracy (paired in space)--the discrepancy between the magnitude of the measured peak one-hour average concentration and the highest one-hour concentration calculated at the same location within three hours (either before or after):

$$A_s = \frac{c_e(\hat{x},t) - c_o(\hat{x},t)}{c_o(\hat{x},t)} \times 100$$

- peak estimation accuracy (paired in time)--the discrepancy between the highest measured concentration at a monitoring station and the highest calculated concentration occurring within the block of nine grid cells immediately surrounding the monitoring location:

$$A_t = \frac{c_e(x,\hat{t}) - c_o(x,\hat{t})}{c_o(x,\hat{t})} \times 100$$

- peak estimation accuracy (unpaired)--the ratio of the maximum one-hour averaged calculated concentration and the maximum one-hour measured concentration (unpaired in space or time):

$$A_U = \frac{c_e(\hat{x},\hat{t}) - c_o(\hat{x},\hat{t})}{c_o(\hat{x},\hat{t})} \times 100$$

- average peak accuracy over all stations (paired in space)--the average value of the spatially-paired peak estimation accuracy measures:

$$\bar{A} = \frac{1}{S}\sum_1^S |A_{si}| = \frac{1}{S}\sum_1^S \frac{|c_e(\hat{x},t) - c_o(\hat{x},t)|}{c_o(\hat{x},t)} \times 100$$

where S is the number of air monitoring stations.

- normalized bias--the average signed normalized deviation of the concentration residuals for all pairs of measured and estimated concentrations above a specified threshold value:

$$\frac{1}{N}\sum_{1}^{N}\frac{c_e - c_o}{c_o}$$

where N is the number of pairs of measured and estimated values.

- mean bias--the average signed deviation of the concentration residuals for all pairs of measured and estimated concentrations above a specified threshold value:

$$\frac{1}{N}\sum_{1}^{N}(c_e - c_o)$$

- normalized error--the average unsigned deviation of the concentration residuals for all pairs of measured and estimated concentrations above a specified threshold value:

$$\frac{1}{N}\sum_{i=1}^{N}\frac{|c_e - c_o|}{c_o}$$

- mean error--the average unsigned deviation of the concentration residuals for all pairs of measured and estimated concentrations above a specified threshold value:

$$\frac{1}{N}\sum_{i=1}^{N}|c_e - c_o|$$

- variance--the variance of all pairs of estimated and measured concentrations above a specified threshold value:

$$\frac{1}{N-1}\sum_{i=1}^{N}(d_i - \bar{d})^2$$

where d_i are the residuals (estimated minus measured values), $\bar{d}$ is the mean of the

residuals, and the summation is over all temporally and spatially paired estimate-observation residuals for which the observed value is above the cutoff concentration level.

Various graphical displays were generated to facilitate the analysis of surface concentration results, including:

- time series plots--displays showing the hourly measured and estimated concentrations at each monitoring station;
- ground level isopleths--spatial displays showing the estimated and measured concentrations at selected hours during the simulation, as well as similar displays depicting the maximum estimated and measured values;
- bias and error plots--displays showing bias vs. concentration and error vs. concentration.

Numerical and graphical assessments of bias, accuracy, and error measures were performed for both O_3 and its precursors (namely NO, NO_2, and VOCs).

Criteria for judging model performance were originally provided in the protocol for this study (see Appendix A). During the course of this investigation, the notion of "pass-fail" performance standards has been replaced by the concept of "thresholds triggering concern" in recent efforts to develop more comprehensive photochemical model evaluation guidance (Reynolds, Roth, and Tesche, 1992, 1994) and in the SARMAP model evaluation program. Basically, if a performance measure exceeds a threshold triggering concern, further diagnostic analyses should be carried out and efforts made to rectify the causes of the problem. At a minimum, there would be a need to carefully assess the adequacy of model performance. We have recast the performance criteria stated in the protocol using thresholds triggering concern to make the evaluations discussed herein consistent with emerging model evaluation practice.

Thresholds triggering concern were established based on Class B performance values, which represent a level of O_3 performance typical of the better (but not necessarily acceptable) model performances seen to date. However, the study team strived to meet a more stringent set of goals

(summarized below) that provided much greater assurance that the model was adequately simulating the important atmospheric and emissions processes. The performance criteria employed in this study may be stated as follows:

- the model's overall performance--for the entire modeling domain and duration of the simulation--should meet the following criteria:
  - peak prediction accuracy (unpaired in space and time): the goal is $\leq \pm 5\%$, and the threshold triggering concern is $\leq \pm 20\%$;
  - normalized bias (paired in space and time): the goal is $\leq \pm 5\%$, and the threshold triggering concern is $\leq \pm 15\%$; and
  - normalized error (paired in space and time): the goal is $\leq 25\%$, and the threshold triggering concern is $\leq 35\%$.
- the model's subregional performance for all important subregions should meet the following criteria:
  - normalized bias (paired in space and time): the goal is $\leq 5\%$, and the threshold triggering concern is $\leq \pm 20\%$; and
  - normalized error (paired in space and time): the goal is $\leq 25\%$, and the threshold triggering concern is $\leq 35\%$.

Model performance measures were calculated for all pairs of observed and estimated values for which at least one member of the pair exceeded the following values:

- O_3 80 ppb
- NO_2 20 ppb
- NO_x 20 ppb

The numerical value for each threshold triggering concern corresponds identically to the performance criteria cited in the protocol (see Appendix A). However, thresholds triggering concern for subregional performance for the normalized bias and error cited in the protocol were 30 and 40 percent, respectively. Upon further consideration of these values, we found no

justification for establishing thresholds triggering concern for subregional performance that are less restrictive than those for overall model performance. Thus, we reset the subregional criteria to correspond to the overall criteria cited above.

To assist in the assessment of model performance, subregions of the modeling domain were identified based on recommendations provided by CARB staff. Air monitoring stations included in each subregion are as follows:

- Region A--Coastal Region

  Anaheim (ANAH)
  Costa Mesa (COST)
  El Toro (TORO)
  Hawthorne (HAWT)
  Long Beach (LGBH)
  Long Beach City College (LBCC)
  Los Alamitos (LSAL)
  West Los Angeles (WSLA)

- Region B--Central Basin

  La Habra (LAHB)
  Los Angeles (CELA)
  Lynnwood (LYNN)
  Pasadena (PASA)
  Pico Rivera (PICO)
  Whittier (WHIT)

- Region C--San Fernando Valley

  Burbank (BURK)
  Reseda (RESE)

- Region D--Eastern Region

  Azusa (AZUS)
  Claremont College (CLAR)
  Fontana (FONT)
  Glendora (GLEN)

Norco (NORC)
Pomona (POMA)
Redlands (REDL)
Riverside-Rubidoux (RIVR)
Rubidoux (RUBI)
San Bernardino (SNBD)
Upland (UPLA)

- Region E--Basin Rim

  Banning (BANN)
  Crestline (CRES)
  Hemet (HEME)
  Perris (PERI)

- Region F--Far Eastern Region

  Palm Springs (PLSP)
  29 Palms (29PL)

- Region G--Lancaster

  Lancaster (LANC)

- Region H--Ventura County

  El Rio-Rio Mesa H.S. (ERIO)
  Ojai (OJAI)
  Piru-2SW (PRU2)
  Simi Valley-Cochran (SIM2)
  Thousand Oaks-Windsor (OAKS)
  Ventura-Emma Wood (EMMA)

- Region I--Victorville and Hesperia

  Hesperia (HESP)
  Victorville (VICT)

Figure 2-1 shows the locations of these air monitoring stations.

If any of the threshold values were exceeded or if the model was not adequately simulating

precursor concentrations or other phenomena in the study domain (as discussed in the next subsection), the study team was to assess the need to conduct further diagnostic analyses. Final determination of the adequacy of model performance rested with the API Air Modeling Task Force and the SCE project representative.

OTHER MODEL ASSESSMENTS

In assessing performance, it is important that the model results be examined to ascertain whether important physical and chemical processes are being adequately simulated. This can be difficult in situations where pertinent data are limited. The SCAQS data base contains measurements of pollutant concentrations aloft and speciated VOC samples. This information has been used in comparisons of ambient measurements and VOC and NO_x emissions inputs and in assessments of how well model estimates agreed with available pollutant measurements collected aloft.

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