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Application of Photochemical Models

Volume III

Recent Sensitivity Tests and other Applications of the LIRAQ Model

APPLICATION OF PHOTOCHEMICAL MODELS

Volume III

Recent Sensitivity Tests and Other Applications of the LIRAQ Model

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PREFACE

This document is one of four volumes intended to provide information relevant to the application of photochemical models in the development of State Implementation Plans. The reports are particularly directed toward agencies and individuals responsible for preparation of non-attainment plans and SIP revisions for ozone. The four volumes are titled as follows:

Application of Photochemical Models

Volume I - The Use of Photochemical Models in Urban Ozone Studies

Volume II - Applicability of Selected Models for Addressing Ozone Control Strategy Issues

Volume III - Recent Sensitivity Tests and Other Applications of the LIRAQ Model

Volume IV - A Comparison of the SAI Airshed Model and the LIRAQ Model

This work is to a large extent based on the photochemical modeling experience gained in the San Francisco Bay Area in support of the 1979 Bay Area Air Quality Plan. The following individuals made significant contributions to this work:

Association of Bay Area Governments	- Ronald Y. Wada (Project Manager) - M. Jane Wong - Eugene Y. Leong
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The authors wish to express their appreciation to John Summerhays, EPA Project Officer in the Source Receptor Analysis Branch of OAQPS, for his thoughtful review and comments on earlier drafts of this report.

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1. SUMMARY

A series of photochemical modeling experiments, using the LIRAQ model applied to the San Francisco Bay Area, was performed to investigate: a) model sensitivity to the spatial resolution of the gridded emissions, b) the impact of future HC and NO controls on the future Bay Area NO2 levels, and c) the future impact of Bay Area HC and NO reductions on O3 in adjacent downwind valleys.

The emission resolution experiments consisted of three simulations wherein emissions were smoothed over a) 5 x 5 km areas, b) 10 x 10 km areas, and c) distributed according to population. It was found that simulated O3 concentrations are sensitive to emission distribution patterns. Changing from 5-km to 10-km resolution changed the O3 maximum concentration by up to 10%. When emissions were distributed proportional to population substantial changes occurred in the timing and magnitude of the O3 maxima. The results suggest that short-cut methods should not be used for source inventory distribution.

The short-term NO2 experiments consisted of simulating O3 and NO2 fields under meteorological conditions favoring high NO2 buildups. Model performance in approximating observed space/time distributions of O3 and NO2 on the prototype day was judged to be adequate. Sensitivity runs were made using three combinations of HC and NO reductions from a projected 1985 inventory. The results suggest that HC control is the most effective strategy for both O3 and NO2. Control of NO tends to increase local O3 and decrease NO2 slightly. NO2 was generally less sensitive to precursor reductions than was O3.

The long range transport experiments consisted of modifying LIRAQ to simulate an expanded 160 x 160 km region that included the Bay Area "source" region and portions of the Sacramento and San Joaquin Valleys as a "receptor" region. We investigated the sensitivity of downwind O3 to varying HC and NO emissions from projected 1985 values. A base year simulation with 1975 emissions yielded reasonable O3 concentrations in the downwind study region on both meteorological prototype days used. The emission sensitivity results showed that for the (26 July 1973) prototype day, downwind O3 was strongly influenced by specification of initial and boundary conditions. It was not possible to assess the downwind effects of Bay Area emissions changes from the simulations that were run in this study. It is believed that such assessments are feasible with proper selection of meteorological prototype conditions and with reasonably accurate estimates of initial and boundary parameters.

2. INTRODUCTION

LIRAQ is a grid-based photochemical model that has been in use for several years in the San Francisco Bay Area. The 1979 Bay Area Air Quality Plan was based on LIRAQ ozone modeling results using historical and projected emission inventories. During that effort, several issues arose which clearly needed more examination than deadlines permitted. These issues included:

- Effectiveness of HC control measures vs. NOx control measures in reducing ozone and NO2 concentrations.
- Long range transport -- effects of local control strategies on downwind receptors, including receptors located outside the standard 100 km by 100 km modeling area.
- Degree of resolution required in the source inventory to produce acceptable modeling results; possibility for savings through use of inventory shortcuts.
- Effects of controlling mobile sources vs. effects of controlling stationary sources.
- Sensitivity of model ozone results to hydrocarbon reactivity classes -- number of classes, distribution of inventory betwen classes, and effects of control measures affecting only certain classes.

These issues are of interest to the modeling community and to many people involved in air pollution control and air quality planning.

The first three issues were of sufficient interest to EPA that a contract was awarded through the Association of Bay Area Governments (ABAG) so that the local modeling group could investigate the importance and effects of certain actions. The experimental plan emerged through an iterative process involving all of the cooperating agencies: EPA, ABAG, the Bay Area Air Quality Management District (BAAQMD), Systems Applications, Inc. (SAI), Lawrence Livermore Laboratories (LLL), and the California Air Resources Board (ARB).

The final experimental design included three separate sections: 1) emission inventory patterns, 2) short-term ambient NO2 concentrations, and 3) long range transport of pollutants.

Effects of emission inventory patterns are addressed in Section 3 of this report. Three different inventory patterns were tested for each of two different years. The 1975 Bay Area inventory represents a baseline case with relatively stringent controls on emissions of organic compounds. A 1985 inventory year was also studied, where very stringent and comprehensive control measures were assumed. The three emissions patterns used for each year were: 5 x 5 km grid resolution, 10 x 10 km resolution, and pure population-based emissions distribution (over a 5 x 5 km grid).

For the short-term NO2 question, a new prototype meteorology day was developed for the LIRAQ model runs. Previous meteorological data had been derived from historical days with high measured ozone levels, regardless of NO2 readings. The day chosen for this project was November 5, 1976, a day with high NO2 (.29 ppm), and only moderate (.13 ppm) ozone. This November day was part of a multi-day NO2 episode that was one of the worst ever experienced in the Bay Area. There was a general interest in model performance for this new application, and a specific interest in the effectiveness of HC and NOx controls on ozone and NO2 predictions. Results are presented in Section 4 of this document.

The goal of the long range transport experiment was to assess the impacts of Bay Area control measures on downwind receptors. California's Central Valley, at a distance of 40 to 60 miles from San Francisco, was the receptor area of interest in this study. The LIRAQ model was modified to cover a larger area, in the hope that long range air quality impacts could be detected and analyzed. Model coverage was increased from a standard 100 x 100 km area, to a 160 x 160 km area, so that the Bay Area and parts of the Central Valley could be accommodated in a single model run. The results of this work are presented Section 5 of the report.

3. MODEL SENSITIVITY TO SPATIAL RESOLUTION IN THE EMISSIONS DATA BASE

PURPOSE

There is a great deal of interest in the degree of data resolution required to produce acceptable photochemical modeling results. This interest is based primarily on cost considerations. Because photochemical models are very data intensive, the choice of spatial and time scales has a critical effect on the total resources that will be required for data collection, input file preparation, computer demands, and output analysis. The photochemical version of LIRAQ has been run with 5-km grid squares in a 20 by 20 array, for a total grid area coverage of 100 km by 100 km. The emissions patterns must be defined, for each pollutant of interest, over the modeling area.

This experiment was designed to test the effects of different techniques for spatial allocations of emissions. Because it is impossible to locate and measure each source of pollutants in a modeling region, some approximations are required in the preparation of emissions inventories. The modeler normally receives an aggregated (regional, annual average) source inventory, which must be allocated over space and time to fit the model data requirements. Some techniques for spatial and temporal resolution have been published by EPA (1974) and Perardi et al. (1979). This project does not consider the technical merits of one or another technique. We are interested only in comparing the model outputs to see first if there are any noticeable differences, and second, if less expensive techniques can provide acceptable results.

Three patterns of emissions distributions were tested for this project:

1. "5 x 5." This is the standard disaggregated inventory used in most LIRAQ runs, including the 1979 Bay Area Air Quality Plan. Point, area, and mobile sources were distributed as nearly as possible to their actual locations in 5 x 5 km grid squares* over a 100 x 100 km region.

2. "10 x 10." For these runs emissions were averaged over 10 km x 10 km grid squares--four times as large as the 5 x 5. The preparation of a 10 x 10 inventory would be somewhat less expensive than a 5 x 5, and there would be a further savings potential in computer time for model execution. As a first estimate, computer time would be one-fourth as much for the same size area, or an area four times as large could be run for the same time.

*Actually most of the data were first compiled by 1 x 1 km grid squares for LIRAQ I.

c. "Pop." In these inventories the model area inventory totals were distributed over the area proportional to population (residential, not employment). One might wish to distribute an aggregated inventory by population, in order to avoid the task of determining the exact locations of a multitude of sources. Because population data are widely available, this technique could be relatively simple and economical for almost any modeling region.

METHODOLOGY

The standard 5 x 5 km gridded emissions inventory was achieved by: 1) direct location of larger point sources (>0.1 ton/day), 2) distribution of small point sources and area sources by association with 19 employment and land use categories, and 3) addition of mobile source emissions derived from a travel model and trip tables. The process has been described in some detail by Perardi et al. (1979). Stationary source emissions are actually maintained on a 1 km grid basis, for use with some (non-reactive) LIRAQ applications. These are aggregatedd to 2 km or 5 km grids, as necessary. Only the 5 km grid has been used for photochemical modeling, because of computer space limitations, with a large number of grid squares and large number of equations to be solved for each grid square and each time step.

The 10 x 10 km grid square inventory was derived from the existing 5 x 5 by averaging groups of four 5 x 5 emission rates into one 10 x 10 emission rate. The model runs still used a 5 x 5 calculation grid but emissions were introduced on a 10 x 10 grid for the entire simulation period. The LIRAQ model was later modified to perform calculations on a larger grid size (8 x 8 km) and those results are discussed in Section 5 of this report. Briefly, it appears that the model is more sensitive to emissions resolution than to calculation grid size.

The population-distributed inventory was prepared by allocating the total emissions for all pollutants over the Bay Region on the basis of population density. The base year population and projections were provided by the local COG, the Association of Bay Area Governments (1977). The original census data covered about 1,000 census tracts over an area of about 20,000 km2. The populated areas are actually only about 6,000 km2, the balance being essentially uninhabited (bays, tidelands, marshes, mountains). Regional emissions were distributed proportional to population over the 6,000 km2 of developed or developable land on a 5 x 5 km grid basis.

The three types of inventories were prepared for each of two years--a 1975 base year and a 1985 control strategy scenario with large reductions in the hydrocarbon inventory.

RESULTS

The aggregated inventory totals and ozone results are shown in Table 3-1. The three different inventories tested (5 x 5, 10 x 10, and pop.) did produce significantly different ozone predictions, especially for the 1975 base year. For the 1985 projections, with comprehensive control strategies and 50% hydrocarbon reductions, the differences were less notable.

The modeling output of fundamental interest is the regionwide ozone maximum, in the second column from the right. This is the highest O3 concentration predicted anywhere in the modeling region at any time of the day. This value changed by about 25% over the three 1975 base year runs, and about 15% in the 1985 runs. The basic O3 patterns are similar in contour shapes because the same meteorology data were input in each run, but the timing, magnitude and spatial resolution of ozone were all affected by the emissions inventory changes. The precursor inventory totals of HC and NO were essentially equal for a given year; only the distribution patterns were changed.

Figure 3-1 shows the regionwide high ozone, as a function of time, for the three 1975 inventories tested. The baseline run, with standard 5 x 5 km inventory, produced the highest O3 prediction of .20 ppm at 1300 hours. The 10 x 10 has the same timing with a .18 ppm maximum. We attribute the difference to a smearing of emissions over the larger areas, with lower resulting cell concentrations of precursors, and lower reaction rates. Figures A4 - A9 in Appendix A show the hydrocarbon* and NO concentration patterns for 0900 hours. These early precursor concentration maps are closely related to emission patterns, which are not directly available in graphic form. Comparing A4 and A6 shows for example the striking dilution of the San Francisco high HC "fingerprint" by the change from 5 x 5 to 10 x 10 emission resolution. This dilution and spreading of emissions takes place over the entire area, and is more evident in areas where high-emissions squares are bordered by low-emissions neighboring squares in the 5 x 5 format. Thus, San Francisco emissions were substantially diluted, while Oakland and San Jose highs were less affected.

The difference between 5 x 5 and Pop. ozone production is even more striking. The high value drops from .20 to .15 ppm and occurs three hours later. In the latter case there is a notable redistribution of emissions. NOx emissions, particularly, are removed from normal point source locations and transferred to (residential) population areas. In the baseline inventory some area sources are distributed on population or population-related variables. Less than 40% of organics and less than 15% of NOx is population related in the baseline 5 x 5 inventories. In the Pop. inventory, by contrast, 100% of each pollutant was distributed by population. The result is that all point source, area, airport and vehicle emissions are transferred to population centers. Cities such as San Francisco, Oakland and San Jose tend to remain as

*Actually a representative LIRAQ hydrocarbon group, "HC2", corresponding to alkanes and less reactive aromatics.

Table 3-1. Inventory Summaries and Ozone Predictions

Inventory Year	Inventory Pattern	Model Inventory [1] Totals (tons/12 hr) HC2 [2]	NO	Model Predictions Regionwide Maximum O3 (ppm)	Time of Occurence (hour)
1975	5 x 5 km	527	202	.20	1300
	10 x 10 km	514	196	.18	1300
	Pop. Distr.	526	202	.15	1600
1985	5 x 5 km	260	172	.13	1500
	10 x 10 km	258	168	.13	1500
	Pop. Distr.	259	169	.11	1500

1. The model inventory is the sum of emissions in the model area for the critical 12 hour period from 4 am, when the simulation begins, to 4 pm, when the latest ozone maximum occurs. The model area is the specific 100 km by 100 km square grid (within the Greater Bay Area inventory region) chosen for LIRAQ model runs.

2. HC2 is one of the three hydrocarbon reactivity classes used in the LIRAQ model. It is representative of total organic emissions and includes about 70% of the total HC mass. Slight variations in the inventory totals for HC2 (and NO) are due to rounding errors from the model inventory summation readouts. Precursor totals for a given year are essentially equal for the three different source inventory patterns.

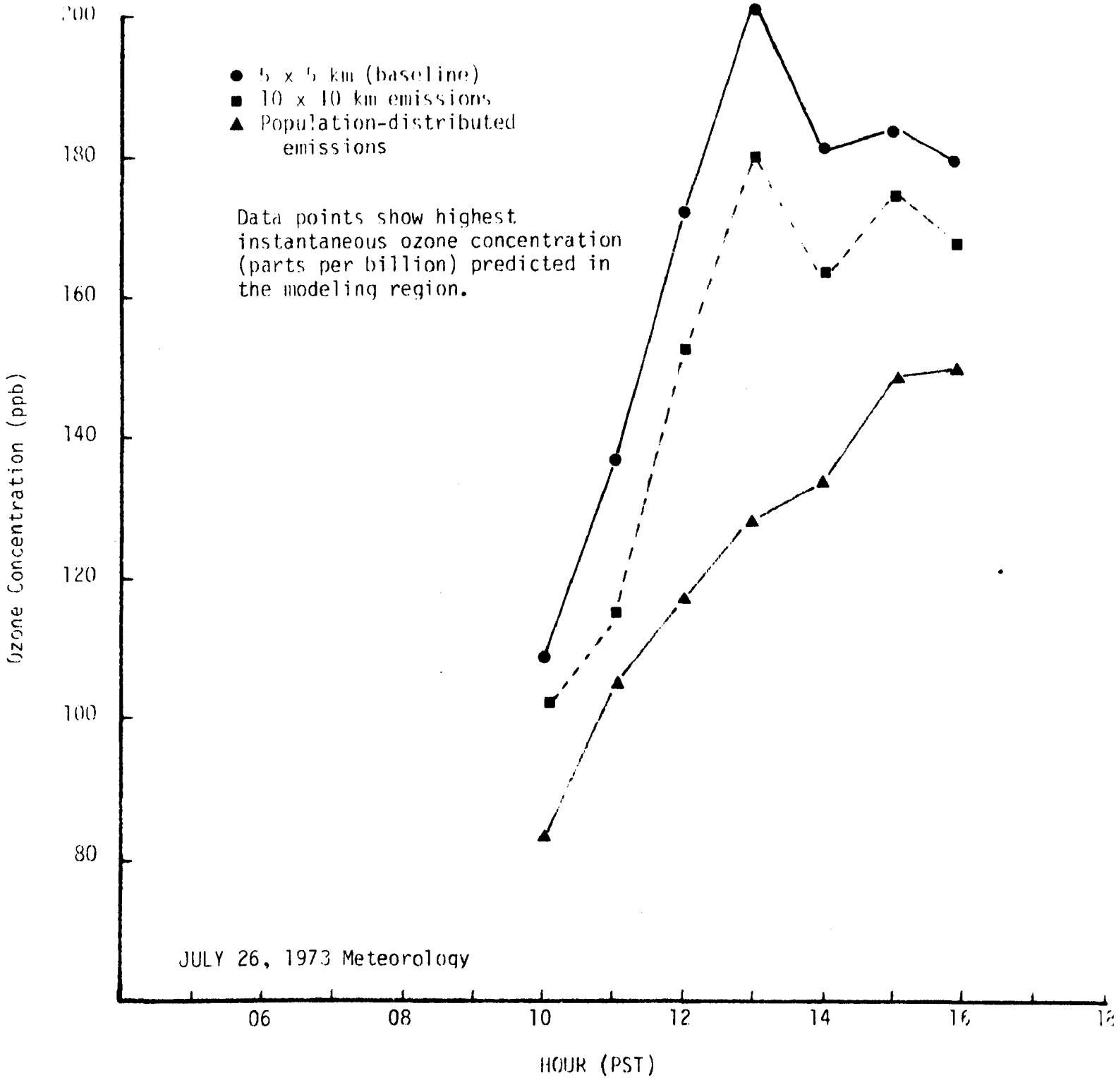

Figure 3-1. Regional ozone maxima from LIRAQ simulations using three spatial distributions of 1975 emissions

high emission areas and may even increase, especially in NOx. The large NOx emissions from power plants and major industries along the Carquinez Straits would be moved to more densely populated areas.

In an area of low HC/NOx ratios, this has the effect of increasing the NOx content of precursor parcels and lowering the expected downwind ozone. It is possible that the long range effects would be to increase O3 formation, but this did not occur within the 100 x 100 km study area.

For the 1985 series, the results are not so clear cut. The difference between the 5 x 5 and 10 x 10 inventory runs is very small: .130 ppm for the 5 x 5, compared to .132 ppm for the 10 x 10. The results are presented to three significant figures in order to show that the 10 x 10 result actually came out higher. This is the opposite of the 1975 result and was not expected. The reversal itself is so small as to be insignificant, but the disappearance of the 1975 difference is of interest. The reduced 1985 inventories resulted in smaller differences overall (.11 to .13 ppm from Pop. to 5 x 5, compared to .15 to .20 ppm for the corresponding 1975 patterns).

In general, models are more credible and useful as they treat more explicitly the relevant physical phenomena. The results of this study show that the model does respond to the degree of physical reality in the inventory. Thus there is a motivation to incorporate as much reality as possible in the source inventory. The final choice of inventory resolution will be determined by a balance of several factors. Among these are the degree of detail available in existing source inventories, project time and budget, size of the region to be modeled, and cost of required computer services.

CONCLUSIONS

- Simulated ozone concentrations from the LIRAQ model are sensitive to the spatial distribution patterns of the NOx and HC emission inventories.
- A change in the resolution of a gridded inventory, from 5 km to 10 km cell length, can produce changes up to 10% in the predicted ozone high.
- Distributing all emissions proportional to population substantially changed the timing and magnitude of the maximum estimated ozone concentrations.
- LIRAQ model performance, with respect to predicting regionwide high hour ozone, was significantly better with more realistic source inventories.
- The results of this work suggest that short-cut methods of source inventory distribution should not be used.

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2. Perardi, T. E., et al., "Preparation and Use of Spatially and Temporally Resolved Emission Inventories in the San Francisco Bay Region," Journal of the Air Pollution Control Association, Vol. 29, No. 4, pp. 358-364, April 1979.

3. U.S. Environmental Protection Agency, "Guidelines for Air Quality Maintenance Planning and Analysis," Volumes 8 and 13, 1974.

4. SENSITIVITY OF SHORT-TERM AMBIENT NO2 CONCENTRATIONS TO REDUCTIONS IN HC AND NO EMISSIONS

PURPOSE AND BACKGROUND

The goals of this study are: 1) to evaluate the LIRAQ photochemical model's usefulness for assessing effects of HC and NO emission controls on ambient NO2 concentrations over time periods of one hour to one day, and 2) to assess the sensitivity of future (1985) ambient NO2 concentrations to HC and NO emission changes under meteorological conditions that produce high NO2 levels.

LIRAQ was useful in the development of the Bay Area's non-attainment plan for O3. Sensitivity analyses using projected future emissions revealed that, while HC reduction is effective for controlling O3, NO reduction tends to increase O3 locally. Because of time and budgetary constraints and because the Federal NO2 standard has never been exceeded in the Bay Area, we did not conduct any NO2 modeling studies.

Models like LIRAQ usually simulate conditions over periods of a day or less and are therefore not well suited for evaluating impacts on long-term standards like the Federal one-year NO2 standard. Over short periods, however, photochemical grid models are appropriate.

LIRAQ simultaneously tracks several of the primary pollutants including CO, NO and three classes of reactive hydrocarbons. It also treats some of their photochemical derivatives including O3 and NO2. LIRAQ had never been applied to the meteorological conditions (usually in early or mid-autumn) when the highest NO2 levels occur. Also, the model's past performance for NO2 was not as good as it was for O3. This result is not surprising when one considers that NO2 performance was a secondary rather than a primary criterion in the development of the model chemistry.

The EPA is considering the adoption of a short-term NO2 standard. California's current one-hour standard of 0.25 ppm is sometimes exceeded in parts of the Bay Area. Therefore it is prudent to evaluate future HC and NO controls in terms of their impacts on both O3 and NO2. Then it will be possible to optimize strategies for meeting air quality goals for both pollutants.

METHODOLOGY

Prototype Day Selection

Selection of a prototype day was based upon two criteria. First, we wanted a day with widespread, sustained high NO2 levels in the Bay Area. Second, the day had to be in 1974, 1975 or 1976 to ensure that the 1975 emission inventory was fairly representative of actual emissions on that day.

The day chosen, 5 November 1976, was the fourth day of a seven-day episode of extremely restrictive dispersion conditions during which daily regional NO2 maxima ranged between 0.24 and 0.30 ppm. In fact, when the duration, intensity and spatial extent of very high levels of NO2, particulates, CO and SO2 are considered, this was perhaps the Bay Area's most severe air pollution episode of the decade. Oxidant levels were only moderate, however, and reached 0.13 ppm on 5 November. This is an unusually high value for the Bay Area so late in the year.

Gridded, mass-consistent flow and inversion base height fields for LIRAQ were generated from analyses of a large number of surface wind measurements, winds and temperature aloft from the Oakland National Weather Service station, solar radiation data from several BAAQMD sites, and a few SODAR soundings provided by SRI International. The MASCON code preprocessed these data to yield the necessary mass flux and inversion base height fields required by LIRAQ. Examples of these preprocessed fields are shown in Appendix B, Figure series B-1 and B-2.

Baseline and Sensitivity Scenarios

A series of simulations was performed 1) to assess LIRAQ's ability to reproduce the space/time distributions of O3 and NO2 observed on 5 November 1976, and 2) to evaluate future (1985) sensitivity of NO2 to changes from projected HC and NO emissions. A "verification" run was required because LIRAQ had never been run using 5 November 1976 meteorological conditions. The 1975 emission inventory was used--no inventory for 1976 was available. Actual differences in emissions between the two years are throught to be small, however.

The 1985 future-year simulations consisted of a baseline run with projected 1985 emissions plus three sensitivity runs with the following emission reductions:

- Strategy 1: 50% reduction in hydrocarbon emissions;
- Strategy 2: 25% reduction in hydrocarbon emissions and 25% reduction in NO emissions;
- Strategy 3: 50% reduction in hydrocarbon emissions and 25% reduction in NO emissions.

This matrix of runs was selected so that we could evaluate NO2 and O3 responses over a wide range of precursor control scenarios. The percent reductions were applied uniformly in space and time throughout the gridded modeling region. Boundary parameters for the 1985 base case were reduced from 1975 levels in proportion to emissions; initial conditions were the same in all runs.

Preliminary Evaluation of Model Performance

Before one can judge the validity and implications of the sensitivity experiments with any confidence one must first determine whether the model does a reasonable job of transforming primary emissions to concentrations of their photochemical derivatives. Tables 4-1 and 4-2 show observed and simulated one-hour averages of O3 and NO2 at eleven BAAQMD monitoring locations throughout the modeling region.

Overall, the observed and simulated O3 values agree very well. The predicted and observed regionwide maxima only differed by one pphm. LIRAQ correctly predicted high concentrations in San Jose, moderate values in Fremont and Livermore and very low values in Concord. Phasing of the hourly values was also good. For example, the time of predicted vs. observed maxima differed by more than one hour at only one station. Only once did an hourly value of the predicted 11-station maximum differ by as much as 3 pphm from observations. Model performance was poor at Pittsburg, where simulated concentrations were highly boundary-condition dependent because of inflow along the northern boundary during much of the day. Vallejo was similarly affected. Elsewhere, LIRAQ underpredicted at San Rafael and Redwood City and overpredicted at San Francisco and Burlingame. However, considering the difficulty of photochemical modeling in an air basin as geographically complex as the Bay Area, model performance for O3 is regarded as encouragingly good.

Agreement for NO2, while not as good as that for O3, was improved when compared with past performance of LIRAQ for other meteorological scenarios. Duewer, et al. (1978) found that, for the 20 August 1973 and 26 July 1973 prototype days, verification statistics for NO2 were weaker than those of any of the other pollutants studied. They noted that NO2 was most strongly affected by boundary conditions (especially the upper boundary), conditions which are usually not accurately known. For the 5 November 1976 simulations, excellent agreement was obtained at San Jose and Fremont. The model overpredicted NO2 along the peninsula from San Francisco to Burlingame and Redwood City. The phasing in this region was reasonably good, however. In the northern and eastern regions (Vallejo, Pittsburg, Concord and Livermore) agreement was poor--at least during parts of the simulation period. A tendency to underpredict at these stations may be related to inflow at the northern and eastern boundaries during much of the period. Overall, the results are encouraging in that agreement is good in much of the NO2-prone portion of the Bay Area.

Emission Sensitivity Results

Review of the sensitivity results for O3 produced few surprises. As was the case with earlier sensitivity experiments using the 26 July 1973 prototype day (De Mandel, et al., 1979), 1985 O3 is very sensitive to HC reduction. Concurrent reduction of NO tends to lessen the effectiveness of HC controls. This is evident in the regionwide O3 hourly maxima shown in Table 4-3. If we examine individually the three areas at which

Table 4-1
Comparison of Observed vs LIRAQ-Simulated Hourly Averages of Ozone (pphm), 5 November 1976 Meteorology, 1975 Emissions

STATION (MAP SYMBOL)		HOUR BEGINNING (PST) 04	05	06	07	08	09	10	11	12	13	14	15	16	17	18	19	20	21	MAX
San Francisco (DSF)	OBS.	0	0	0	0	0	0	1	1	1	1	1	0	0	0	0	0	0	0	1
	LIRAQ	0	0	0	0	0	1	2	3	4	4	3	1	0	0	0	0	0	0	4
Burlingame (DBU)	OBS.	0	0	0	0	0	0	0	1	1	2	2	2	1	0	0	0	0	0	2
	LIRAQ	0	0	0	0	0	0	1	1	2	4	5	4	1	0	0	0	0	0	5
Redwood City (DRC)	OBS.	1	1	1	1	2	3	3	5	7	8	9	7	4	3	3	3	3	2	9
	LIRAQ	0	0	0	0	0	1	1	2	3	4	5	4	2	0	0	0	0	0	5
San Jose (DSJ)	OBS.	0	0	0	0	1	1	3	4	9	10	11	3	4	1	1	1	1	1	11
	LIRAQ	0	0	0	0	0	0	1	3	8	12	11	9	5	1	0	0	0	0	12
Fremont (DFR)	OBS.	1	1	1	1	1	1	2	4	6	6	7	6	3	1	1	1	1	1	7
	LIRAQ	0	0	0	0	0	1	2	3	5	6	6	5	4	2	1	0	0	0	6
Richmond (DRM)	OBS.	1	1	1	1	1	1	2	3	2	2	2	1	1	1	1	1	1	0	3
	LIRAQ	0	0	0	0	0	1	2	3	4	4	3	2	1	0	0	0	0	0	4
San Rafael (DSR)	OBS.	0	0	0	1	1	2	3	3	4	4	4	2	1	1	1	1	1	1	4
	LIRAQ	0	0	0	0	0	0	1	1	2	2	2	2	1	0	0	0	0	0	2
Vallejo (DVA or DVT)	OBS.	0	0	0	0	2	3	3	3	3	4	5	5	2	0	0	0	0	0	5
	LIRAQ	0	0	0	0	0	1	1	2	2	2	1	1	0	0	0	0	0	0	2
Pittsburg (DPT)	OBS.	0	0	0	0	3	-	1	5	6	7	7	3	0	0	0	0	0	0	7
	LIRAQ	0	0	0	0	0	1	1	0	0	0	0	0	0	0	0	0	0	0	1
Concord (DCO)	OBS.	0	0	0	0	0	1	1	1	2	1	1	1	0	0	0	0	0	0	2
	LIRAQ	0	0	0	0	0	1	2	2	2	2	1	1	0	0	0	0	0	0	2
Livermore (DLI)	OBS.	0	0	0	0	0	1	2	4	5	5	5	4	2	1	0	0	0	0	5
	LIRAQ	0	0	0	0	1	2	4	6	6	6	6	5	4	3	2	1	0	0	6
11 STATION MAXIMUM	OBS.	1	1	1	1	3	3	3	5	9	10	11	8	4	3	3	3	3	2	11
	LIRAQ	0	0	0	0	1	2	4	6	8	12	11	9	5	3	2	1	0	0	12

Table 4-2
Comparison of Observed vs LIRAQ-Simulated
Hourly Averages of NO_2 (pphm), 5 November 1976 Meteorology,
1975 Emissions

STATION (MAP SYMBOL)		HOUR BEGINNING (PST) 04	05	06	07	08	09	10	11	12	13	14	15	16	17	18	19	20	21	MAX
San Francisco (DSF)	OBS.	7	8	8	8	9	14	16	15	10	14	13	11	12	11	12	11	9	10	16
	LIRAQ	5	8	11	14	19	34	37	29	27	27	26	25	23	19	16	16	16	16	37
Burlingame (DBU)	OBS.	9	10	8	9	12	10	9	18	10	--	--	21	21	15	14	14	15	12	21
	LIRAQ	4	5	6	7	7	8	11	14	16	18	21	25	30	30	29	29	29	29	30
REDWOOD CITY (DRC)	OBS.	2	2	2	2	3	8	10	12	9	10	6	8	12	15	14	13	11	9	15
	LIRAQ	5	5	6	7	7	9	10	11	11	11	12	14	18	20	19	17	17	16	20
SAN JOSE (DSJ)	OBS.	10	7	8	10	13	17	22	24	18	--	--	16	19	23	26	27	26	19	27
	LIRAQ	6	8	11	11	12	15	23	29	29	24	20	20	24	27	25	24	25	25	29
FREMONT (DFR)	OBS.	4	5	4	4	5	9	9	9	7	7	9	10	12	13	12	12	11	10	13
	LIRAQ	4	5	6	6	6	7	9	9	7	7	9	12	16	14	12	11	12	12	16
RICHMOND (DRM)	OBS.	6	6	5	6	6	6	7	8	7	6	7	8	9	9	8	8	8	8	9
	LIRAQ	3	3	4	4	5	6	8	8	9	9	10	10	9	9	6	5	5	5	10
SAN RAFAEL (DSR)	OBS.	5	6	6	8	10	7	3	4	--	3	4	8	10	9	9	8	7	6	10
	LIRAQ	3	4	6	6	7	8	11	12	13	13	14	15	16	13	11	10	10	10	16
VALLEJO (DVA or DVT)	OBS.	7	7	7	6	6	--	--	--	--	--	3	3	7	9	9	9	9	9	9
	LIRAQ	2	2	4	4	4	5	5	4	4	3	2	2	3	2	2	2	2	2	5
PITTSBURG (DPT)	OBS.	7	7	7	8	9	4	4	6	4	3	4	4	8	13	11	11	9	9	13
	LIRAQ	3	4	4	4	4	5	7	8	8	7	6	6	6	6	5	4	4	4	8
CONCORD (DCO)	OBS.	4	4	4	5	7	9	10	7	6	9	9	9	9	10	9	8	8	7	10
	LIRAQ	3	4	4	4	4	4	4	4	5	5	6	6	6	6	6	5	6	6	6
LIVERMORE (DLI)	OBS.	3	3	3	4	6	7	7	7	6	6	6	7	9	9	9	8	7	7	9
	LIRAQ	3	3	3	4	4	5	5	4	3	3	2	2	2	2	2	3	4	4	5
11 STATION MAXIMUM	OBS.	10	10	8	10	13	17	22	24	18	14	13	21	21	23	26	27	26	19	27
	LIRAQ	6	8	11	14	19	34	37	29	29	27	26	25	30	30	29	29	29	29	37

Table 4-3. Sensitivity of Bay Area O_3 maxima to HC and NO emission reductions, based on LIRAQ simulations using 1985 emissions and 5 November 1976 meteorology

Time (PST)	Ozone Concentration (ppb)			
	1985 Baseline	50% HC Reduction	25% HC & 25% NO Reduction	50% HC & 25% NO Reduction
0800	11	11	10	11
0900	24	24	23	24
1000	43	43	42	43
1100	56	56	55	56
1200	64	64	65	64
1300	72	65	71	68
1400	96	66	77	68
1500	104	63	85	65
1600	80	57	72	58
1700	54	48	56	50
1800	41	37	41	39
1900	28	26	28	28
2000	19	18	20	19
2100	13	12	14	13
2200	9	9	10	9

O3 highs developed (see Figure B-3) the results are similar except in the Livermore Valley. Table 4-4 shows that precursor controls strongly affect O3 in and near the Bay Area's major population centers. Simulated O3 in the Livermore Valley, however, was primarily determined by initial and boundary conditions and was insensitive to controls (see also Figures B-5 and B-7).

Tables 4-5 and 4-6 show equivalent analyses of NO2 sensitivity to HC and NO reductions. The results indicate that HC control is also effective for reducing NO2. Control of NO also reduces NO2, but to a much smaller degree. We also note NO2 is generally less responsive to precursor controls than is O3. The somewhat different results for the Santa Clara Valley NO2 "high" are suspect because the high center appears to have drifted out of the modeling region by 1700 PST in two of the simulations with emissions reductions (see Figures B-4, B-6 and B-8 for more details). The concentrations in the Santa Clara Valley may also have been more influenced by boundary conditions than those in the central Bay Area.

Results of Previous Simulations

The LIRAQ sensitivity runs that were performed for the 1979 Bay Area Air Quality Plan (ABAG, et al., 1979) using the 26 July 1973 prototype day yielded results for O3 and NO2 that are comparable to those reported here. Table 4-7 summarizes these results. Again, NO2 is much more sensitive to HC control than to NO control. The comparability of the NO2 sensitivity results is interesting in that the two prototype days were meteorologically quite different and the resultant NO2 concentrations and time profiles were also quite different at most locations. We also note that, except for the Livermore Valley, O3 was somewhat more sensitive to HC controls in the 5 November simulations than in the 26 July simulations.

CONCLUSIONS

1. Model performance for the 5 November 1976 "NO2 day" was excellent for O3 and, in many NO2-prone locations, adequate for NO2. Because the model is able to reproduce observed NO2 concentrations fairly well it is reasonable to select it as an instrument for evaluating the sensitivity of NO2 to precursor emissions.*

*Nevertheless, NO2 performance was only a secondary consideration in the development of LIRAQ's photochemical reaction set. Thus further investigation of the model's ability to simulate NO2 response to emissions (where smog results would provide the basis for comparison) would be desirable.

Table 4-4. Ozone Sensitivity to Emission Reduction Strategies* in Selected Bay Area Subregions, 1500 PST, 5 November 1976 Meteorology

a) Maximum O3 Concentration (ppb)

Bay Area Subregion	1975 Baseline	1985 Baseline	Strategy 1	Strategy 2	Strategy 3
San Francisco	126 pbb	83.6 ppb	14.9 ppb	69.2 ppb	26.9 ppb
Santa Clara Vl.	135 pbb	104.3 ppb	21.0 ppb	85.0 ppb	37.8 ppb
Livermore Valley	70.5 ppb	68.6 ppb	62.9 ppb	67.4 ppb	64.8 ppb

b) Percent O3 Change From 1985 Baseline

Bay Area Subregion	Strategy 1	Strategy 2	Strategy 3
San Francisco Bay	-82%	-17%	-68%
Santa Clara Valley	-80%	-19%	-64%
Livermore Valley	- 8%	- 2%	- 6%

*Strategy 1: 50% reduction in hydrocarbon emissions
Strategy 2: 25% reduction in hydrocarbon emissions and 25% reduction in NO emissions
Strategy 3: 50% reduction in hydrocarbon emissions and 25% reduction in NO emissions

Table 4-5. Sensitivity of Bay Area NO_2 maxima to HC and NO emission reduction strategies*, based on LIRAQ simulations using 1985 emissions and 5 November 1976 meteorology

Hour (PST)	NO_2 Concentration (ppb)			
	1985 Baseline	Strategy 1	Strategy 2	Strategy 3
0400	48	48	48	48
0500	68	70	66	66
0600	93	94	81	81
0700	154	155	125	125
0800	175	174	140	140
0900	220	186	170	149
1000	371	221	278	199
1100	287	183	218	165
1200	272	182	221	178
1300	280	204	230	198
1400	268	219	211	205
1500	280	220	216	200
1600	322	220	249	200
1700	311	220	247	220
1800	299	200	236	220
1900	287	200	228	200
2000	276	200	240	200
2100	294	205	240	180
2200	297	210	243	200

*Strategy 1: 25% reduction in hydrocarbon emissions
Strategy 2: 25% reduction in hydrocarbon emissions and 25% reduction in NO emissions
Strategy 3: 50% reduction in hydrocarbon emissions and 25% reduction in NO emissions

Table 4-6. NO2 Sensitivity to Emission Reduction Strategies* in Selected Bay Area Subregions, 1700 PST, 5 November 1976 Meteorology

a) Maximum NO2 Concentration

Bay Area Subregion	1975 Baseline	1985 Baseline	Strategy 1	Strategy 2	Strategy 3
S. F. Peninsula	397 pbb	311 ppb	190 ppb	247 ppb	181 ppb
Oakland/East Bay	318 pbb	282 ppb	173 ppb	225 ppb	173 ppb
Santa Clara Vl.	359 ppb	303 ppb	230 ppb	246 ppb	230 ppb

b) Percent NO2 Change From 1985 Baseline

Bay Area Subregion	Strategy 1	Strategy 2	Strategy 3
S. F. Peninsula	-39%	-21%	-42%
Santa Clara Valley	-39%	-20%	-39%
Livermore Valley	-24%	-19%	-24%

*Strategy 1: 25% reduction in hydrocarbon emissions
Strategy 2: 25% reduction in hydrocarbon emissions and 25% reduction in NO emissions
Strategy 3: 50% reduction in hydrocarbon emissions and 25% reduction in NO emissions

Table 4-7. Effect of NO and HC emission reductions on Bay Area O_3 and NO_2 maxima (based on LIRAQ simulations using 26 July 1973 meteorology and 1985 emissions projections*)

Emission Changes		Resultant Concentration Changes	
% HC Reduction	% NO Reduction	% O_3 Change	% NO_2 Change
0	40	+33	-14
40	0	-55	-30
40	20	-36	-35
80	0	-80	-55
80	40	-70	-60

Source: Waterland, et al., 1978.

* Here, an earlier 1985 baseline inventory was used that included regionwide emissions of 782 tons/day of HC and 725 tons/day of NO_x (as NO_2). Elsewhere in this chapter a revised 1985 baseline inventory, with 835 tons/day HC and 721 tons/day NO_x was used. The change resulted from a revision in the EPA emission factors for mobile sources.

2. Based on Bay Area LIRAQ simulations using projected 1985 emissions, we conclude that:

   a) HC controls are effective for both O3 and NO2;

   b) NO controls increase O3 levels and produce relatively small reductions in NO2; and

   c) NO2 is less sensitive to controls than O3.

REFERENCES

1. Association of Bay Area Governments, Bay Area Air Quality Management District, and Metropolitan Transportation Commission, "1979 Bay Area Air Quality Plan," January 1979.

2. De Mandel, R. E., L. H. Robinson, J. S. L. Fong and R. Y. Wada, "Comparisons of EPA Rollback, Empirical/Kinetic, and Physicochemical Oxidant Relationships in the San Francisco Bay Area," J. Air Pollution Control Assoc., 29, pp. 352-358, April 1979.

3. Duewer, W. H., M. C. MacCracken and J. J. Walton, "The Livermore Regional Air Quality Model: II. Verification and Sample Application in the San Francisco Bay Area," J. Appl. Meteor., 17, pp. 273-311, March 1978.

4. Waterland, L. R., K. J. Lim, K. G. Salvesen, R. M. Evans, E. B. Higginbotham and H. B. Mason, "Environmental Assessment of Stationary Source NOx Control Technologies--Second Annual Report," Accurex Corporation Report TR-78-116, July 1978.

5. MODELING THE DOWNWIND EFFECTS OF CHANGING BAY AREA HC AND NOx EMISSIONS

PURPOSE

The LIRAQ photochemical simulations used in the development of the 1979 Bay Area Air Quality Plan (Association of Bay Area Governments, et al., 1979) indicated that local NOx reductions might actually increase Bay Area ozone concentrations. An inverse relationship between ozone and NOx is possible in regions with low HC - NOx ratios. Before making a final judgment on the desirability of NOx controls, however, it is advisable to evaluate the effects of local emission changes on downwind air basins.

The work described in this section was designed to:

1) Expand the LIRAQ modeling region such that transport can be simulated from the Bay Area to the north and east as far as Stockton and Sacramento.

2) Evaluate model performance in the expanded modeling region under the contrasting meteorological conditions of 26 July 1973 and 20 August 1973.

3) Assess the sensitivity of ozone in the Central Valley (i.e., the Sacramento and San Joaquin Valleys) to Bay Area emissions under the restrictive meteorological conditions of 26 July 1973. (This was the prototype day used in the development of the 1979 Bay Area Air Quality Plan.)

METHODOLOGY

The Modeling Region

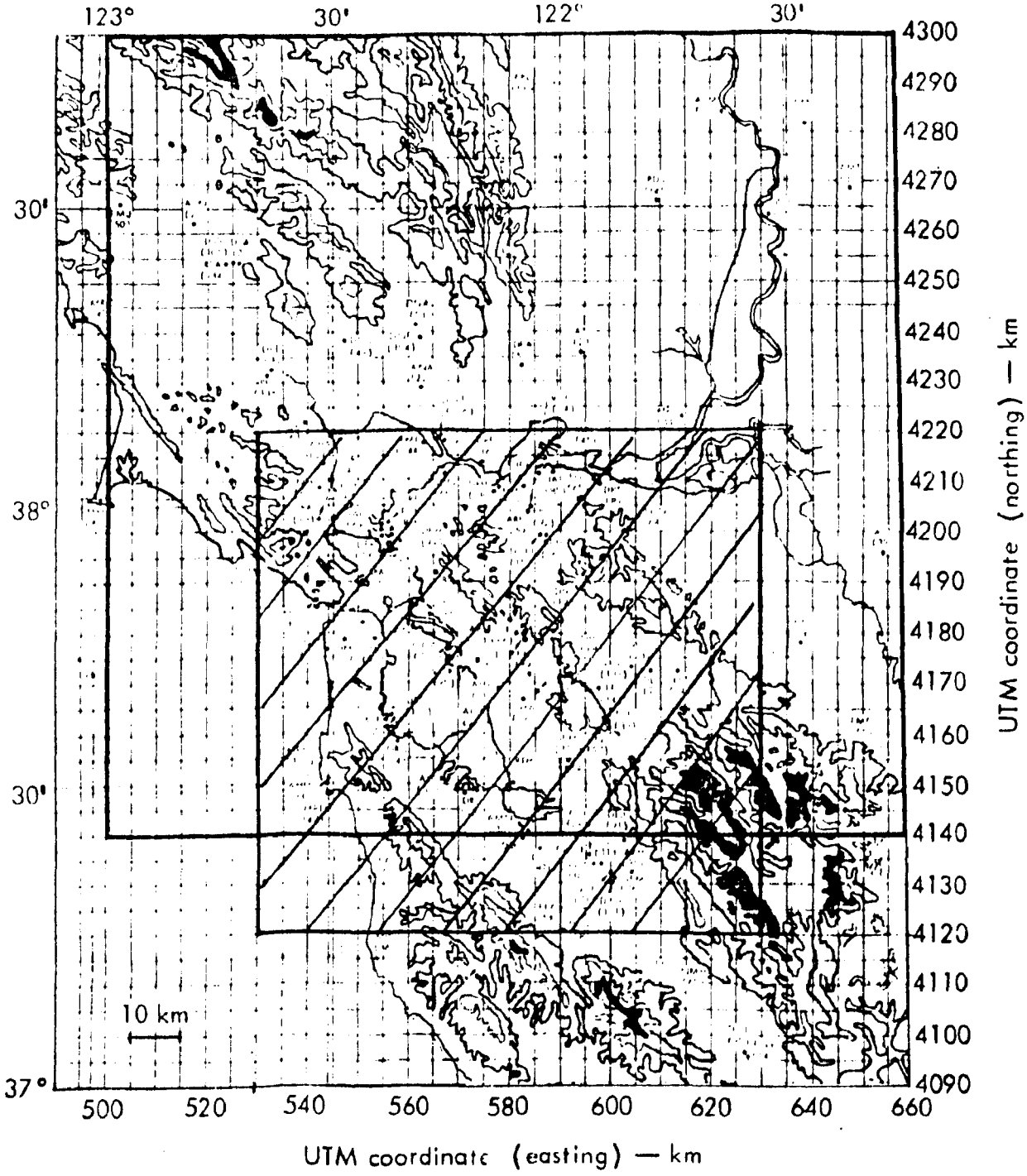
In order to simulate transport from the Bay Area to the Central Valley the LIRAQ modeling region was expanded to a 160 x 160 km area that included the central Bay Area "source" region and Sacramento and Stockton as potential receptor locations. Because of computer limitations the LIRAQ-2 photochemical model is currently limited to 400 grid cells. Therefore it was necessary to increase the grid cell size from the 5 x 5 km used in previous work to 8 x 8 km. The old 100 x 100 km region and the new 160 x 160 km region are shown in Figure 5-1.

Meteorological Input Fields

It was also necessary to modify the inputs to the MASCON preprocessor for the two prototype days that were simulated. The MASCON code calculates mass-consistent gridded fields of mass flux and inversion base height. It also generates solar flux fields interpolated from a limited number of pyranometer measurements made at BAAQMD stations.

Figure 5-1. Enlarged 160 x 160 km Long-Range Transport Study Area and 100 x 100 km Region Used in Previous Bay Area LIRAQ Simulations.

(The 8-km cells used in the enlarged study area are not shown.)



Legend:

Enlarged 160 x 160 km Study Area.

100 x 100 km Region where most previous LIRAQ runs were made.

Unexpected, time-consuming problems associated with the generation of 8 x 8 km MASCON files on the Lawrence Berkeley Laboratories (LBL) computer forced postponement of the long range transport simulations until late in the contract period.

Emissions Inventory

Gridded emission inputs for all previous Bay Area LIRAQ simulations were limited to the nine county jurisdictional area of the BAAQMD. The expanded modeling region includes a large area outside of this jurisdiction. In order to generate gridded emissions for the exogenous region, county totals (in tons/day) for the five major pollutants (particulates, HC, NOx, SO2 and CO) were obtained from the California Air Resources Board (CARB) (Bradley, 1979). County source inventories, provided for both 1975 and 1985, are shown in Table 5-1.

Because of contractual time constraints and limited data availability a simplified method was used for spatial distribution of emissions. First, undevelopable land areas (e.g., mountain ridges, marshland, bays) were identified from U.S. Geological Survey maps. Next, county population totals were distributed over the developable land. Population projections for 1985 were obtained from the California Department of Finance (DOF, 1978). The emissions were distributed into 1 x 1 km grid cells based on population. Finally, the 1 x 1 km gridded emissions were aggregated into 8 x 8 km cells. As an illustration of the resultant emissions pattern, Figure 5-2 shows the 24-hour distribution of nitric oxide emission rates for 1975.

The temporal distribution of emissions was based primarily upon data supplied by Systems Applications, Incorporated (SAI). In 1978 SAI prepared hourly emission estimates, from 0500 to 1800 PST, of both stationary and mobile sources in the Sacramento area (Reid, 1979). BAAQMD personnel used this and other information to develop the profiles of hourly variations in mobile, stationary-source and total emissions shown in Figure 5-3. The temporal distribution of emissions within the Bay Area was the same as that used in previous simulations. A detailed discussion of the preparation of gridded emissions in the Bay Area is presented by Perardi, et al., 1979.

Initial and Boundary Conditions

As a result of expanding the modeling region, it was necessary to modify the background pollutant concentrations specified along the southern and eastern boundaries for the 26 July 1973 prototype day. These values are important because:

1) there was inflow along portions of these boundaries for part of the simulation period,

2) inflow along the northern half of the eastern boundary directly affects pollutant concentrations in the regions of greatest interest (Sacramento/Stockton), and

Table 5-1. Source Inventory Totals for the Sacramento/San Joaquin Valley Area Used in LIRAQ Transport Studies

a) 1975

Area \ Pollutant	Emissions in Tons/Day				
	Part.	HC	NO_x	SO_2	CO
Sacramento County	33.9	132.0	76.6	5.6	567.0
San Joaquin County[1]	40.5	57.8	34.6	10.2	210.0
Solano County[2]	9.4	7.6	6.3	.4	35.3
Yolo County	27.8	23.0	15.1	2.1	104.0
Total	111.6	220.4	132.6	18.3	916.3
Bay Area AQMD	133.6	748.0	567.0	654.6	1,842.5
Grand Total	245.2	968.4	699.6	672.9	2,758.8

b) 1985

Area \ Pollutant	Emissions in Tons/Day				
	Part.	HC	NO_x	SO_2	CO
Sacramento County	36.8	92.9	70.5	6.5	205.6
San Joaquin County[1]	48.7	45.3	34.9	15.4	134.0
Solano County[2]	11.0	5.6	6.5	.4	24.0
Yolo County	31.9	19.0	16.0	2.7	79.4
Total	128.4	162.8	127.9	25.0	566.4
Bay Area AQMD	147.8	557.6	455.0	647.9	2,192.4
Grand Total	276.2	720.4	582.9	672.9	2,758.8

[1] 80% of total county emissions (20% are estimated to be outside of the study area).

[2] Emissions only from the portion of the county outside of the BAAQMD.

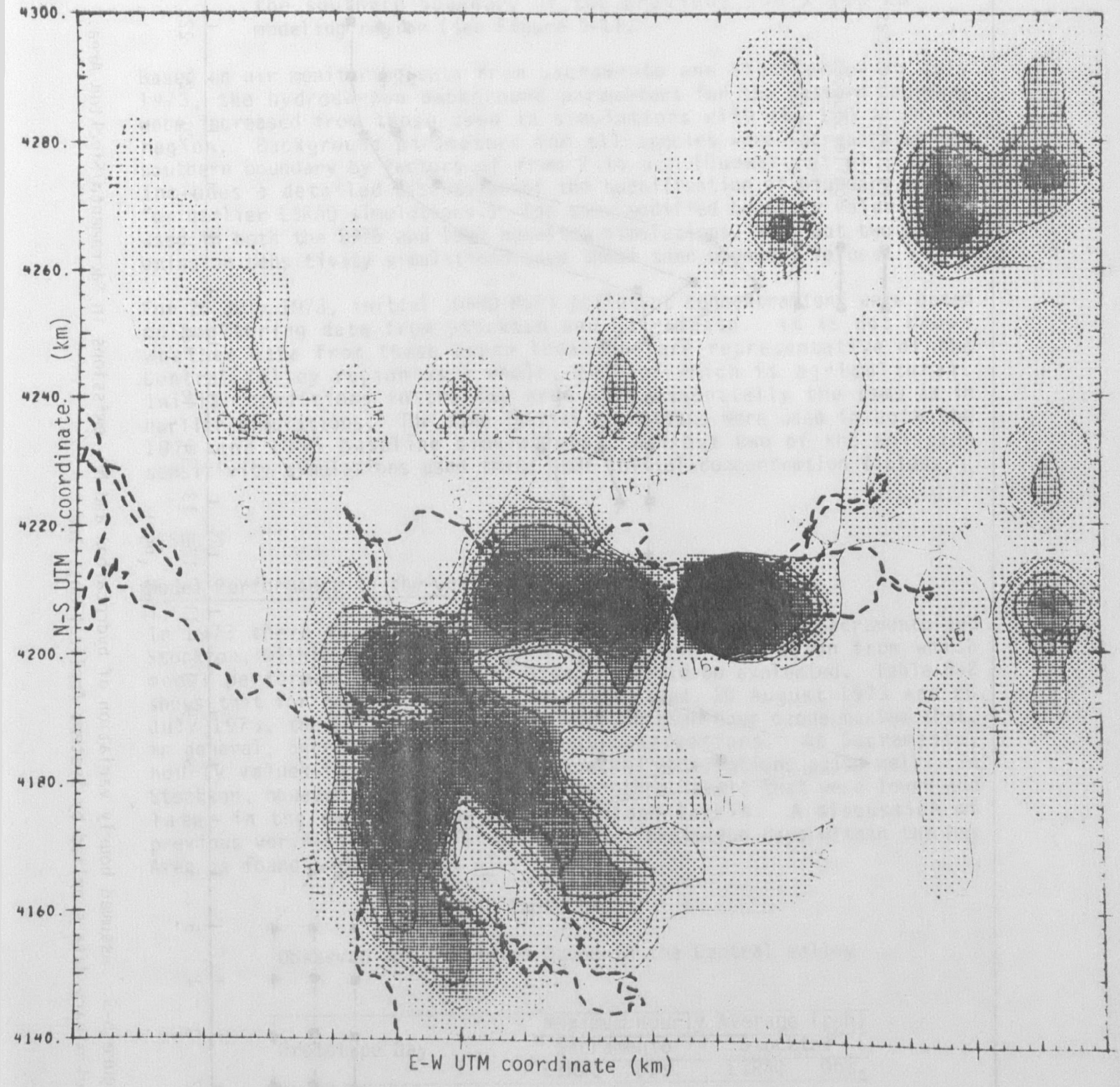


Figure 5-2. Spatial distribution of 24-hour mean emission rates for Nitric Oxide, 1975 emissions inventory (units: grams per second per grid square, and each grid square is 64 km^2).

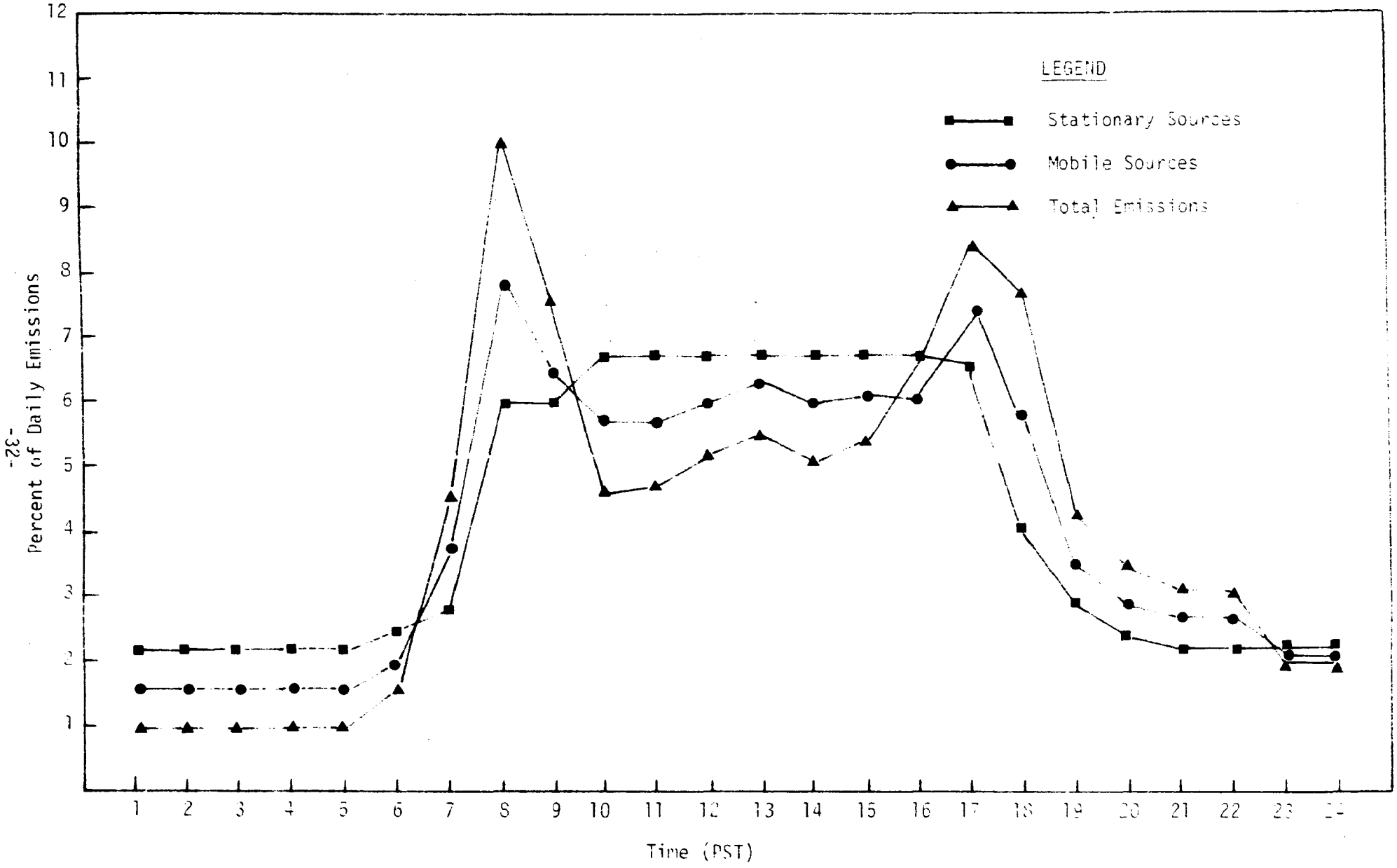


Figure 5-3. Assumed hourly variation of hydrocarbon and NO_x emissions in Sacramento/Stockton Area. Source: Preliminary data supplied by Systems Applications, Inc.

3) the expanded region excludes the heavily populated Santa Clara Valley to the south, and inflow from this region contains higher pollutant concentrations than flow into the southern boundary of the previous 100 x 100 km modeling region (see Figure 5-1).

Based on air monitoring data from Sacramento and Stockton on 26 July 1973, the hydrocarbon background parameters for the eastern boundary were increased from those used in simulations with the 100 x 100 km region. Background parameters for all species were increased at the southern boundary by factors of from 2 to 6. (Duewer, et al., 1978, includes a detailed discussion of the specification of boundary values for earlier LIRAQ simulations.) The same modified boundary values were used in both the 1975 and 1985 baseline simulations. All but two of the emission sensitivity simulations used these same boundary values.

For 26 July 1973, initial (0600 PST) pollutant concentrations were based on monitoring data from Stockton and Sacramento. It is not known whether data from these urban locations are representative of the Central Valley region as a whole, much of which is agricultural. Initial conditions in the Bay Area were essentially the same as in earlier simulations. The same initial conditions were used in both the 1975 and 1985 baseline simulations. All but two of the emission sensitivity simulations used these same initial concentration fields.

RESULTS

Model Performance in the Central Valley

In 1973 there were just two ozone monitoring sites, in Sacramento and Stockton, within the expanded 160 x 160 km modeling region from which model performance in the Central Valley could be evaluated. Table 5-2 shows that for the two prototype days simulated, 20 August 1973 and 26 July 1973, the 1975 baseline runs produced high-hour ozone maxima that, in general, agreed reasonably well with observations. At Sacramento, hourly values for the 26 July 1973 tracked observations quite well. In Stockton, however, LIRAQ predicted peak ozone levels that were lower and later in the day than the observed ozone levels. A discussion of previous verification studies of these two prototype days within the Bay Area is found in Duewer, et al., 1978.

Table 5-2

Observed vs. Predicted Ozone in the Central Valley

Prototype Day	Maximum Hourly Average (ppb)			
	Sacramento		Stockton	
	LIRAQ	Obs.	LIRAQ	Obs.
26 July 1973	110	120	110	150
20 August 1973	70	90	90	80

Comparability of 5 x 5 km and 8 x 8 km Baseline Simulations

In order to determine the degree to which simulations with the enlarged region and 8 km cells agree with earlier local simulations with 5-km cells, LIRAQ runs with both grids were compared for two prototype days. Generally the region common to both grids displayed similar, but not identical, ozone concentration fields. This can be seen by comparing Figures 5-4 and 5-5, which depict 1300 PST ozone contours from simulations with the standard and expanded modeling regions, respectively, on the relatively well-ventilated 20 August 1973 prototype day. Similarly, Figures 5-6 and 5-7 provide a comparison for the more stagnant and polluted conditions of 26 July 1973. Differences between these two fields are on the order of 10 percent, and are probably due to both the change in grid size and to the modified boundary conditions that were needed for this prototype day. Similar differences were found between the 5 x 5 km and 10 x 10 km simulations discussed in Section 3.

Sensitivity of Central Valley Ozone to Bay Area Emissions

A series of simulations was performed using the expanded modeling region in an attempt to assess the sensitivity of Central Valley ozone to changes in Bay Area precursor emissions. The baseline simulation represented a 1985 control strategy scenario with large reductions in Bay Area hydrocarbon emissions. Initial and boundary conditions were the same as those used in the 1975 baseline simulations.

Figures 5-8 and 5-9 show sample output from the 1985 baseline simulation and from a simulated reduction of Bay Area hydrocarbon emissions by 60% from the baseline levels. The two ozone fields differ only slightly over the Bay Area in that neither the pattern nor the location of the 'fingerprint' changed, and the peak ozone value (0.06) shifted to the northwest but did not significantly change in magnitude. The two ozone fields are nearly identical in the Central Valley. The same can be said for the 1975 and 1985 baseline simulations (see Figures 5-7 and 5-8) and for several other simulations in which precursor emissions were changed significantly. Clearly the effects of boundary and/or initial conditions overwhelm the effects of Bay Area emissions in this series of simulations.

Two additional runs were made in which emissions were reduced throughout the modeling region and in which proportionate reductions were made in initial and boundary values. Sample output from each run, one representing a 43% hydrocarbon and 20% NOx reduction from the 1985 base case and the other representing a 60% hydrocarbon-only reduction, are shown in Figures 5-10 and 5-11. Ozone concentrations were significantly different in those runs, but it is difficult to assess the relative impacts of reduction in emissions, initial conditions and boundary conditions.

SUMMARY AND CONCLUSIONS

The completion of an operational version of LIRAQ-2 for the 160 x 160 km expanded modeling region, complete with 1975 and 1985 emissions

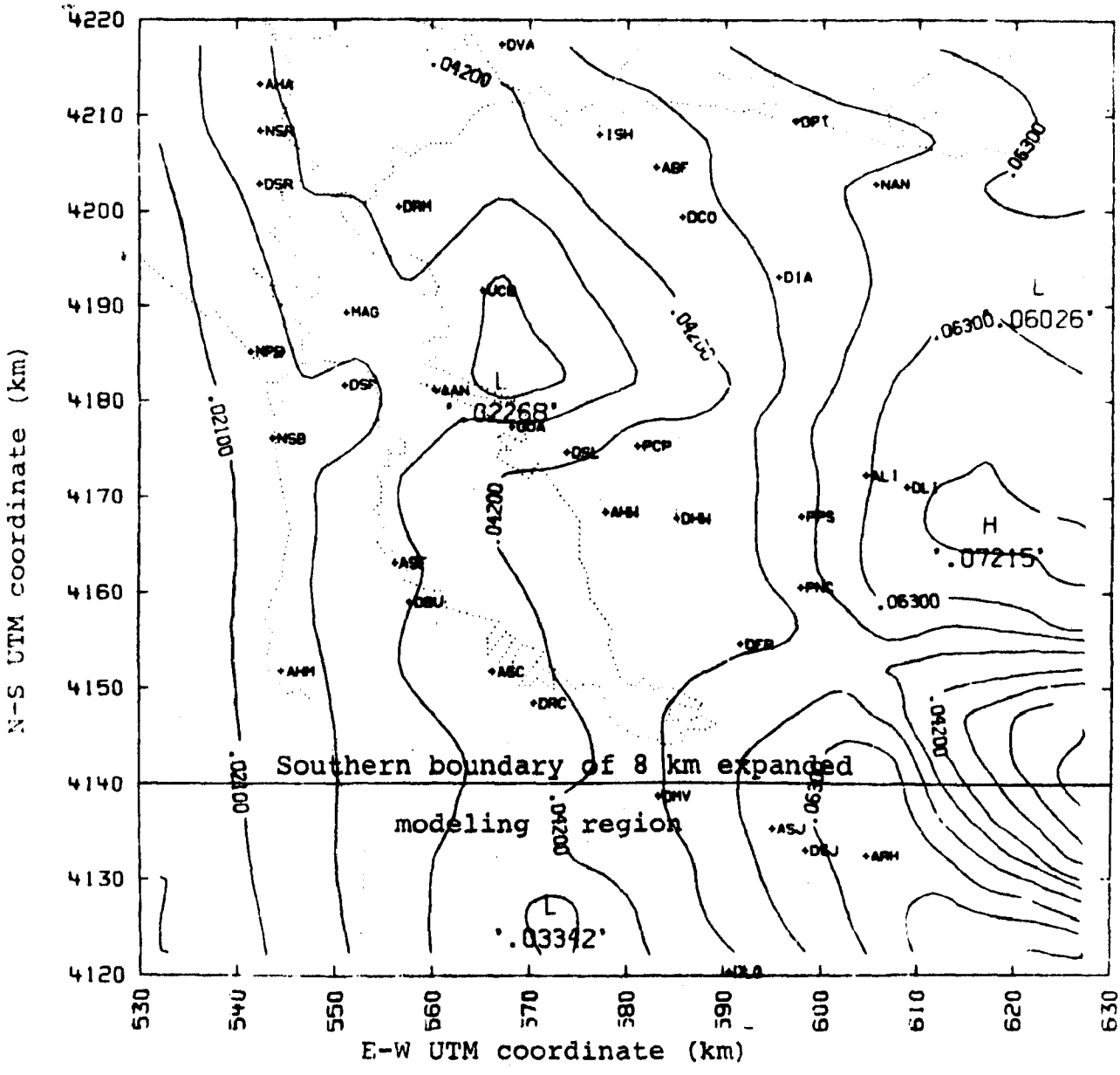


Figure 5-4. 1300 PST surface ozone concentration field, 20 August 1973 meteorology, 1975 emissions, standard gridded region with 5 x 5 km grid cells.

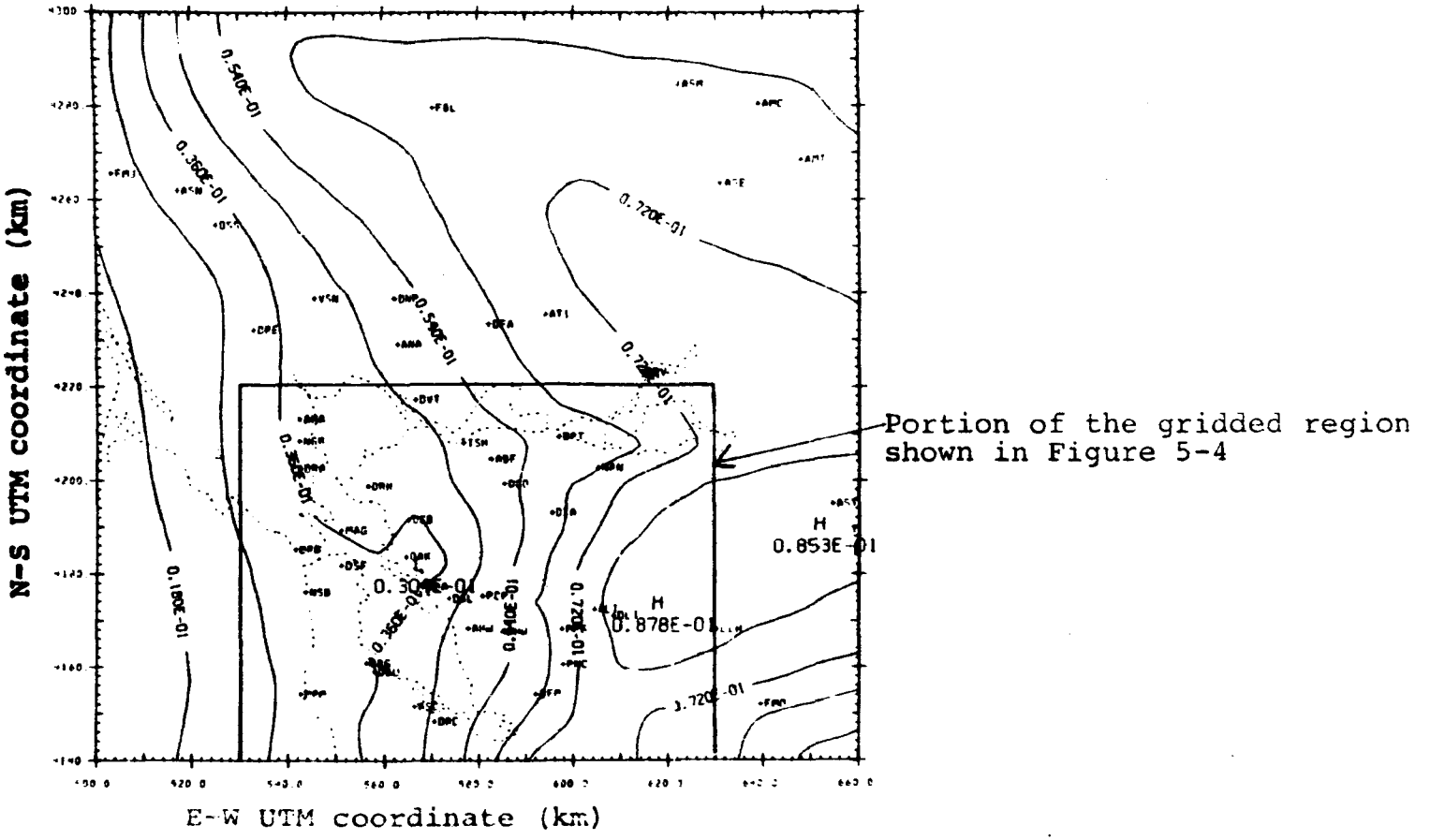


Figure 5-5. 1300 PST surface ozone concentration field, 20 August 1973 meteorology, 1975 emissions, with the expanded 8 x 8 km gridded region.

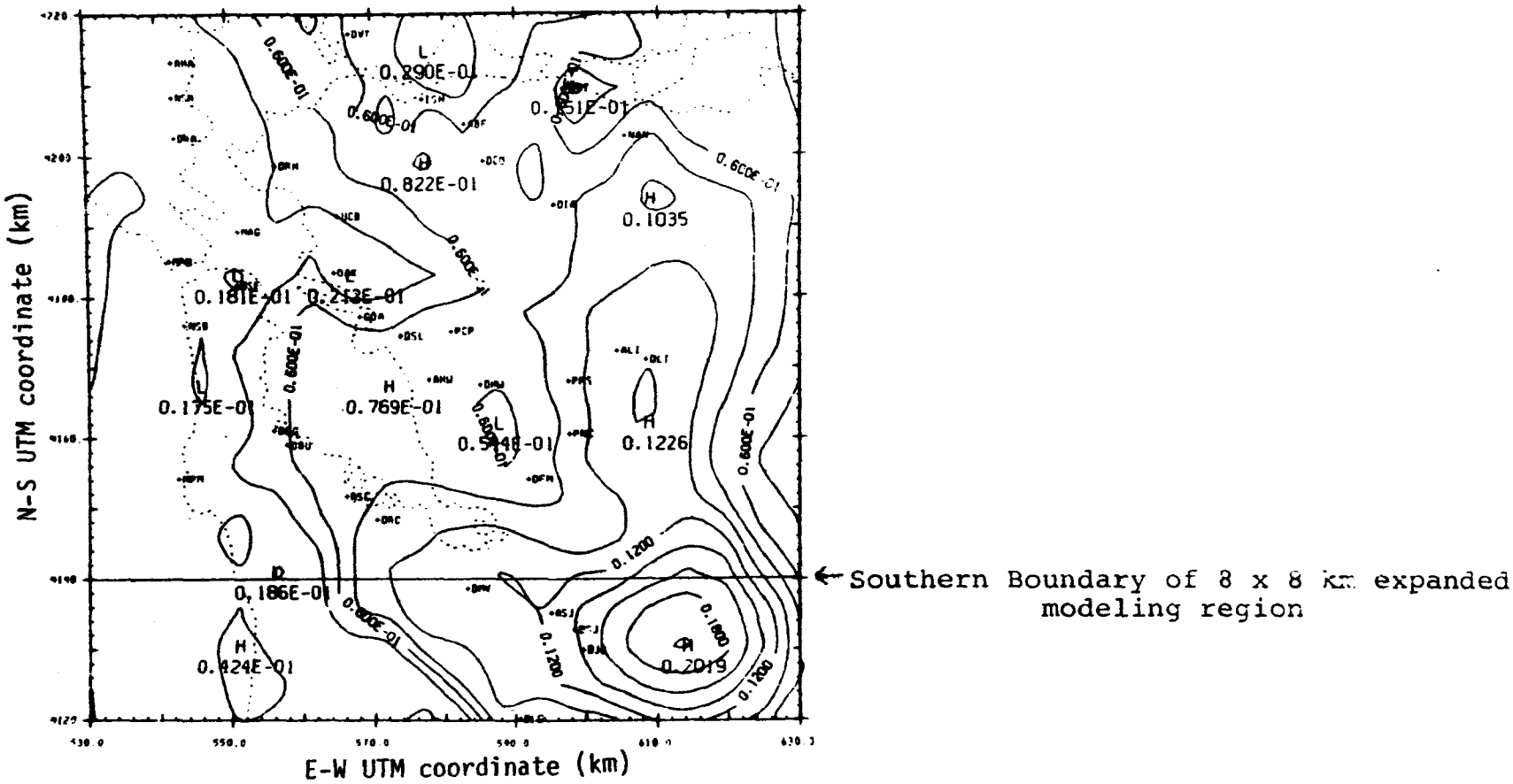


Figure 5-6. 1300 PST surface ozone concentration field, 26 July 1973 meteorology, 1975 emissions, standard gridded region with 5 x 5 km grid cells.

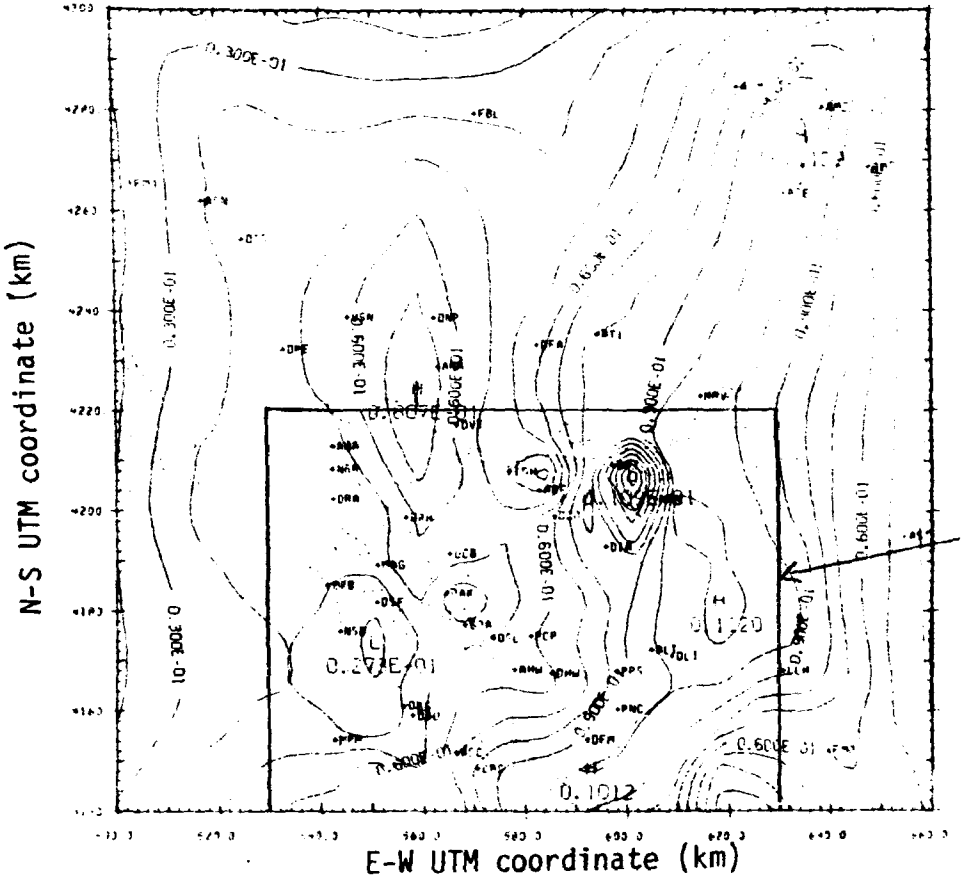


Figure 5-7. 1300 PST surface ozone concentration field, 26 July 1973 meteorology, 1975 emissions, with the expanded modeling region of 8 x 8 km cells. (The 'fingerprint' ozone low near Pittsburg is associated with the quenching effects of large NO_x emissions from nearby power plants.)

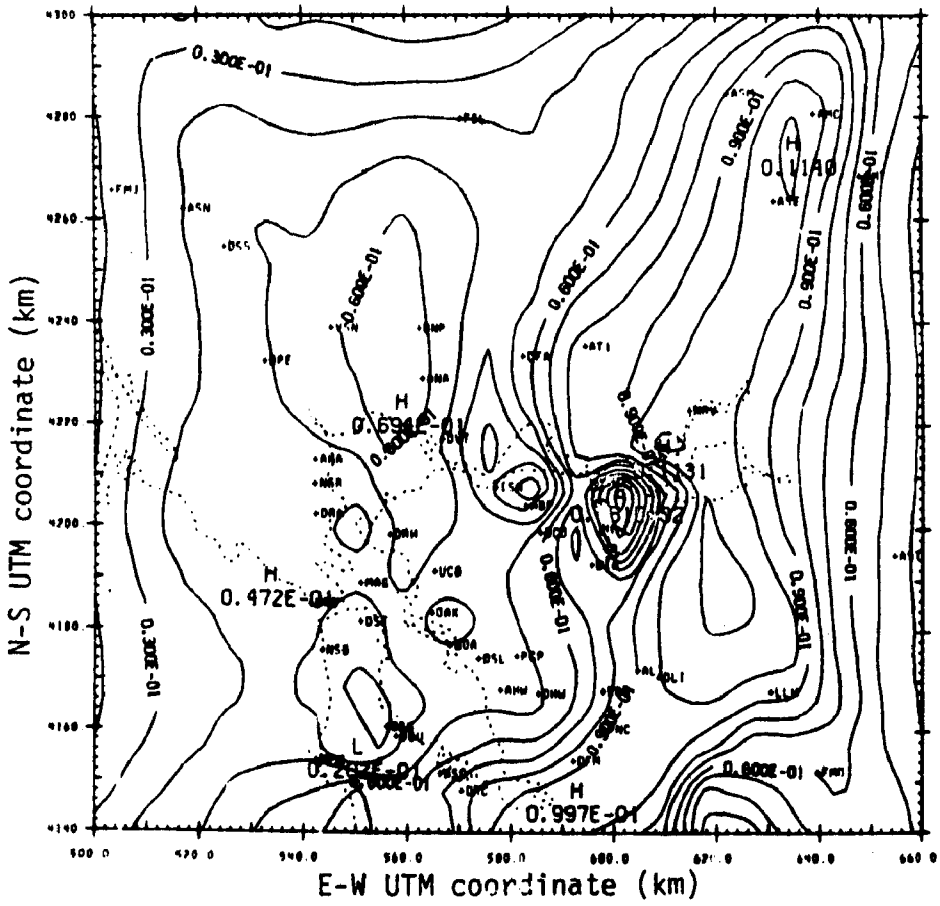


Figure 5-8. 1300 PST surface ozone concentration field, 26 July 1973 meteorology, 1985 baseline emissions.

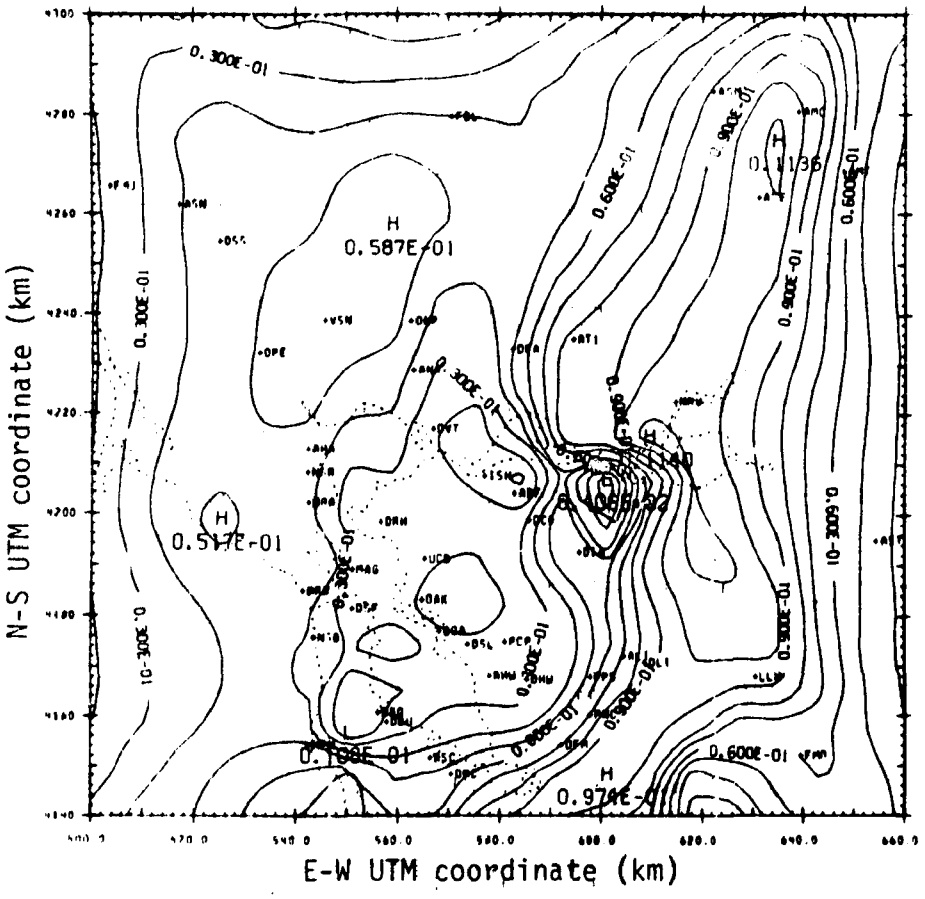


Figure 5-9. 1300 PST surface ozone concentration field, 26 July 1973 meteorology, 60% HC reduction from 1985 baseline (Bay Area only).

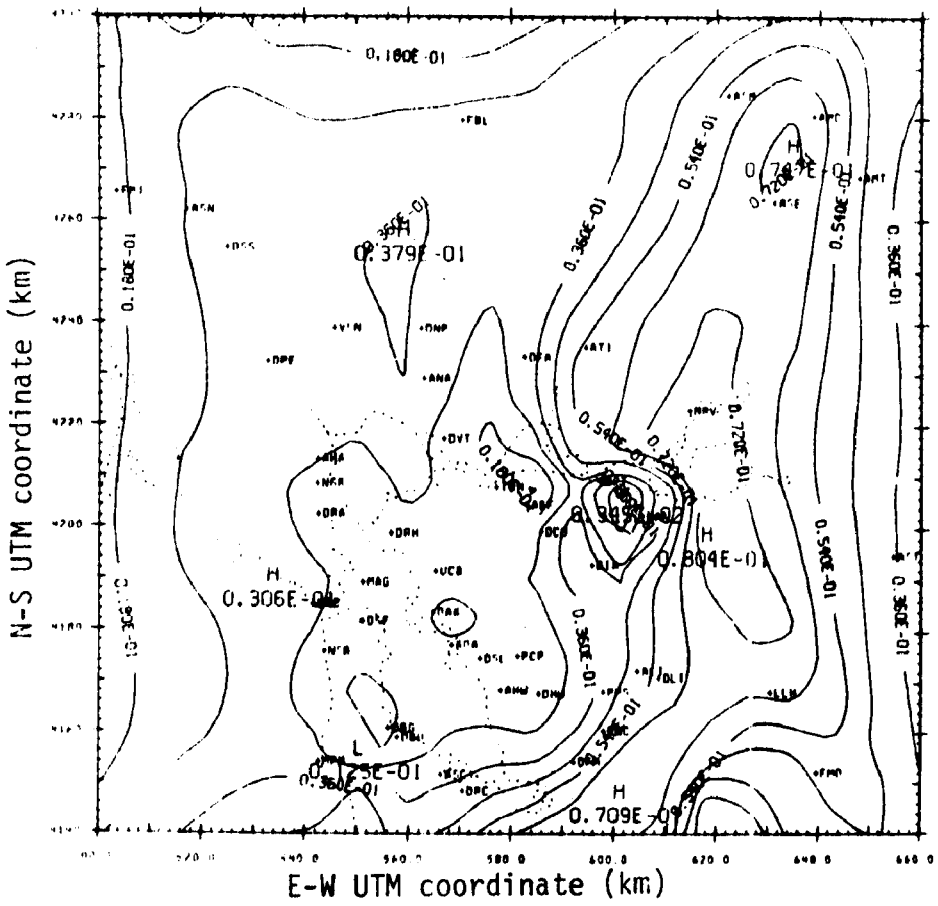


Figure 5-10. 1300 PST surface ozone concentration field, 26 July 1973 meteorology, 43% hydrocarbon and 20% NO reduction from all 1985 baseline emissions, boundary values and initial conditions.

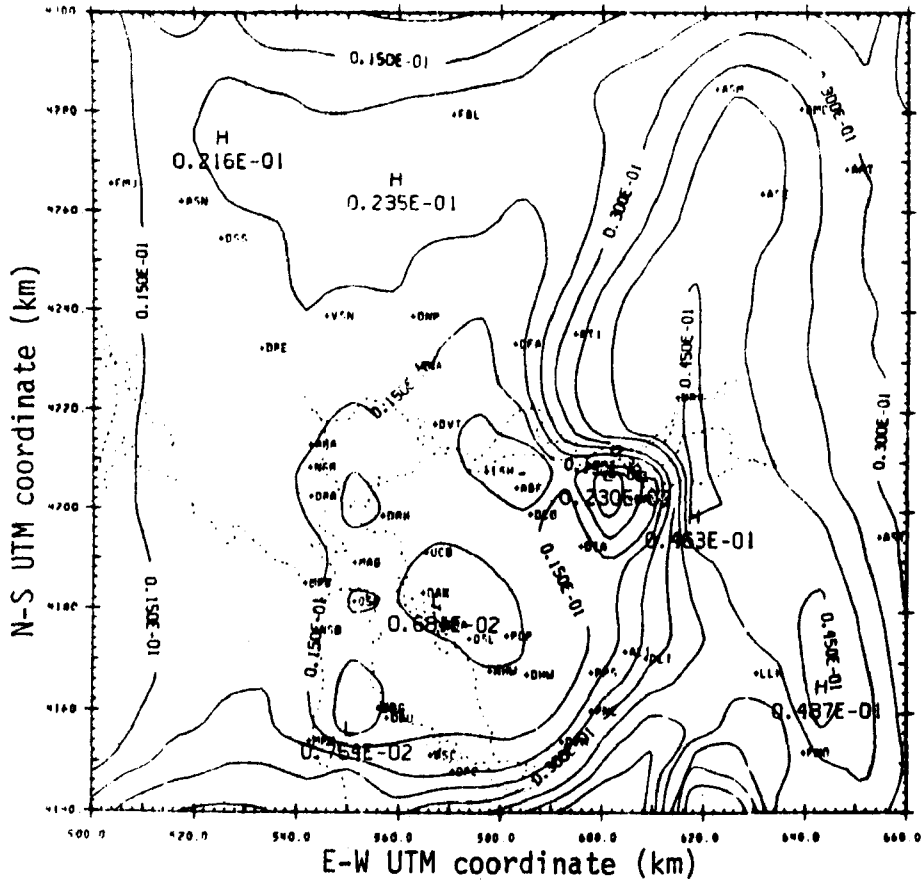


Figure 5-11. 1300 PST surface ozone concentrations, 26 July 1973 meteorology, 60% hydrocarbon reduction from all 1985 baseline emissions, boundary values and initial conditions.

inventories for adjacent areas north and east of the Bay Area, represents an important addition to our photochemical modeling capabilities. Unfortunately the simulations to date did not provide a definitive assessment of the downwind impact of Bay Area precursor emission changes. Valuable modeling information was gained however, and is summarized as follows:

1. Central Valley ozone concentrations resulting from simulations using 1975 emissions and two 1973 prototype days were reasonably close to observed levels on those days.

2. Model performance does not appear to have changed greatly as a result of the coarser (8-km) grid and revised boundaries of the enlarged 160 x 160 km modeling region. This was determined by comparing parallel simulations (same emissions, same meteorology) using the 100 x 100 km and 160 x 160 km modeling regions. In the subregion common to both regions ozone fields were generally similar for each of two prototype days. Significant differences did occur locally near parts of the southern boundary of the enlarged modeling region and near the large NOx sources in the Pittsburg area.

3. Initial and boundary conditions dominated some of the 1985 simulations to the extent that Central Valley ozone was unaffected by large percentage changes in Bay Area HC and NOx emissions under 26 July 1973 meteorological conditions. Inflow along the eastern boundary may have produced a significant boundary influence in the Sacramento area. The fact that simulations with large differences in emissions and fixed initial and boundary conditions produced similar ozone values throughout the modeling region suggests that initial conditions (or perhaps conditions at the upper boundary) dominated the production of ozone.

4. The accuracy of the boundary and initial-condition values used in the simulations is not known. The values are reasonable in that they are based on observations (albeit sparse) taken on 26 July 1973. The simulations using 1975 emissions produced reasonable results and thus there is no obvious evidence of large errors.

5. For the 1985 simulations initial and boundary values of some pollutants should be reduced because anthropogenic emissions will be lower than they were in 1973. It is not necessarily true, however, that the reductions should be proportional to reductions in the emissions inventories. It is quite possible that, as controls become more and more effective in the future, an increasingly significant fraction of ambient

concentrations of some pollutants will be due to natural or other sources that are not accounted for in current or projected emission inventories.

6. It will be necessary to conduct further studies before we can assess adequately the downwind effects of Bay Area emissions.

RECOMMENDATIONS

The authors believe that LIRAQ, now operational over an extended modeling region, can be an effective tool for evaluating the effects of transport from the Bay Area. Such an evaluation could best be accomplished by a program of study that includes the following elements:

1. Past meteorological records should be surveyed to find those meteorological prototype days having the greatest potential for Bay Area/Central Valley interaction. One would hope to find days on which there were high O3 levels in the Valley and general west-to-east flow over the modeling region. It is expected that the day(s) selected would be less influenced by inflow along the eastern boundary than was 26 July 1973. It may be desirable to conduct a multi-day simulation. The Bay Area's impact downwind is likely to be greatest on the day after peak ozone levels in the Bay Area when the onshore pressure gradient intensifies enough to induce transport of air into the Central Valley.

2. For future simulations it will be important to make initial and boundary values as accurate as possible. It is hoped that improved estimates will be possible as a result of extensive Central Valley field studies conducted by Pacific Gas and Electric Company in the summer of 1979.

3. Finally, for any given prototype day, systematic tests should be conducted of model sensitivity to varying emissions, boundary conditions and initial conditions.

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2. Bradley, Richard, California Air Resources Board, private communication, 1979.

3. California Department of Finance, "1978 Population Estimates of California Cities and Counties," Report 78 E-1, Sacramento, May 1978.

4. Duewer, W. H., M. C. MacCracken and J. J. Walton, "The Livermore Regional Air Quality Model: II. Verification and Sample Application in the San Francisco Bay Area," J. Appl. Meteor., 17, pp. 273-311, 1978.

5. MacCracken, M. C. and G. D. Sauter, editors, "Development of an Air Pollution Model for the San Francisco Bay Area," Final Report, Lawrence Livermore Laboratory Rep. UCRL-51920.

6. Perardi, T. E., M. Y. Kim, E. Y. Leong and R. Y. Wada, "Preparation and Use of Spatially and Temporally Resolved Emission Inventories in the San Francisco Bay Region," J. Air Poll. Control Assoc., 29, pp. 358-364, 1979.

7. Reid, L. E., private communication, Systems Applications, Incorporated, San Rafael, CA, 1979.

APPENDIX A

Ozone, Hydrocarbon and Nitric Oxide Concentration Maps
for Different Source Inventory Distribution Patterns

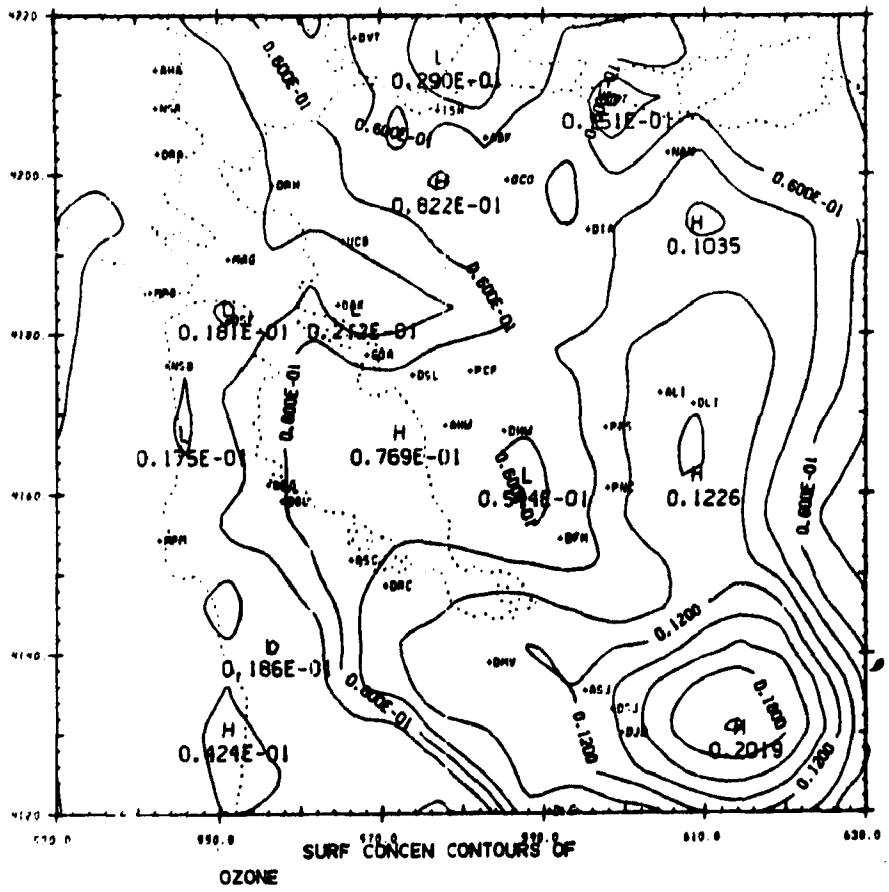


Figure A-1. 1300 PST surface ozone (ppm), 1975 5 x 5 km emission pattern.

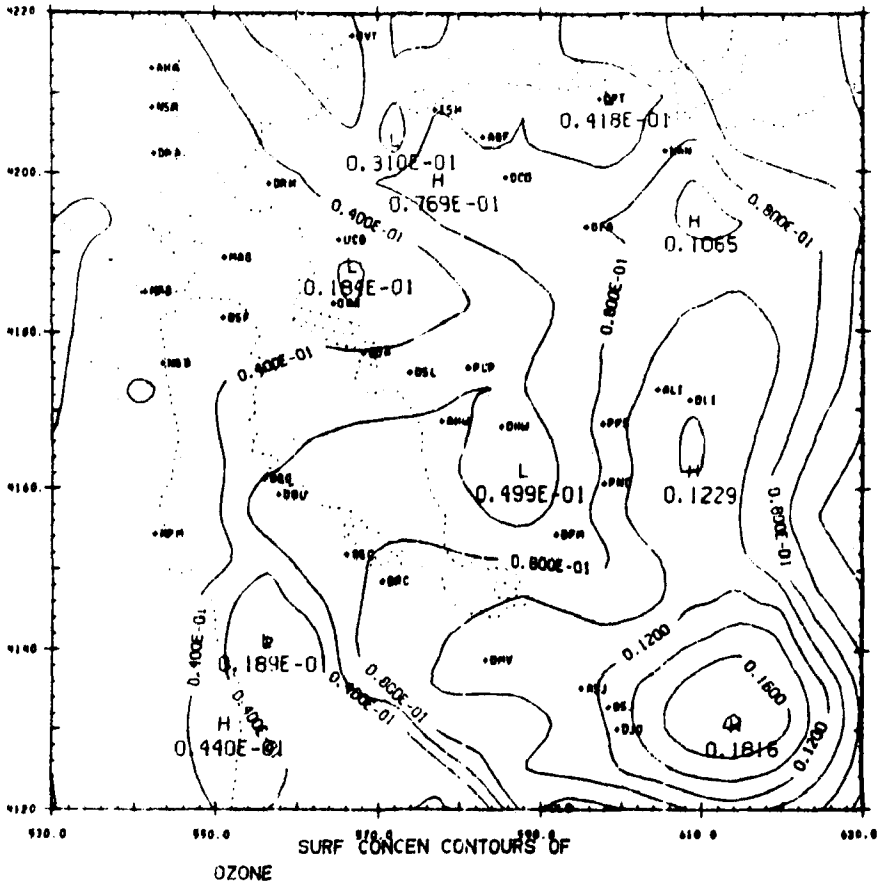


Figure A-2. 1300 PST surface ozone (ppm), 1975 10 x 10 km emission pattern.

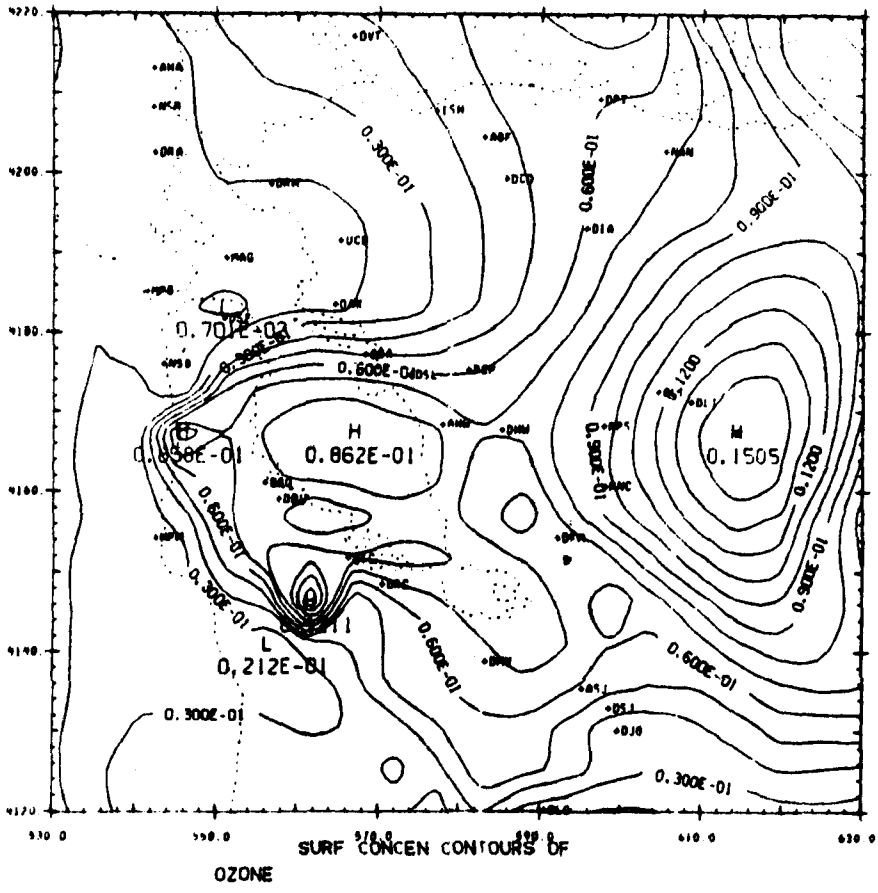


Figure A-3. 1600 PST surface ozone (ppm), 1975 pop. emission pattern.

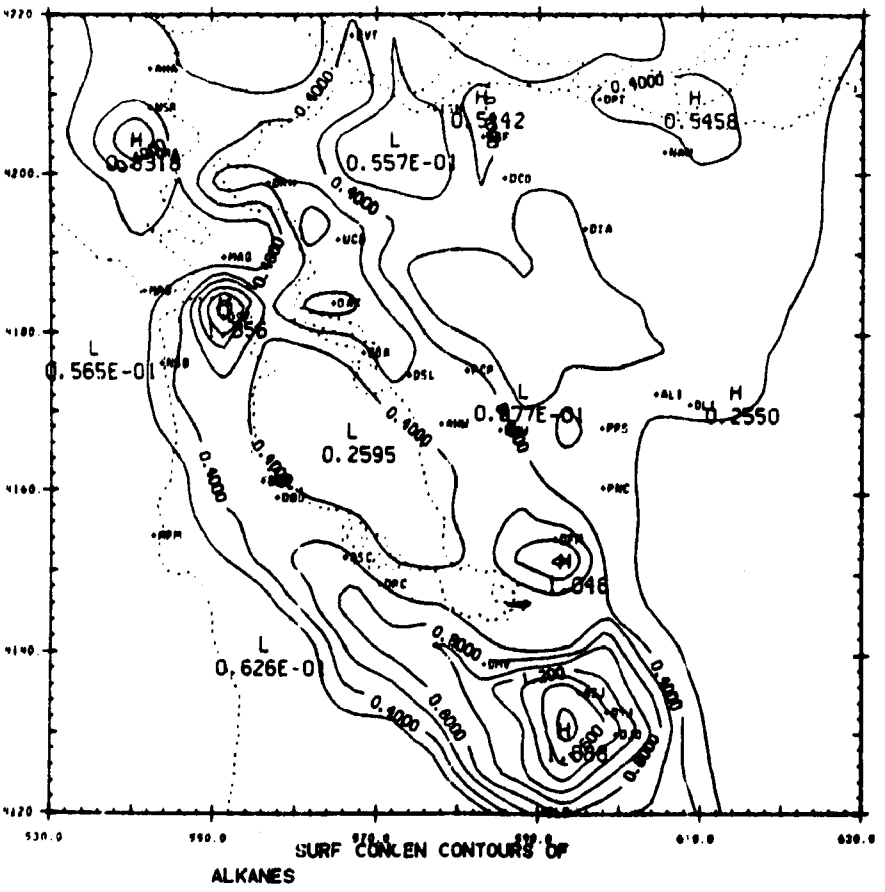


Figure A-4. 900 PST surface alkanes (ppm), 5 x 5 km emission pattern.

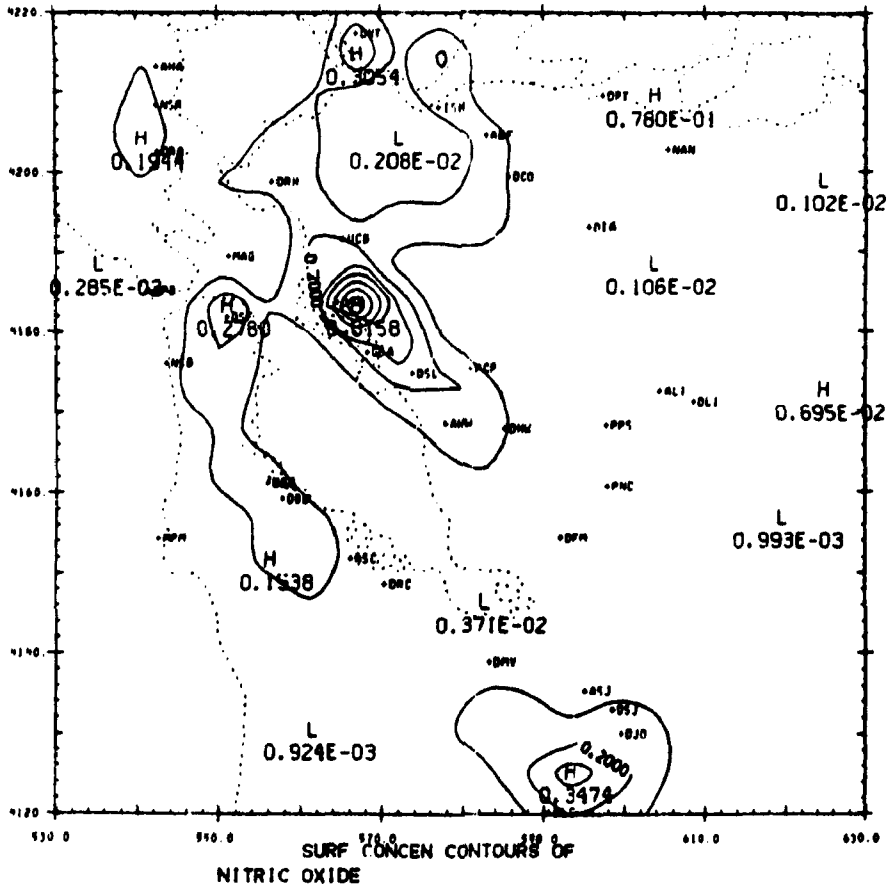


Figure A-5. 900 PST surface NO (ppm), 1975
5 x 5 km emission pattern.

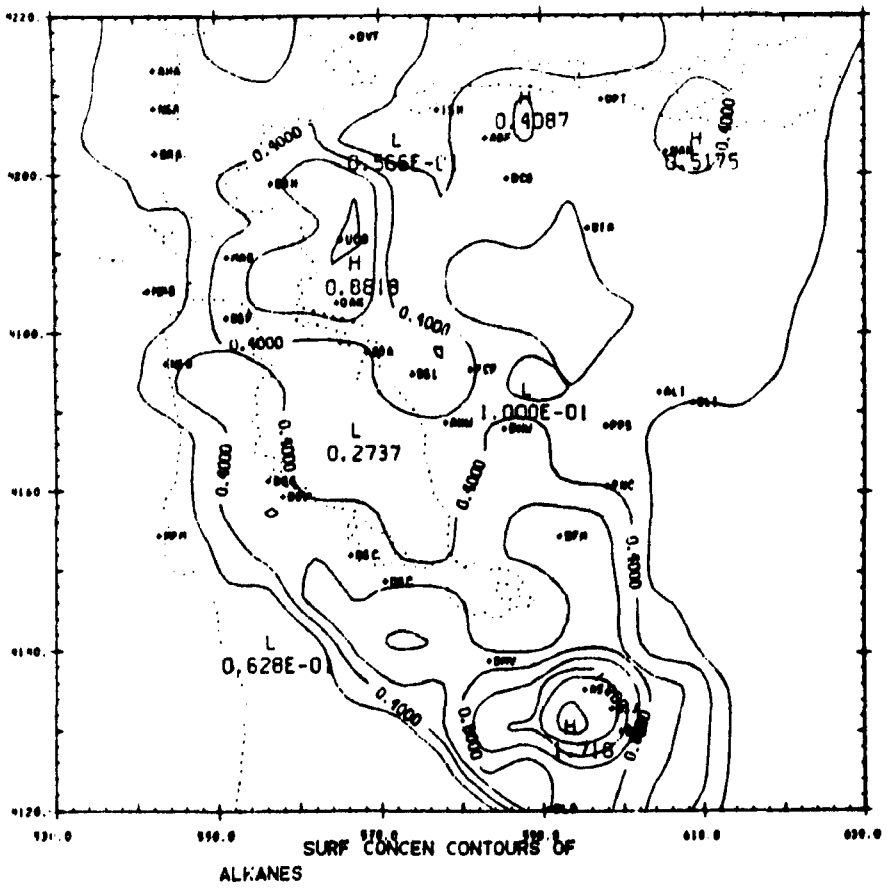


Figure A-6. 900 PST surface alkanes (ppm), 1975 10 x 10 km emission pattern.

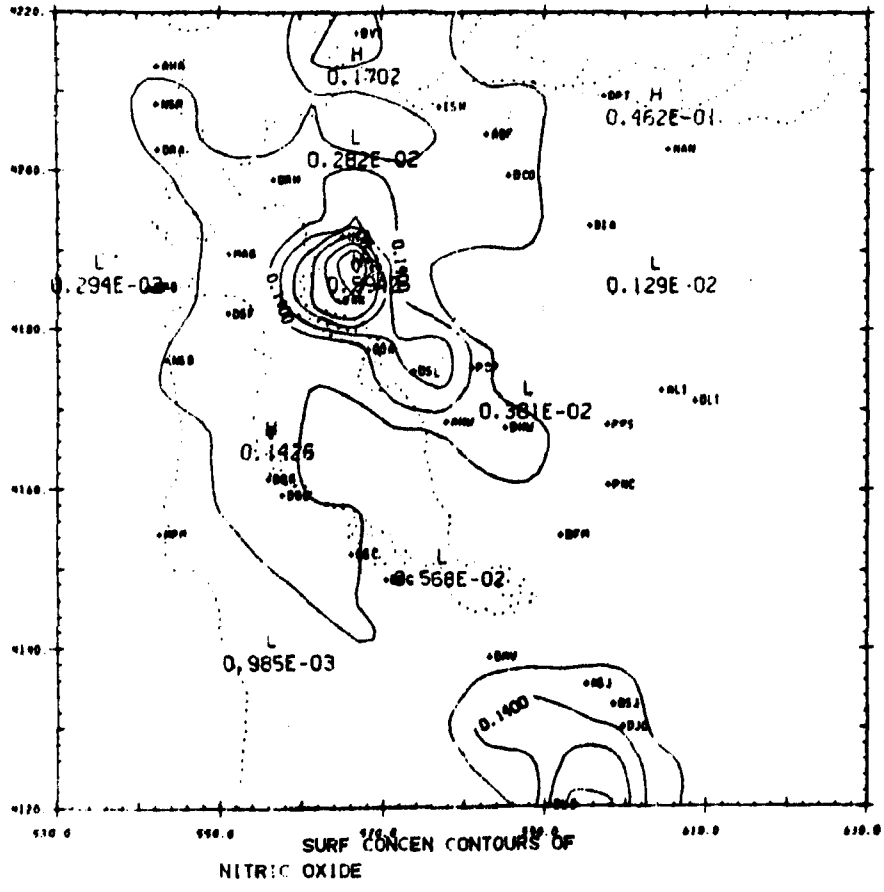


Figure A-7. 900 PST surface NO (ppm), 1975 10 x 10 km emission pattern.

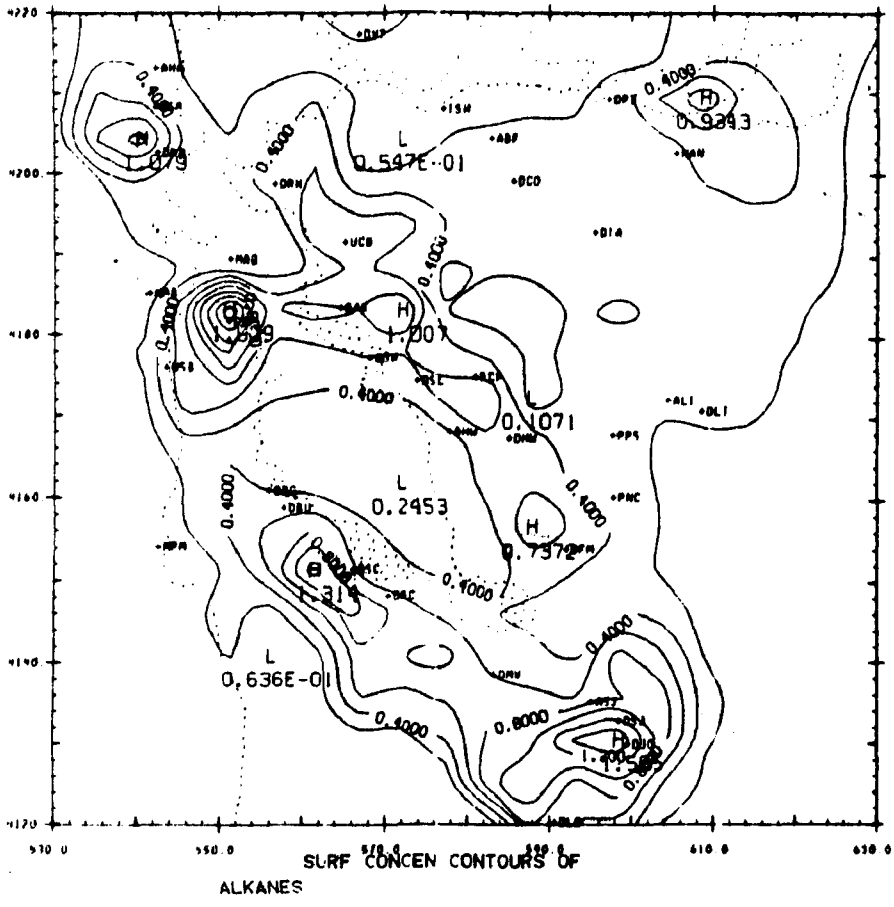


Figure A-8. 900 PST surface alkanes (ppm), 1975 pop. emission pattern.

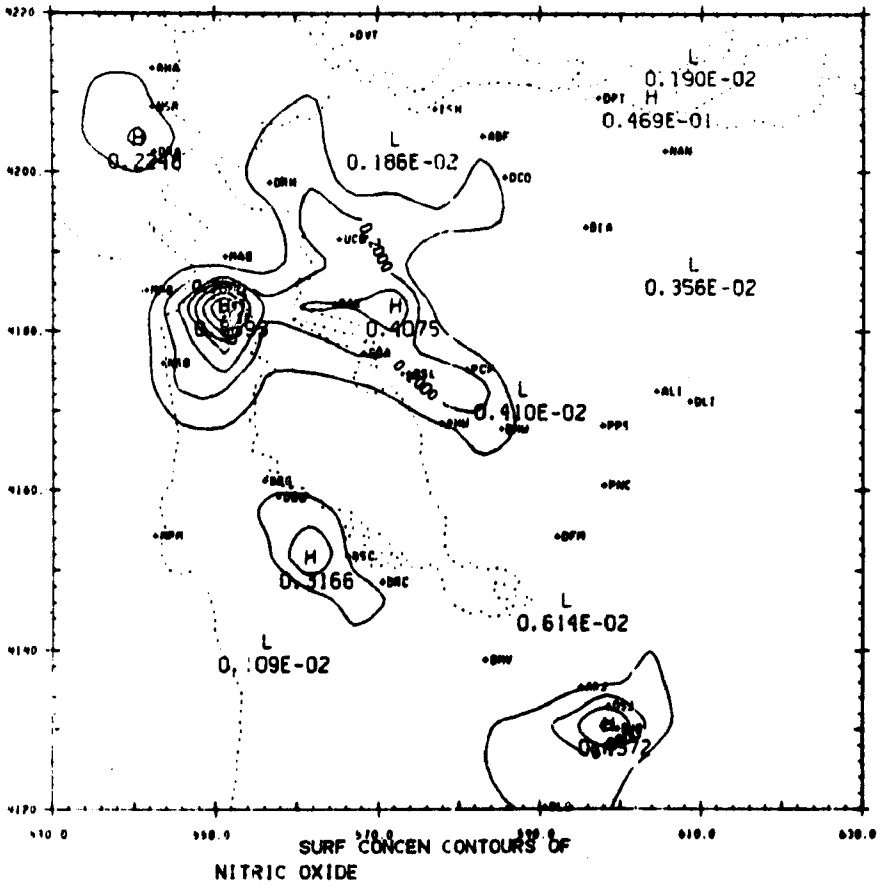


Figure A-9. 900 PST surface NO (ppm), 1975 pop. emission pattern.

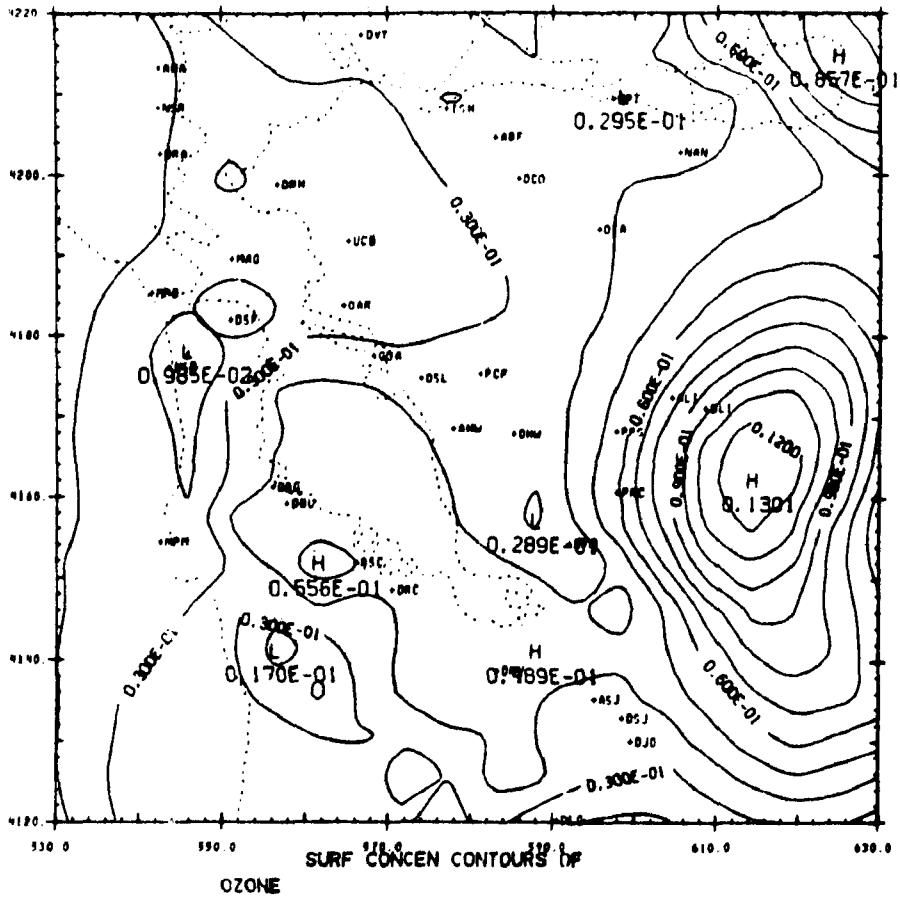


Figure A-10. 1500 PST surface ozone (ppm), 1985 5 x 5 km emission pattern.

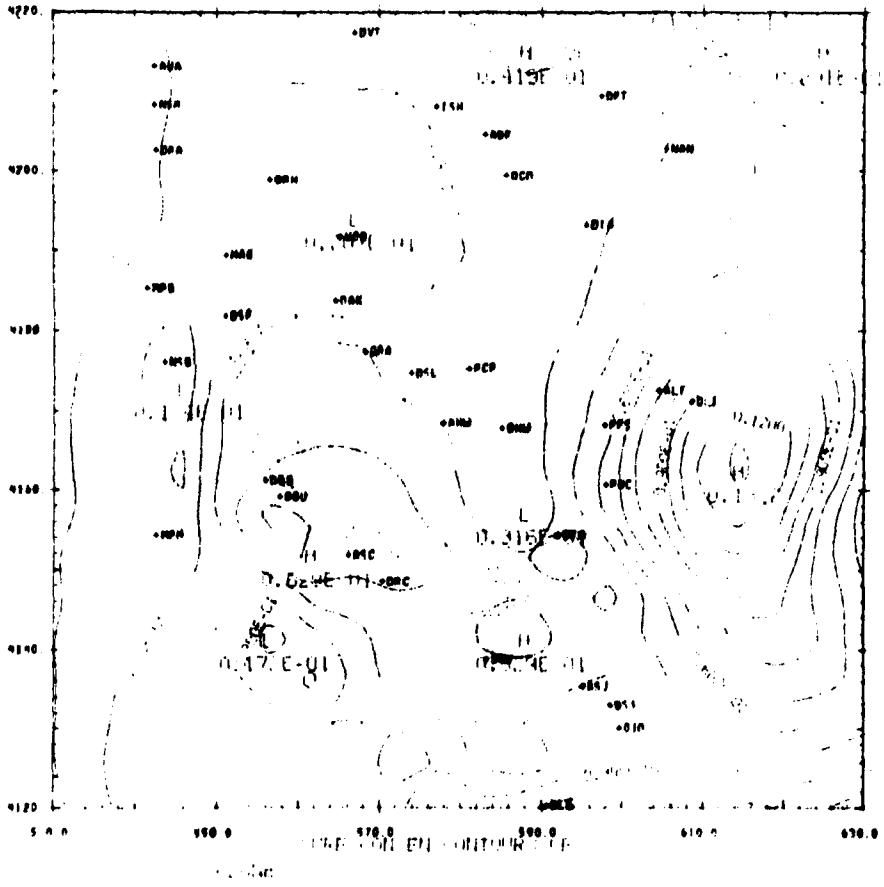


Figure A-11. 1500 PST surface ozone (ppm), 1985
10 x 10 km emission pattern

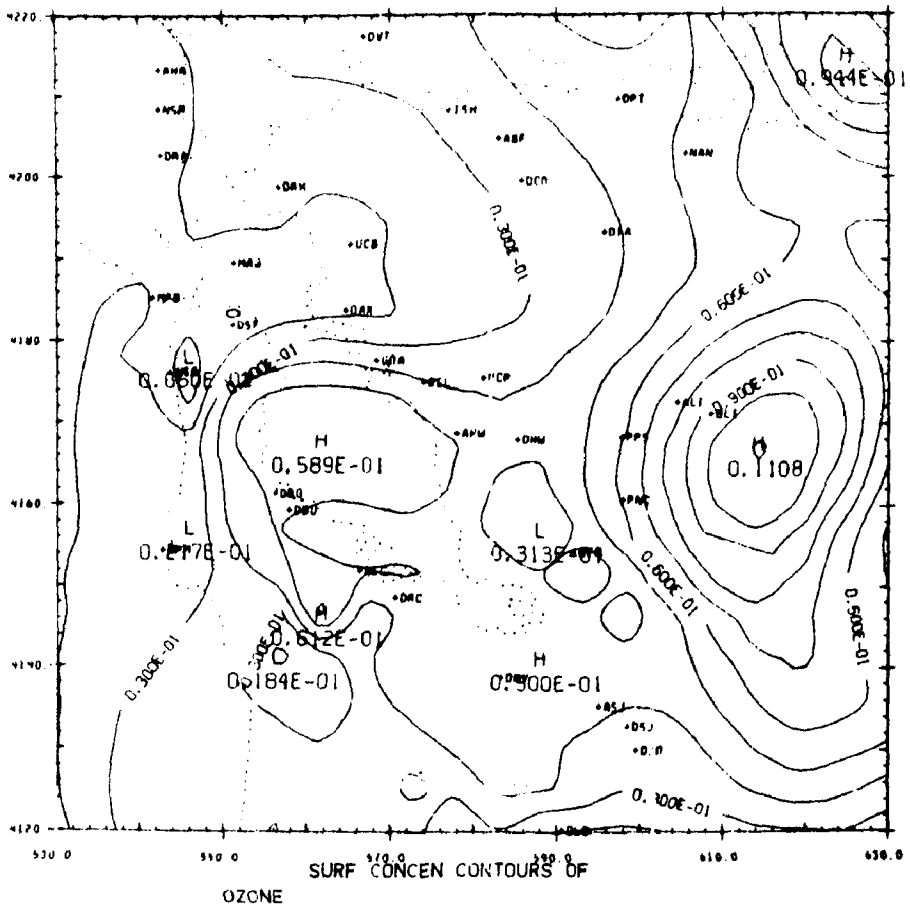


Figure A-12. 1500 PST surface ozone (ppm), 1985 pop. emission pattern.

APPENDIX B

- MASCON-Generated Mass Flux and Inversion Base Height Maps for the 5 November 1976 Prototype Day
- Selected Maps and Time Histories of O3 and NO2 for the 1985 Baseline and Sensitivity Simulations

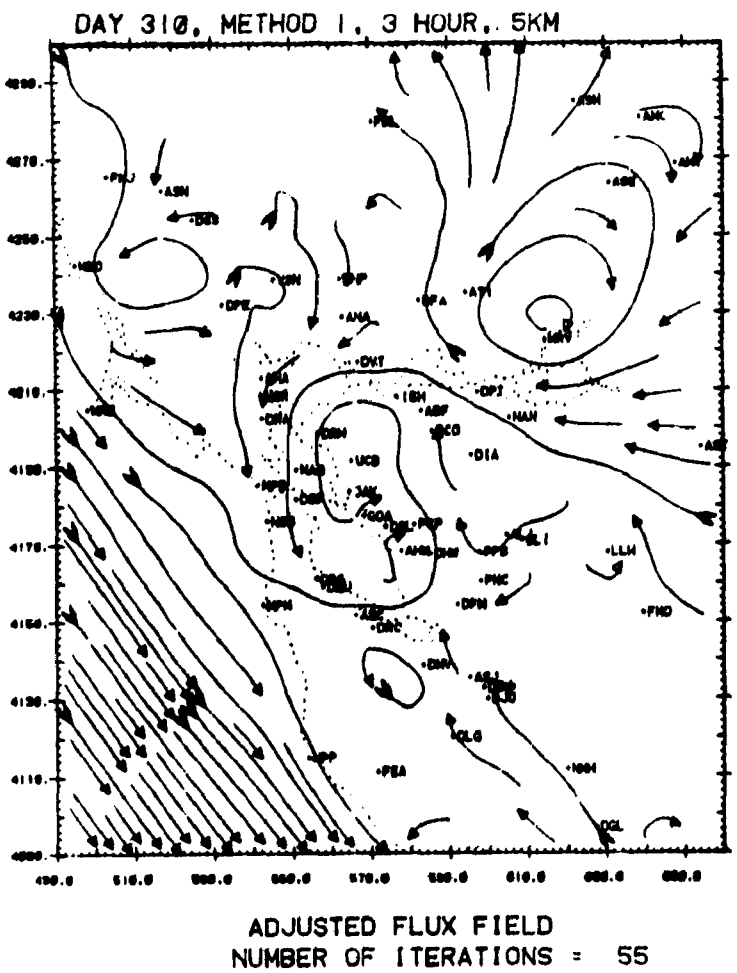


Figure B-1a. Mass Flux streamline computer analysis for 0530 PST, November 5, 1976

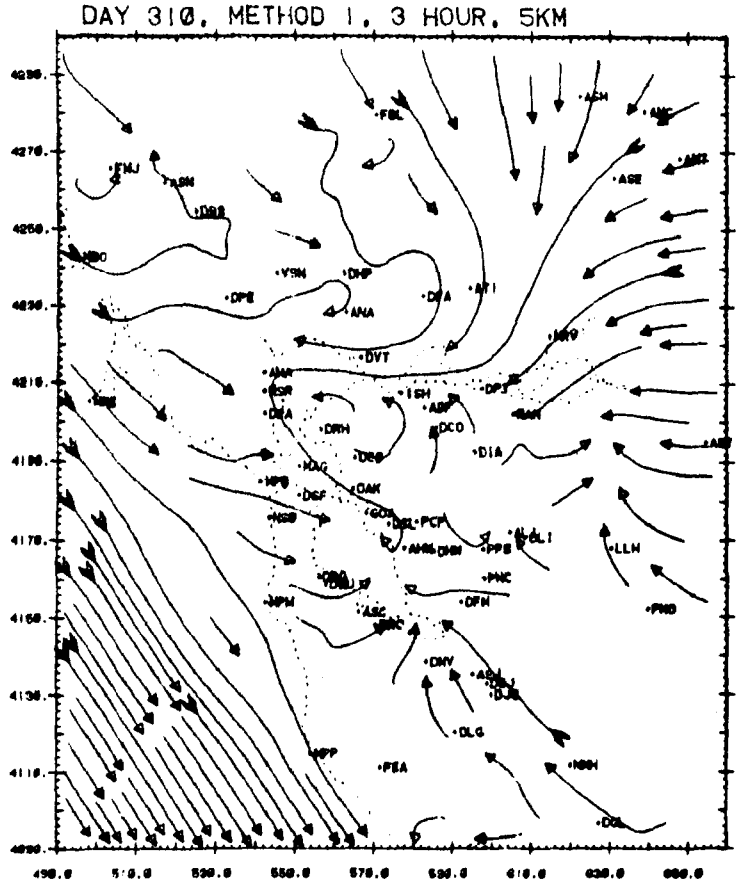


Figure B-1b. Mass Flux streamline computer analysis for 0830 PST, November 5, 1976

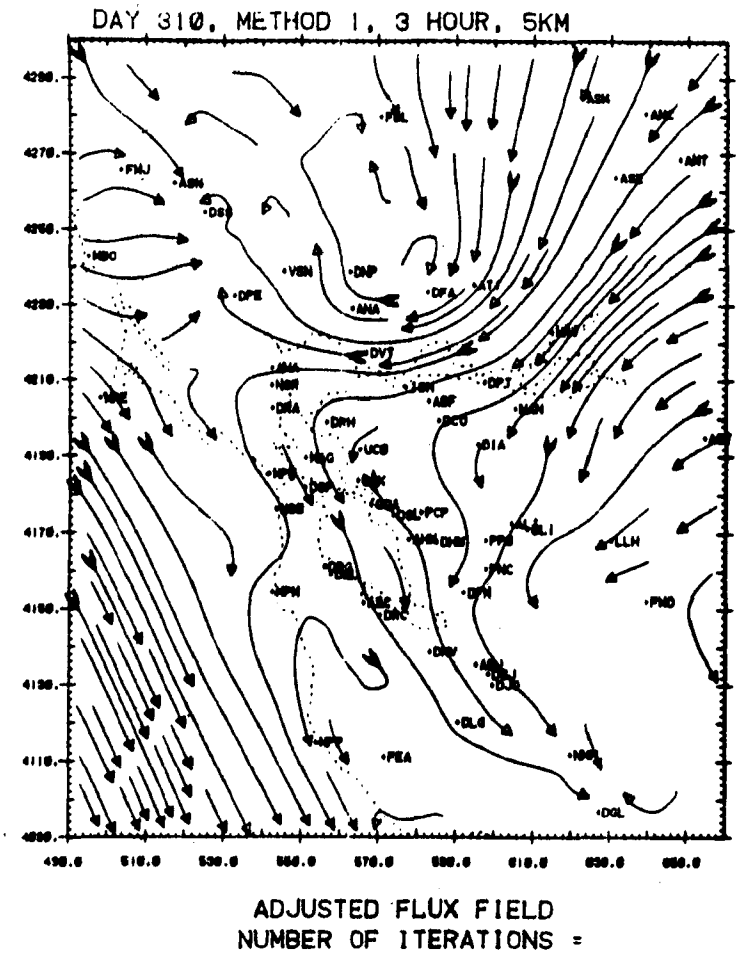


Figure B-1c. Mass Flux streamline computer analysis for 1130 PST, November 5, 1976

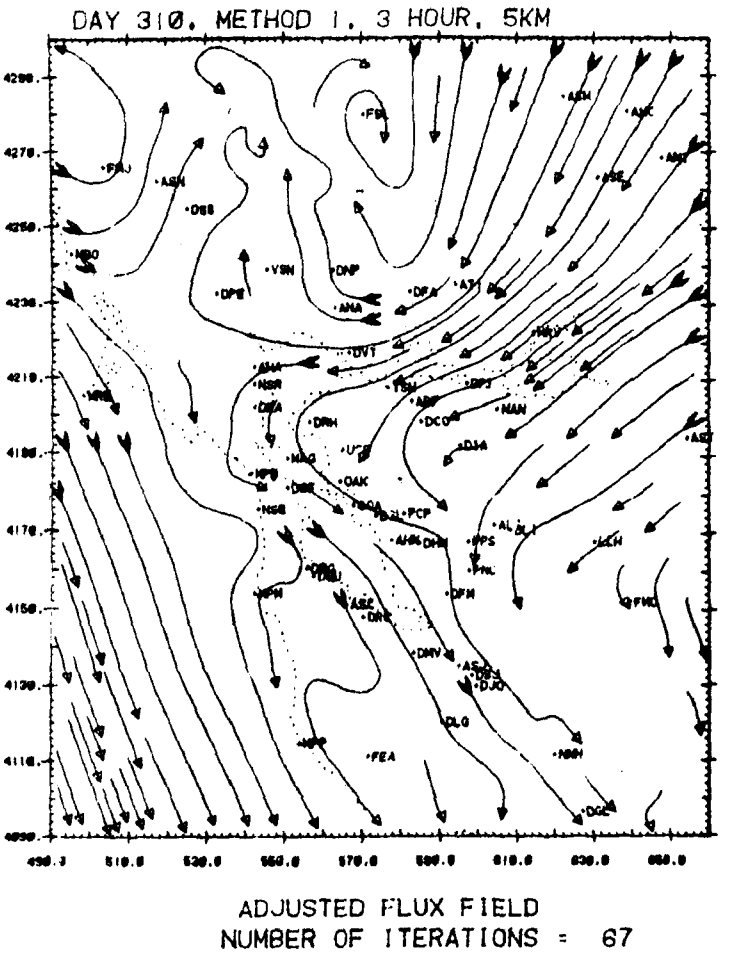


Figure B-1d. Mass Flux streamline computer analysis for 1430 PST, November 5, 1976

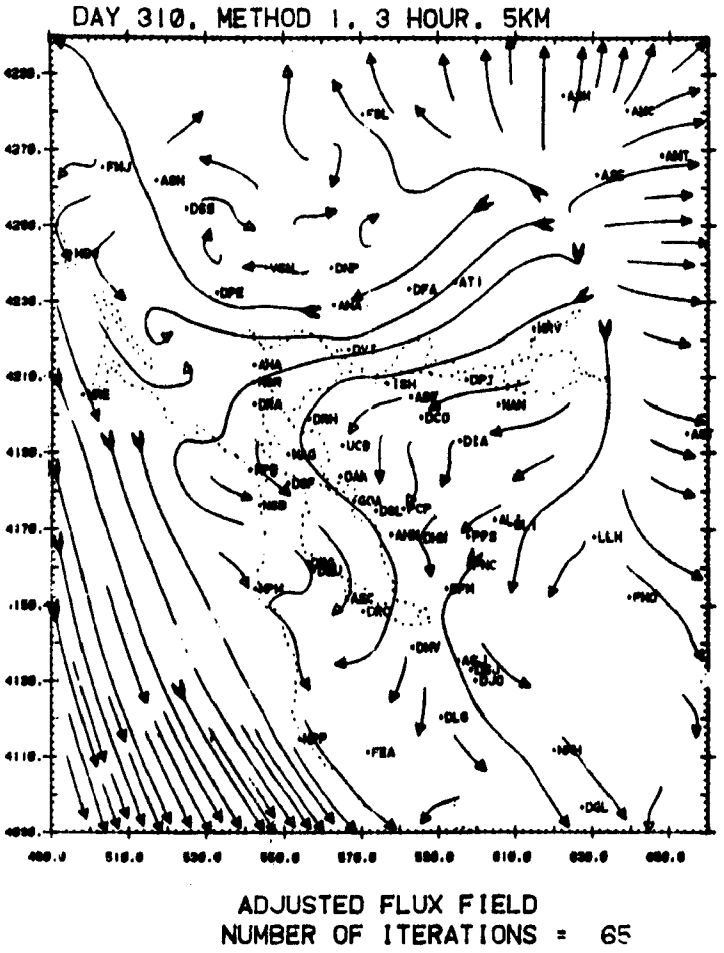


Figure B-1e. Mass Flux streamline computer analysis for 1730 PST, November 5, 1976

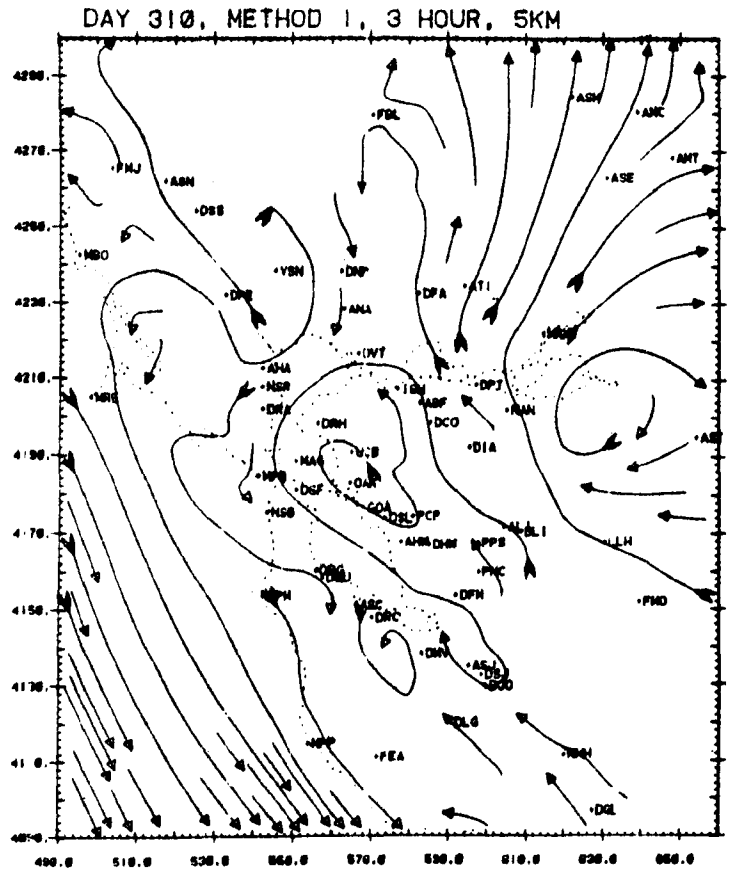
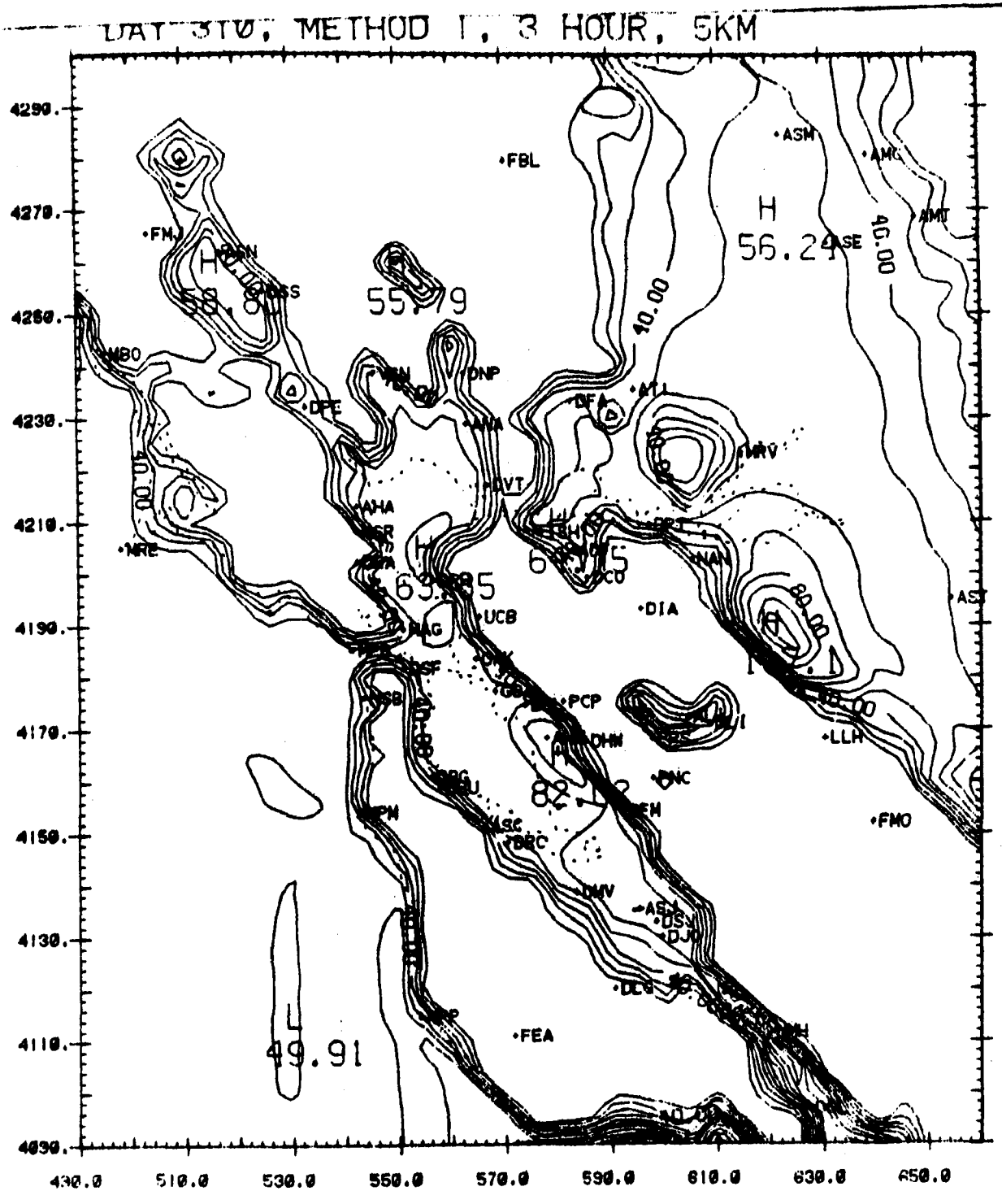


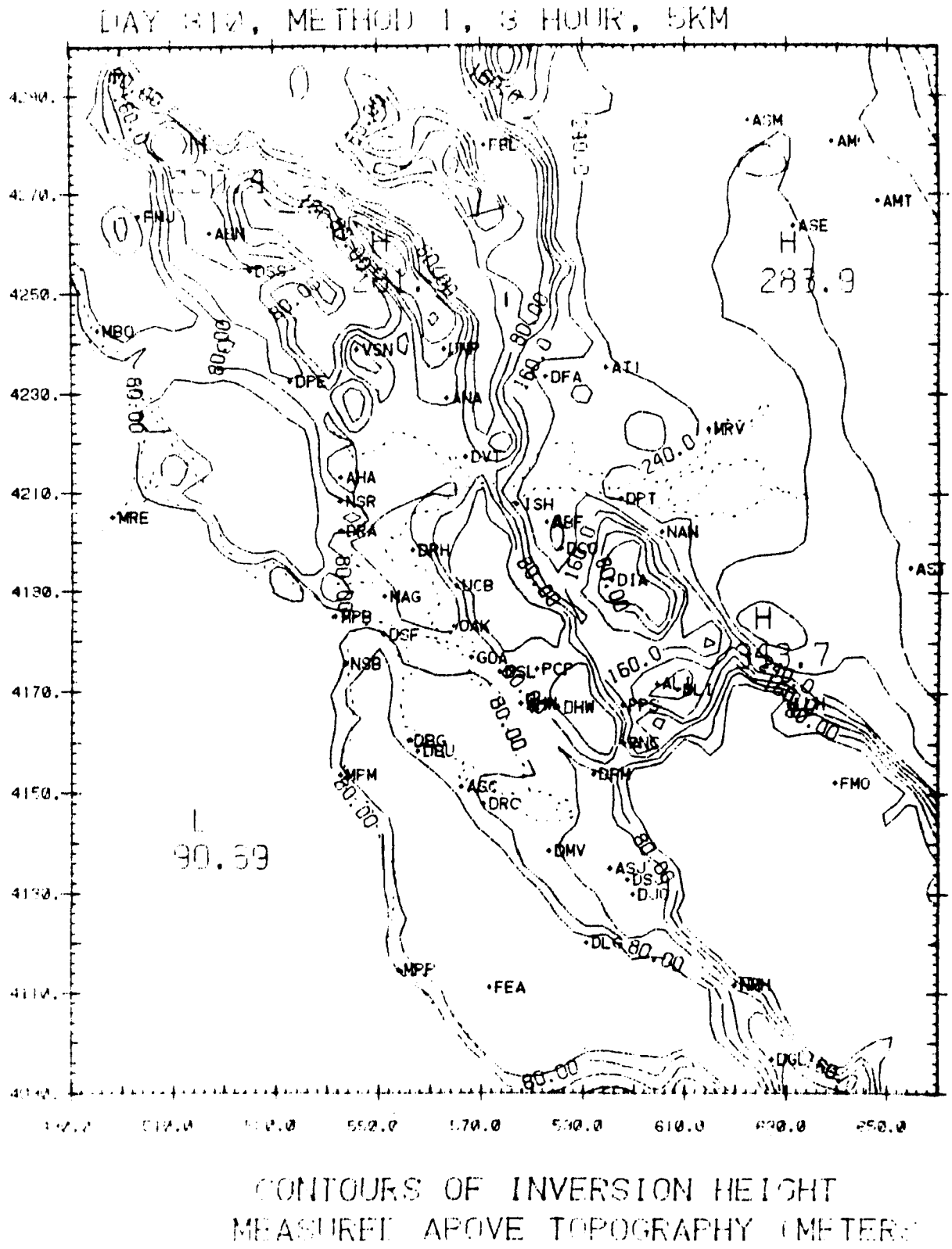
Figure B-1f. Mass Flux streamline computer analysis for 2030 PST, November 5, 1976



CONTOURS OF INVERSION HEIGHT
MEASURED ABOVE TOPOGRAPHY (METERS)

SCALE= 5.0 KM

Figure B-2a Inversion base height (above topography) analysis for 0700 PST, November 5, 1976



CONTOURS OF INVERSION HEIGHT
MEASURED ABOVE TOPOGRAPHY (METERS

Figure B-2b. Inversion base height (above topography) analysis for 1600 PST, November 5, 1976

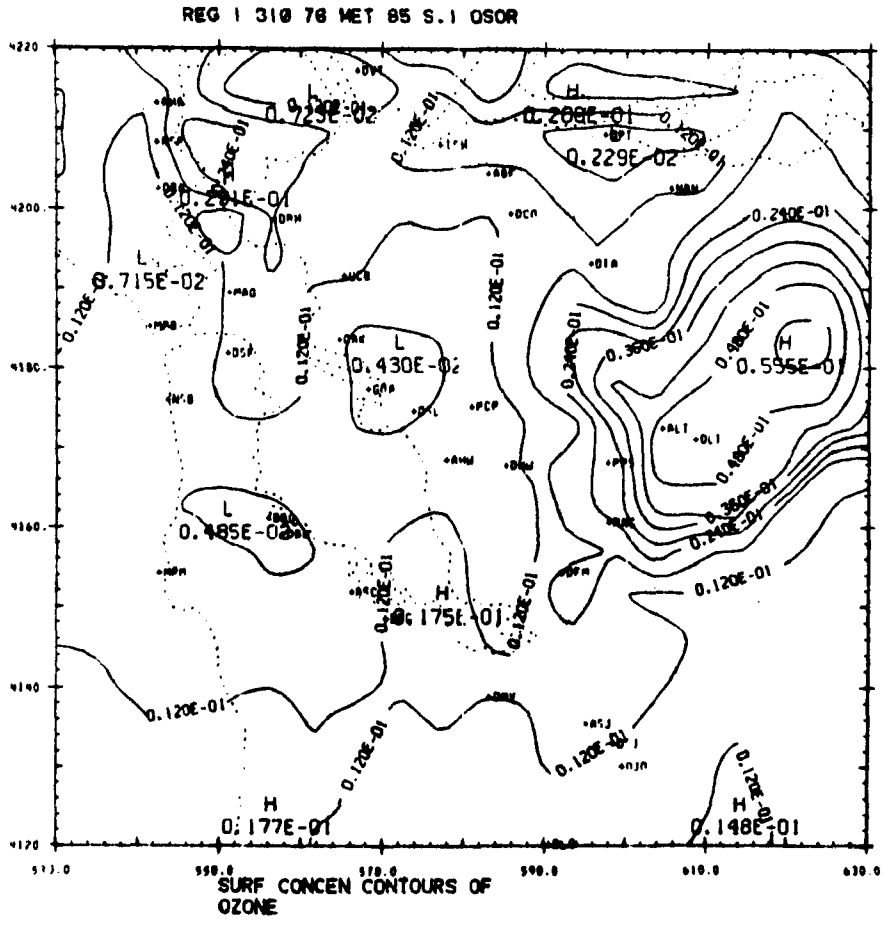


Figure B-3a 1100 PST surface ozone (ppm), 1985 baseline emissions, 5 November 1976 meteorology

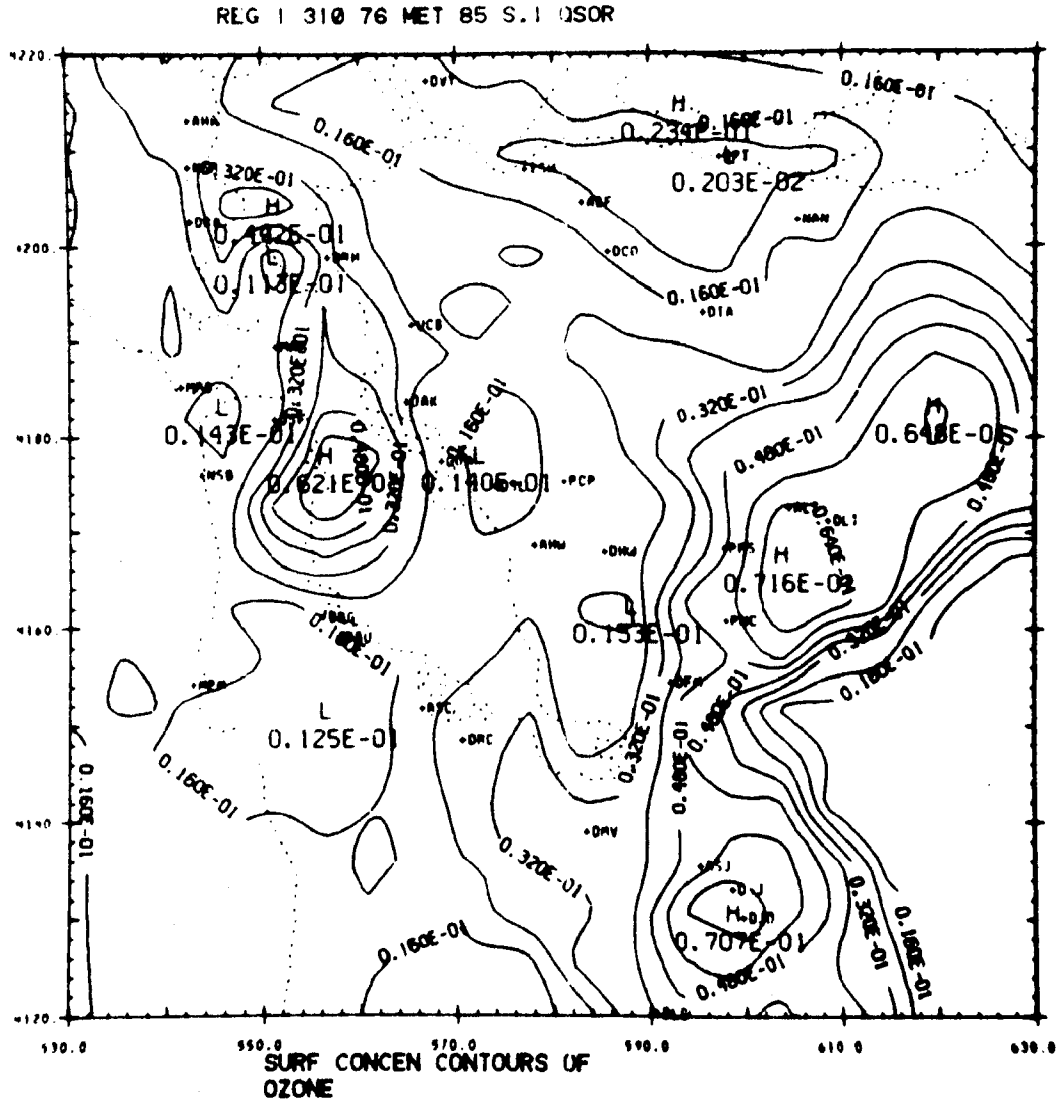


Figure B-3b. 1300 PST surface ozone (ppm), 1985 baseline emissions, 5 November 1976 meteorology

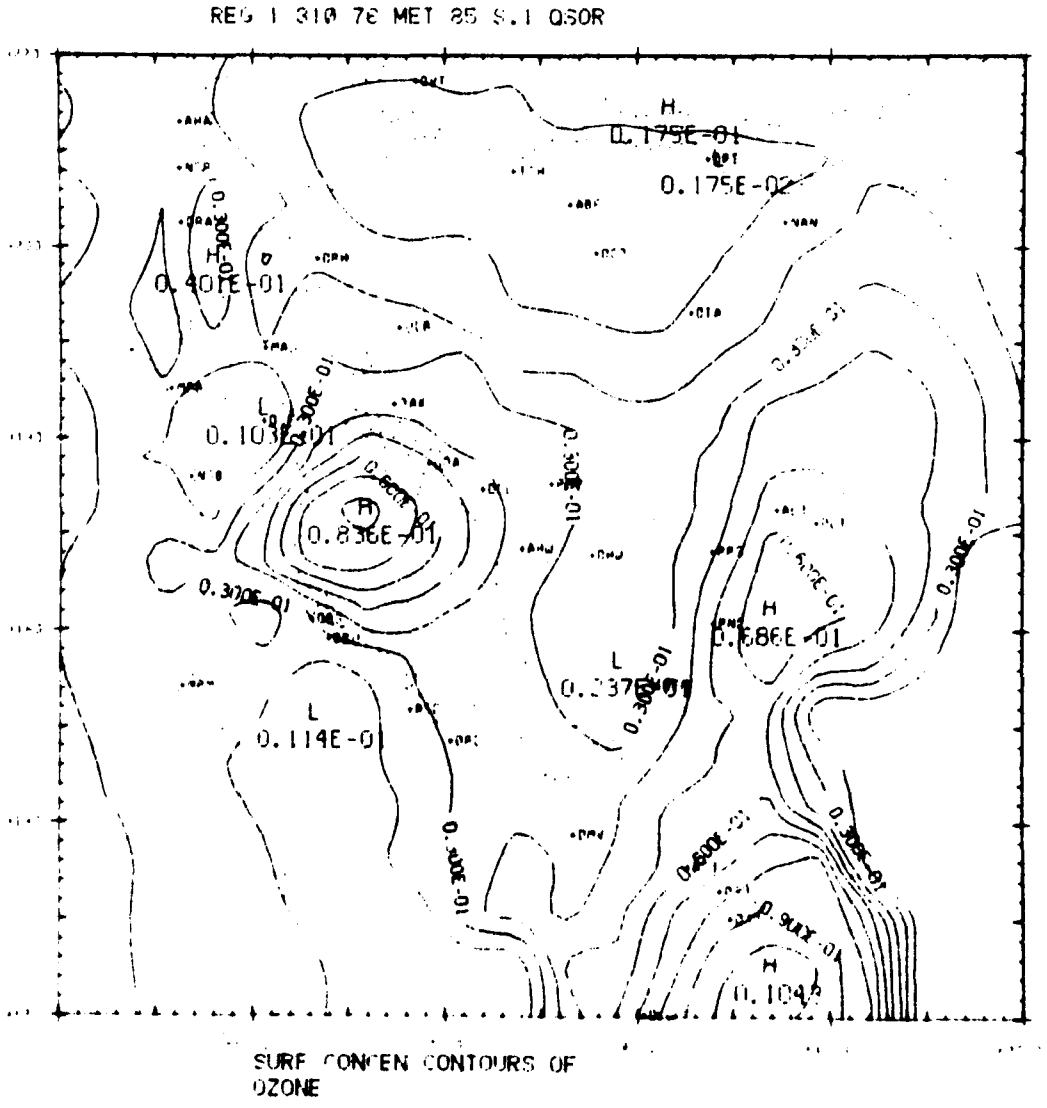


Figure B-3c. 1500 PST surface ozone (ppm), 1985 baseline emissions, 5 November 1976 meteorology.

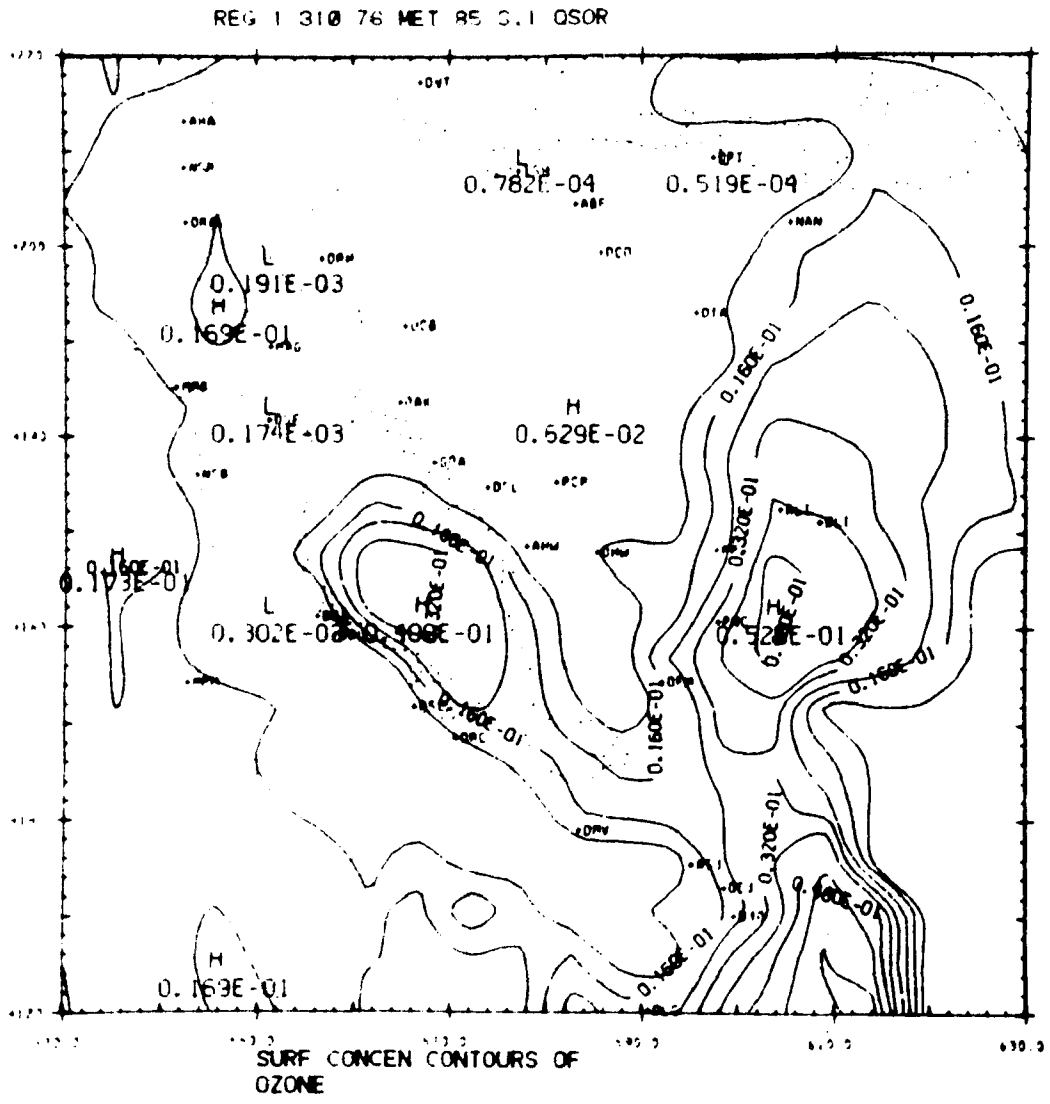


Figure B-3d. 1700 PST surface ozone (ppm), 1985 baseline emissions, 5 November 1976 meteorology.

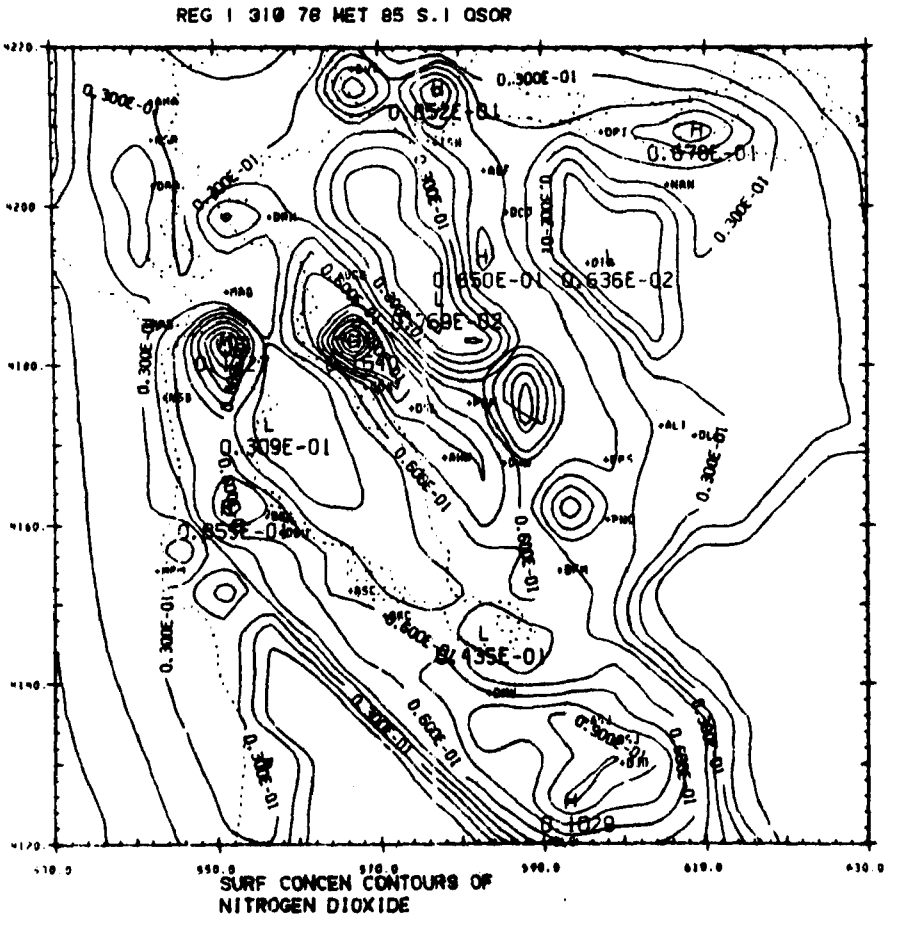


Figure B-4a 0700 PST surface NO_2 (ppm), 1985 emissions, 5 November 1976 meteorology

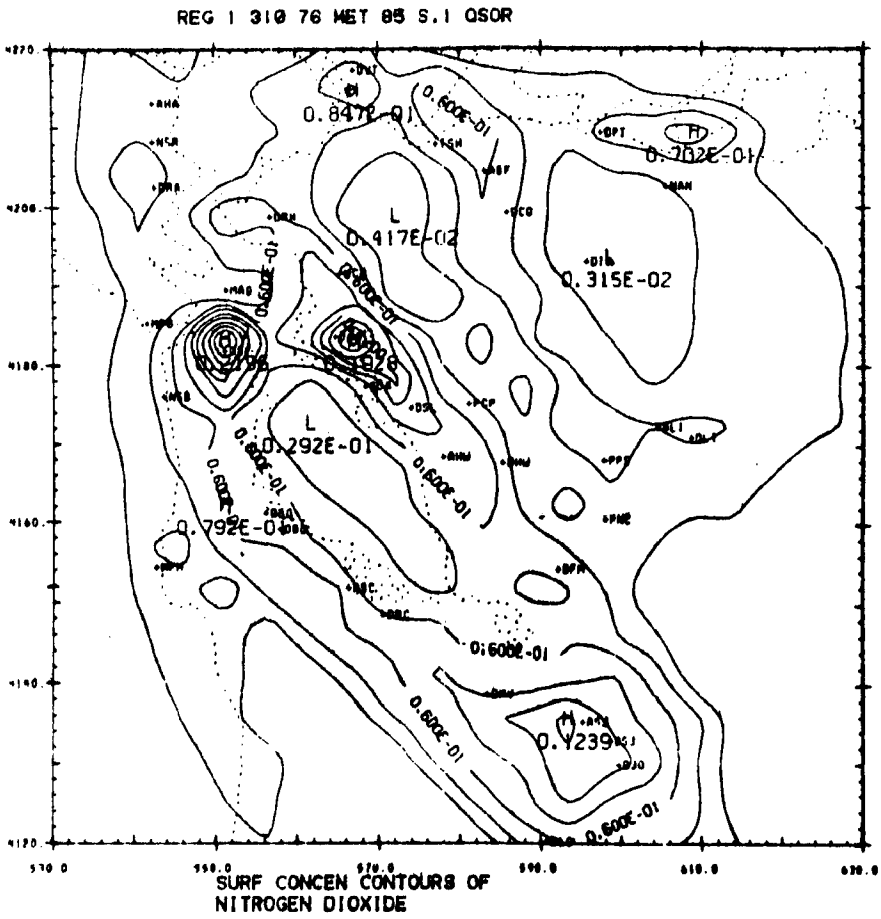


Figure B-4b 0900 PST surface NO_2 (ppm), 1985 emissions, 5 November 1976 meteorology

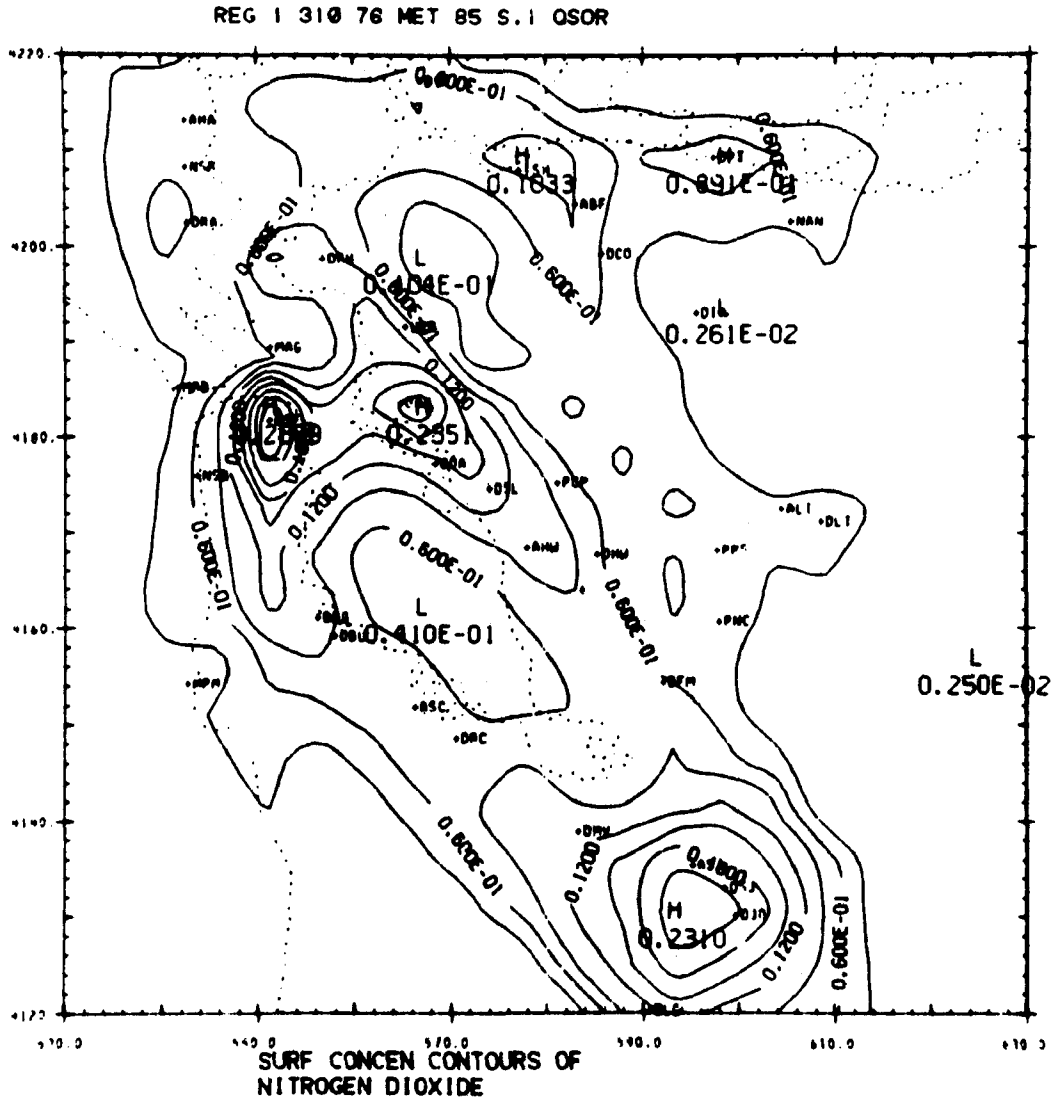


Figure B-4c. 1100 PST surface NO_2 (ppm), 1985 emissions, 5 November 1976 meteorology

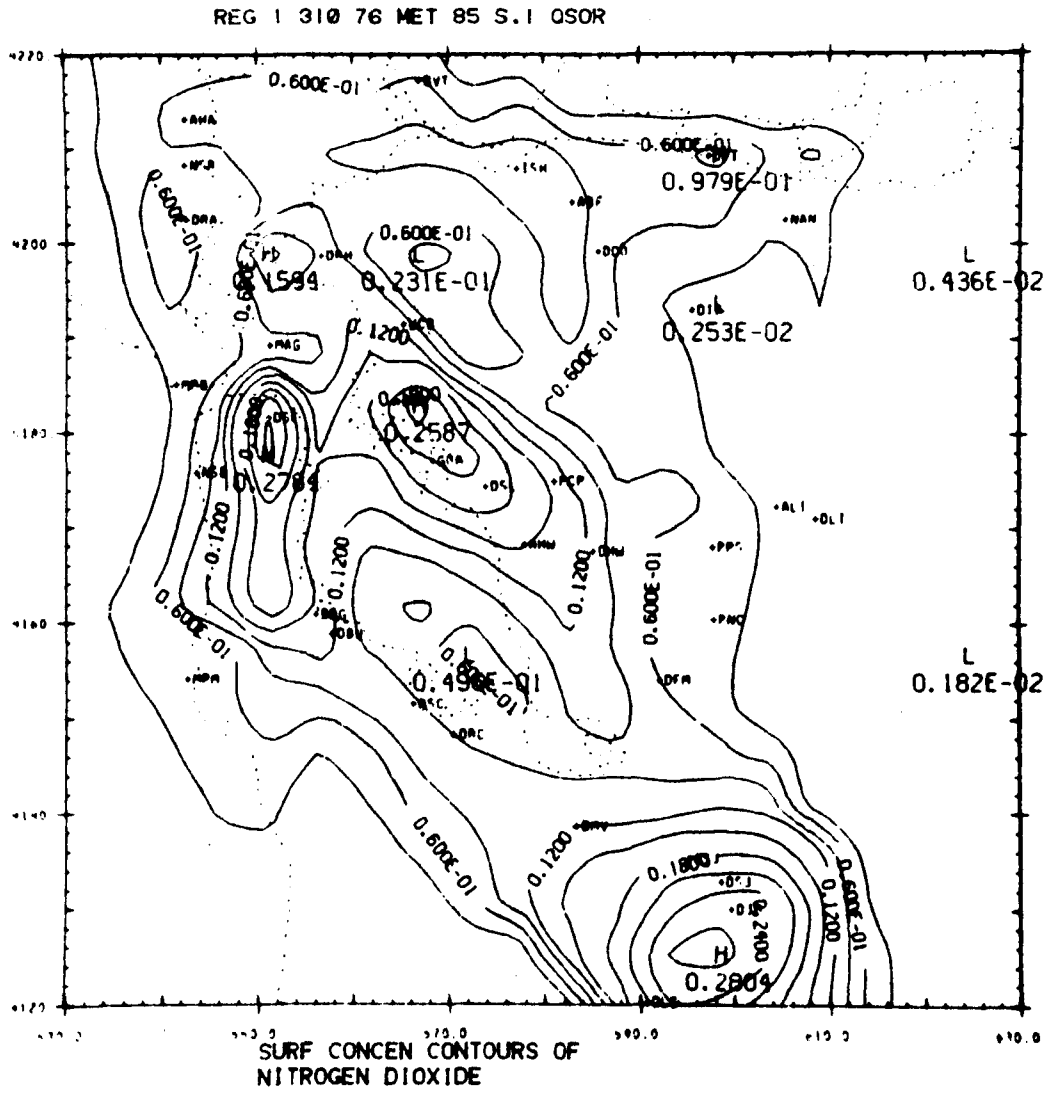


Figure B-4d. 1300 PST surface NO_2 (ppm), 1985 emissions, 5 November 1976 meteorology

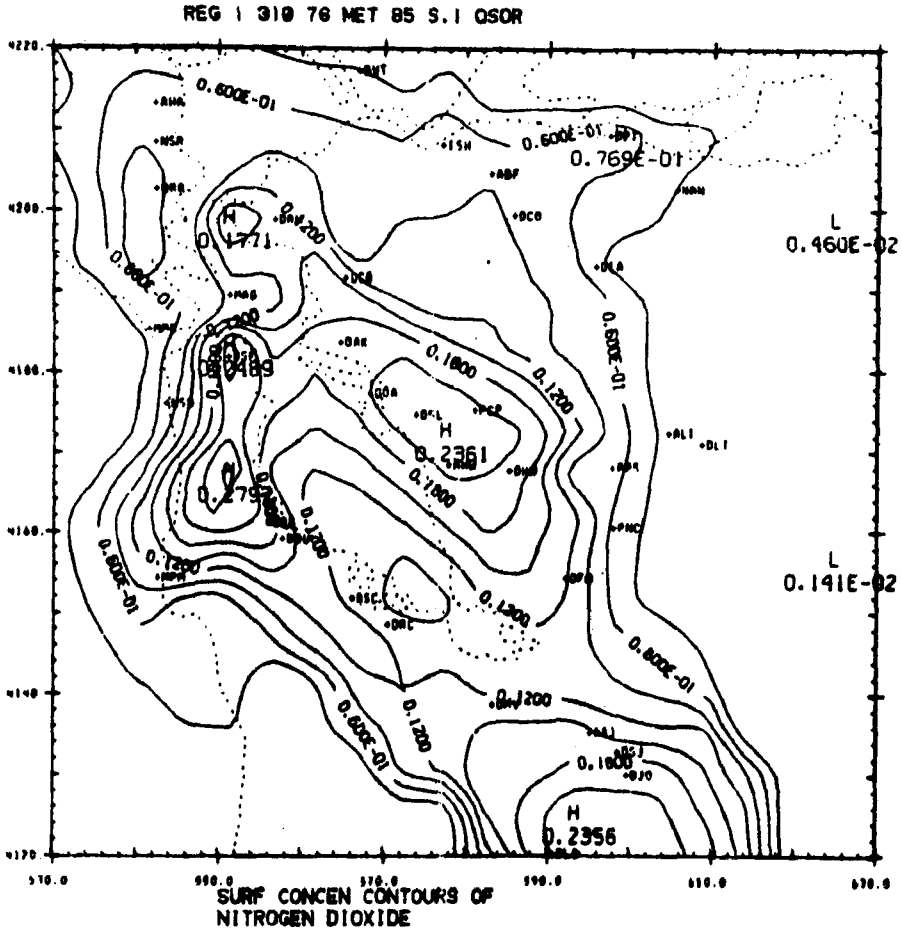


Figure B-4e 1500 PST surface NO_2 (ppm), 1985 emissions, 5 November 1976 meteorology

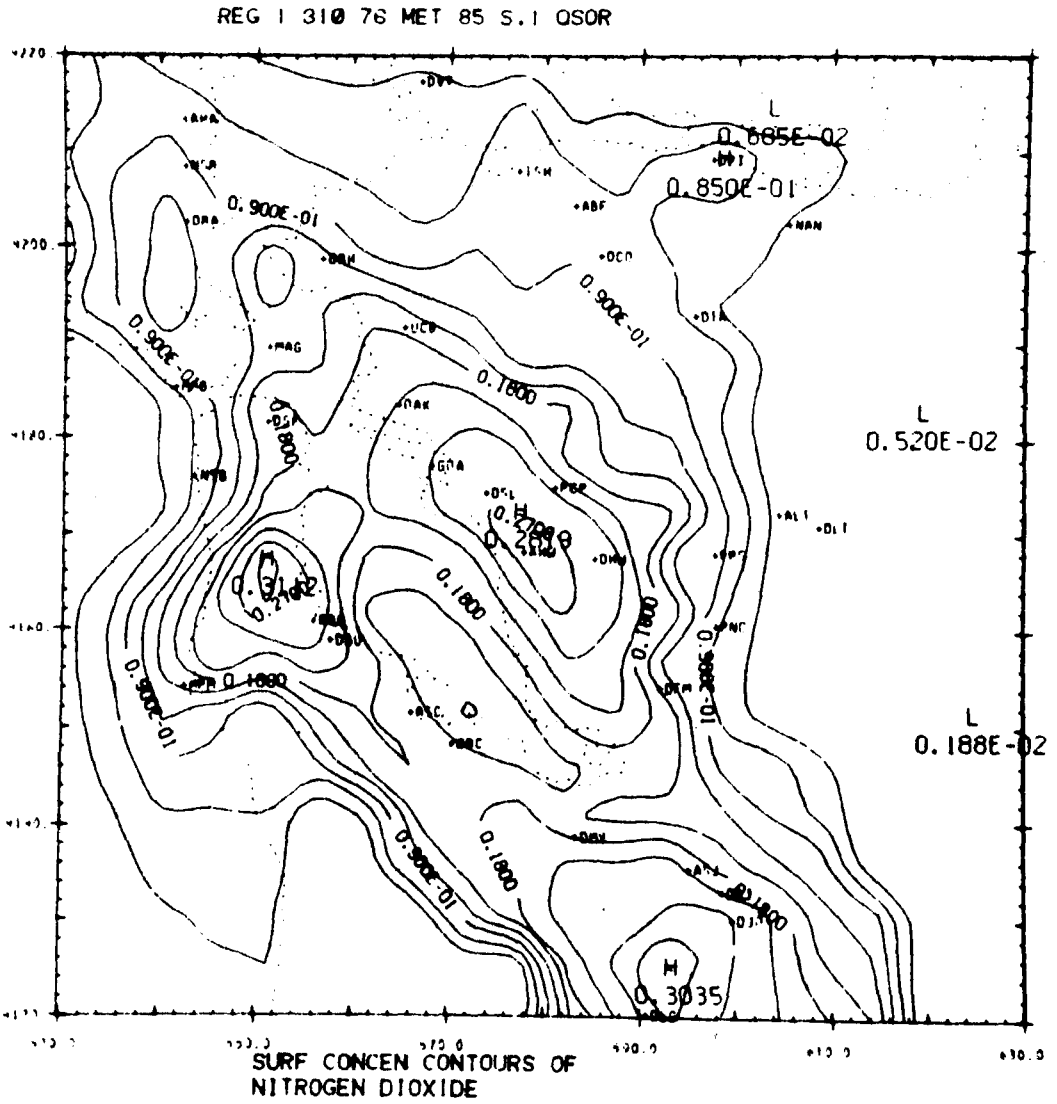


Figure B-4f. 1700 PST surface NO_2 (ppm), 1985 emissions, 5 November 1976 meteorology

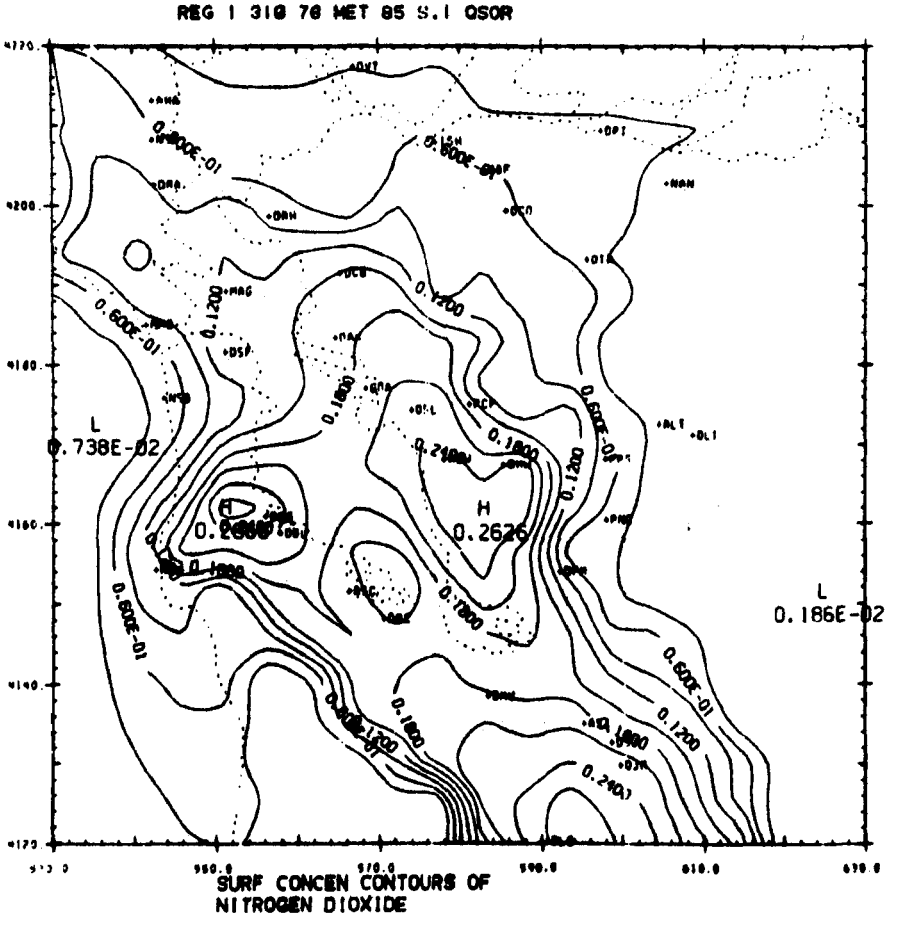


Figure B-4g 1900 PST surface NO_2 (ppm), 1985 emissions, 5 November 1976 meteorology

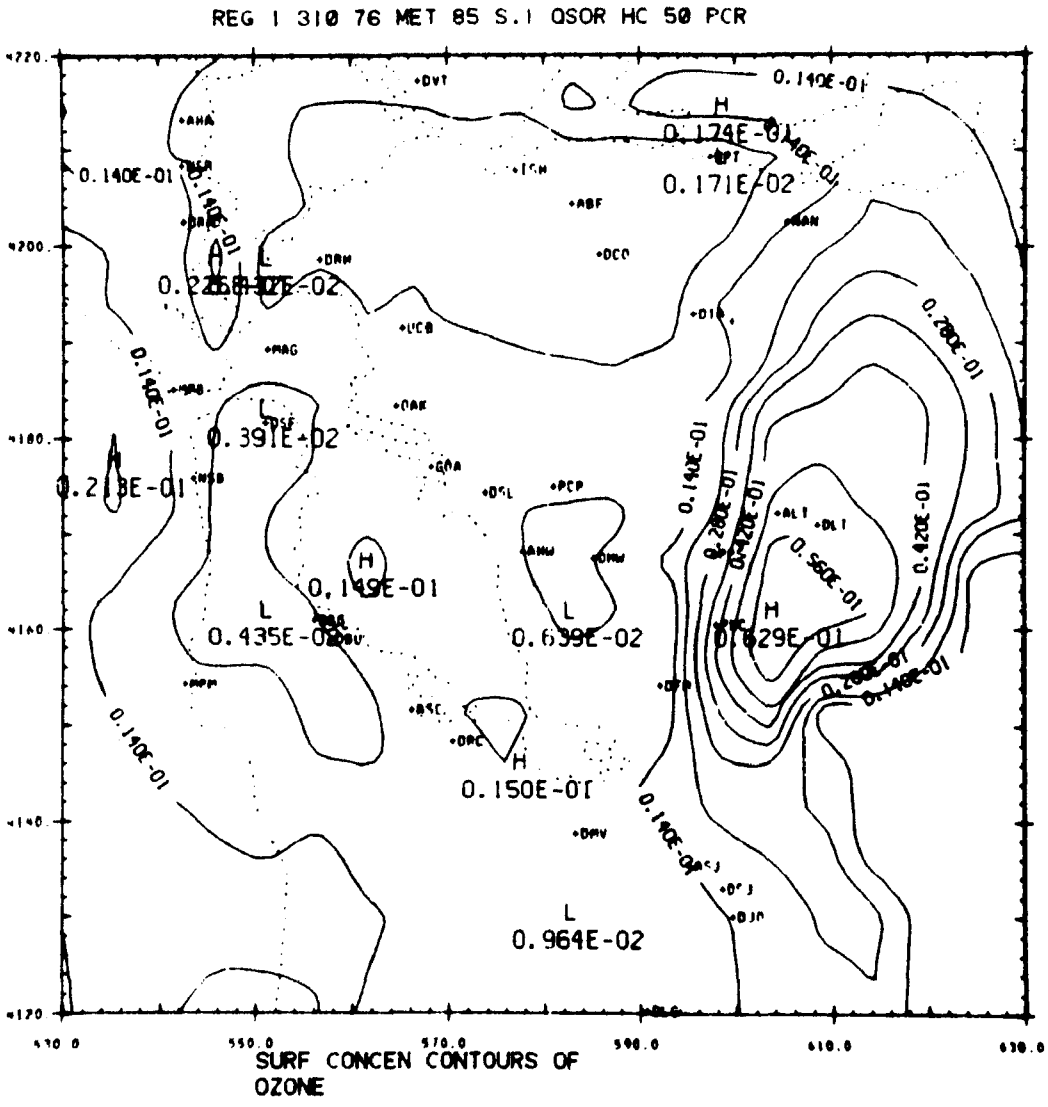


Figure B-5a. 1500 PST surface ozone, 50% HC emission reduction from 1985 baseline, 5 November 1976 meteorology.

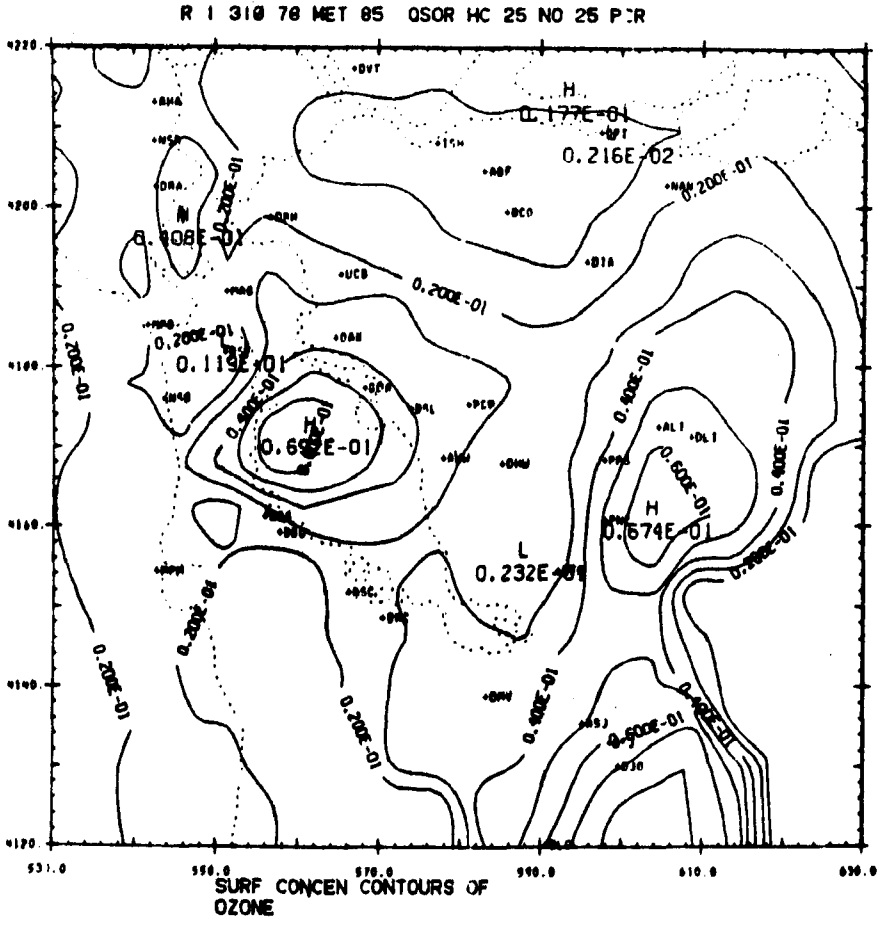


Figure B-5b. 1500 PST surface ozone, 25% HC and 25% NO emission reduction from 1985 baseline, 5 November 1976 meteorology.

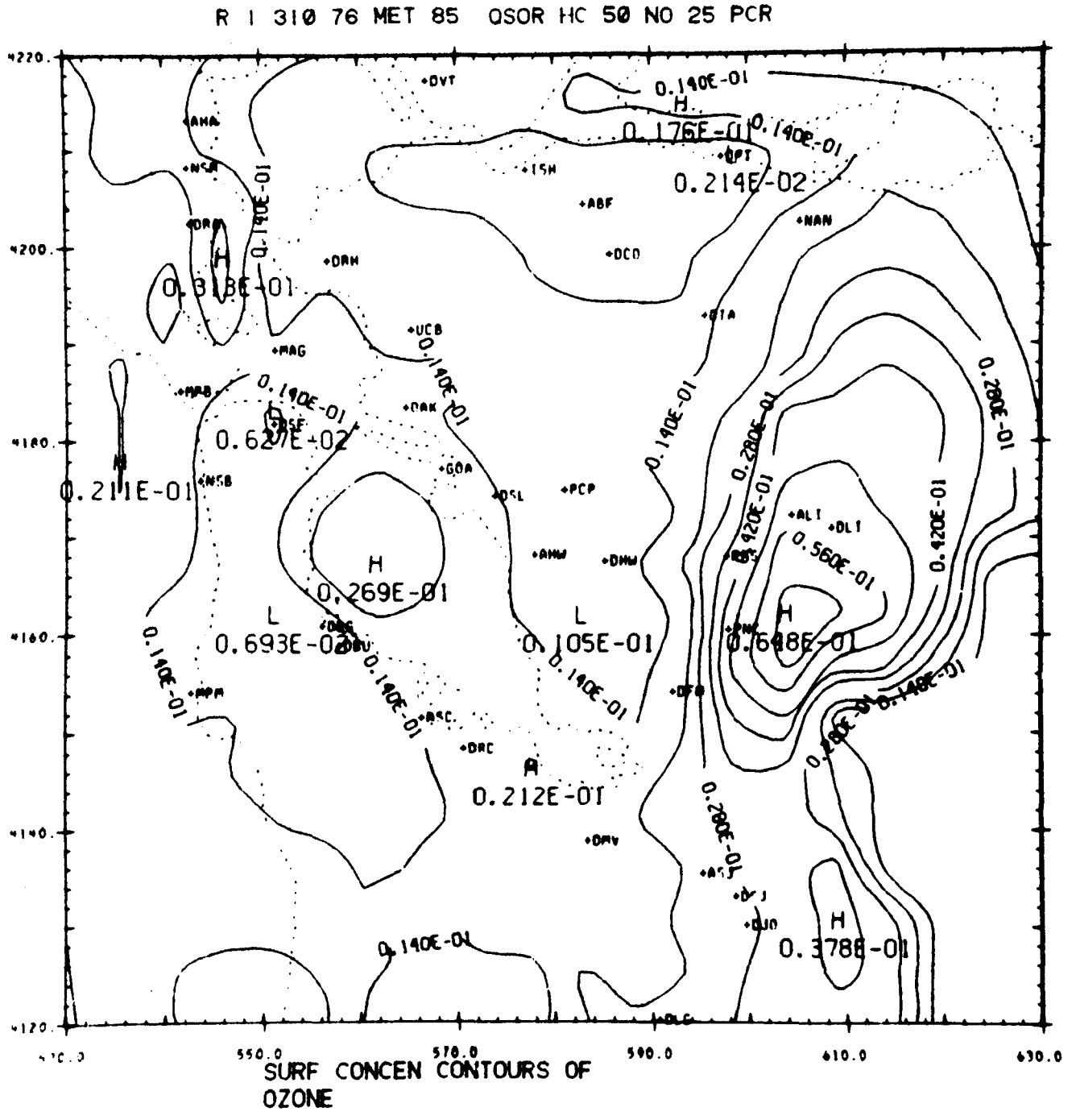


Figure B-5c. 1500 PST surface ozone, 50% HC and 25% NO emission reduction from 1985 baseline, 5 November 1976 meteorology.

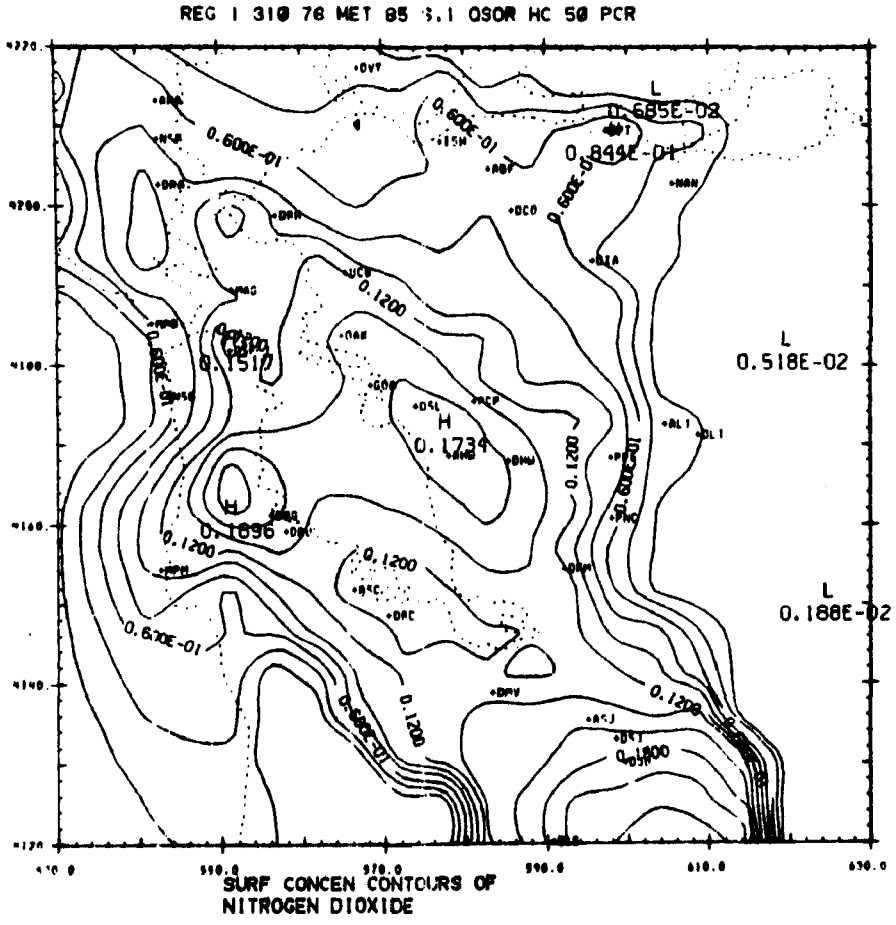


Figure B-6a 1700 PST surface NO_2 (ppm), 50% HC emission reduction from 1985 baseline, 5 November 1976 meteorology

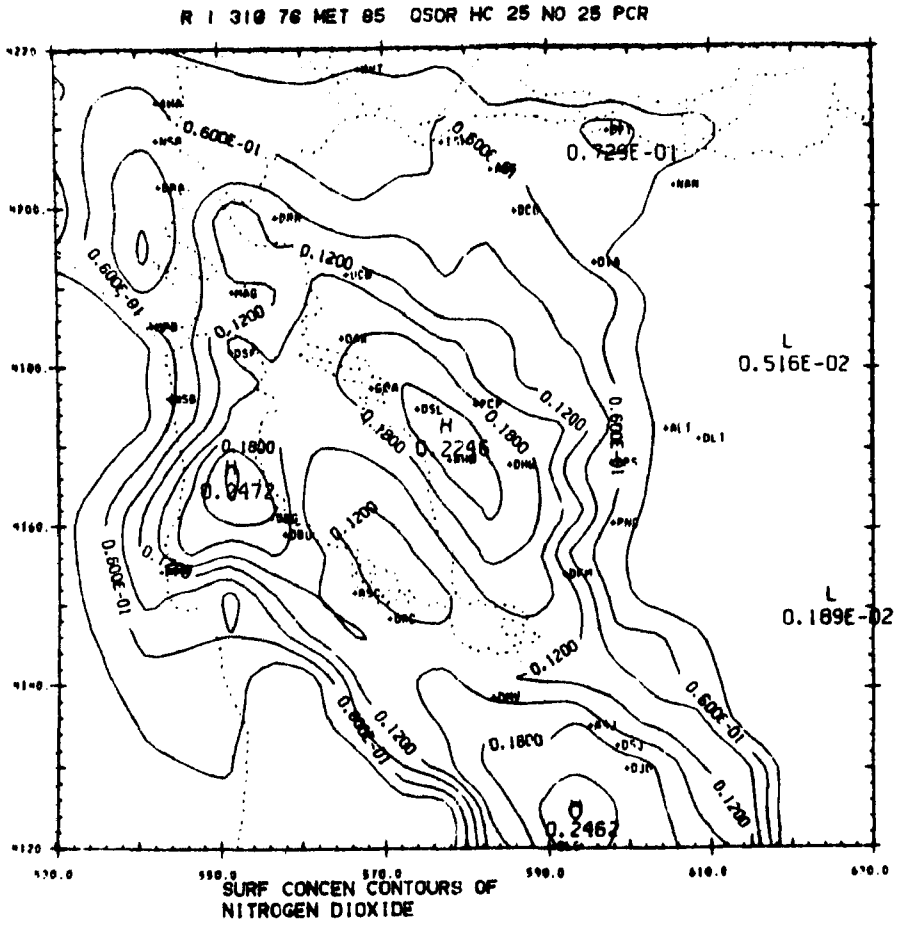


Figure B-6b 1700 PST surface NO_2 (ppm), 25% HC and 25% NO emission reduction from 1985 baseline, 5 November 1976 meteorology

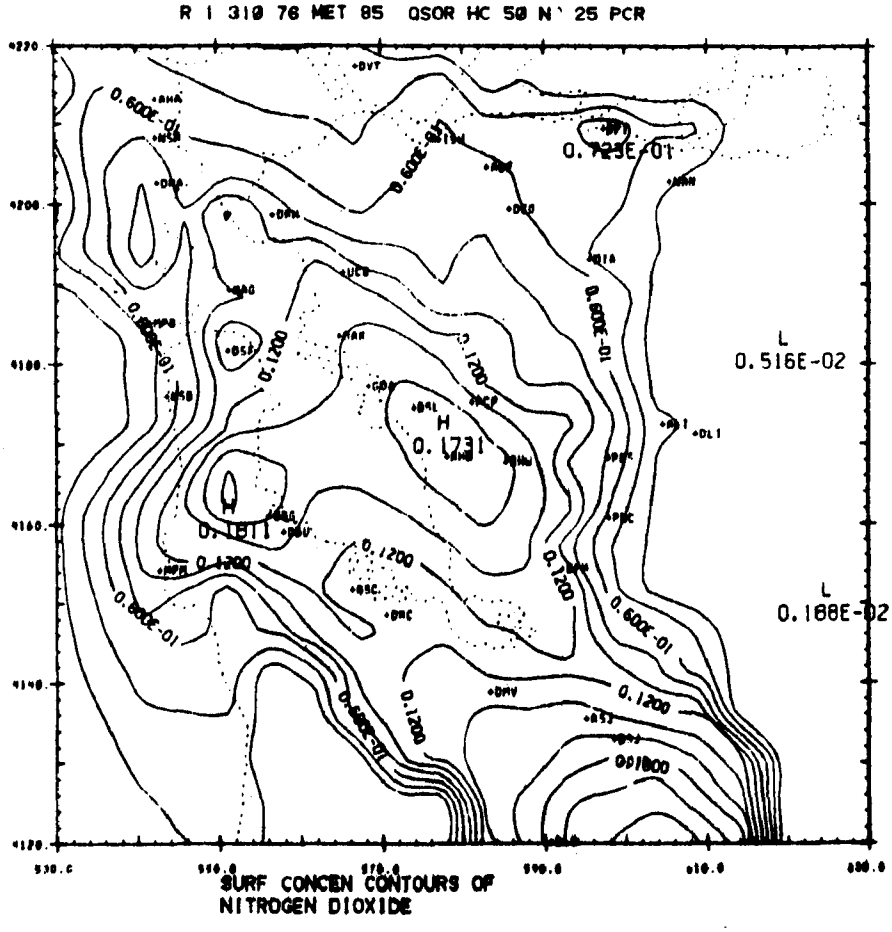


Figure B-6c 1700 PST surface NO_2 (ppm), 50% HC and 25% NO emission reduction from 1985 baseline, 5 November 1976 meteorology

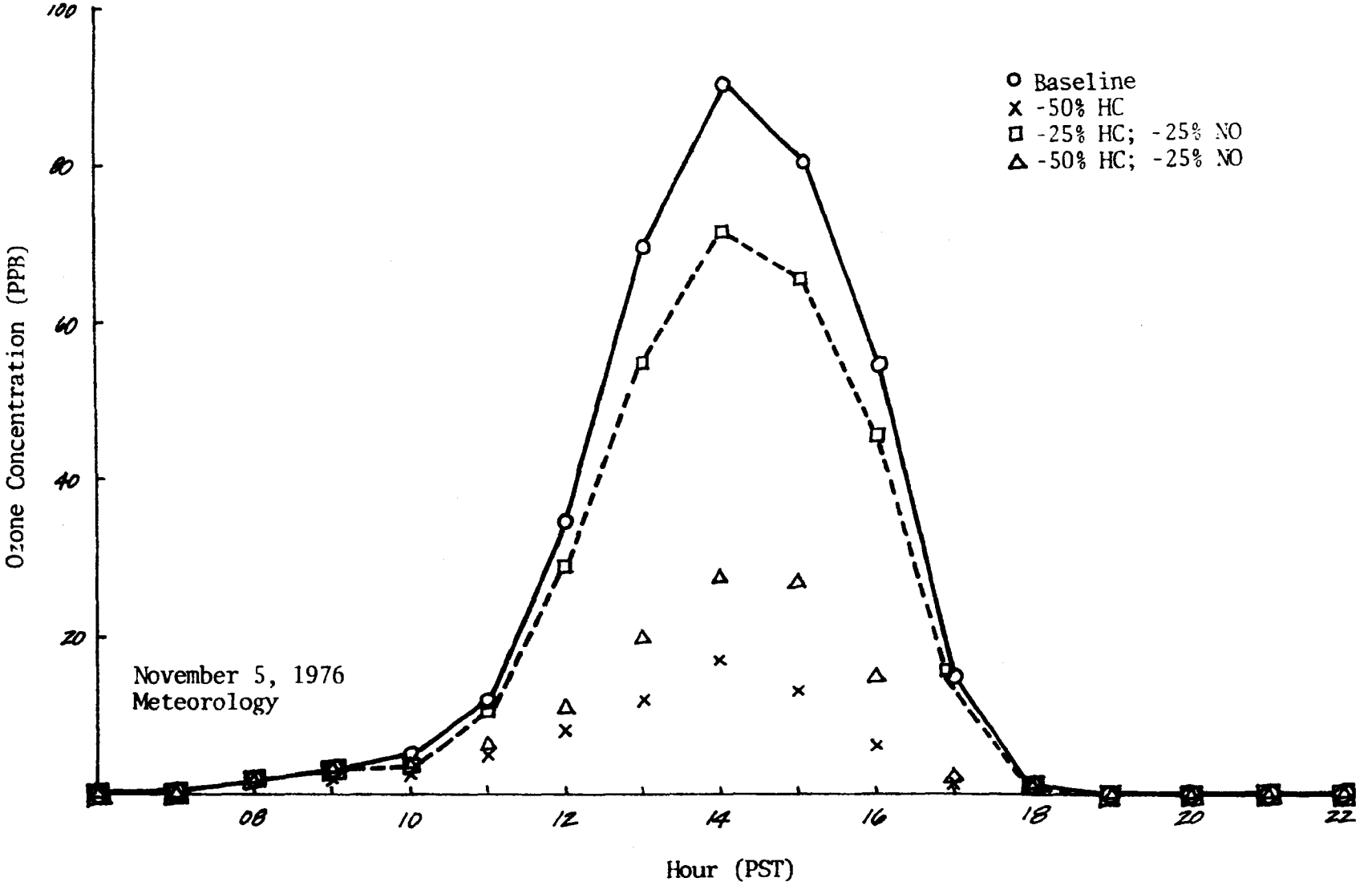


Figure B-7a. Hourly ozone concentrations at San Jose (DSJ) from LIRAQ simulations using 1985 baseline emissions and three combinations of HC and NO reductions.

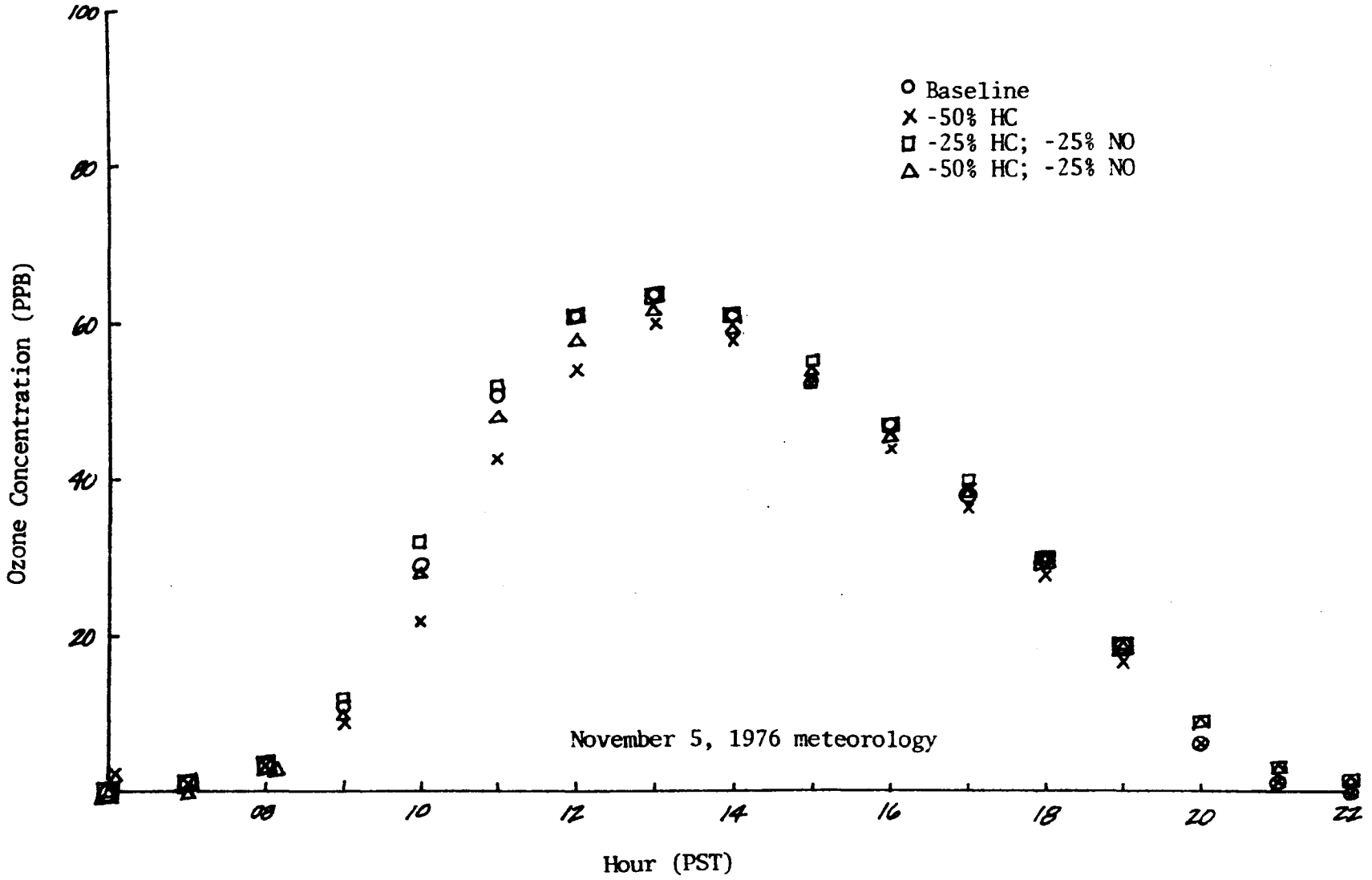


Figure B-7b. Hourly ozone concentrations at Livermore (DLI) from LIRAQ simulations using 1985 baseline emissions and three combinations of HC and NO reductions.

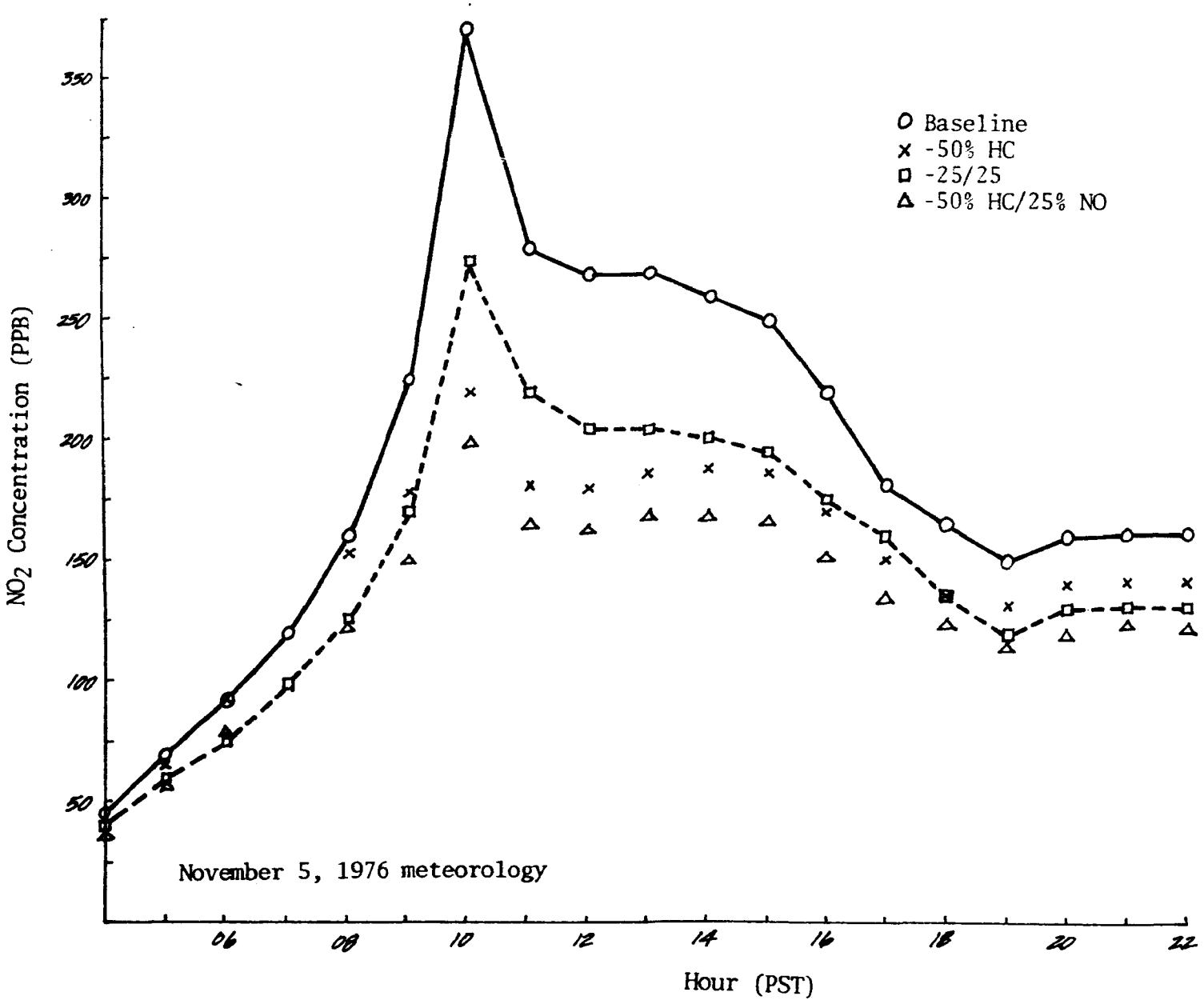


Figure B-8a. Hourly NO_2 concentration at San Francisco (DSF) from LIRAQ simulations using 1985 baseline emissions and three combinations of HC and NO reductions.

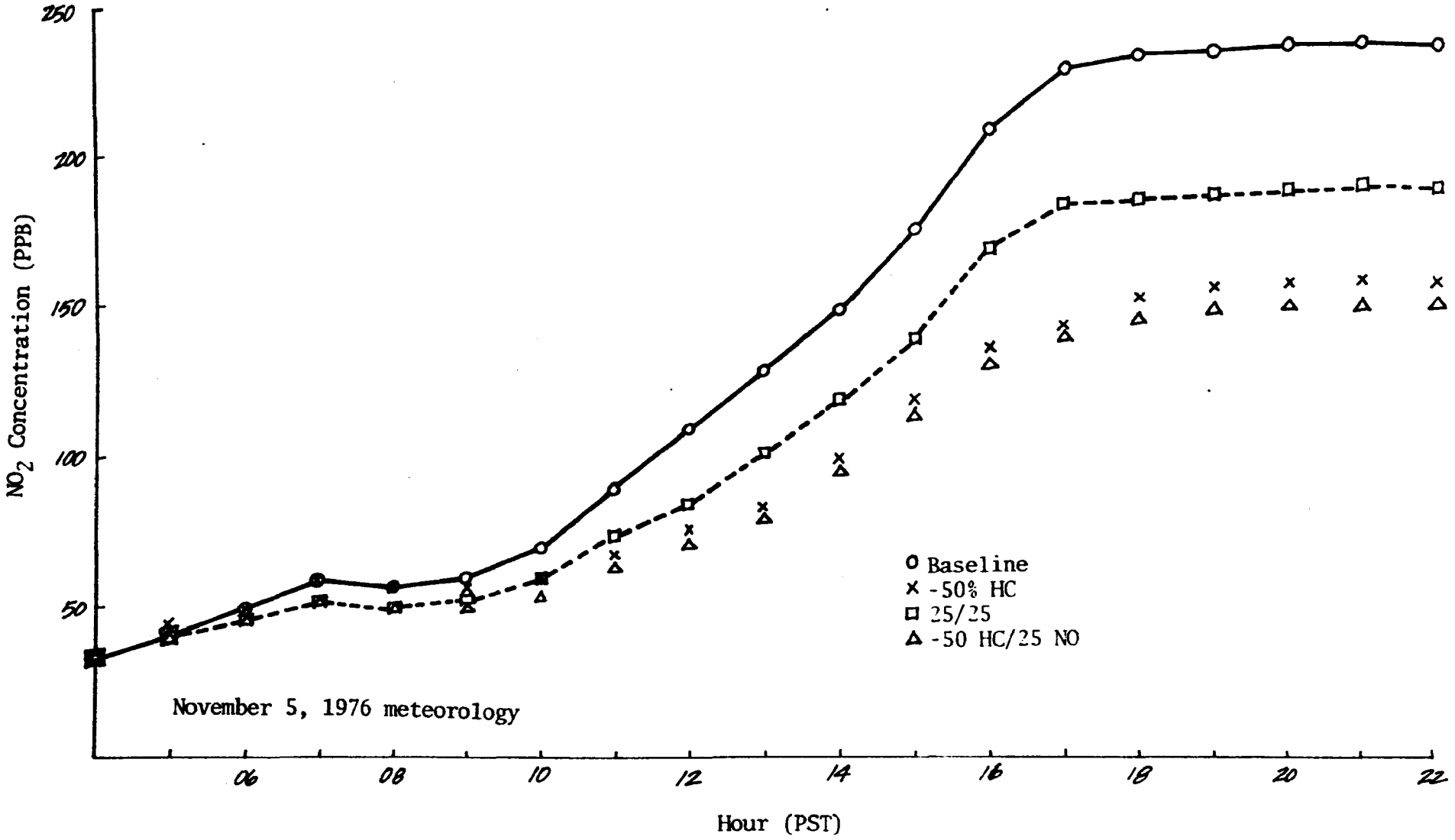


Figure B-8b. Hourly NO_2 concentrations at Burlingame (DBU) from LIRAQ simulations using 1985 baseline emissions and three combinations of HC and NO reductions.

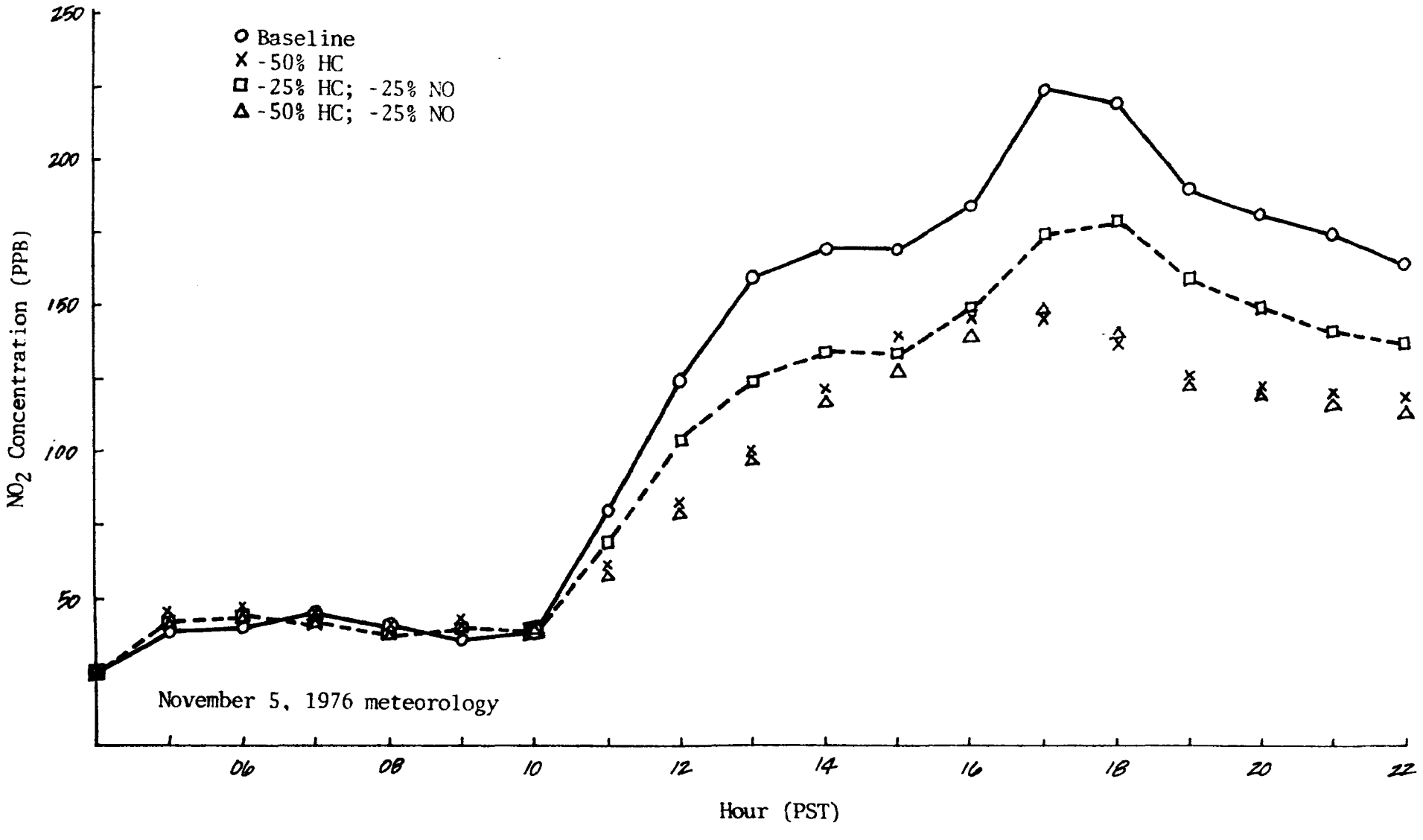


Figure B-8c. Hourly NO_2 concentrations at Oakland airport (AOA) from LIRAQ simulations using 1985 baseline emissions and three combinations of HC and NO reductions.

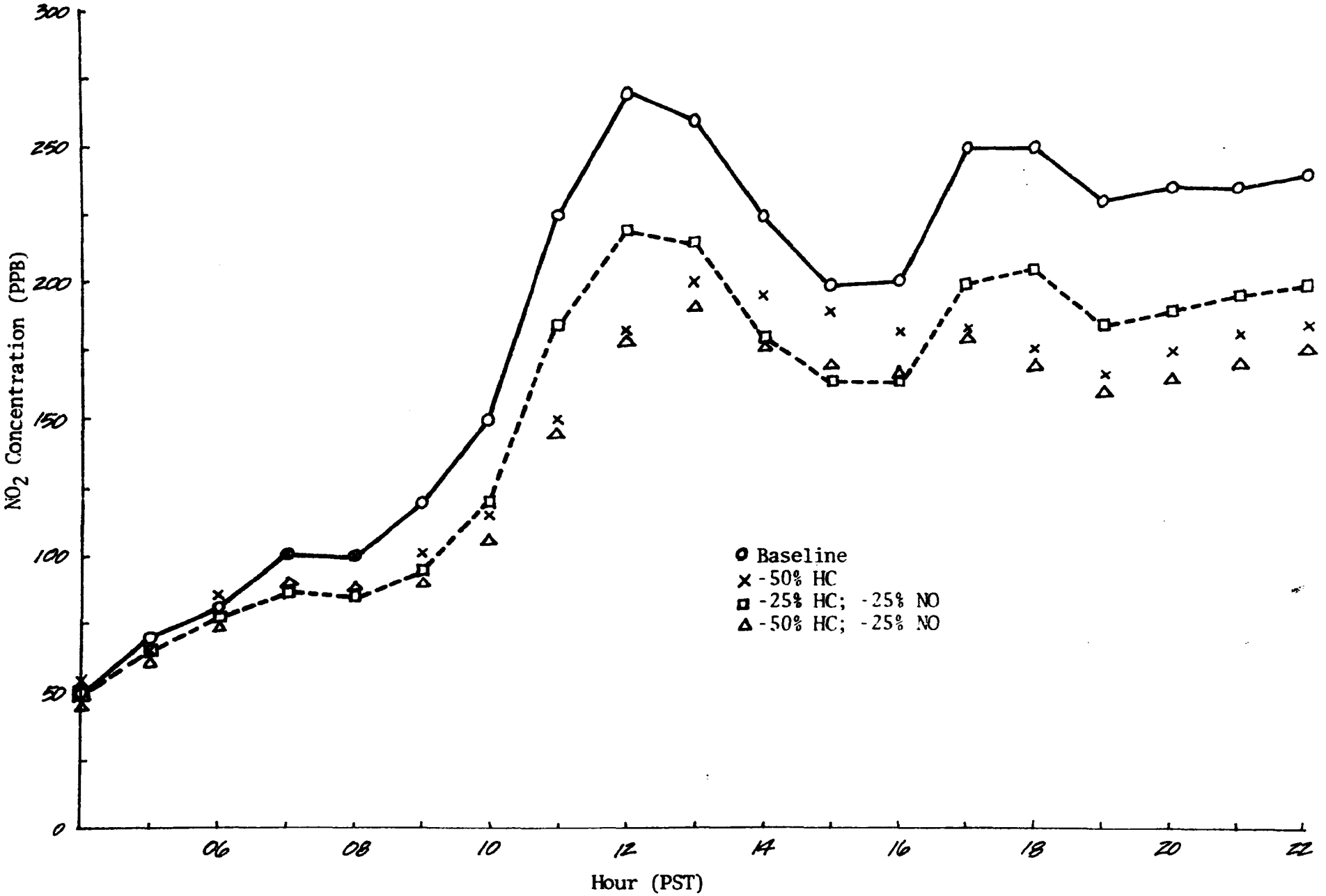


Figure B-8d Hourly NO_2 concentrations at San Jose (DSJ) from LIRAQ simulations using 1985 baseline emissions and three combinations of HC and NO reductions

APPENDIX C

Selected Mass Flux Streamline and Inversion Base Height Fields for the 20 August 1973 and 26 July 1973 Prototype Days.

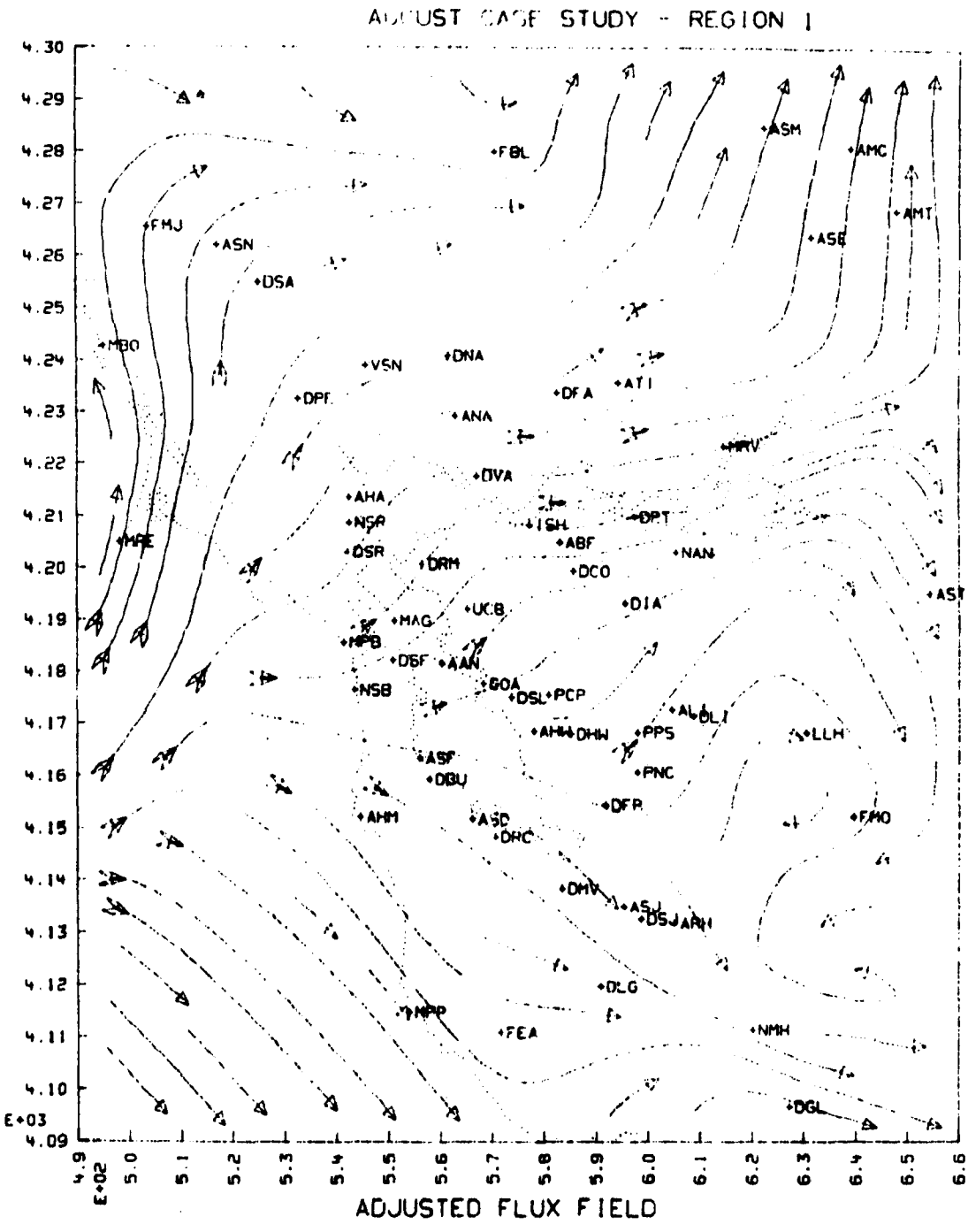


Fig. C-1a. Mass flux streamline computer analysis for 0830, August 20, 1973.

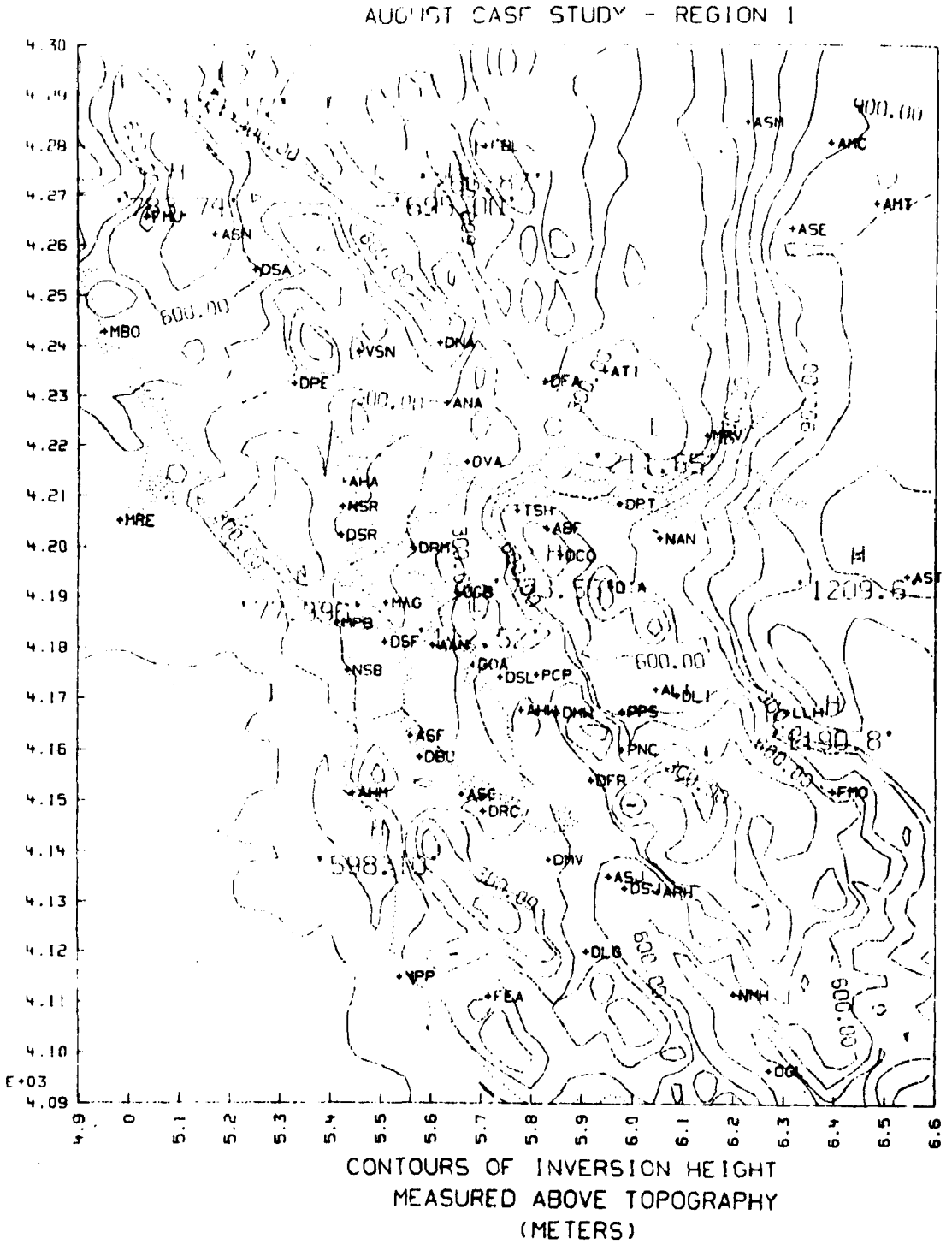


Fig. C-1b. Inversion base height (above topography) analysis for 0830, August 20, 1973.

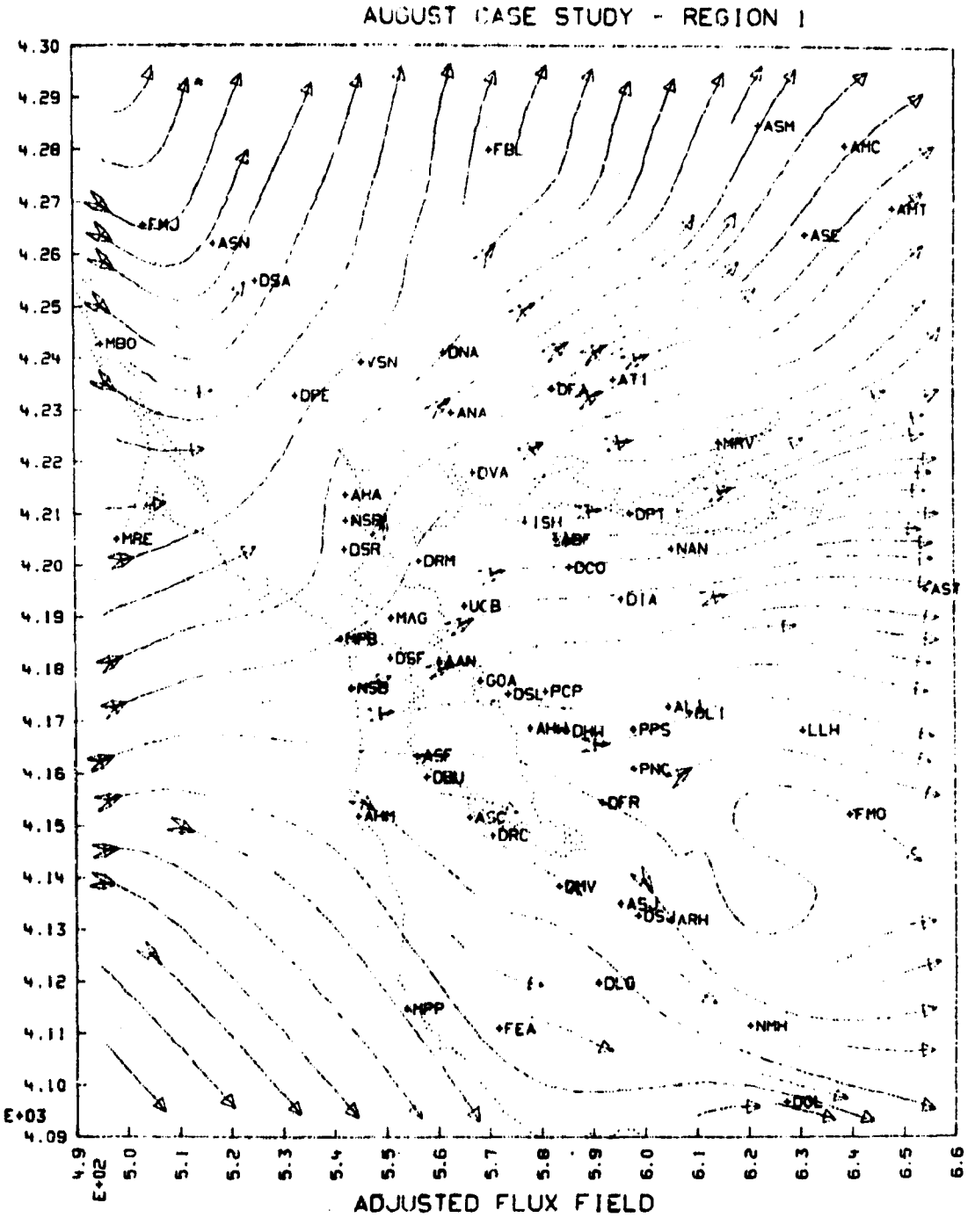


Fig. C-1c. **Mass flux streamline computer analysis for 1430, August 20, 1973.**

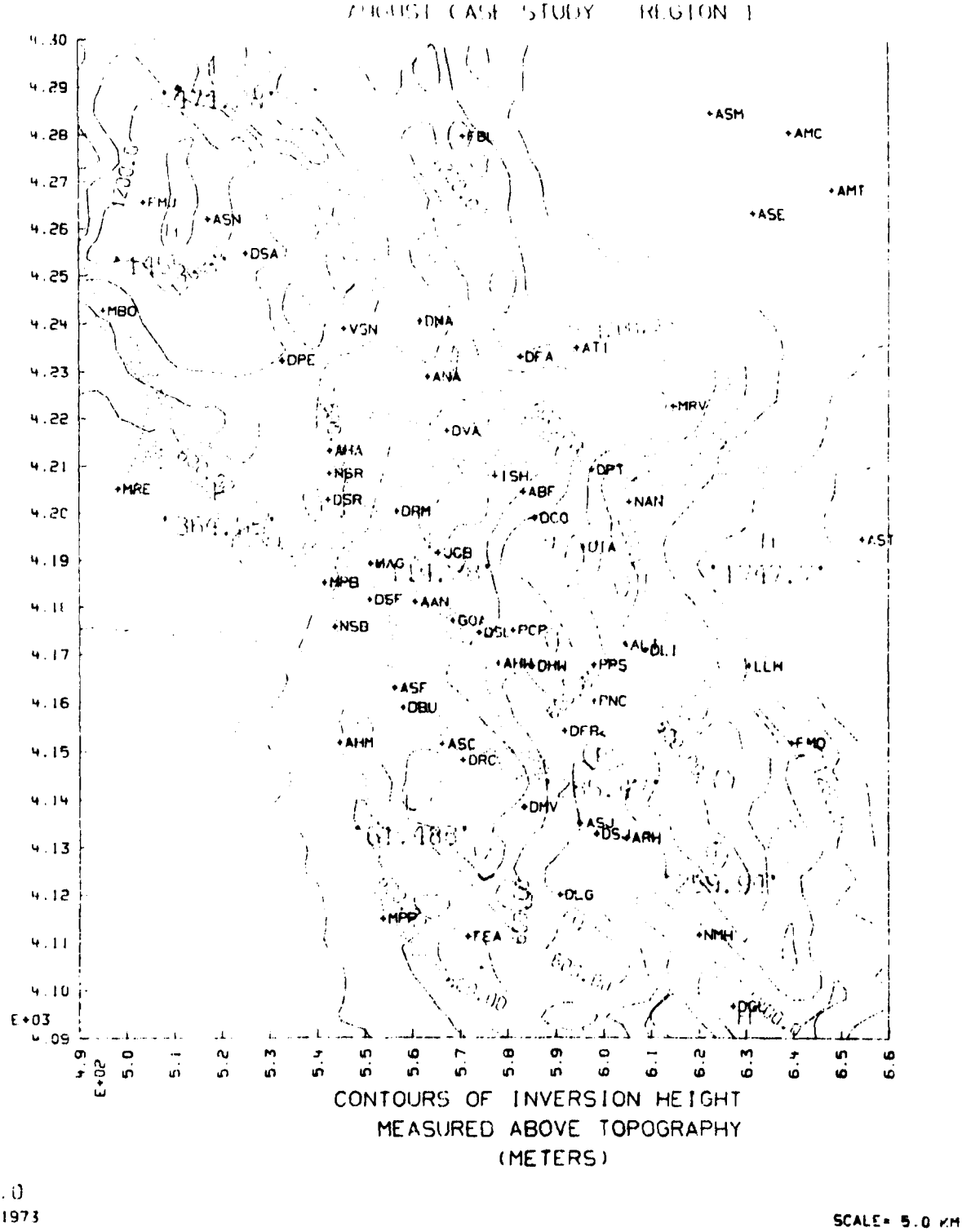


Fig. C-1d. Inversion base height (above topography) analysis for 1430, August 20, 1973.

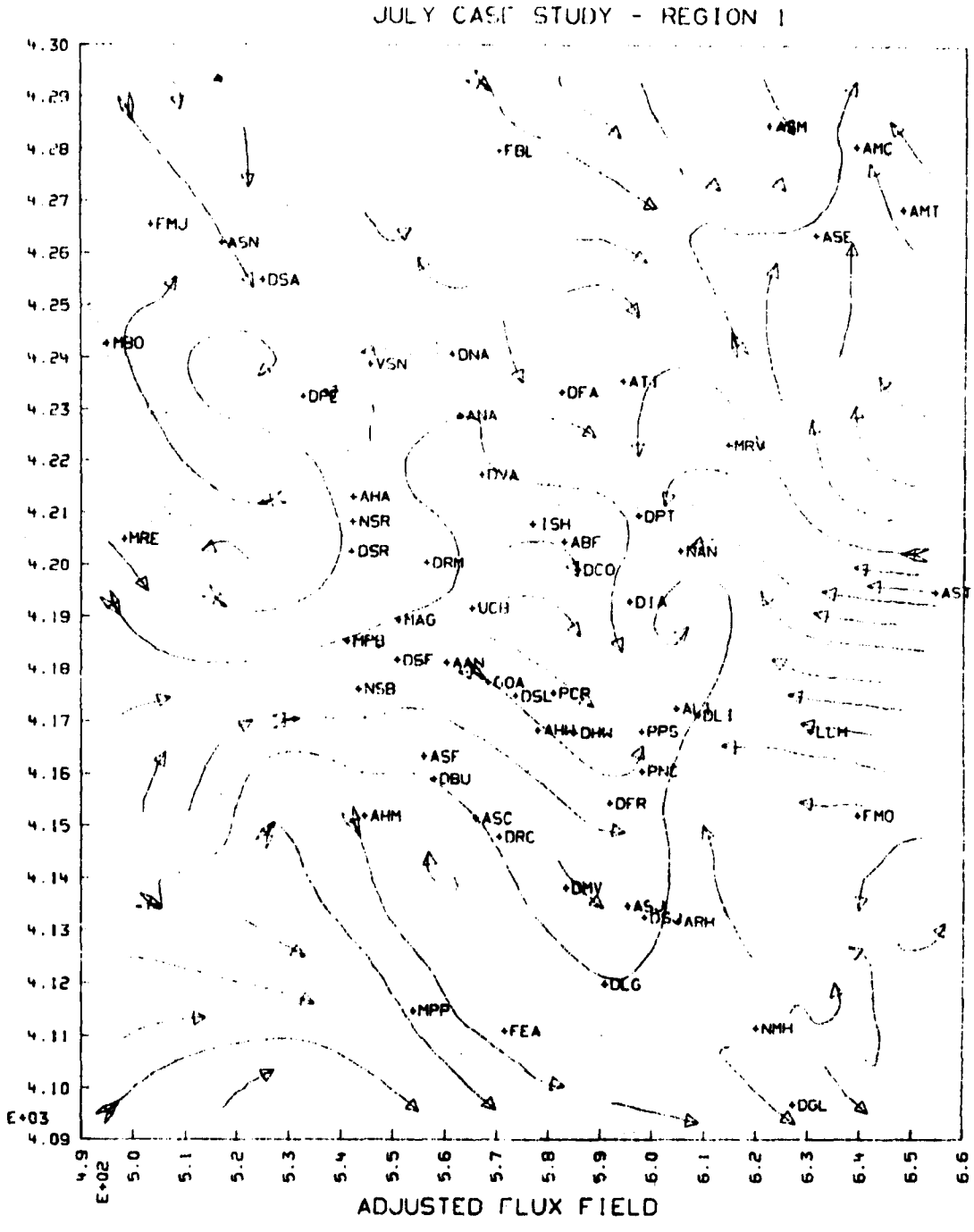


Fig. C-2a **Mass flux streamline computer analysis at 0830 on July 26, 1973.**

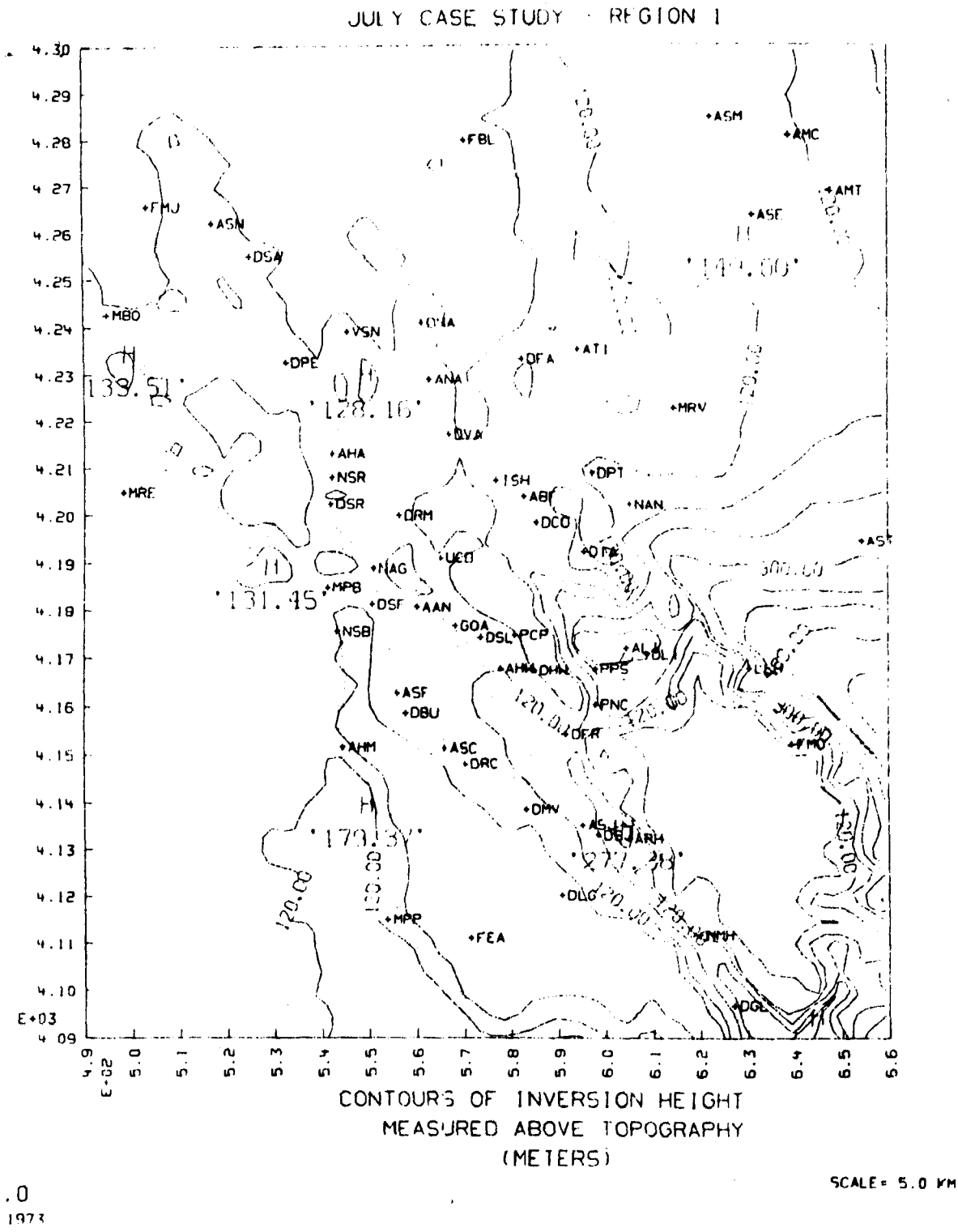


Fig. C-2b Inversion base height (above topography) analysis at 0830 on July 26, 1973.

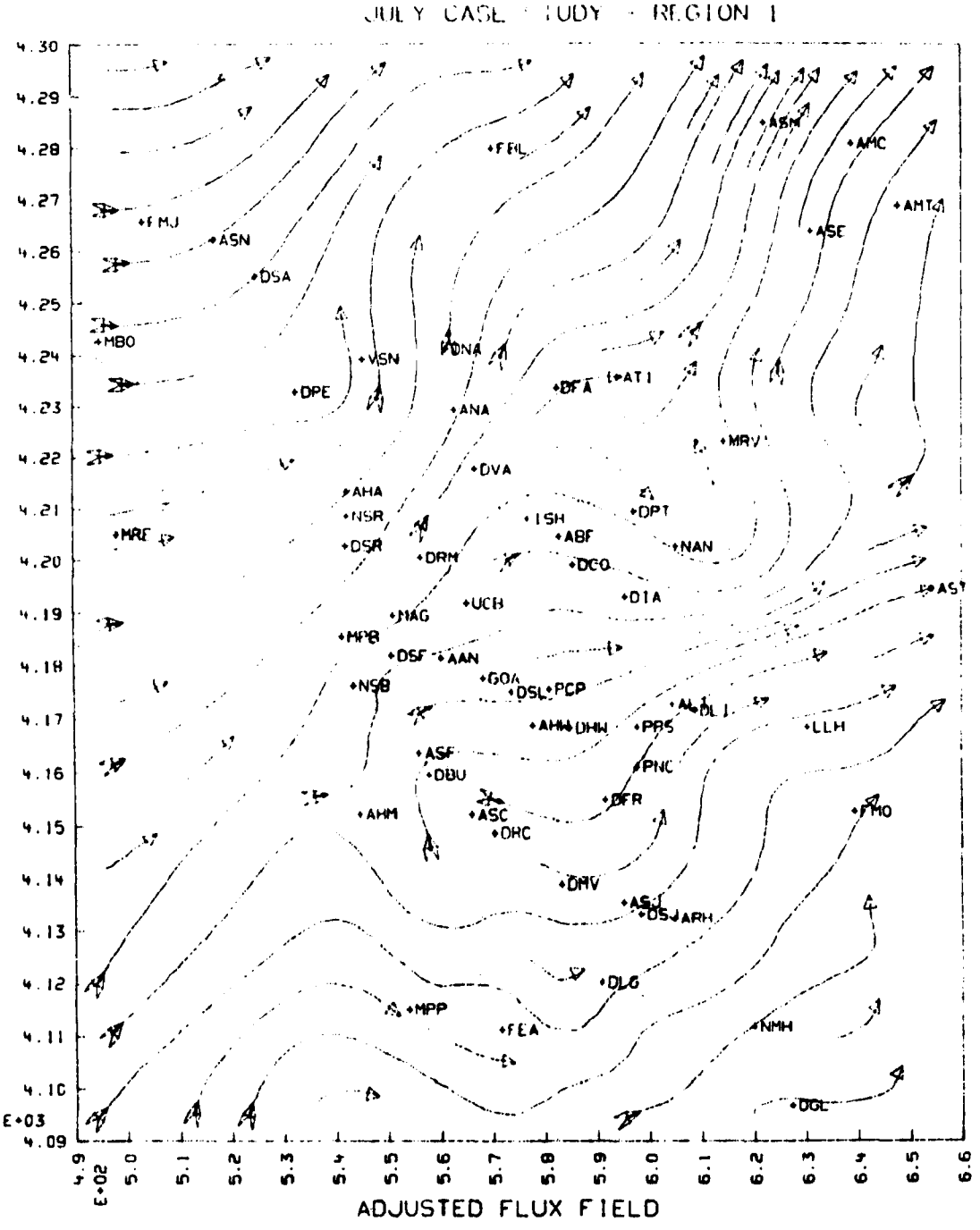


Fig. C-2c **Mass flux streamline computer analysis at 1430 on July 26, 1973.**

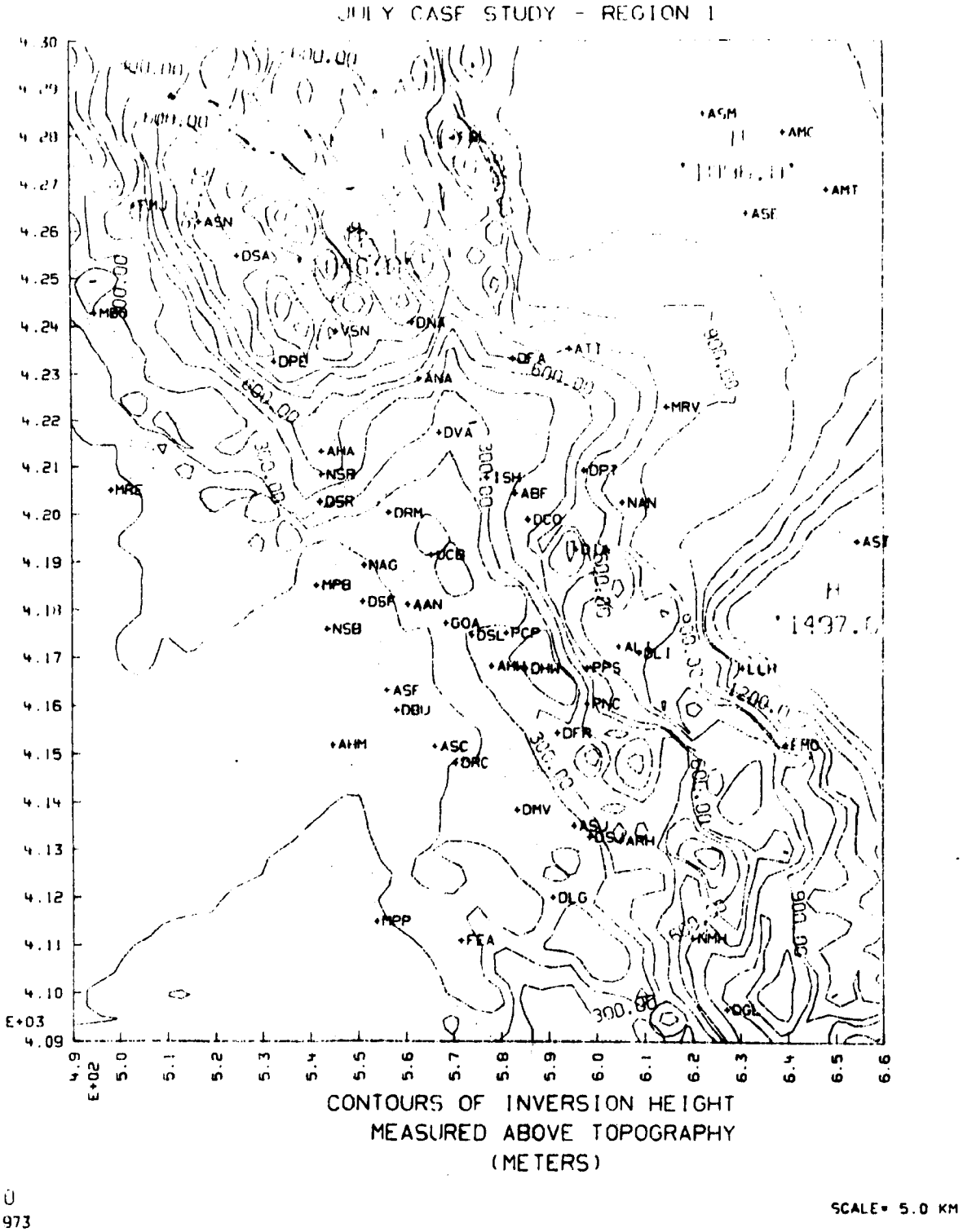


Fig. C-2d Inversion base height (above topography) analysis at 1430 on July 26, 1973.

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(Please read Instructions on the reverse before completing)

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16. ABSTRACT

A series of photochemical modeling experiments, using the LIRAQ model applied to the San Francisco Bay Area, was performed to investigate: a) model sensitivity to the spatial resolution of the gridded emissions, b) the impact of future HC and NO controls on the future Bay Area NO_2 levels, and c) the future impact of Bay Area HC and NO reductions on O_3 in adjacent downwind valleys.

The emission resolution experiments consisted of three simulations wherein emissions were smoothed over a) 5 x 5 km areas, b) 10 x 10 km areas, and c) distributed according to population. Changing from 5 km to 10 km resolution changed the O_3 maximum concentration by up to 10%. When emissions were distributed proportional to population substantial changes occurred in the timing and magnitude of the O_3 maxima.

The short-term NO_2 experiments consisted of simulating O_3 and NO_2 fields under meteorological conditions favoring high NO_2 buildups. Sensitivity runs were made which suggest that HC control is the most effective strategy for both O_3 and NO_2.

The long range transport experiments consisted of modifying LIRAQ to simulate an expanded 160 x 160 km region that included portions of the Sacramento and San Joaquin Valleys as a "receptor" region. The results showed that for the prototype day used, downwind O_3 was more strongly influenced by initial and boundary conditions than by Bay Area emissions changes.

17. KEY WORDS AND DOCUMENT ANALYSIS

a. DESCRIPTORS	b. IDENTIFIERS/OPEN ENDED TERMS	c. COSATI Field/Group
Photochemical Modeling SIP Development		

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