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UCRL - 76198
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CONF-750533--1

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# LIVERMORE REGIONAL AIR QUALITY MODEL (LIRAQ-1)

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Keith E. Grant

October 1975

This paper was prepared for presentation at
First Conference on Regional and Mesoscale Modeling, Analysis, and
Prediction of the American Meteorological Society,
May 6-9, 1975, Las Vegas, Nevada

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UCRL-76198

# LIVERMORE REGIONAL AIR QUALITY MODEL (LIRAQ-1)*

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## ABSTRACT

The Livermore Regional Air Quality (LIRAQ) model is an Eulerian grid model developed for use in assessing the regional air quality of a region with temporally and spatially varying meteorology in complex terrain. The first implementation of this approach is embodied in the LIRAQ-1 model and is intended for use with either simple chemical systems or relatively inert pollutants. The basic model formulation is based on the conservation of mass equation integrated vertically from the surface to the base of an inversion layer, thereby creating a single layer model with a grid structure established in the two horizontal dimensions. Surface pollutant concentrations are related to vertical average concentrations using a logarithmic profile. Atmospheric transport, inversion height, source emissions and topography are all prescribed. Data for the San Francisco Bay Area obtained during 1973 have been used in validation studies

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*This work was performed under the auspices of the U. S. Energy Research & Development Administration under contract No. W-7405-Eng-48 and supported in part by the National Science Foundation under agreement (AG-412).

## INTRODUCTION

With the support of the Research Applied to National Needs (RANN) program of the National Science Foundation, the Lawrence Livermore Laboratory (LLL) has been developing a regional air quality model for use by the Bay Area Air Pollution Control District (BAAPCD). NASA Ames Research Center (ARC) has also been supported mainly to provide aircraft data for model verification.

Our objective in this model development program has consisted of several elements, each of which we have had to be cognizant of during our work. This paper will focus briefly on each of them:

1. The model must be oriented to the needs of the user agency and readily useable by them;
2. Meeting the user needs in a region as spatially and temporally complex as the Bay Area (shown in Fig. 1) with its complex atmospheric chemistry and within the time constraints of the objective has necessitated some assumptions in model development; and
3. Model verification in the Bay Area is a necessary prerequisite to model utilization in application studies.

## MODEL PURPOSE AND STRUCTURE

Without attempting to preempt the options of the BAAPCD, let me indicate briefly what we have perceived as potential applications of the model.

These include:

1. Assessment of the present air quality pattern;
2. Capability for assessing the effectiveness of alert, short-term, long-term control strategies; and
3. Capability for assessing the potential effects of various land use and growth patterns.

Of particular interest in each of these cases with respect to our modeling effort are the regional effects of photochemical pollutants.

In response to these perceived needs we have developed the Livermore Regional Air Quality (LIRAQ) model. The LIRAQ model is actually a suite of codes, processors, and data banks which can be applied to solve a particular problem for the user. We originally envisioned a rather disparate set of codes requiring some substantial user participation. Discussions with the BAAPCD indicated they wanted to focus on problem formulation and analysis of the results. Thus, we have developed a structure which greatly simplifies the user's interaction with the model, as shown in Fig. 2.

Briefly, as implemented at LLL the user interacts with a problem formulator which interrogates the user via teletype for such information as grid size, pollutants of interest, modifications to the source file, choice of meteorological data set, output mode and so on. An executive routine then selects the appropriate data files from libraries of available data files, modifies the files as appropriate, chooses between the LIRAQ-1 model and the LIRAQ-2 model (Wuebbles, et al., 1975), runs the problem and sends the output to the user. The present status of this structure is that the BAAPCD has exercised nearly final versions of the model on the LLL computer via telephone coupler. We are now in the process of converting the whole structure to the Lawrence Berkeley Laboratory computer system. Their operating system will necessitate minor changes in the program interrelationships shown in Fig. 2 which will not be apparent to the user.

The models are set up to deal with either a 1, 2 or 5 km grid size, all referenced in terms of a Universal Transverse Mercator (UTM) coordinate system. Within limits of the number of grid elements, the grid can be located almost arbitrarily over the region (see Fig. 3); as for example, 5 km over the whole region, 2 km in the south Bay, or 1 km over an inland valley.

Once the grid is located, the model selects the appropriate topographic and geographic data, which have been developed from USGS data. Figure 4 shows a simulated three-dimensional plot of the topography of the area with 5 km resolution. A source inventory file can then be selected which includes emission information for several types of sources: (1) mobile sources (based on a cooperative effort with the Metropolitan Transportation Commission); (2) point sources (divided into surface and elevated); (3) airports; and (4) population based sources (based on census tract data under a cooperative effort with the Association of Bay Area Governments). Point sources are assumed spread over the grid square in which they are emitted. Each source type includes a temporal pattern, and source files are being projected for various future years to allow use in land use planning. The pollutants included in the data file are CO, NO, three categories of hydrocarbons [HC1 (mainly alkenes), HC2 (mainly alkanes), and HC4 (mainly aldehydes)], $SO_2$ and particulate. These latter two are not presently treated by our model, but emission data are available in the data base. For studying particular land use applications, the source inventory can be modified in various ways based on user input to the problem formulator.

The model does not try to predict the meteorological fields, a research topic which has been discussed in some detail at this meeting. Rather, meteorological data are generated from data collected on particular observation days and adjusted in a mass consistent sense using the MASCON model described by Dickerson (1975). Thus, the model is supplied with wind fields, mixing depth, horizontal diffusion coefficients, and surface vertical diffusion coefficients at three hour intervals. The variables are then interpolated between these times. Initial concentrations based on observed data are also supplied for the time at which the user wants to start the model calculation. This has posed problems in the Bay Area since observations are typically from urban areas and are not generally applicable in the many undeveloped parts of the region.

The two air quality models which are available are LIRAQ-1 and LIRAQ-2, with a comparison of their capabilities shown in Table 1. LIRAQ-1 is intended for use on non-photochemically active species (such as CO) or for pollutants for which only source and transport processes want to be studied (possibly NO and some hydrocarbons). Such relatively straightforward photochemical schemes as those used by Eschenroeder and Martinez (1972) could be included. The solution method for the advection is explicit using the flux corrected transport (FCT) method of Boris and Book (1973), generalized to treat time and space varying mixing depth. This makes the solution method at least second order accurate in terms of spatial differencing.

The LIRAQ-2 model, described by Wuebbles, et al. (1975), is intended to treat photochemically active species. Because of the number of species and reactions, it is more limited in the number of grid elements which can be treated and the transport is only solved using a first order accurate differencing scheme.

## PHYSICAL BASIS OF THE LIRAQ MODEL

Both the LIRAQ-1 and LIRAQ-2 models are based on the same physical representation of an air quality region. The basic equation to solve is the continuity equation for each of the N species, as reviewed recently by Reynolds, et al. (1973) and given in Fig. 5. For several reasons, including first the need to somewhat simplify the three-dimensional model to suit user and computer needs; second, the general lack of knowledge about the vertical structure within the well-mixed layer; and third, the difficulty of representing both topography and changing mixing layer depth in terms of a vertical grid structure, we have chosen to simplify the problem by integrating the continuity equation vertically through the well-mixed layer. The resulting geometry is shown conceptually in Fig. 6. In doing this we make some assumptions about the vertical structure below the inversion, as listed in Fig. 7.

If we now carry out the vertical integration we end up with a new mass continuity equation appropriate for the well mixed layer where the depth H can change in space and time. This form of the equation is given in Fig. 8, where the terms represent advection, vertical flux through the inversion (due to ablation, reformation and gradient flow through the inversion) eddy fluctuations, sources, and reactions.

As indicated earlier the flux and inversion height terms are provided based on the mass-consistent wind field analysis described by Dickerson (1975). In the LIRAQ-1 model we have emphasized the treatment of the source and transport terms, using a second order accurate finite differencing scheme, and we take the reaction term to be zero. Further details on the mathematical formulation will be available in the Final Report on this project (MacCracken and Sauter, 1975).

## MODEL RESULTS

One of the major tasks of this project has been to develop the appropriate data bases to allow verification of the model. The initial verification study is for an air pollution episode on July 26-27, 1973. This was actually the last day of a three day period with relatively high photochemical air pollution, but measurements were only available in sufficient detail for July 26.

The results in this paper give preliminary model results for carbon monoxide concentrations during the 24 hour period beginning at 0400 July 26. Simulation results for both 2 and 5 km grid resolution have been carried out. The 5 km simulation was limited to a grid of 14 by 16 grid squares, while the 2 km results cover a slightly larger region. Regional surface air quality patterns (Fig. 9) early in the simulation from the 5 km grid run show the expected correlation with the emission pattern. Results from an early 2 kilometre study (Fig. 10) show an even stronger correlation of surface concentrations with sources, as would be expected, and quite high peak concentrations in heavily urbanized areas.

Time histories of concentration for some stations show very good agreement and for others rather disappointing agreement (Figs. 11-13). We do not yet have enough experience with these simulations to determine whether the problem lies with the model, with the emission inventory associated with off highway traffic, with representativeness of station location (e.g., the San Francisco station is atop a seven story building), or any of numerous other potential problem areas. Nonetheless, we have carried out some initial statistical assessments. Correlation coefficients at individual stations range from 0.15 to 0.85. The low value in Fremont (Fig. 12), however, appears to be in large part a result of the limited variation in the observations, resulting in a nearly constant pollutant level through the day. Collectively, the correlation coefficient for 199 hourly average data points for which comparison is possible is 0.59.

## SUMMARY

The LIRAQ model is actually a suite of interconnected models designed to be applied to air quality and land use planning questions by the BAAPCD. This paper has briefly reviewed the status of the LIRAQ-1 model, which is designed to treat non-reacting pollutants. In general, the pattern of observed air quality is well represented, and to a large extent so are actual magnitudes. Further model verification by both LLL and the BAAPCD should provide the basis for model utilization by the BAAPCD.

## ACKNOWLEDGEMENTS

The development and utilization of this model has been greatly aided by the efforts of Ted Stullich.

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## DIFFERENCES BETWEEN THE

## LIRAQ-1 AND LIRAQ-2 MODELS

| VARIABLE | LIRAQ-1 CAPABILITY | LIRAQ-2 CAPABILITY |
|---|---|---|
| POLLUTANT | NON-REACTIVE | REACTIVE |
| MAXIMUM GRID LIMITS | 45 X 50 | 20 X 20 |
| ACCURACY OF SPATIAL DIFFERENCING SCHEME | SECOND ORDER | FIRST ORDER |
| NUMBER OF SPECIES | $\leq 4$ | 15 ACTIVE<br>4 STEADY STATE |

TABLE 1.

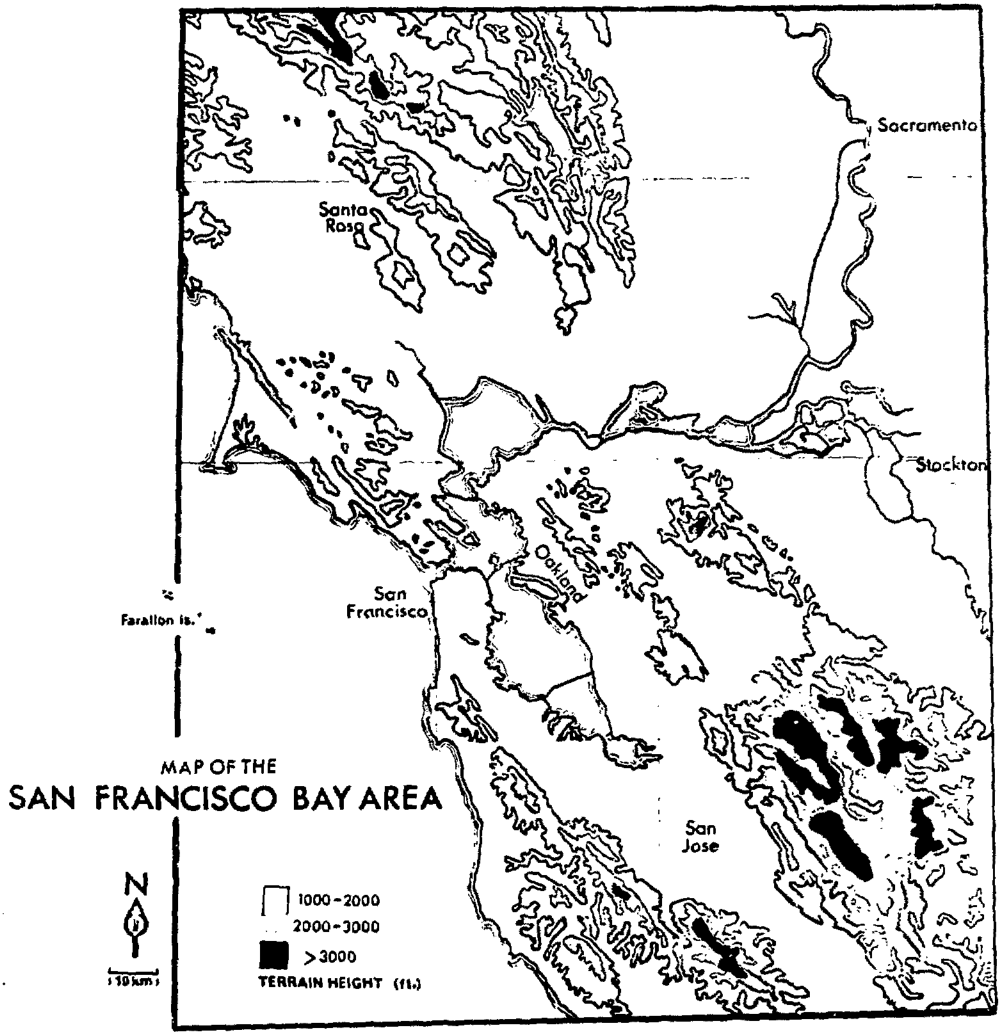

Sacramento
Santa Rosa
Stockton
Oakland
San Francisco
Farallon Is.
San Jose
MAP OF THE
SAN FRANCISCO BAY AREA
N
10 km
1000-2000
2000-3000
>3000
TERRAIN HEIGHT (ft.)

FIGURE 1

## LIRAQ MODEL OPERATION

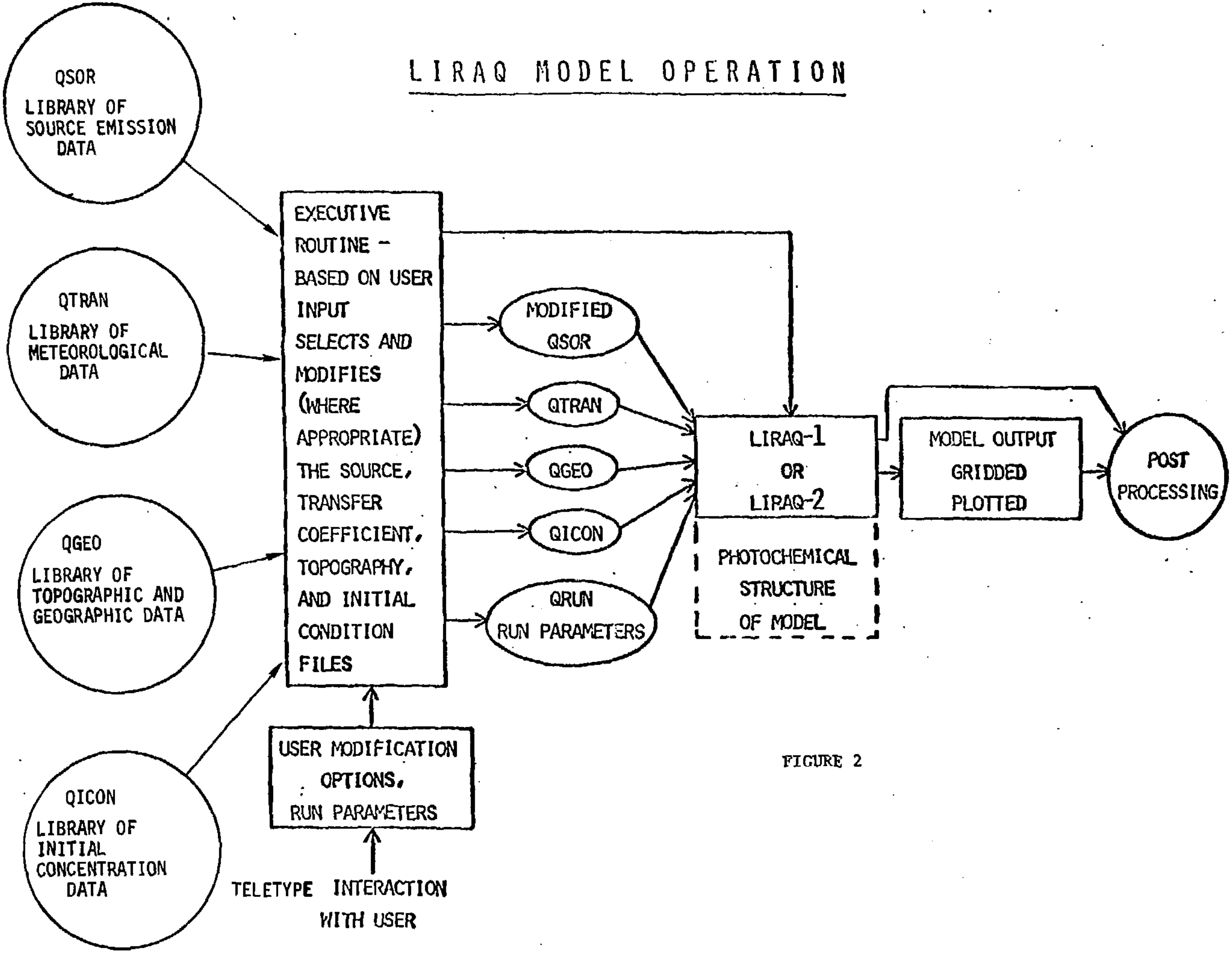


FIGURE 2

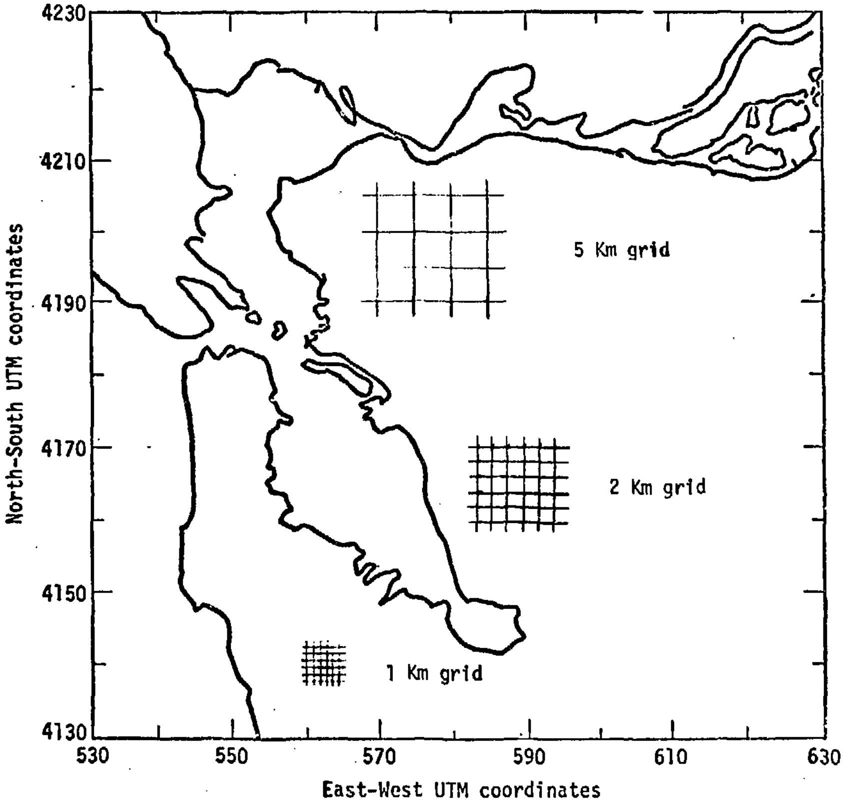

4230
4210
4190
4170
4150
4130
530
550
570
590
610
630
North-South UTM coordinates
East-West UTM coordinates
5 Km grid
2 Km grid
1 Km grid

FIGURE 3

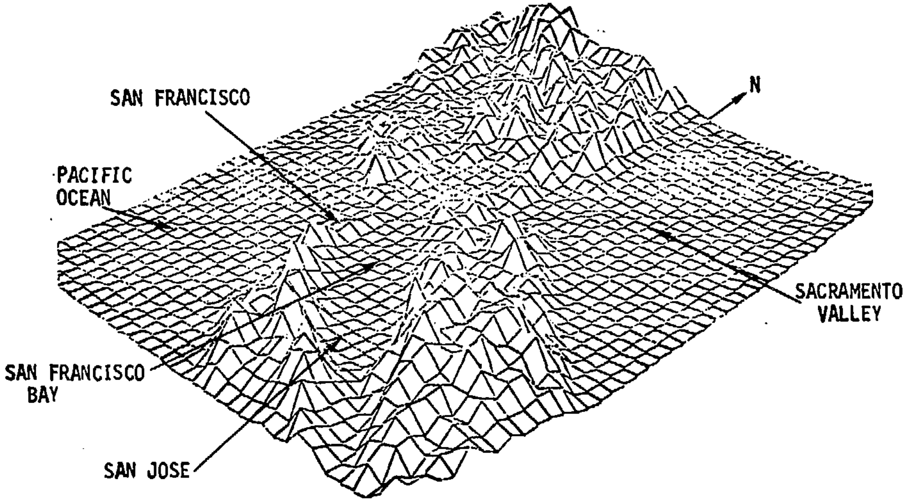

SAN FRANCISCO
PACIFIC OCEAN
N
SAN FRANCISCO BAY
SAN JOSE
SACRAMENTO VALLEY

FIGURE 4

## GENERALIZED CONTINUITY EQUATION

$$\frac{\partial c_i}{\partial t} + \frac{\partial}{\partial x}(uc_i) + \frac{\partial}{\partial y}(vc_i) + \frac{\partial}{\partial z}(wc_i) =$$

$$\frac{\partial}{\partial x}\left(K \frac{\partial c_i}{\partial x}\right) + \frac{\partial}{\partial y}\left(K \frac{\partial c_i}{\partial y}\right) + \frac{\partial}{\partial z}\left(K_z \frac{\partial c_i}{\partial z}\right) + \frac{S_i}{\rho} + R_i\ (c_1,\ldots,c_N)$$

where

| | |
|---|---|
| $u,v,w$ | Cartesian frame velocities |
| $c_i$ | concentration of species i |
| $S_i$ | non-reaction related sources and sinks of species i |
| $R_i$ | chemical and photochemical reaction sources and sinks for species i |
| $K$ | horizontal eddy diffusion coefficient |
| $K_z$ | vertical eddy diffusion coefficient |
| $\rho$ | air density |

FIGURE 5

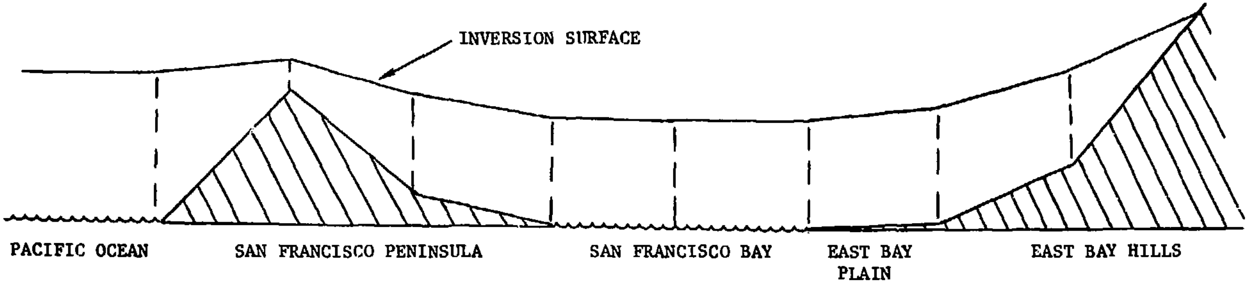

INVERSION SURFACE
PACIFIC OCEAN
SAN FRANCISCO PENINSULA
SAN FRANCISCO BAY
EAST BAY PLAIN
EAST BAY HILLS

FIGURE 6.

## FIGURE 7

## ASSUMPTIONS FOR DEVELOPMENT OF LIRAQ

1. Power law wind profile applicable in well-mixed layer

$$u(x,y,z,t) = u_0(x,y,t) \left(\frac{z}{z_0}\right)^n$$

2. Logarithmic pollutant profile in well mixed layer such that

$$c_i(x,y,z,t) = a(x,y,t) + b(x,y,t) \ln \frac{z}{z_0}$$

where derive a and b from conditions that

$$\bar{c}(x,y,t) \cong \frac{1}{H(x,y,t)} \int_{z_0}^{H(x,y,t)} c(x,y,z,t)\, dz$$

and vertical equilibrium boundary condition for surface

$$K_z(x,y,z_0,t) \left.\frac{dc_i}{dz}\right|_{z=z_0} + \frac{q_i}{\rho} - v_D\, c_i(x,y,z_0,t) = 0$$

3. Horizontal eddy diffusion coefficient

$$K = \bar{K}(x,y,t) = \frac{1}{H} \int_{z_0}^{H} K(x,y,z,t)\, dz$$

where

$$K(x,y,z,t) = \varepsilon^{1/2}\, \sigma^{4/3}$$

$$\varepsilon = \varepsilon_0 \frac{z_0}{z} \left(\frac{u}{u_0}\right)^3$$

$$\sigma = 0.7\, \Delta x = 0.7\, \Delta y$$

## FIGURE 8
## CONTINUITY EQUATION AS
## VERTICALLY INTEGRATED THROUGH WELL-MIXED LAYER

$$\frac{\partial}{\partial t}(H\bar{c}_i) + \frac{\partial}{\partial x}\{H\bar{c}_i\bar{u} \cdot (1+\beta_i)\} + \frac{\partial}{\partial y}\{H\bar{c}_i\bar{v} \cdot (1+\beta_i)\} + W_i =$$

$$\frac{\partial}{\partial x}\{K\frac{\partial}{\partial x}(H\bar{c}_i)\} + \frac{\partial}{\partial y}\{K\frac{\partial}{\partial y}(H\bar{c}_i)\} + \frac{S_i}{\rho} + HR_i(\overline{c_1},\ldots,\overline{c_N})$$

where

$$\beta_i = \frac{n}{n+1}\ \frac{b_i}{c_i}$$

$$W_i = \begin{cases} -w(x,y,H,t)c_i(x,y,H,t) & W \geq 0 \\ -w(x,y,H,t)c_i(\text{above inversion}) & W < 0 \end{cases}$$

and where applicable in the term $R_i$

$$\overline{c_j c_k} = \overline{c_j}\,\overline{c_k}\ \{1 + (\frac{n+1}{n})^2\ \beta_j\beta_k\}$$

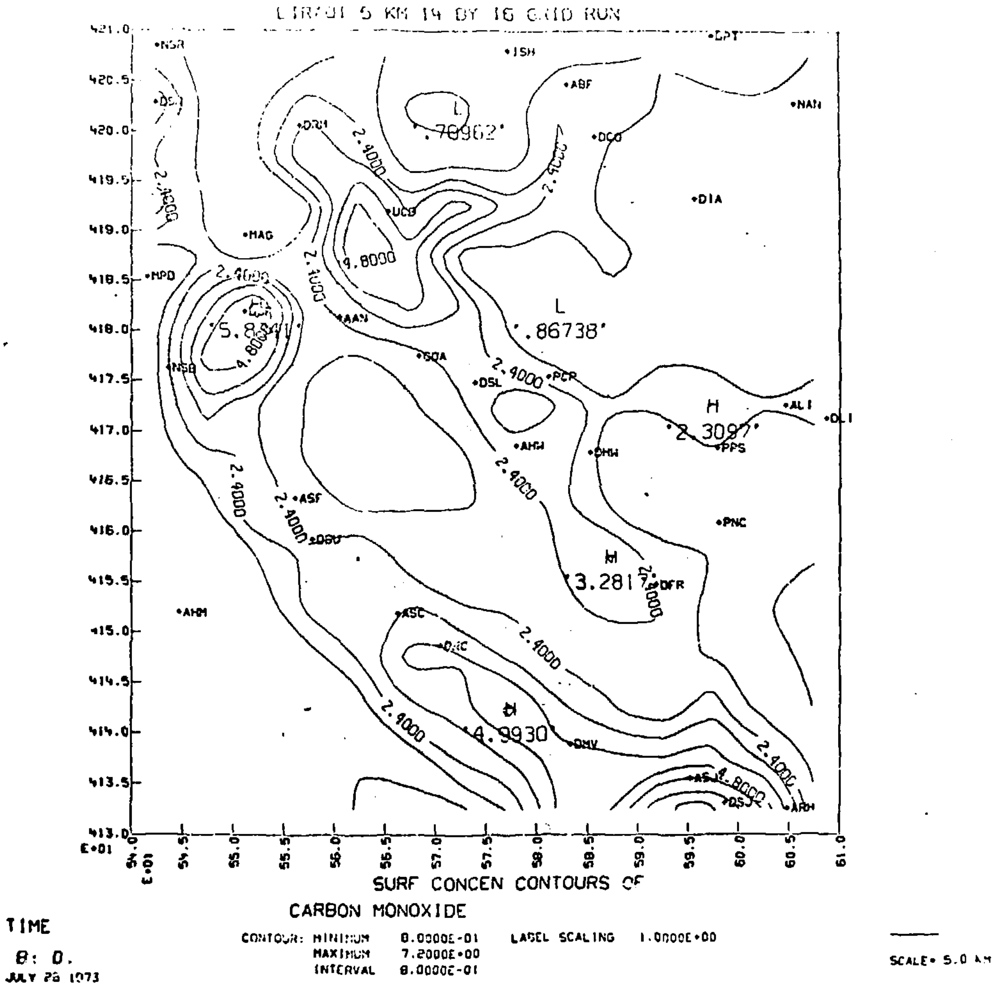

LIRAQ1 5 KM 14 BY 16 GRID RUN
421.0
420.5
420.0
419.5
419.0
418.5
418.0
417.5
417.0
416.5
416.0
415.5
415.0
414.5
414.0
413.5
413.0
E+01
54.0
54.5
55.0
55.5
56.0
56.5
57.0
57.5
58.0
58.5
59.0
59.5
60.0
60.5
61.0
10+3
NSR
DSJ
DRM
MAG
MPD
UCB
AAN
GOA
DSL
PCP
ISH
ABF
DCO
DIA
DPT
NAN
ALI
DLI
PPS
DMW
AHW
PNC
ASF
DGU
DFR
AHM
ASC
DMC
DMV
ASJ
DSJ
ARH
L
.70962
L
.86738
H
2.3097
H
3.2817
H
4.9930
H
5.8841
2.4000
4.8000
SURF CONCEN CONTOURS OF
CARBON MONOXIDE
CONTOUR: MINIMUM 0.0000E-01
MAXIMUM 7.2000E+00
INTERVAL 8.0000E-01
LABEL SCALING 1.0000E+00
TIME
8: 0.
JULY 26 1973
SCALE= 5.0 KM

FIGURE 9

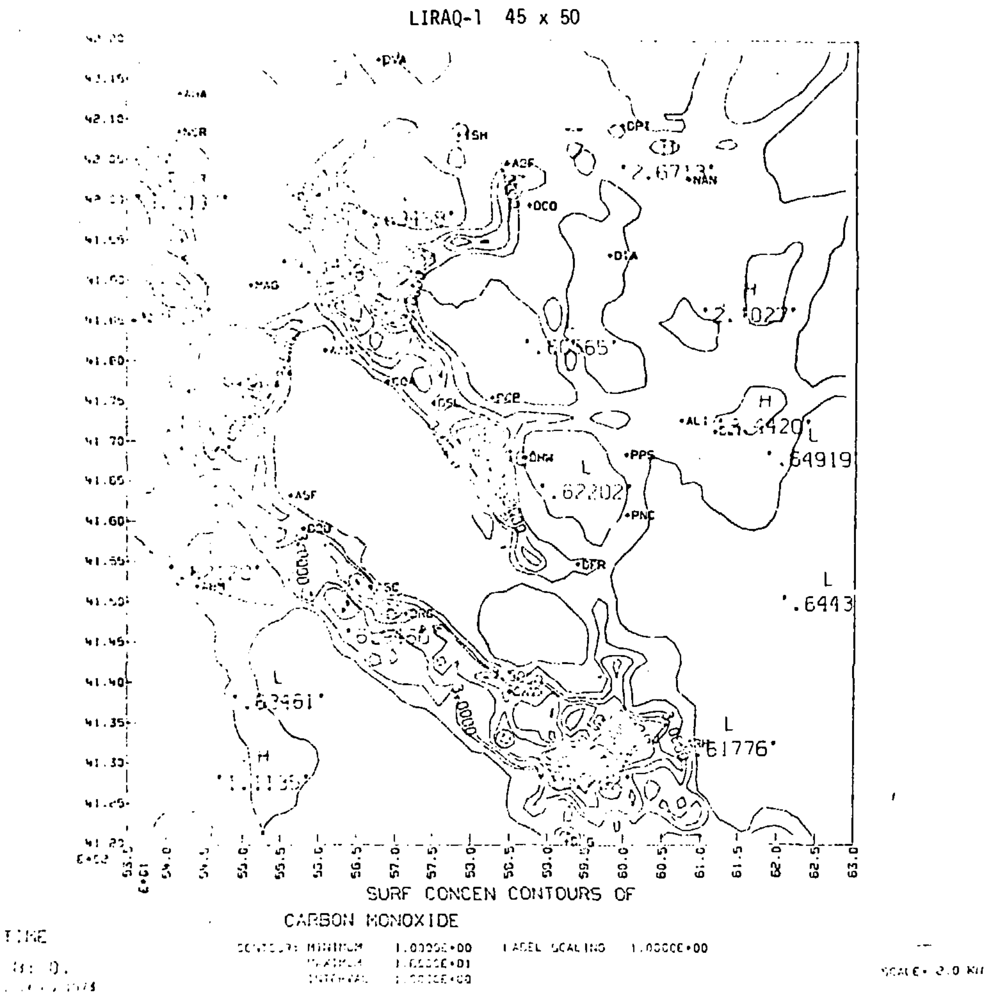

LIRAQ-1 45 x 50
SURF CONCEN CONTOURS OF
CARBON MONOXIDE
TIME
CONTOUR: MINIMUM 1.0000E+00
MAXIMUM 1.6500E+01
INTERVAL 1.0000E+00
LABEL SCALING 1.0000E+00
SCALE= 2.0 KM
PVA
SH
CPI
ASE
DCO
NAN
DIA
MAG
CCA
CSL
SCB
ALI
PPS
PNC
DHW
DFR
ASF
DCO
SC
L
H
2.6713
2.027
.60565
.62202
.64919
.6443
.62461
.61776
1.1135
3.0000
41.20
41.25
41.30
41.35
41.40
41.45
41.50
41.55
41.60
41.65
41.70
41.75
41.80
41.85
41.90
41.95
42.00
42.05
42.10
42.15
42.20
53.5
54.0
54.5
55.0
55.5
56.0
56.5
57.0
57.5
58.0
58.5
59.0
59.5
60.0
60.5
61.0
61.5
62.0
62.5
63.0
E+02
E+01

FIGURE 10

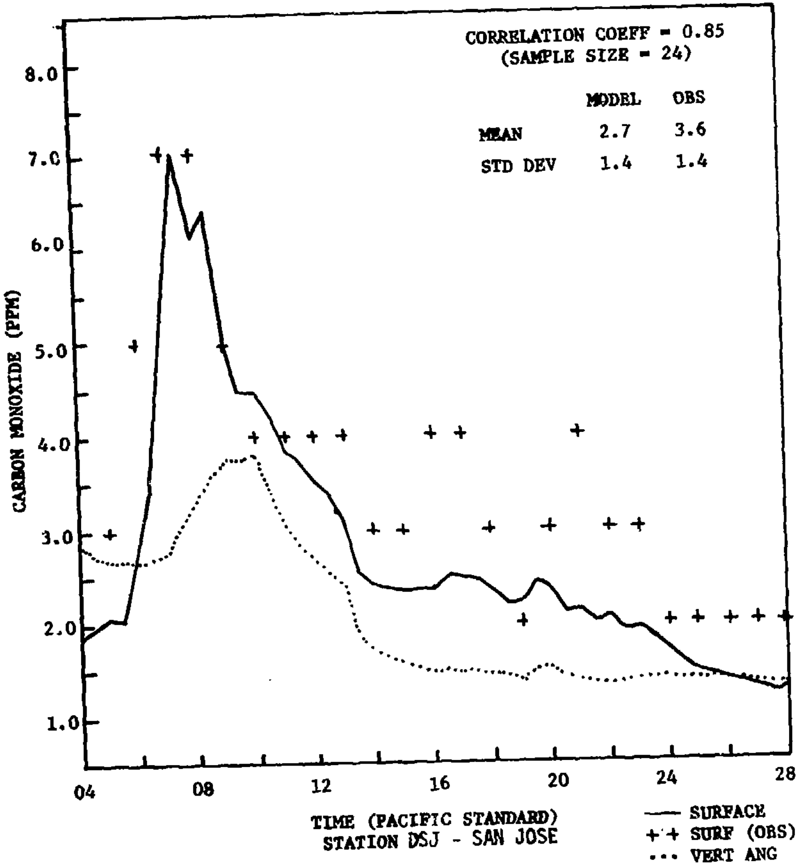
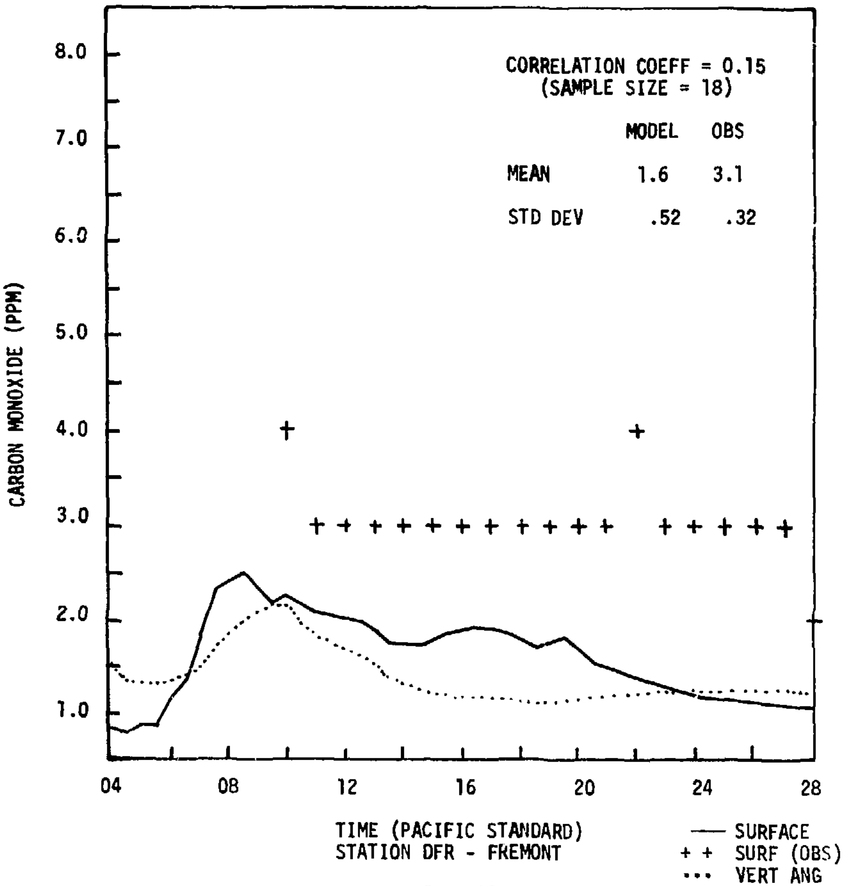

CORRELATION COEFF = 0.85
(SAMPLE SIZE = 24)
MODEL
OBS
MEAN 2.7 3.6
STD DEV 1.4 1.4
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
CARBON MONOXIDE (PPM)
04
08
12
16
20
24
28
TIME (PACIFIC STANDARD)
STATION DSJ - SAN JOSE
SURFACE
+ + SURF (OBS)
... VERT ANG

FIGURE 11



CORRELATION COEFF = 0.15
(SAMPLE SIZE = 18)
MODEL
OBS
MEAN
1.6
3.1
STD DEV
.52
.32
CARBON MONOXIDE (PPM)
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
04
08
12
16
20
24
28
TIME (PACIFIC STANDARD)
STATION DFR - FREMONT
SURFACE
+ + SURF (OBS)
... VERT ANG

FIGURE 12

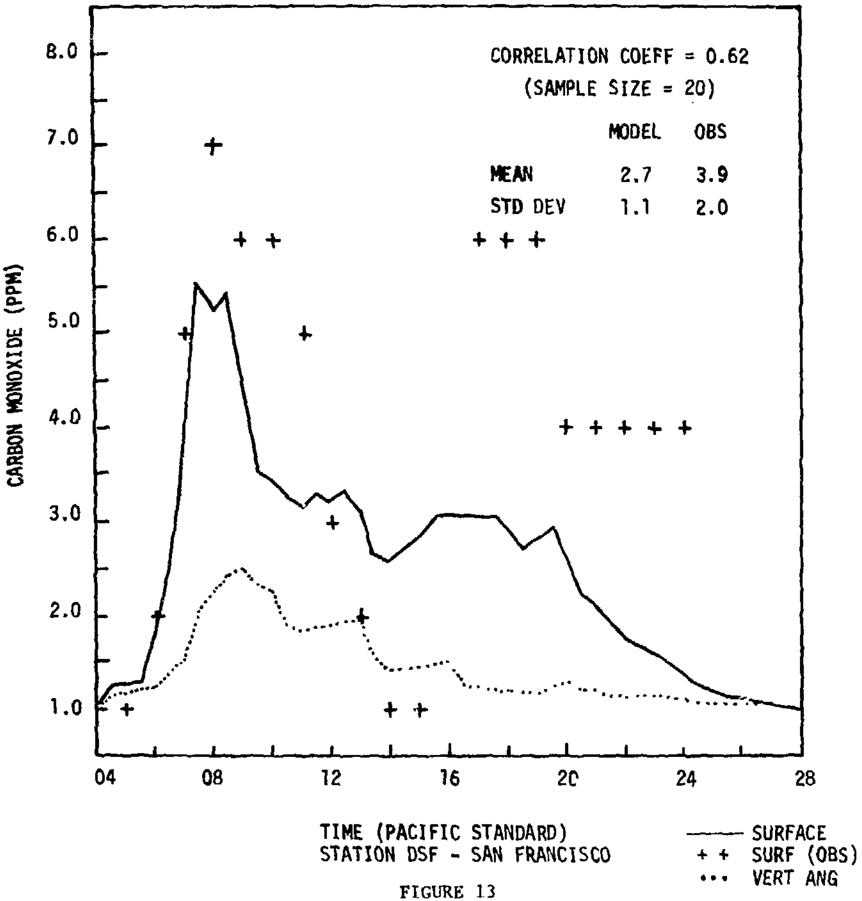

CORRELATION COEFF = 0.62
(SAMPLE SIZE = 20)
MODEL OBS
MEAN 2.7 3.9
STD DEV 1.1 2.0
CARBON MONOXIDE (PPM)
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
04
08
12
16
20
24
28
TIME (PACIFIC STANDARD)
STATION DSF - SAN FRANCISCO
SURFACE
+ + SURF (OBS)
• • • VERT ANG

FIGURE 13