

# APPLICATION OF COMPUTER SIMULATION TECHNIQUES TO PROBLEMS IN AIR POLLUTION

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The need for a rationale for deciding between alternative air pollution control strategies has been apparent for many years, yet to date, none exists. The utility and power of the techniques of systems analysis and numerical or computer simulation have been known for many years, yet, only recently, have they been applied to problems in air pollution.

In planning an epidemiological study of the effects of various pollutants it is reasonable to consider the potential contribution of simulation models of pollutant distributions. One such model has been utilized in this laboratory to simulate the distribution of total oxidants in the South Coast Air Basin in California. The advantages are clear in that knowledge of the spatial distribution of pollutants allows calculation of dose rates for the entire population within the mapped area. This in turn removes the important constraint, requiring that the sample population be located within a certain radius of an air monitoring station.

The computer program produces maps which graphically illustrate spatially disposed information, both qualitative and quantitative. As such, it is suited to a broad range of applications with only minor alterations. Raw data of any kind, be it physical, social, medical, economic, and so forth, may be related, manipulated, weighted and arrayed in any desired fashion. The concept, general design, and mathematical model for the program were first developed in 1963 by Howard T. Fisher at Northwestern Technological Institute. Since then, many others, too numerous to mention, have generously contributed ideas and improvements to the program.

The notion of mapping is that of graphically depicting spatially disposed quantitative information, in our case, concentration of total oxidants. The data consists of triplets  $(X, Y, Z)$  where  $X$  and  $Y$  are the abscissa and the ordinate data which define a point on the map surface and  $Z$  is the concentration of total oxidants at that point. The  $X, Y$  data must be continuous. Concentration data is also continuous, that is, is defined for every point  $X, Y$  on the map by a continuous mathematical function. Restricting ourselves in this way, the map which results is a contour map.

The program uses a "gravity" interpolation function, where, essentially, the concentration at an unknown point  $(X, Y)$  is directly proportional to the

weighted sum of all the known concentrations on the map. The weighting factor is the inverse square of the distance between the unknown concentration and the known concentration, hence the name "gravity" model.

In Figure 1 the shaded area depicts the region which was mapped. It is bounded on the south and west by the Pacific Ocean and on the north and east by the 1500 foot elevation contour. The area lies within the South Coast Air Basin, contains twenty air quality monitoring stations (represented by the filled circles), and has a population of about 9.7 million people. Figure 2 illustrates the ten concentration ranges represented by ten shades of gray. Owing to the uncertainty in printing and reproduction, these same ten ranges are also represented by a number between zero and nine. The levels of greatest interest, of course, are level 4 (0.05 to 0.09 ppm) which contains the health related federal ambient air quality standard for total oxidant (0.08 ppm); level 5 (0.09 to 0.15 ppm) which contains the State of California health related ambient air quality standard for total oxidant (0.1 ppm); level 7 (0.25 to 0.35 ppm) which contains the Riverside County school alert level (0.27 ppm)—0.35 ppm for Los Angeles County—at which point school children are brought indoors and restrained from strenuous physical activity; and last, level 9 (0.45 to 0.54 ppm) which contains the Los Angeles County first alert level (0.5 ppm).

The maps, Figures 3-36, are produced, utilizing actual oxidant measurements obtained through the cooperation of the Air Pollution Control Districts of Los Angeles, San Bernardino, Orange, and Riverside Counties. The data are hourly averages, hence are directly relatable to health effects based on dosage. There is one map for each hour of the day for thirty-four continuous hours on August 21, and 22, 1969, starting at 6:00 a.m. on the 21st.

The maps are self explanatory, however, certain features and trends are worth pointing out. At 6:00 a.m. (Figure 3), the basin in general is at essentially background levels of oxidant, except for a small region at the east end, bounded by Riverside, San Bernardino, Corona, Chino, and Pomona, where the total oxidant is slightly elevated. The reason for this elevated oxidant in this region is not completely clear as yet. This condition does recur later on, after the sun has and can be seen every hour between 7:00 p.m. (Figure 16) on the 21st and 6:00 a.m. (Figure 27) on the 22nd.

By 7:00 a.m. (Figure 4) almost right at sun-up, areas in Pasadena and southwestern Riverside are experiencing oxidant levels in excess of health related federal ambient air quality standards. At 8:00 a.m. (Figure 5) more than half of the area studied is engulfed by air which exceeds federal standards. If one assumes a uniform population distribution over the entire region, then by 9:00 a.m. (Figure 6) about 70 per cent of the population, slightly less than seven million people are breathing substandard air.

At 10:00 a.m. (Figure 7) the central portion of the basin as well as areas to the north around Burbank and Pasadena are experiencing levels in excess of the Riverside County school alert level. People in these areas should begin restraining strenuous physical activity. By 11:00 a.m. (Figure 8) the maximum oxidant

readings are obtained, and if we again assume a uniform population distribution, everyone in the basin is breathing substandard air, and about three million of these persons should according to advice given by some physicians, curtail any form of vigorous activity. Note that between the hours of 11:00 a.m. to 1:00 p.m. (Figures 8 through 10) the entire air shed equals or exceeds the health related federal ambient air quality standard for total oxidant.

Starting at 1:00 p.m. (Figure 10) and going to 6:00 p.m. (Figure 15) one can observe two phenomena occurring simultaneously; first, a decrease in the rate of build up of oxidant, it apparently peaked between 11:00 a.m. and 12 noon; second, an increase in the effect of wind on the oxidant distribution. It is quite apparent that during the afternoon hours, the wind velocity has increased, and is moving the material from west to east. The sharp decrease in oxidant between 5:00 p.m. (Figure 14) and 7:00 p.m. (Figure 16) is consistent with the fact that the sun has set and the mechanism for oxidant production has been removed. By 7:00 p.m. (Figure 16) the basin in general has returned to near background levels of total oxidant.

Except for the apparent anomaly noted earlier, occurring in the eastern end of the basin, the oxidant levels remain at or near background throughout the night from 8:00 p.m. (Figure 17) to 6:00 a.m. (Figure 27) the following morning. Between 6:00 a.m. (Figure 27) and 7:00 a.m. (Figure 28) the sun rises and oxidant begins rising immediately. The pattern repeats itself, the following day being very much like the preceding one. The series continues to 3:00 p.m. (Figure 36) on August 22, 1969. One last input of information regarding this segment of data: the meteorology observed on August 21 and 22, 1969 was quite typical of the late summer season.

It should be noted that this series of maps, simulating actual concentration distributions of total oxidants, condenses into rapidly digestible form, an enormous amount of information. The implications are clear in terms of a much wider choice of sample populations. The specific method used here only begins to illustrate the enormous power of the more general technique of simulation modelling.

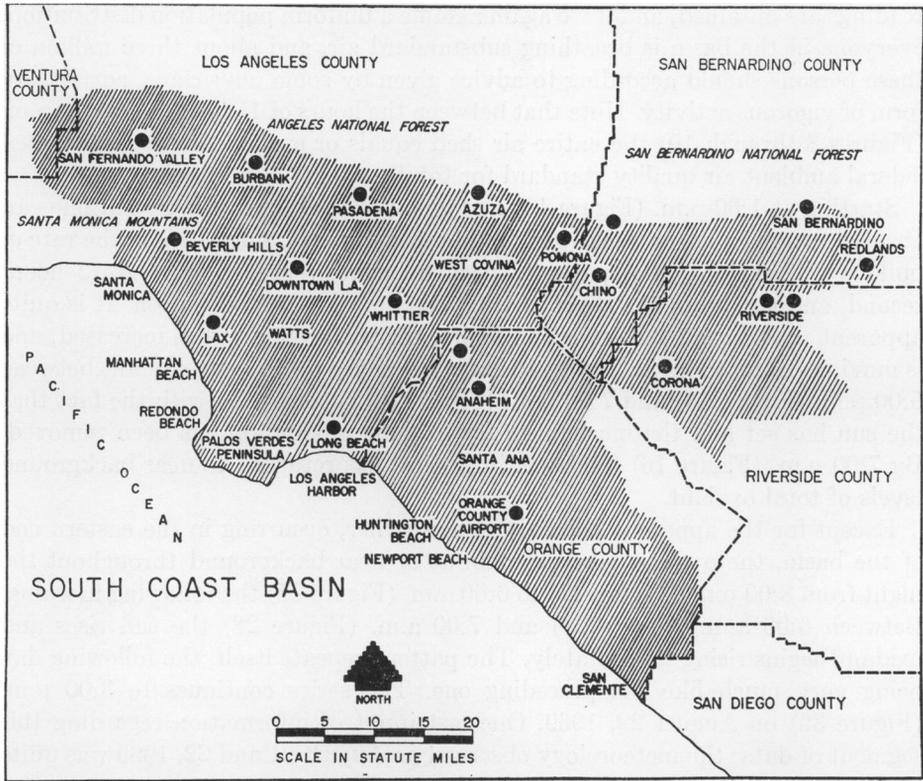


FIGURE 1

South Coast Air Basin study area, southern California.

**OXIDANT CONTOURS  
IN THE  
SOUTH COAST BASIN  
COMPUTER GENERATED**

Levels	Total Oxidant (ppm)	Levels	Total Oxidant (ppm)
 0	0.00 - 0.01	 5	0.09 - 0.15
 1	0.01 - 0.02	 6	0.15 - 0.25
 2	0.02 - 0.03	 7	0.25 - 0.35
 3	0.03 - 0.05	 8	0.35 - 0.45
 4	0.05 - 0.06	 9	0.45 - 0.54

FIGURE 2

Explanation of shadings for Figures 3 through 36.

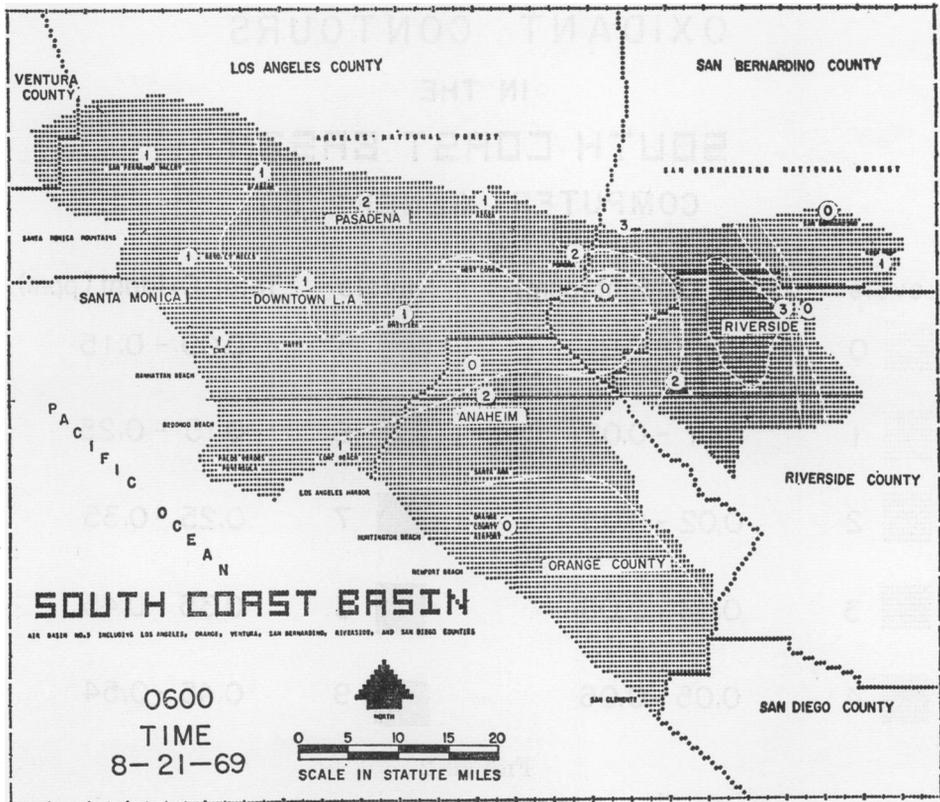


FIGURE 3

Extent of oxidant level at 0600 on August 21, 1969.

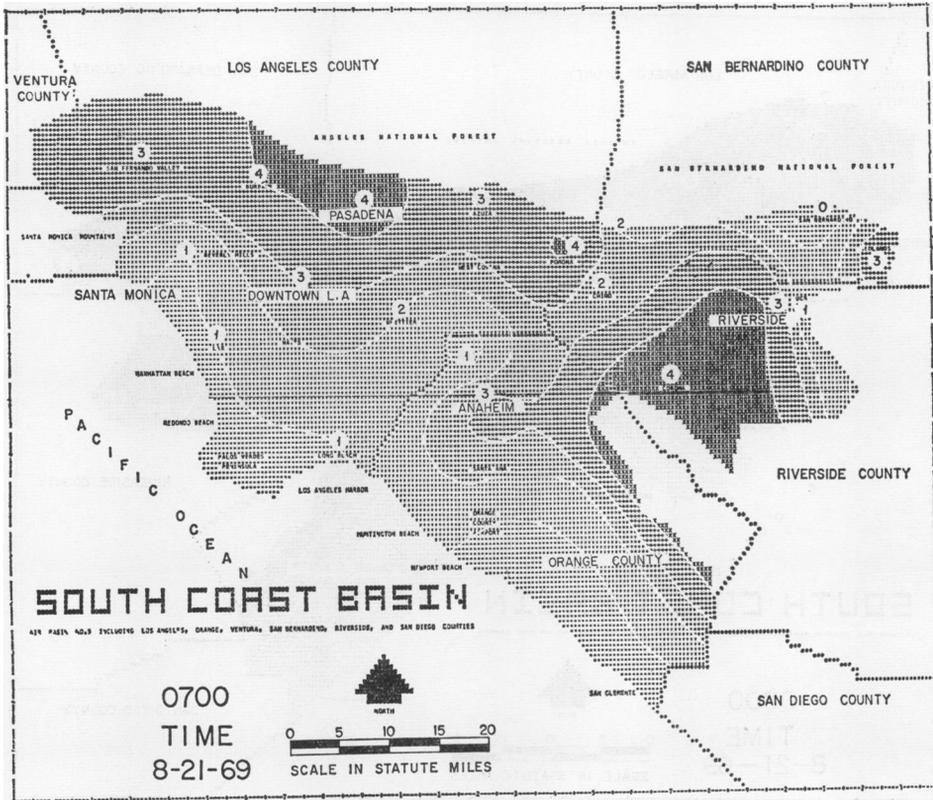


FIGURE 4  
Extent of oxidant level at 0700 on August 21, 1969.

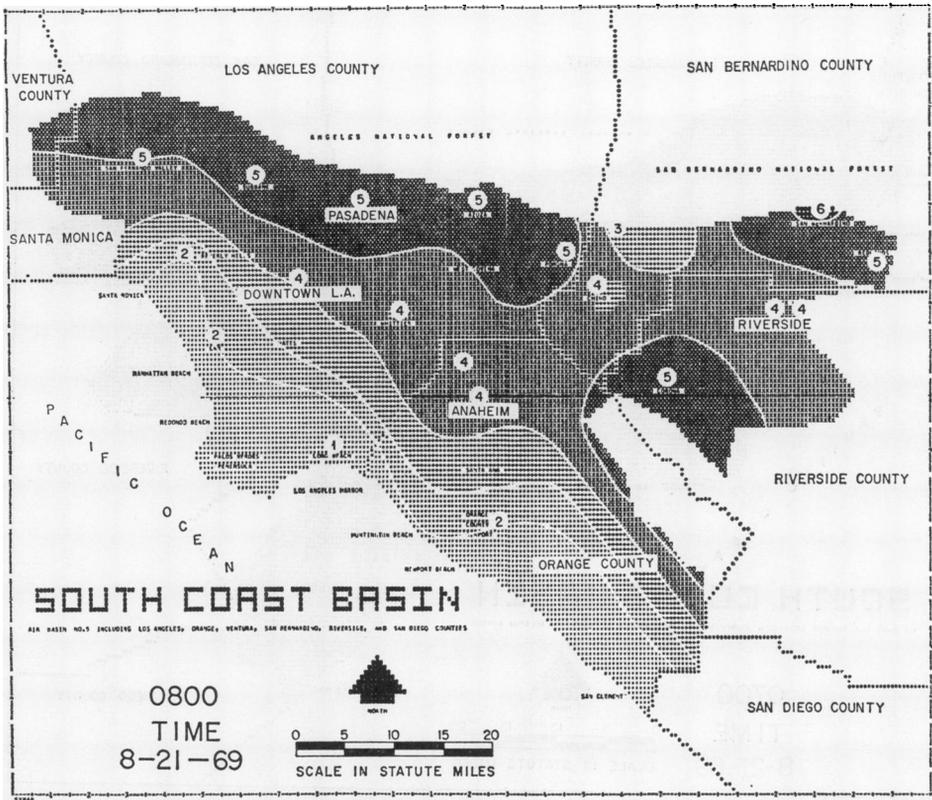


FIGURE 5

Extent of oxidant level at 0800 on August 21, 1969.

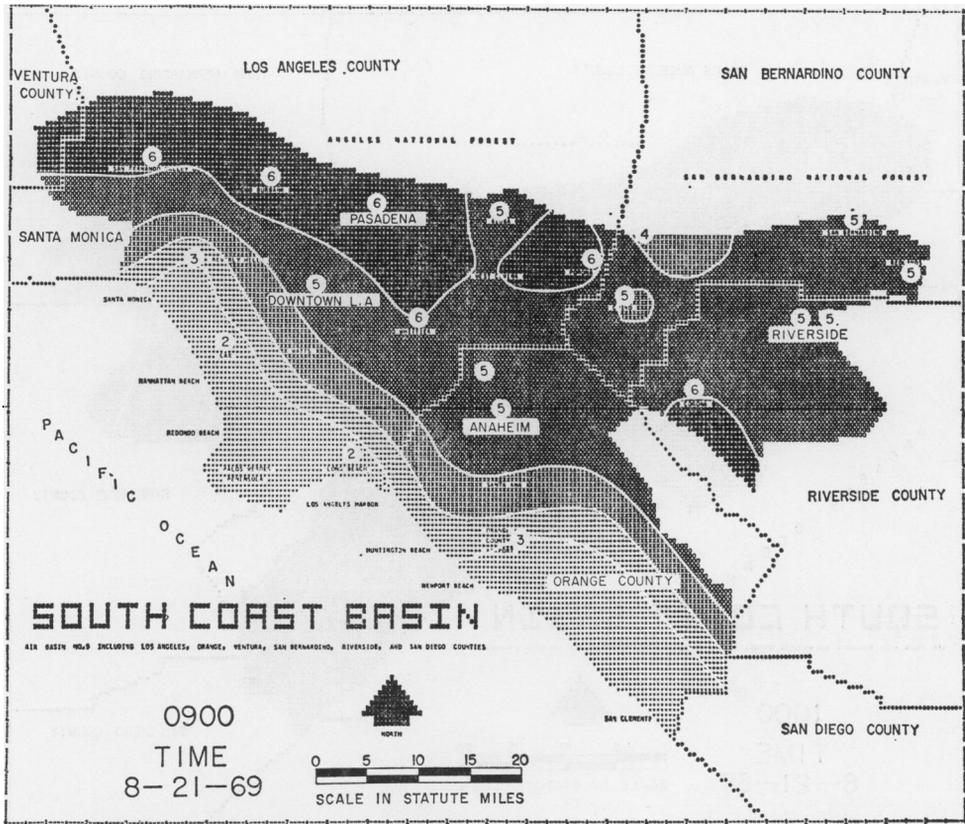


FIGURE 6  
Extent of oxidant level at 0900 on August 21, 1969.

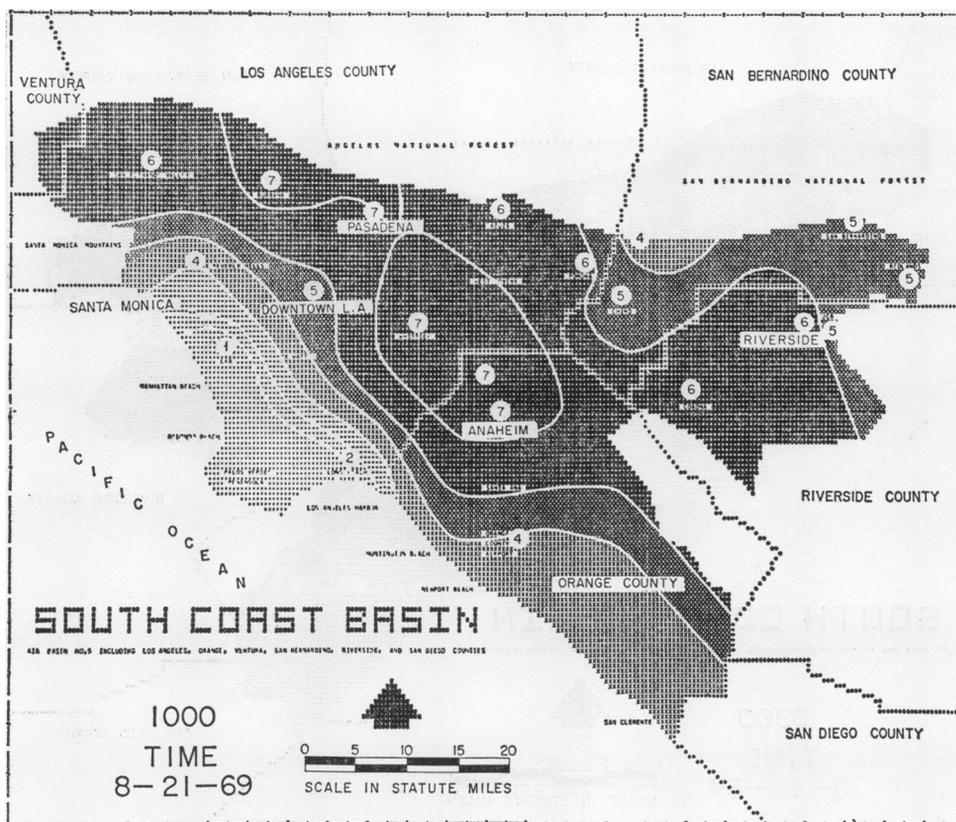


FIGURE 7

Extent of oxidant level at 1000 on August 21, 1969.

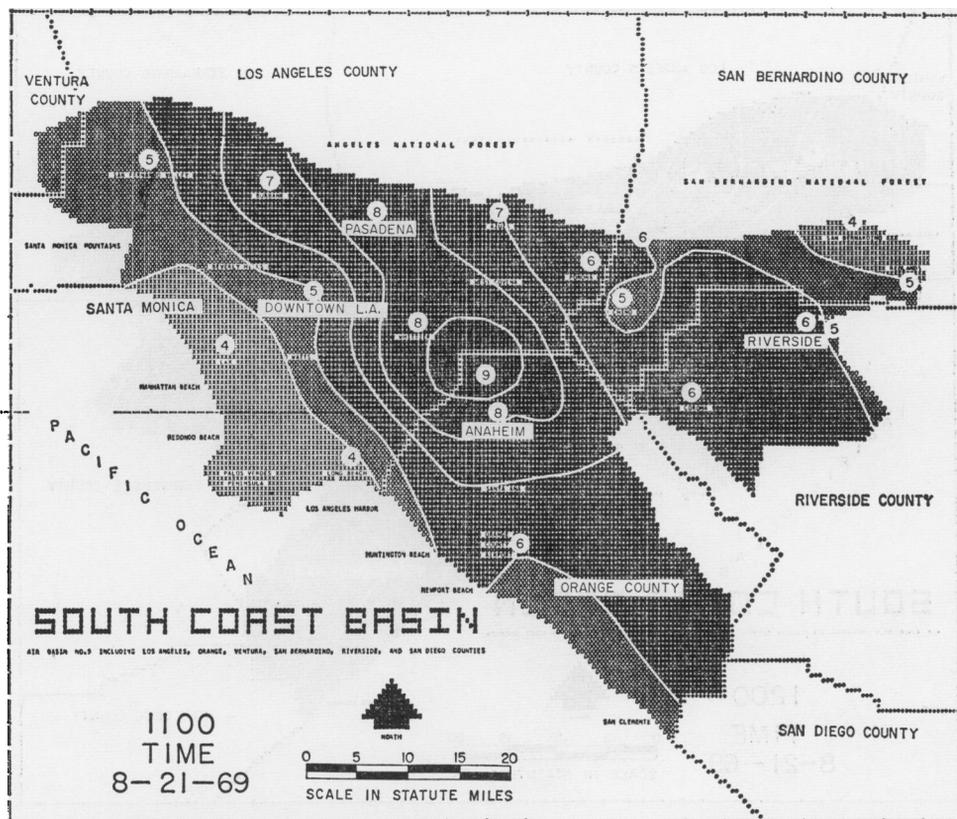


FIGURE 8  
Extent of oxidant level at 1100 on August 21, 1969.

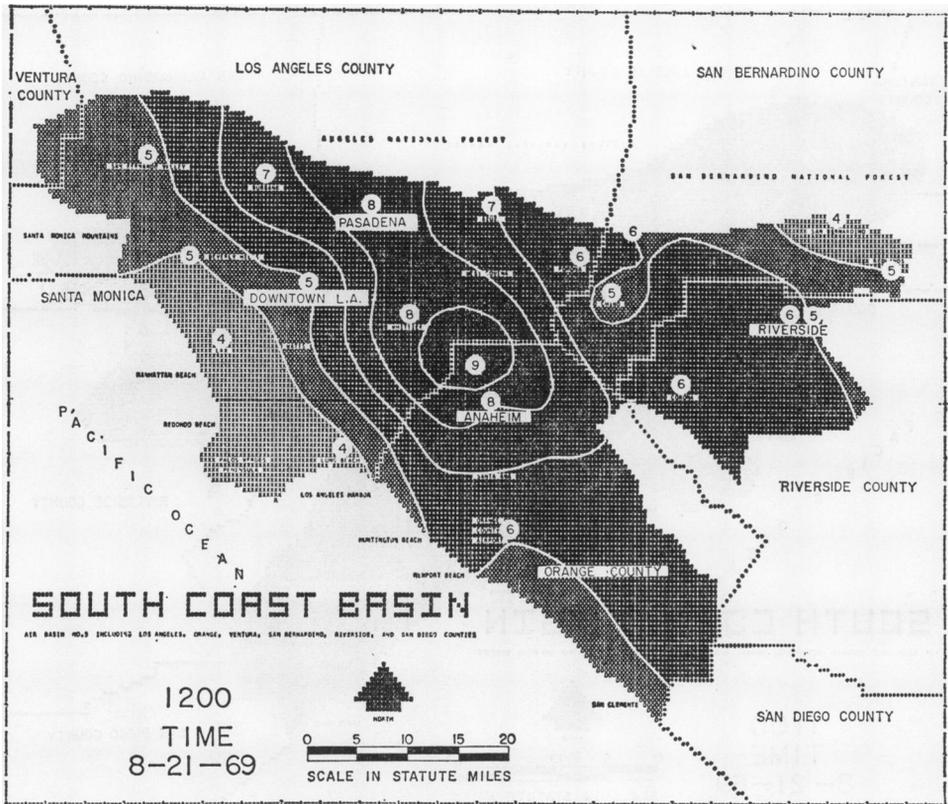


FIGURE 9

Extent of oxidant level at 1200 on August 21, 1969.

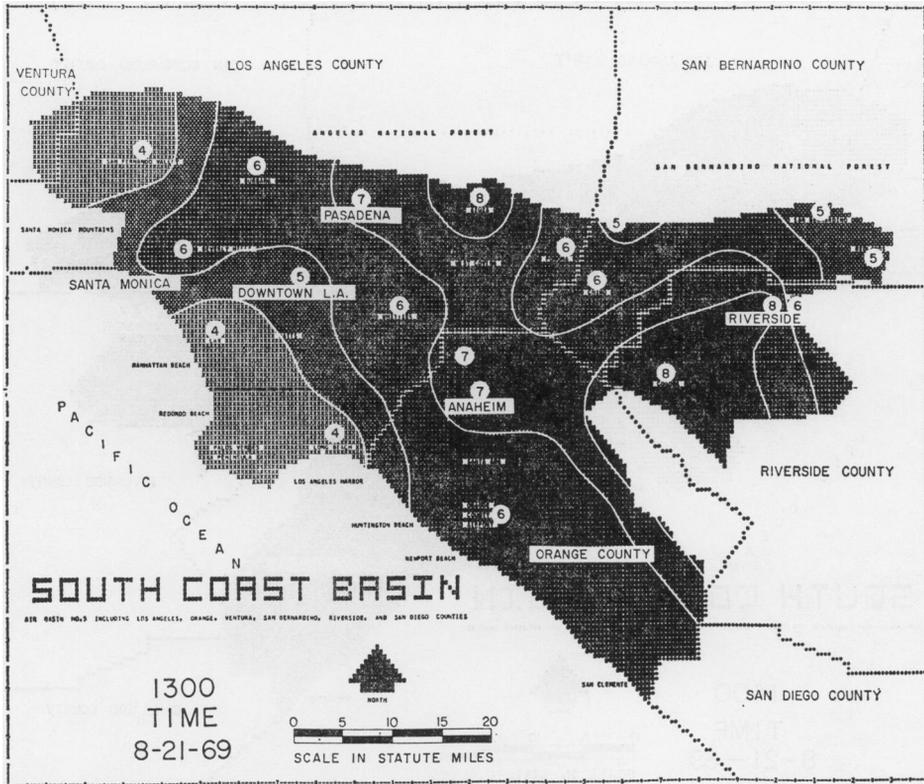


FIGURE 10

Extent of oxidant level at 1300 on August 21, 1969.

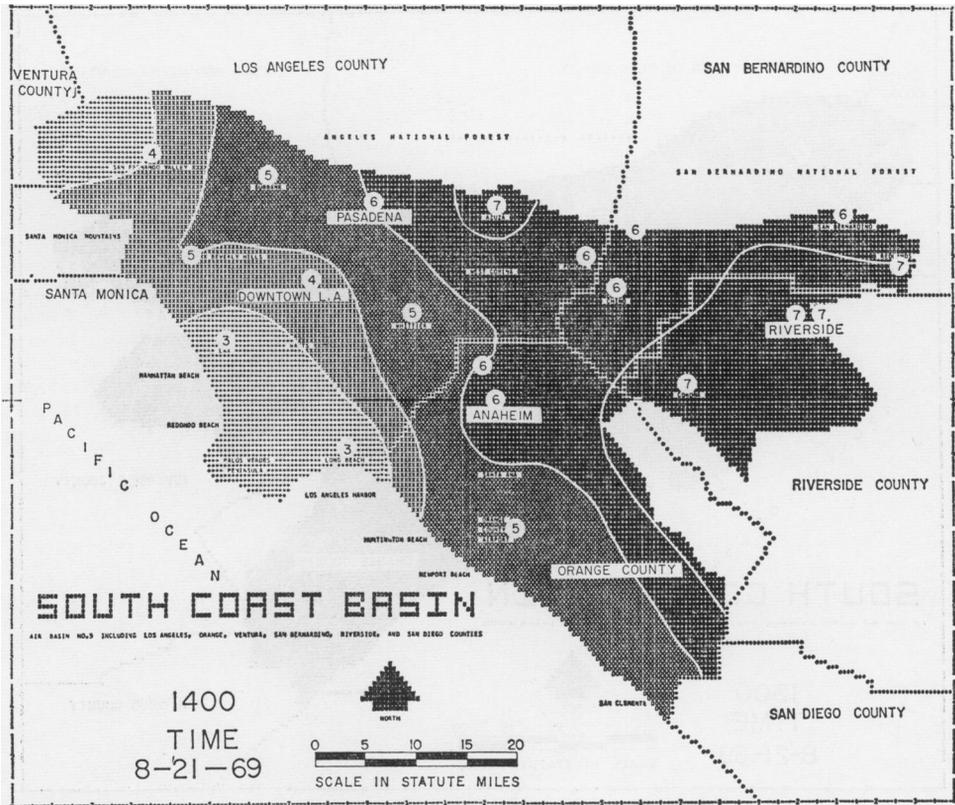


FIGURE 11

Extent of oxidant level at 1400 on August 21, 1969.

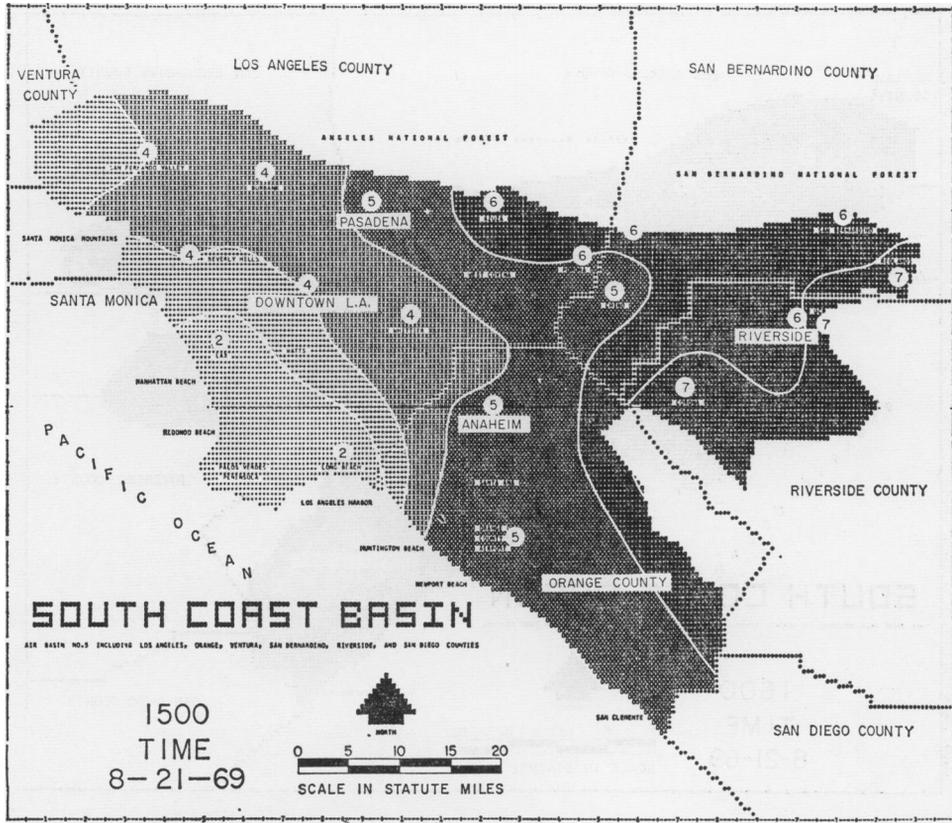


FIGURE 12  
Extent of oxidant level at 1500 on August 21, 1969.

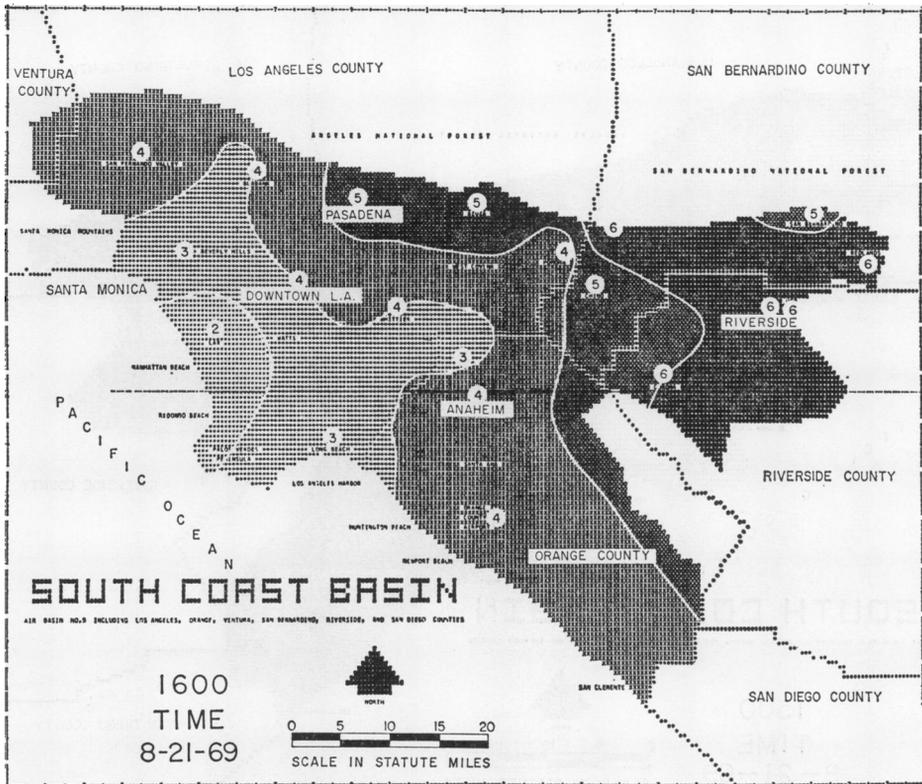


FIGURE 13

Extent of oxidant level at 1600 on August 21, 1969.

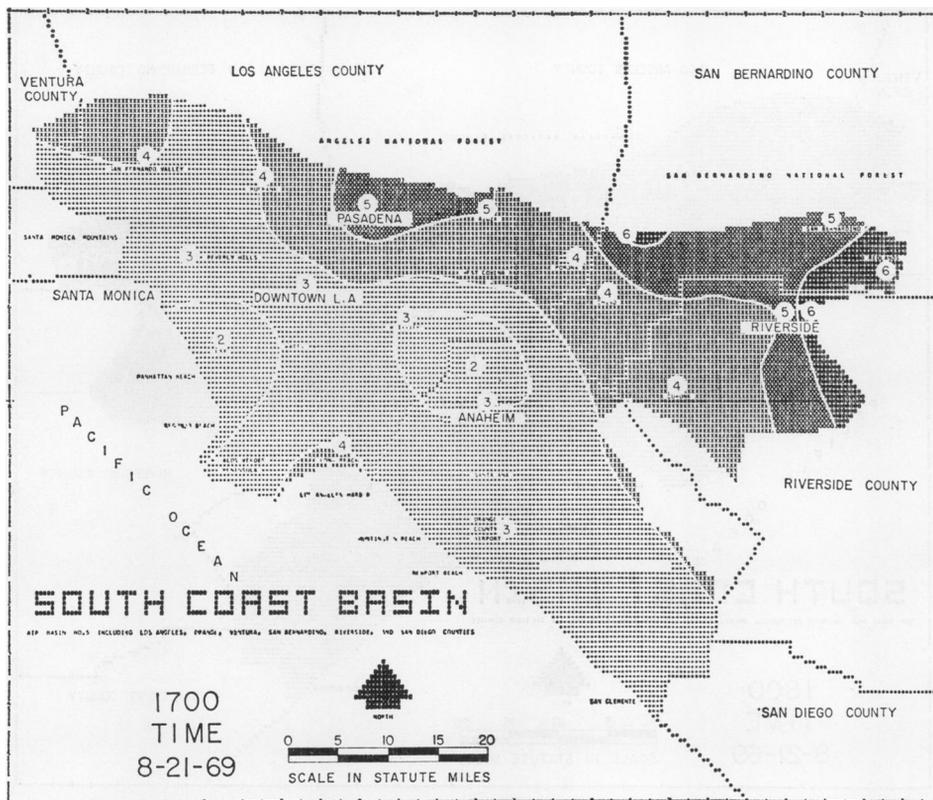


FIGURE 14  
Extent of oxidant level at 1700 on August 21, 1969.

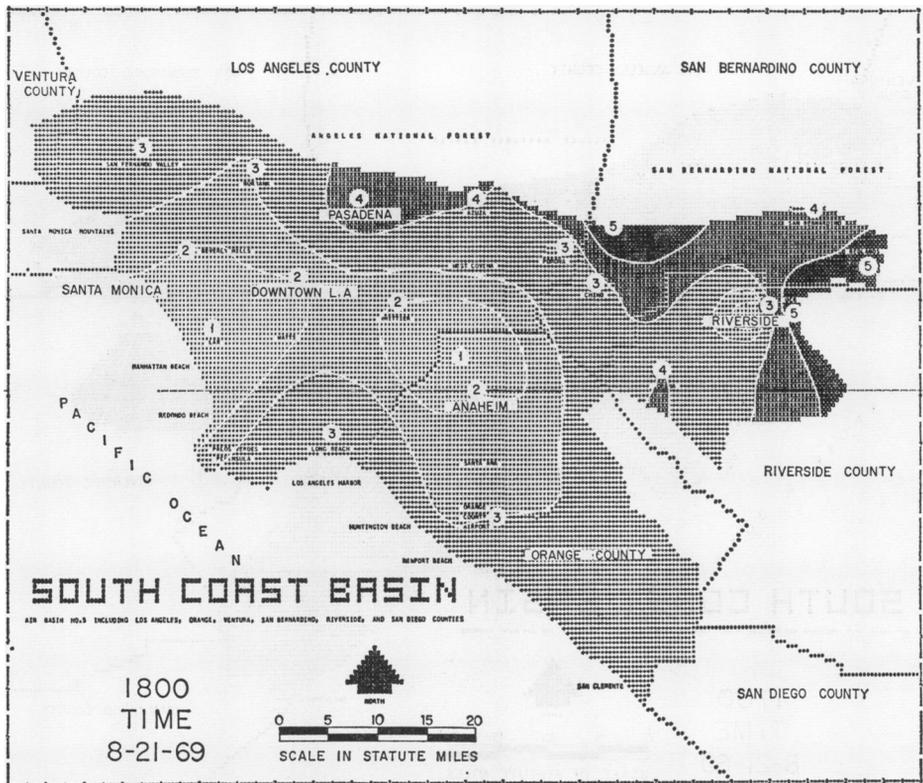


FIGURE 15

Extent of oxidant level at 1800 on August 21, 1969.

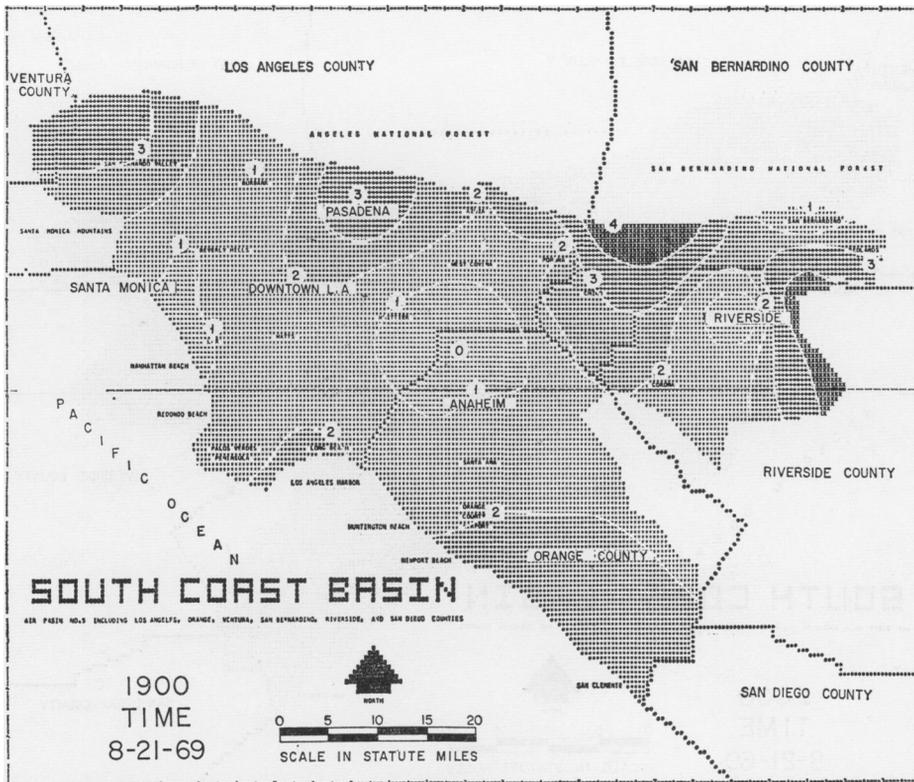


FIGURE 16  
Extent of oxidant level at 1900 on August 21, 1969.

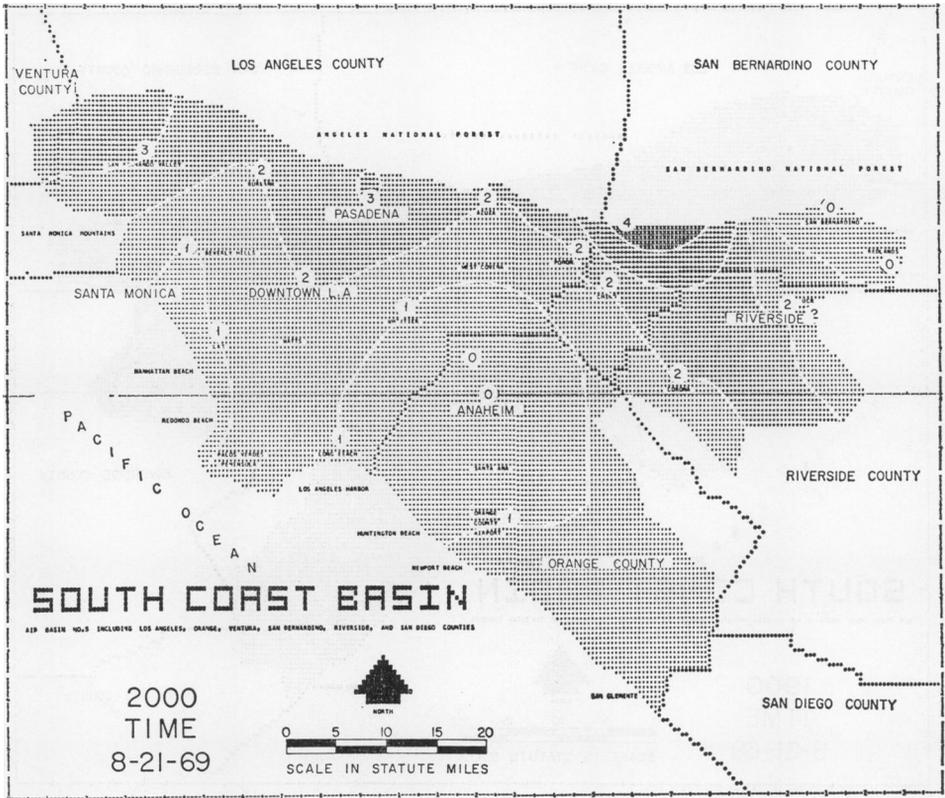


FIGURE 17  
Extent of oxidant level at 2000 on August 21, 1969.

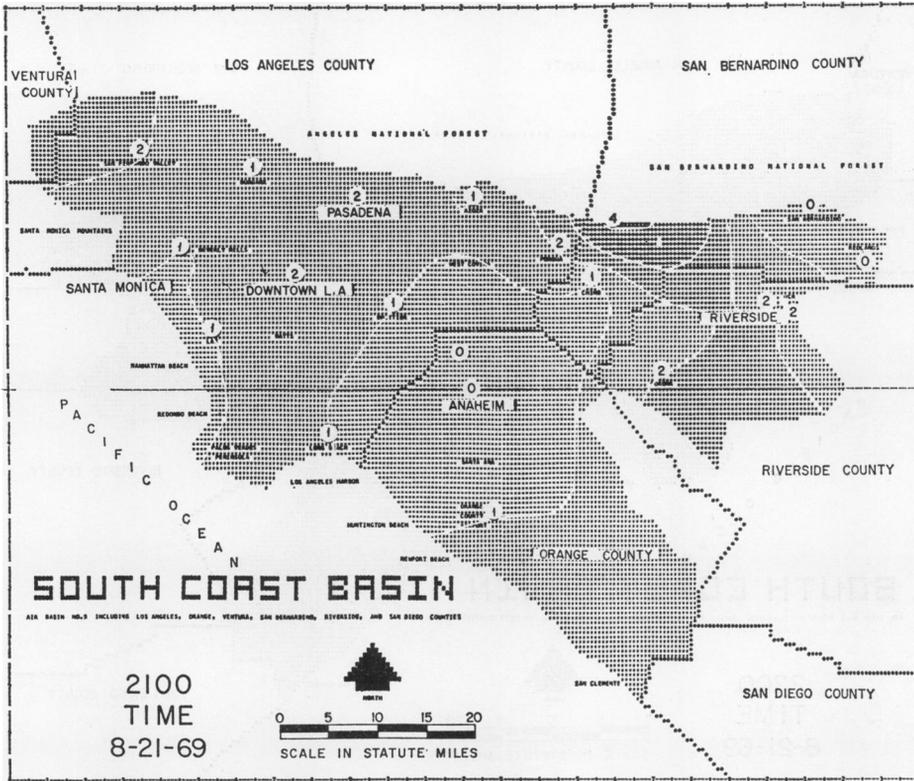


FIGURE 18  
Extent of oxidant level at 2100 on August 21, 1969.

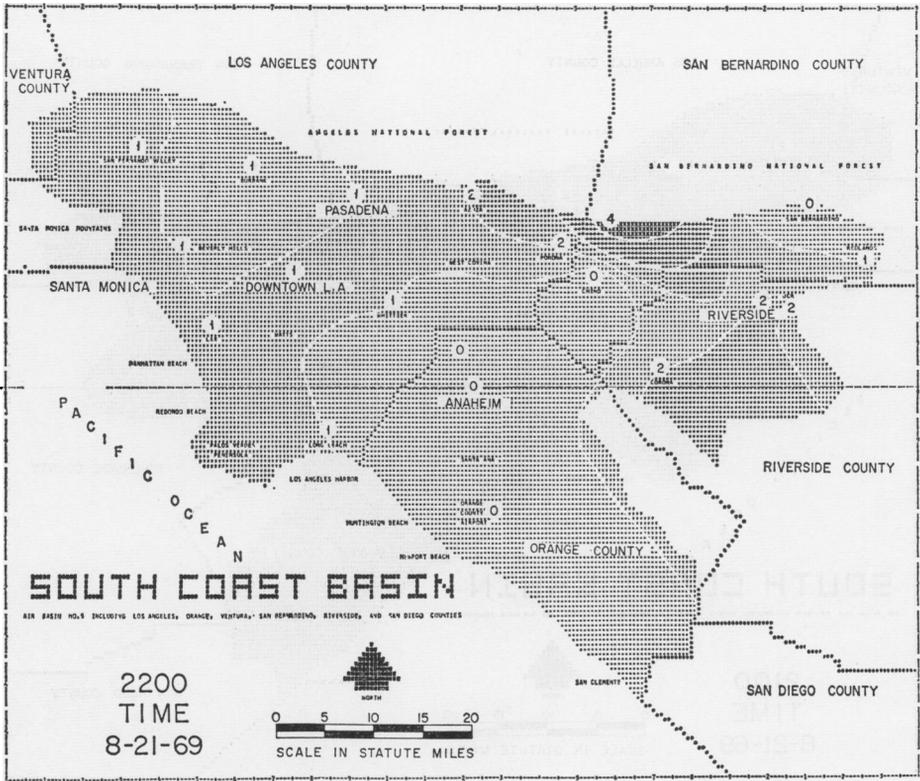


FIGURE 19

Extent of oxidant level at 2200 on August 21, 1969.

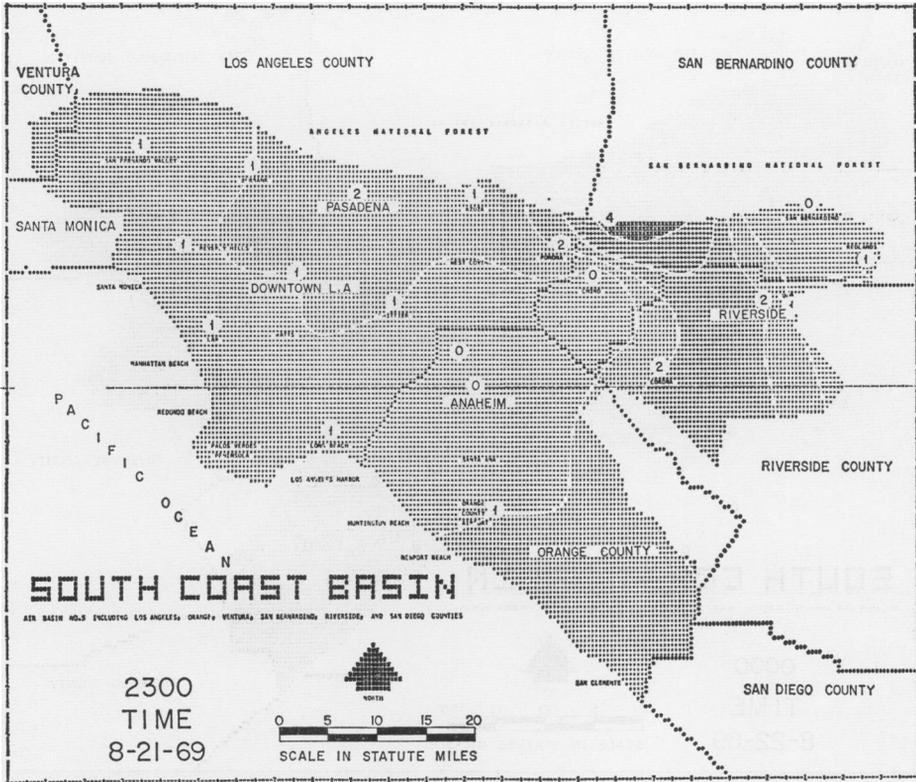
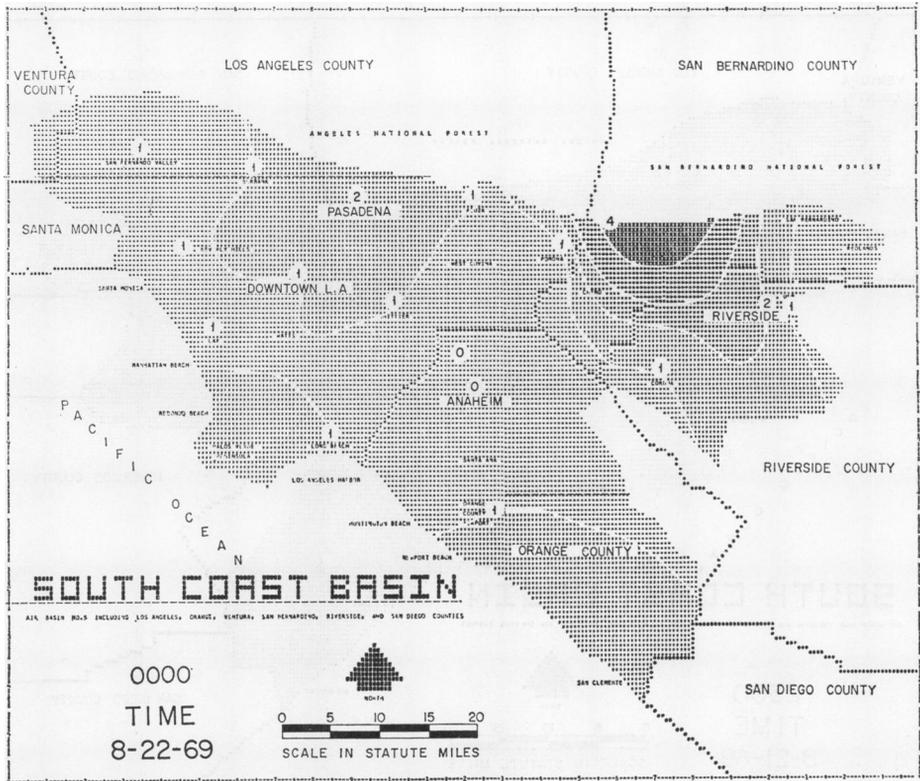


FIGURE 20  
Extent of oxidant level at 2300 on August 21, 1969.



**FIGURE 21**

Extent of oxidant level at 0000 on August 22, 1969.

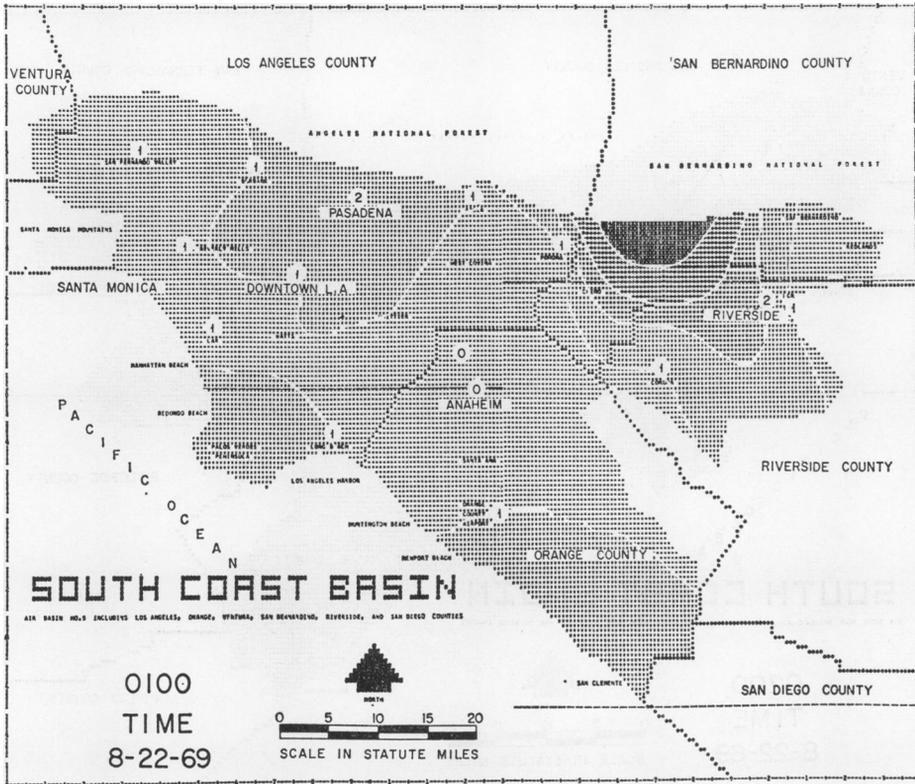


FIGURE 22

Extent of oxidant level at 0100 on August 22, 1969.

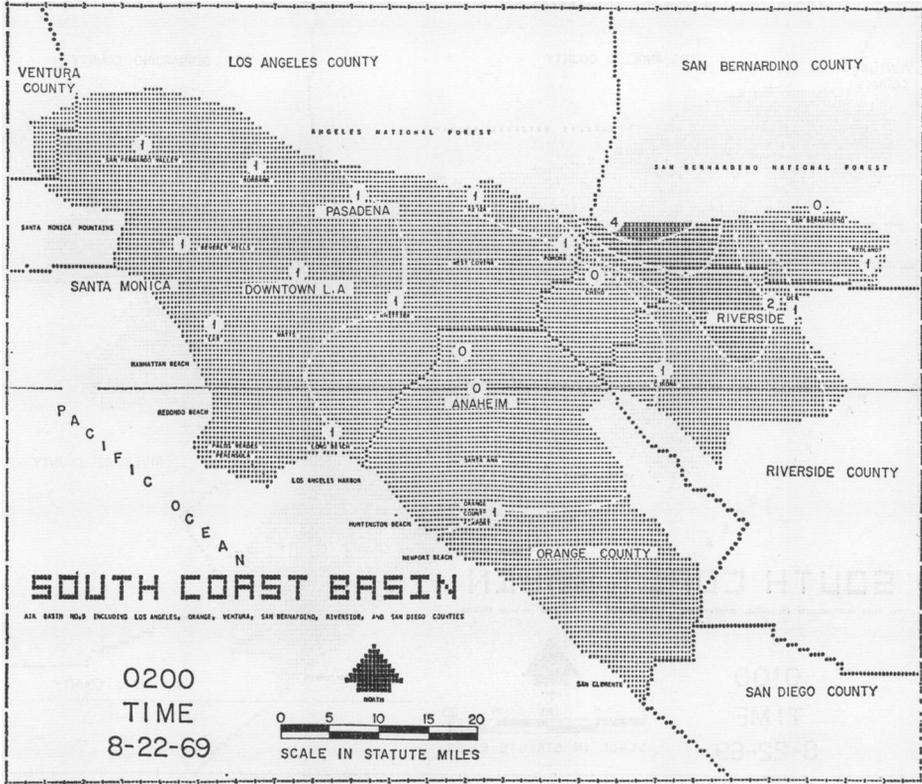


FIGURE 23

Extent of oxidant level at 0200 on August 22, 1969.

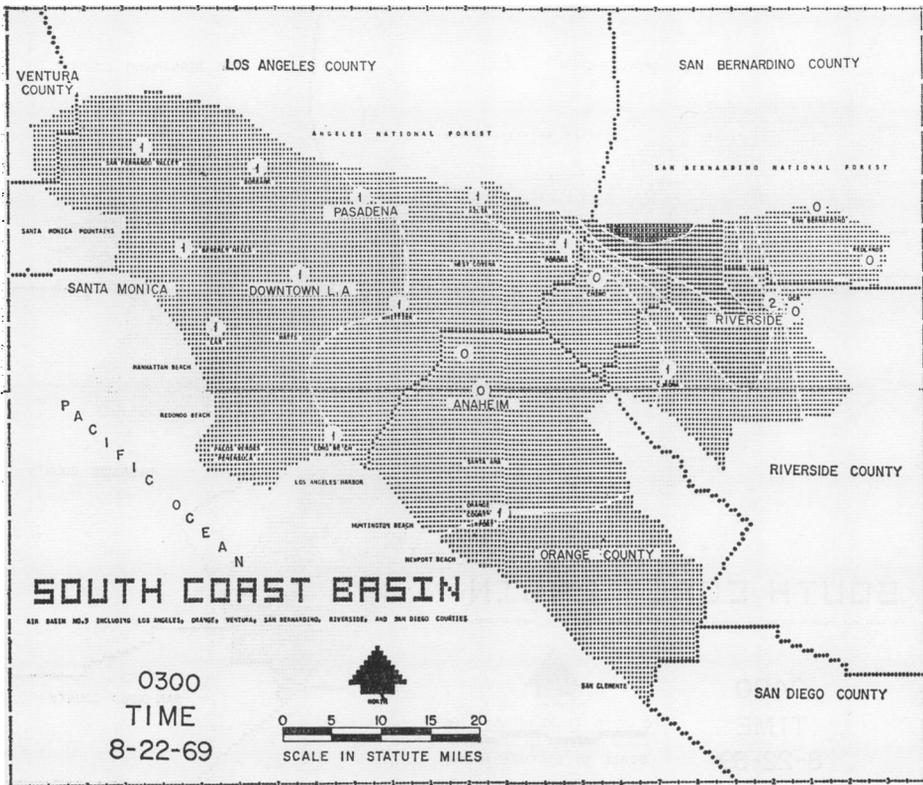


FIGURE 24

Extent of oxidant level at 0300 on August 22, 1969.

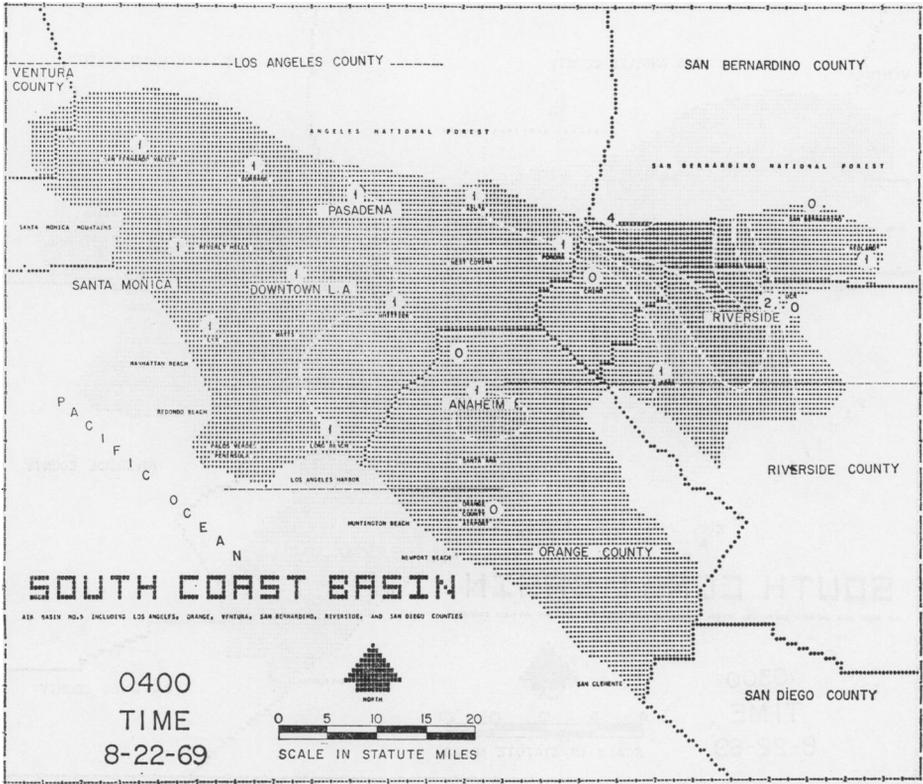


FIGURE 25

Extent of oxidant level at 0400 on August 22, 1969.

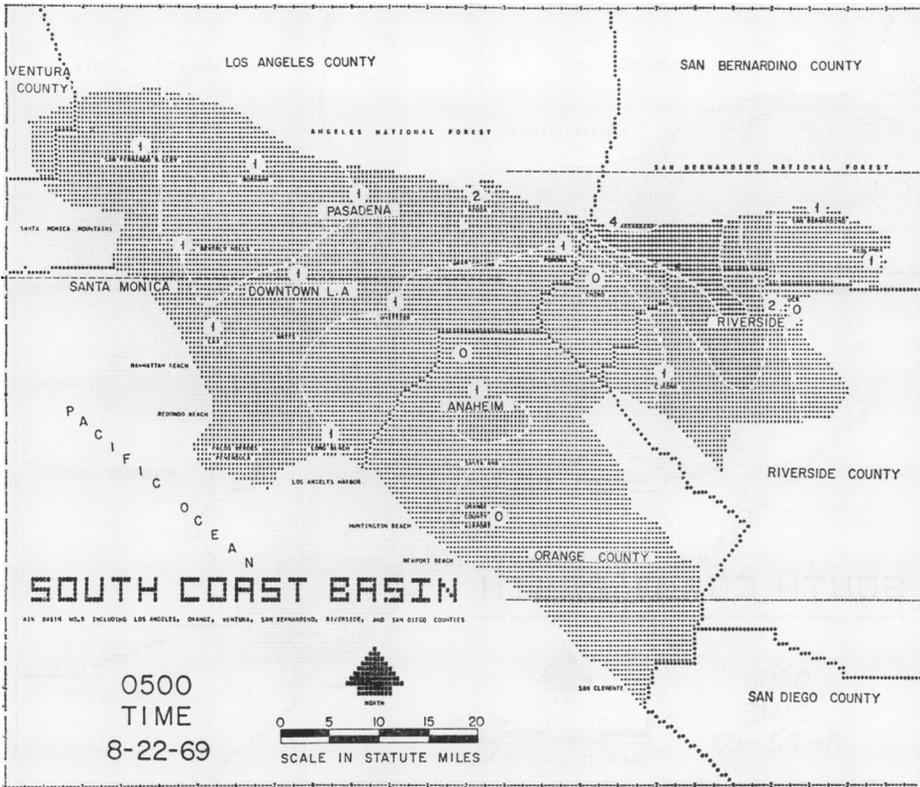


FIGURE 26  
Extent of oxidant level at 0500 on August 22, 1969.

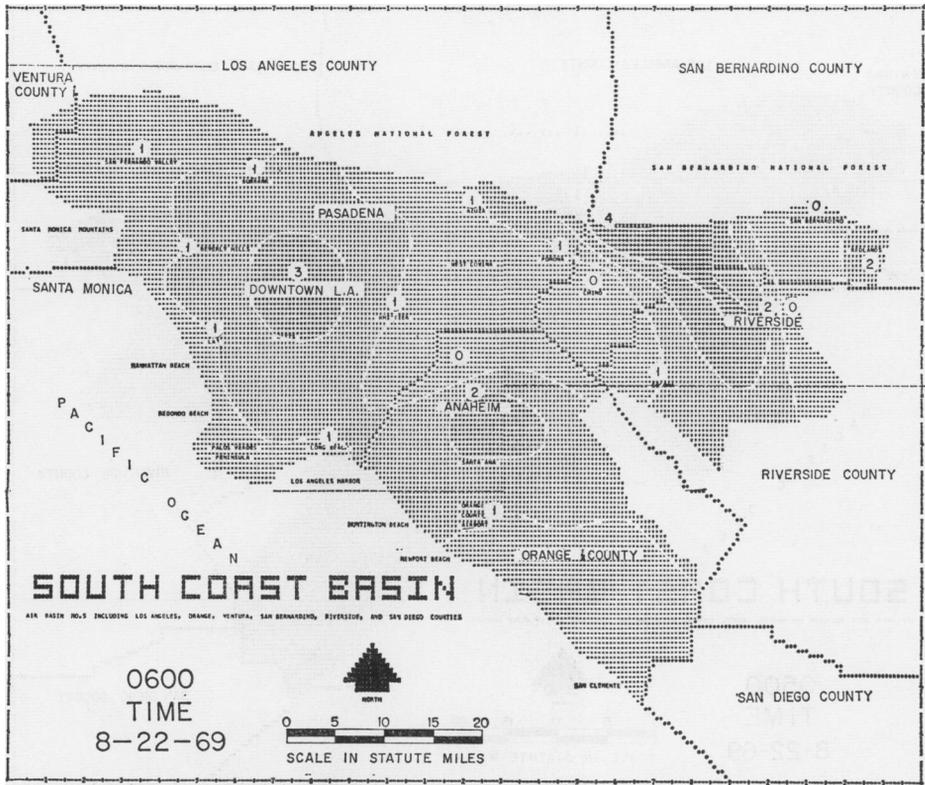


FIGURE 27

Extent of oxidant level at 0600 on August 22, 1969.

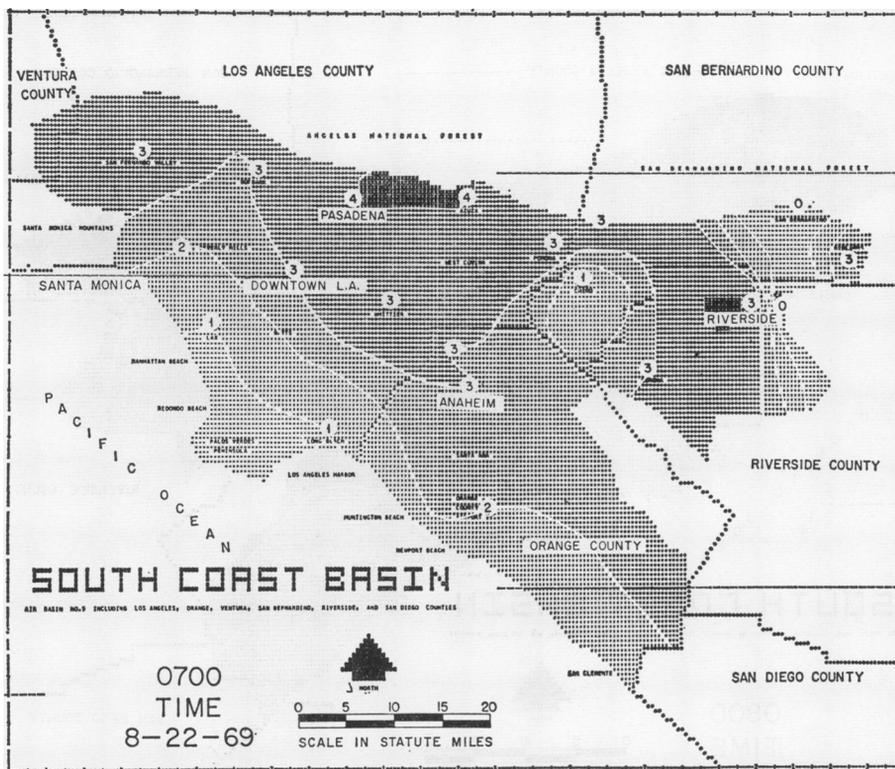


FIGURE 28  
Extent of oxidant level at 0700 on August 22, 1969.

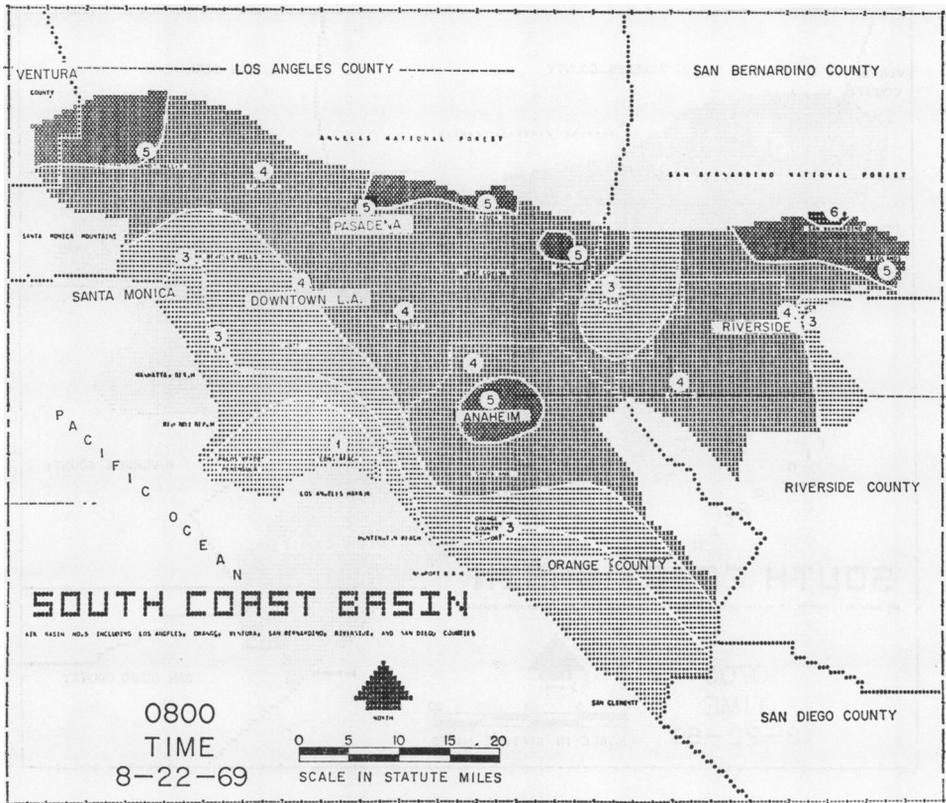


FIGURE 29

Extent of oxidant level at 0800 on August 22, 1969.

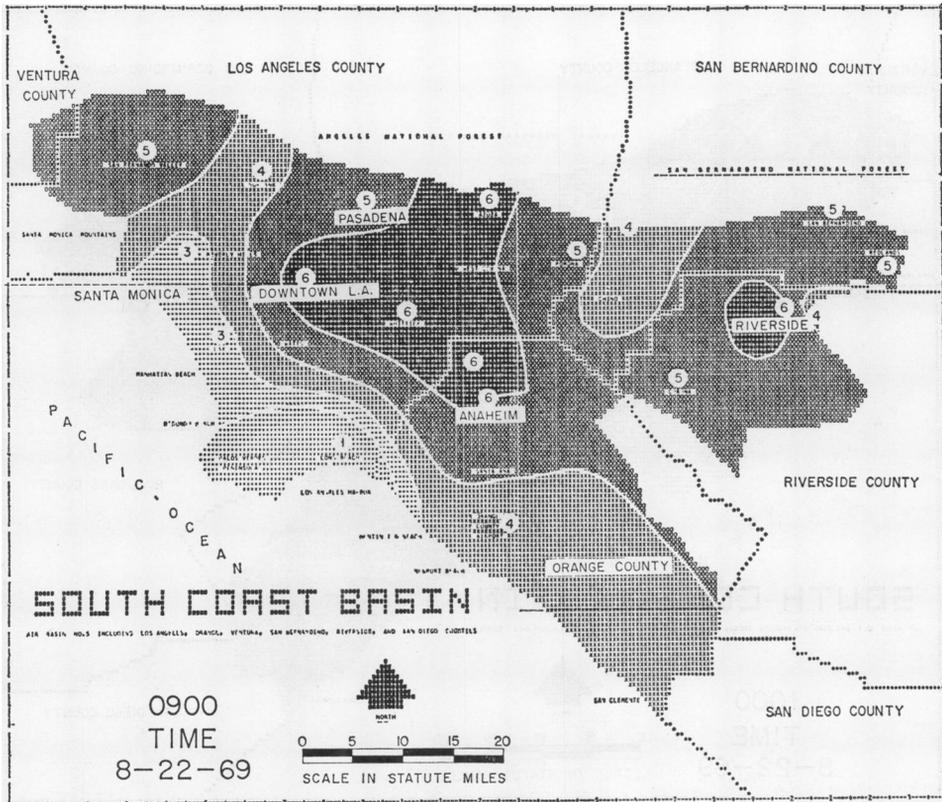


FIGURE 30  
Extent of oxidant level at 0900 on August 22, 1969.

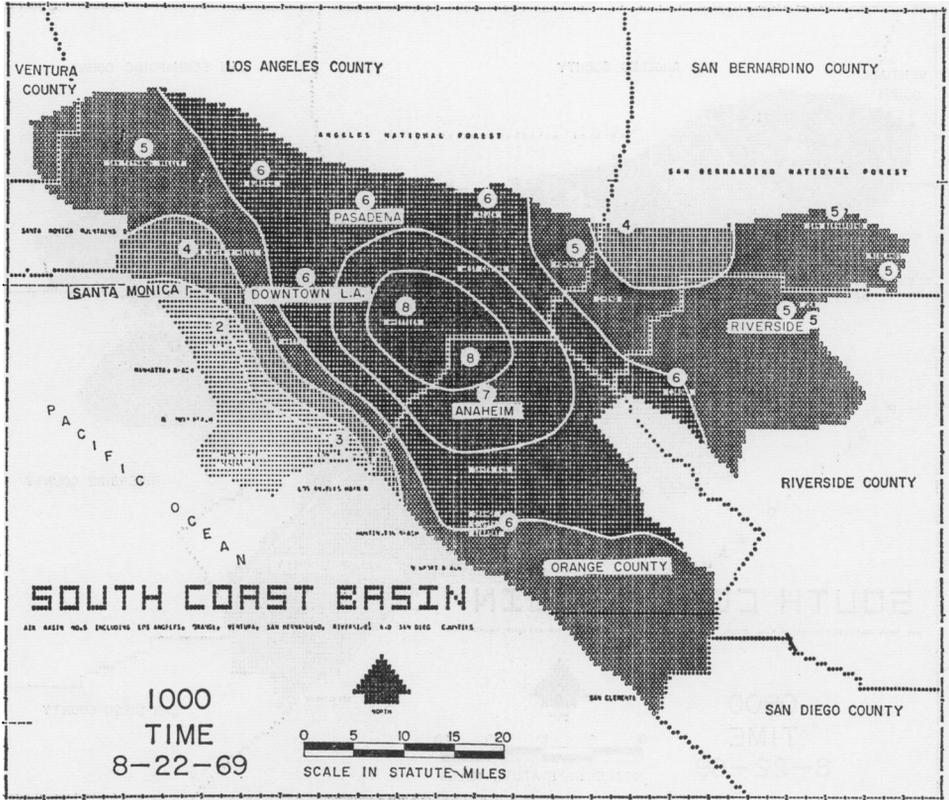


FIGURE 31

Extent of oxidant level at 1000 on August 22, 1969.

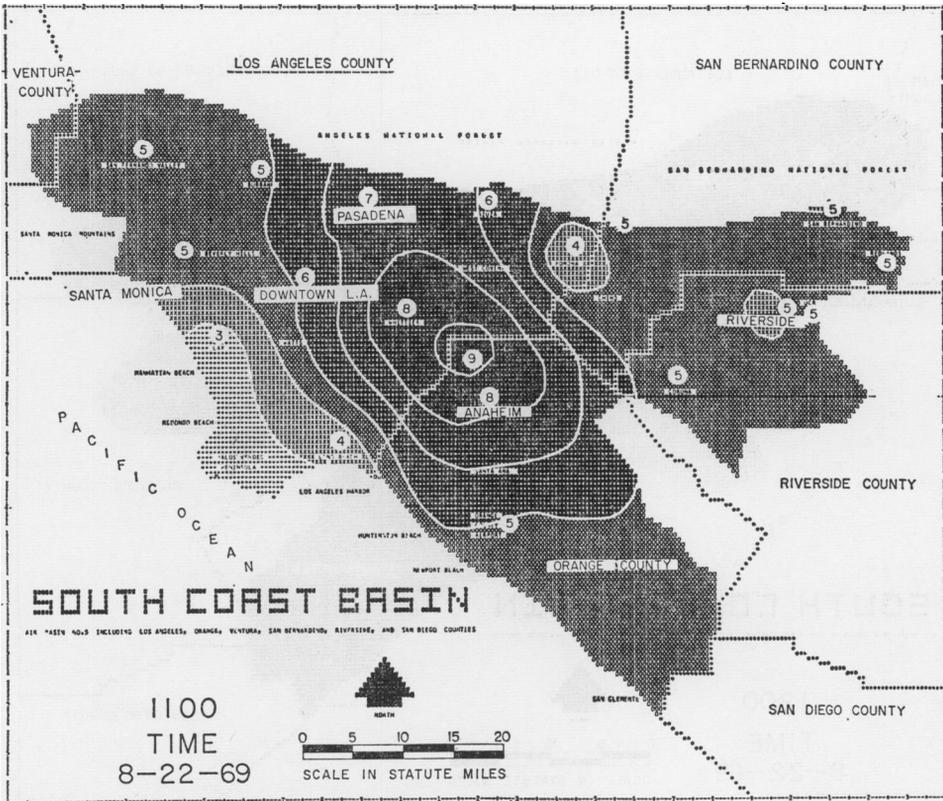


FIGURE 32  
Extent of oxidant level at 1100 on August 22, 1969.

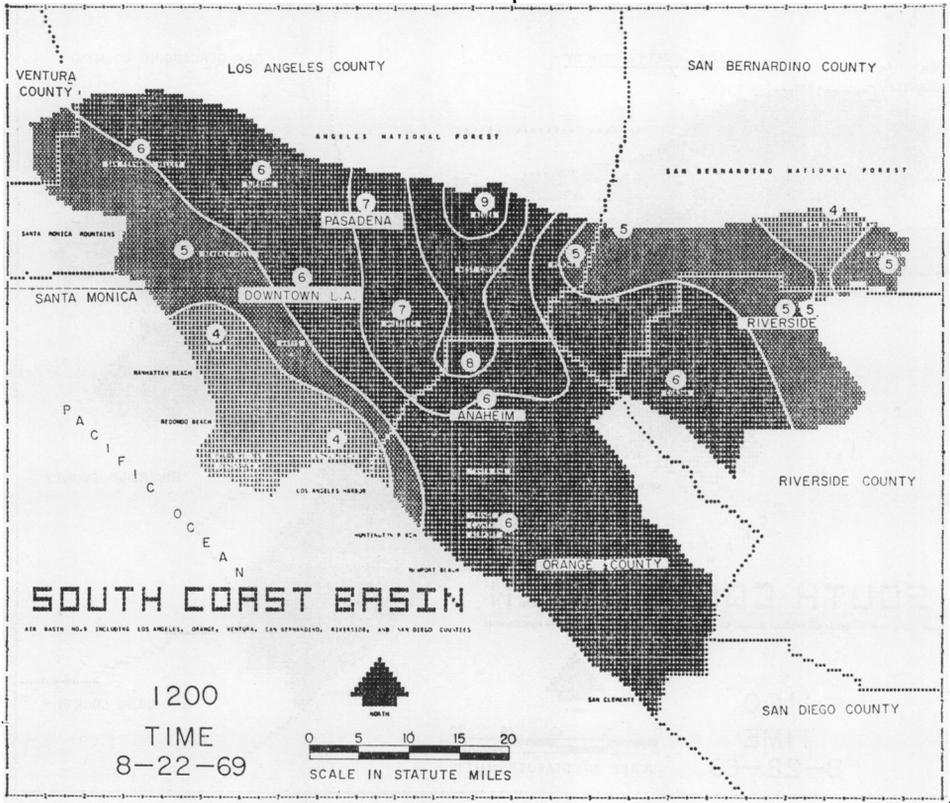


FIGURE 33

Extent of oxidant level at 1200 on August 22, 1969.

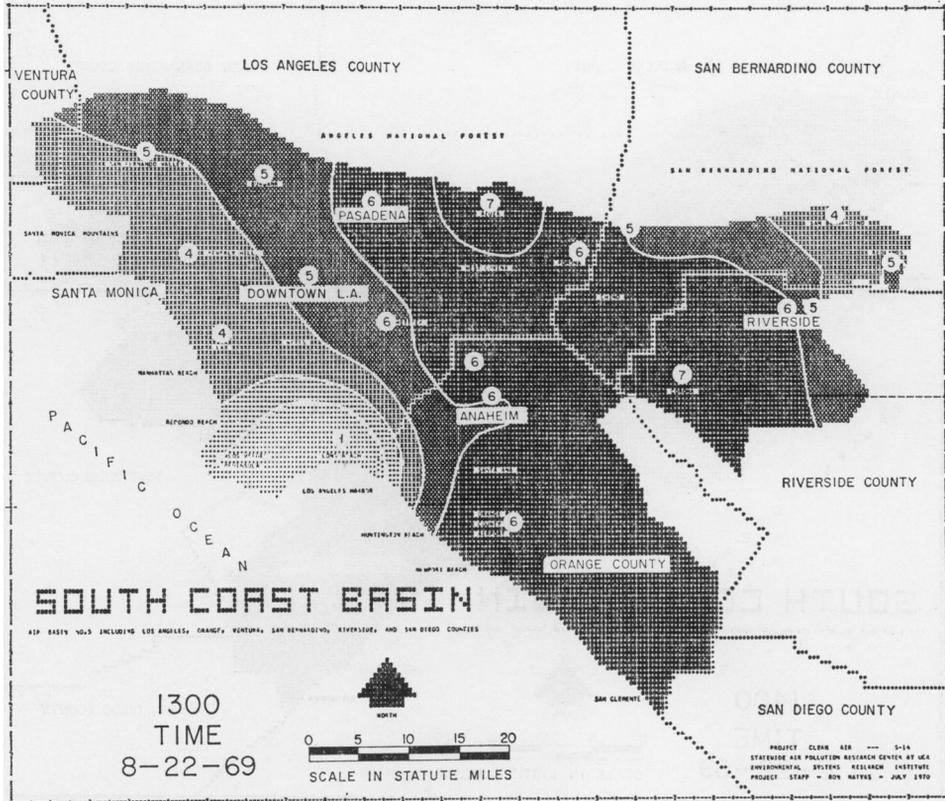


FIGURE 34

Extent of oxidant level at 1300 on August 22, 1969.

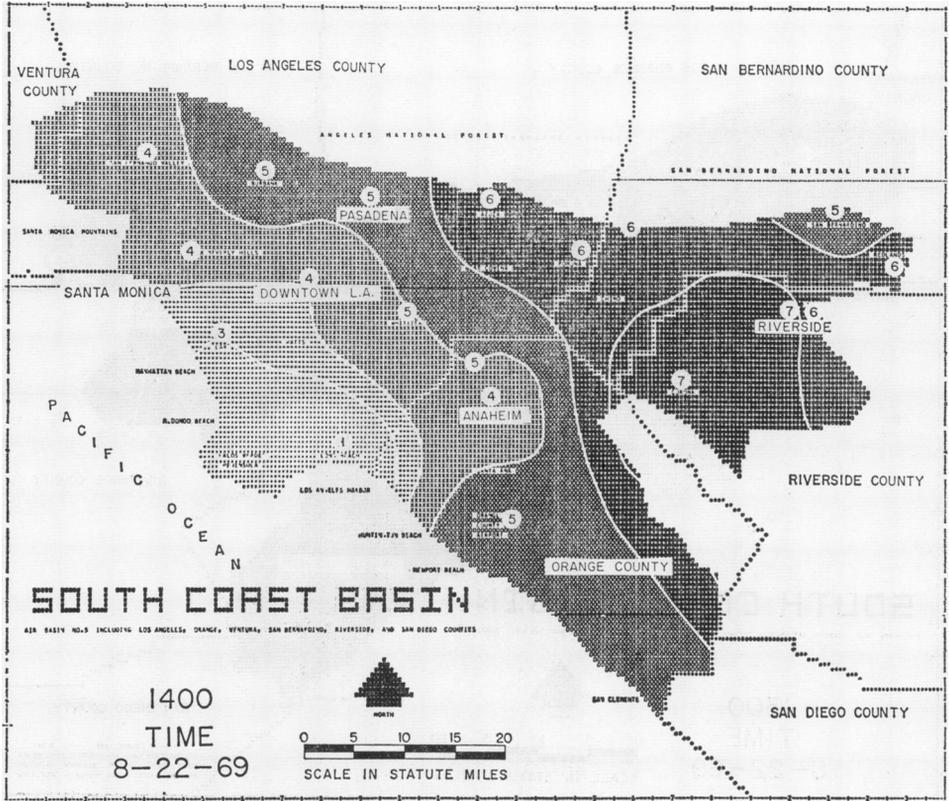
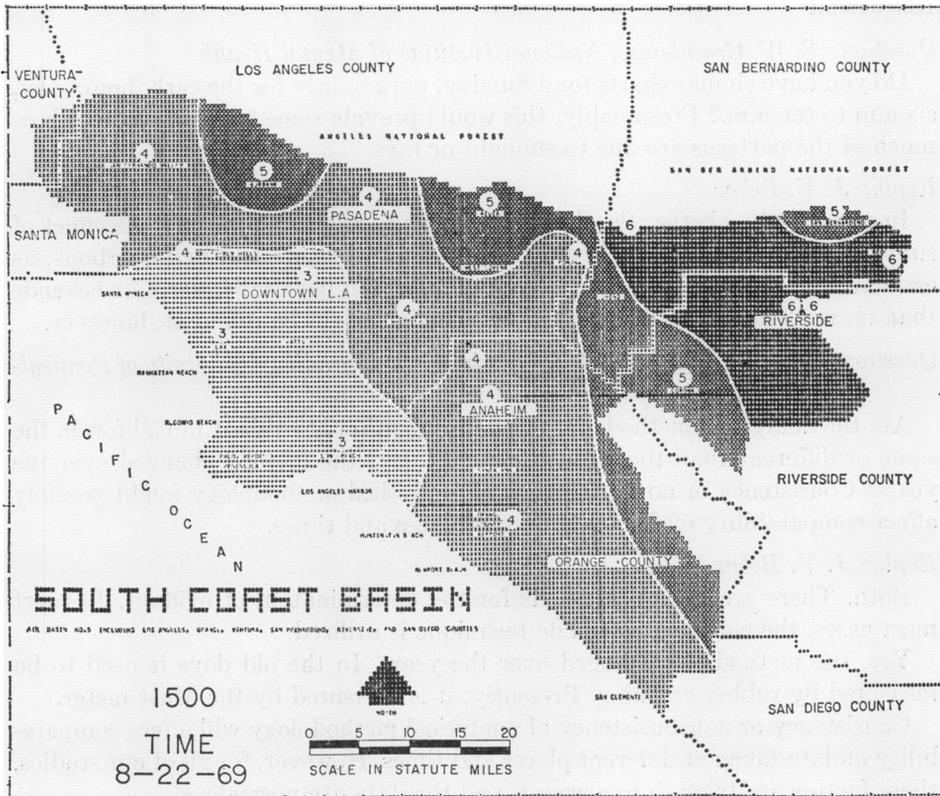


FIGURE 35

Extent of oxidant level at 1400 on August 22, 1969.



**FIGURE 36**  
Extent of oxidant level at 1500 on August 22, 1969.

**Discussion**

*Question: S. W. Greenhouse, National Institute of Mental Health*

Do you have similar charts for a Sunday, particularly for the early hours, say, six a.m. to ten a.m.? Presumably, this would provide some base line data of how much of the patterns are due to sunlight or rays.

*Reply: J. V. Behar*

In response to whether Sunday measurements might reflect only the effect of sunlight, note that the primary emissions of nitric oxide and hydrocarbons, as estimated by carbon monoxide, are only about ten per cent lower on weekends than on weekdays. The distribution by location might be different, however.

*Question: R. J. Hickey, Institute for Environmental Studies, University of Pennsylvania, Philadelphia*

Are the analytical methods for the determination of oxidant in California the same or different than the method of PHS? Has the method changed over the years? Consistency or nonconsistency of analytical methodology might possibly affect comparability of data in different places and times.

*Reply: J. V. Behar*

Both. There are several methods for the determination of oxidant. In most most cases, the colorimetric iodide technique is utilized.

Yes, the method has changed over the years. In the old days it used to be measured by rubber cracking. Presently, it is measured by the Mast meter.

Consistency or nonconsistency of analytical methodology will affect comparability of data taken at different places and times. However, for all of our studies, these factors are taken into account, and the data are normalized.

*Question: J. F. Finklea, Environmental Protection Agency, Durham, N.C.*

Scattered observations from eastern conifer forests indicate that background levels of oxidants may, on occasion, reach up to one half to two thirds of the national ambient air quality standard for photochemical oxidants (0.08 ppm).

*Reply: J. V. Behar*

I agree.

*Question: V. L. Sailor, Brookhaven National Laboratory*

Could you please explain briefly what you mean by oxidants?

*Reply: J. V. Behar*

Oxidants are generally thought to be composed by approximately 80–90% ozone, some NO<sub>2</sub>, and some peroxyacetyl nitrate.

*Question: B. E. Vaughan, Ecosystems Department, Battelle Memorial Institute, Richland, Wn.*

In discussing toxic effects, it is important to realize that there is a question of environmental degradation and overall ecological effect. A datum for toxicity in any one animal or a datum for toxicity in a particular plant may not be an adequate measure of environmental degradation.

*Reply: J. V. Behar*

I agree. It ought to be pointed out that the technique here involves study of the dose rates and not the toxicities.

*Question: H. L. Rosenthal, School of Dentistry, Washington University*

Dr. Went has recently shown that the atmosphere in wooded areas contained large amounts of terpenoid and hydrocarbon emissions from plants. Do you have any information concerning the levels of oxidants in primeval areas due to such emissions? What can be considered an adequate background of oxidant acceptable for human life? In view of our evolutionary development, should a level of zero oxidants be advisable? (Dr. Goldsmith commented that zero levels are not really attempted.)

*Reply: J. V. Behar*

No, we do not have information concerning levels of oxidants in primeval areas. We do have measurements in forested areas located downwind from large urban centers, and measurements indicate that the levels of oxidants from the slopes of the wooded areas may be higher than in the general urban atmosphere. Reference: *Project Clean Air*, Vol. 2, University of California Task Force and Assessments, September 1970. See S-20, in the bibliography.

I do not feel qualified to answer Dr. Rosenthal's second question. As for the third, zero oxidant level is not attainable, in principle, since there is background level independent of human activity; precisely what that level is presumably in the range 0.02–0.05 ppm.

*Question: R. W. Gill, Department of Biology, University of California, Riverside*

What method was used to fit contour lines to data from only 20 stations?

*Reply: J. V. Behar*

This was stated in the paper.