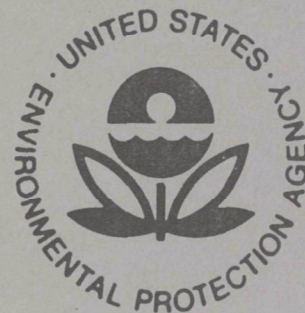


EPA-R4-73-030f

July 1973

ENVIRONMENTAL MONITORING SERIES

**URBAN AIR SHED PHOTOCHEMICAL
SIMULATION MODEL STUDY**
VOLUME II - USER'S GUIDE AND DESCRIPTION
OF COMPUTER PROGRAMS



Office of Research and Development
U.S. Environmental Protection Agency
Washington, D.C. 20460

**URBAN AIR SHED PHOTOCHEMICAL
SIMULATION MODEL STUDY
VOLUME II - USES'S GUIDE AND DESCRIPTION
OF COMPUTER PROGRAMS**

by

S. D. Reynolds

Systems Applications, Inc.
9418 Wilshire Boulevard
Beverly Hills, California 90212

Contract No. 68-02-0339
Program Element No. 1A1009

EPA Project Officer: Herbert Viebrock

Meteorology Laboratory
National Environmental Research Center
Research Triangle Park, North Carolina 27711

Prepared for

OFFICE OF RESEARCH AND DEVELOPMENT
U.S. ENVIRONMENTAL PROTECTION AGENCY
WASHINGTON, D.C. 20460

July 1973

This report has been reviewed by the Environmental Protection Agency and approved for publication. Approval does not signify that the contents necessarily reflect the views and policies of the Agency, nor does mention of trade names or commercial products constitute endorsement or recommendation for use.

TABLE OF CONTENTS

	<u>Page</u>
INTRODUCTION	1
I. SYSTEM OVERVIEW	3
II. DESCRIPTION OF THE PROGRAMS	10
A. The Emissions Data Preparation Program	10
1. Program Objective and Capabilities	10
2. Program Structure	11
3. Input Data Requirements	13
4. Program Output	14
B. The Meteorological Data Preparation Program	14
1. Program Objective and Capabilities	14
2. Program Structure	16
3. Input Data Requirements	17
4. Program Output	17
C. The Atmospheric Pollution Simulation Program	17
1. Program Objective and Capabilities	17
2. Program Structure	18
3. Input Data Requirements	28
4. Program Output	29
D. The Data Plotting Program	29
1. Program Objective and Capabilities	29
2. Program Structure	31
3. Input Data Requirements	38
4. Program Output	38
III. OPERATING PROCEDURES	39
A. General Information and Instructions	39
B. Program Operating Characteristics	40
1. The Emissions Data Preparation Program	40
2. The Meteorological Data Preparation Program	50

	<u>Page</u>
3. The Atmospheric Pollution Simulation Program	50
4. The Data Plotting Program	66
IV. LISTINGS, SYMBOL GLOSSARIES, AND SAMPLE OUTPUT . . .	71
A. The Emissions Data Preparation Program	72
1. Program Listing	72
2. Symbol Glossary	80
3. Sample Output	86
B. The Meteorological Data Preparation Program . .	90
1. Program Listing	90
2. Symbol Glossary	95
3. Sample Output	97
C. The Atmospheric Pollution Simulation Program .	100
1. Program Listing	100
2. Symbol Glossary	135
3. Sample Output	149
D. The Data Plotting Program	166
1. Program Listing	166
2. Symbol Glossary	179
3. Sample Output	185
REFERENCES	189

INTRODUCTION

The simulation model described in Volume I of this report is a dynamic model that was developed to predict ground level concentrations of inert and photochemically reactive atmospheric contaminants and their variations in space and time. Since the governing equations that comprise the model are coupled, nonlinear, second-order partial differential equations, a numerical, rather than analytical, solution is required. In addition, a comprehensive emissions and meteorological data base is needed to exercise the model. Clearly, a model of this computational complexity must be implemented on a digital computer. It is the purpose of the User's Guide to describe both the overall and specific operational characteristics of the computer programs which embody the model.

To realize the full utility of the model, the computer programs have been structured for general use, and not for exclusive application to a particular airshed. Thus, the inputs to the programs are parameters which specify the characteristics of the region to be modeled. For any specific application, minor modification of the codes may be required to account for individual airshed characteristics which are not treated in the general formulation of the model or codes. Since the simulation study of Los Angeles, reported in Volume I, is the first extensive application of the model, the codes included in this Guide reflect some of the characteristics which are unique to the Los Angeles airshed. In Section III, we discuss the alterations that we have made in the general codes in order to perform the present study.

As a part of this modeling effort, we have developed an airshed simulation package consisting of four computer programs. Three of the programs are subsidiary to the main program, which is used to predict ground level pollutant concentrations. We note that there are a large number and variety of inputs to an airshed model. As a result, we have written two specialized programs which perform specific tasks involving input data. One program carries out operations dealing with meteorological input data, while the other processes pollutant emissions inputs. The third subsidiary program prepares plots of the results predicted by the main airshed simulation program. We have found that structuring the system in this manner greatly simplifies its use.

The User's Guide is segmented into four sections. In Section I, we present an overview of the airshed simulation package. The main objective is to explain the basic computational structure of the package, indicating the function of all programs. To illustrate the manner in which a typical airshed simulation is performed, we describe the step-by-step application of each program, discussing required inputs, calculations performed, and use of the program output.

Section II is devoted to a detailed description of the individual programs, focusing on objectives, structure and capabilities. Since complete disclosures of all algorithms are included in Volume I of this report and in Roth et al. (1971), this discussion will deal only superficially with the technical content of the model. When appropriate, we refer the user to related sections in either or both of the reports cited for an expanded discussion of the topic.

The successful implementation of the airshed simulation package requires detailed knowledge of individual program operating procedures. In Section III, we present a complete set of instructions for the use of all programs. Computing system information is given, including program size, computing time, and hardware requirements. Since a large volume of data, provided as punched cards, is input to the programs, we have formulated a set of tables depicting the data-deck setup for every program. The tables include a detailed description of the input parameters, their units, and the format of each card.

Finally, listings of all programs are provided in Section IV. In addition, we have compiled for each program a symbol glossary describing important variables and their definitions. The glossary, in conjunction with the comments contained in the program, is intended for use as an aid in identifying the function of any particular section of the code. The symbol glossary is located immediately after the listing of the program. Following the glossary, we include several typical examples of program output.

In a practical sense, the computer codes may be viewed as FORTRAN representations of the algorithms and ideas presented in Volume I of this report and its earlier companion report. Thus, in order to fully appreciate the technical content of the programs, the user should be thoroughly familiar with Volume I and its Appendices, and with Roth et al. (1971) and its associated Appendices. Of course, anyone primarily interested in the technical aspects of the model will find the discussions in the reports cited of greater benefit and interest than the general descriptions included in the User's Guide.

For those who are interested in obtaining general information regarding the computational structure or capabilities of the programs, the discussions in Sections I and II of this Guide should prove sufficient. Individuals responsible for actually operating any or all of the programs should read the entire User's Guide, Sections II, III, and IV being of particular interest.

I. SYSTEM OVERVIEW

In this section, we describe the overall operating structure of the airshed simulation package. Before presenting this discussion, however, we briefly outline the major components of the model.

- a. Emissions. An emissions inventory must be prepared for all chemical species of interest. This involves calculating the total mass of pollutant emitted from automobiles, aircraft, and fixed sources into each ground level grid cell.
- b. Meteorology. Meteorological inputs of wind speed, wind direction, and mixing depth are specified at the center of all grid cells.
- c. Chemical kinetic mechanism. A chemical kinetic mechanism is required if any of the species of interest react in the atmosphere. The mechanism is used to determine the rate at which pollutant concentrations change due to chemical reaction.

The nonlinear, coupled partial differential equations expressing the conservation of mass of each pollutant comprise the governing equations of the model. Individual reaction rate expressions (from the kinetic mechanism) are incorporated into the equations, and emissions and meteorological data are inputs to the model. The solution is carried out by numerically integrating the governing equations on a three dimensional grid overlaying the modeling region to obtain the temporal variation of pollutant concentrations at each cell on the grid. The ground level grid layout used for the Los Angeles simulation study is shown in Figure 1.

The model developed in this study is embodied in four computer programs. The most important of these is the Atmospheric Pollution Simulation Program (APSP), which is used for predicting concentrations of air contaminants at the grid cells comprising the region to be modeled. We have also developed two specialized data preparation programs to process the large volume of emissions and meteorological input data. Digitized wind and mixing depth maps are input to the Meteorological Data Preparation Program (MDPP). This information is processed and placed in the Meteorological Data File (MDF). Emissions from automobiles, aircraft, and fixed sources are all combined in the Emissions Data Preparation Program (EDPP) to produce an array of total pollutant fluxes into each ground level grid cell. These fluxes are then placed in the Emissions Data File (EDF). The two data files serve as the primary mechanism for input of meteorological and source data to the APSP.

Validation of the model involves comparison of simulated concentration predictions with actual field measurements. As an aid in making these comparisons, we developed a Data Plotting Program (DPP). This program is used to prepare plots of both predicted and measured concentrations as a function of time. A Calcomp Plotter is employed to produce the plots, although any other plotter may be substituted after making the appropriate software alterations.

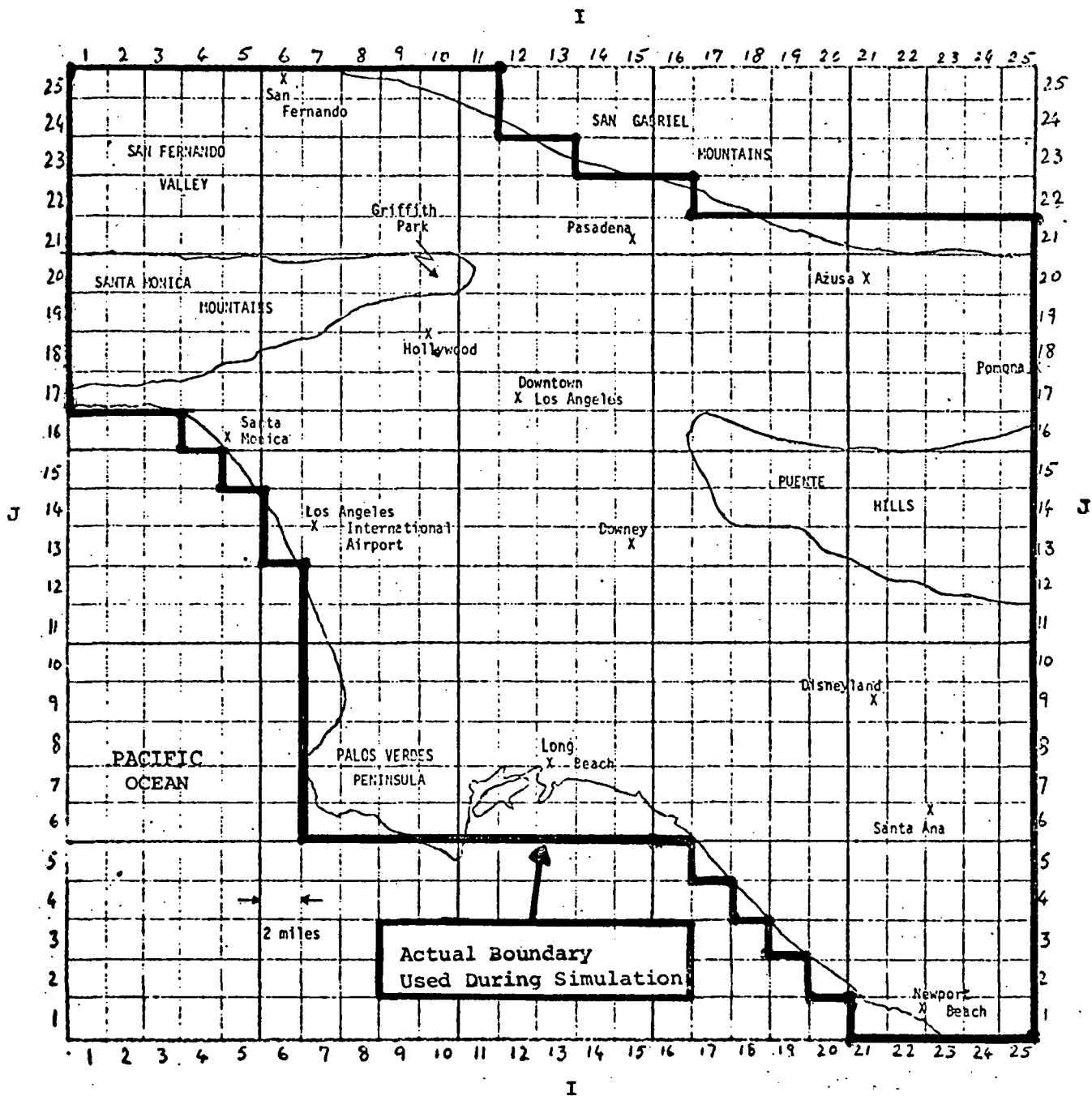
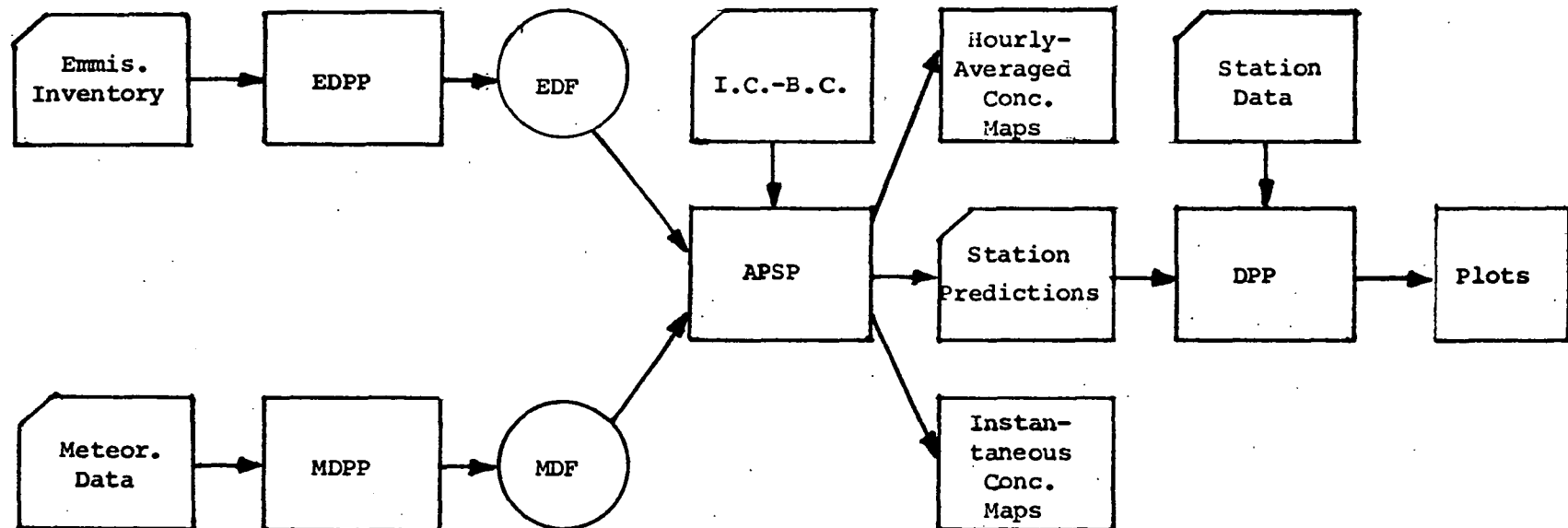


FIGURE 1
THE MODELING REGION

FIGURE 2
SYSTEM FLOW DIAGRAM



- APSP - Atmospheric Pollution Simulation Program
- DPP - Data Plotting Program
- EDPP - Emission Data Preparation Program
- EDF - Emissions Data File
- I.C.-B.C. - Initial and Boundary Conditions, and Other Program Operating Parameters
- MDPP - Meteorological Data Preparation Program
- MDF - Meteorological Data File

In Figure 2, we summarize the overall structure of the airshed simulation package, indicating the flow of information to and from each program. To operate the system, wind and mixing depth maps are prepared and transferred to punched cards. This information is input to the MDPP, which is used to create the MDF. Next, a complete emissions inventory is assembled. Once this inventory is digitized, the EDF is established by the EDPP.

After the two input data files are created, initial and boundary conditions are determined and placed on punched cards. In addition, operating parameters for the APSP are also specified on punched cards and included in the data-deck with the initial and boundary conditions. The APSP is then used to perform the airshed simulation. Pollutant concentrations are predicted at each grid cell, and using these values, an estimate is obtained for the predicted contaminant level at each air quality monitoring station. The results of the simulation are presented in three forms:

- 1) "instantaneous"* ground level concentration maps for all species printed at regular time intervals, such as once an hour - see Figure 3.
- 2) printed hourly-averaged ground level concentration maps for all species - see Figure 4.
- 3) punched cards containing hourly-averaged pollutant concentrations predicted at each air quality monitoring station.

The punched cards from the APSP, along with cards containing the actual pollutant concentrations measured at the stations, serve as the input data to the DPP. This program is used to prepare the final plots, which illustrate the model's performance.

At this point it may not be clear why all four programs are not integrated into one large program. This may be accomplished, for example, by writing each program as a subroutine and creating a small driving program. The reasons for structuring the system in its present form are based mainly on computing and user-oriented considerations. Once a particular data file is created, it may be employed many times while changes are made in the other data file, thus eliminating unnecessary data processing. Consider the following two cases. One emissions inventory may, for example, be used in conjunction with various meteorological conditions, which is in effect the procedure adopted when model validation runs are made for several different days. Similarly, one set of meteorological conditions may be combined with different emissions inventories to test the effectiveness of emission control strategies.

While the two cases discussed above are illustrative of the computational savings inherent in the present package structure, user-oriented considerations are even more important. To successfully perform an airshed simulation, all inputs to the model must be specified correctly.

*An "instantaneous" concentration is a concentration predicted at a particular time during the course of the numerical integration.

FIGURE 3. TYPICAL COMPUTER DISPLAY OF THE INSTANTANEOUS GROUND LEVEL CONCENTRATIONS

03 GROUND LEVEL CONCENTRATIONS (PPHM) AT 1100.00 PST																									
1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	
25	3.5	4.3	4.2	3.9	3.7	3.8	6.3	17.6	27.2	24.5	10.7														
24	3.5	3.8	3.7	3.8	4.0	6.7	14.3	29.5	38.0	36.7	24.0														
23	3.0	3.0	3.0	3.0	4.3	10.1	17.9	25.5	35.8	43.4	36.6	23.1	12.0												
			RESEDA																						
22	2.1	2.5	2.6	2.6	4.7	8.5	12.7	18.9	30.5	41.4	41.2	32.7	21.5	12.4	10.1	11.5									
21	1.7	2.8	3.1	2.9	3.2	6.0	10.5	16.5	23.5	31.6	36.3	36.1	28.5	19.1	13.4	12.2	12.2	12.5	12.0	10.4	8.2	6.2	5.1	4.5	4.2
20	3.3	4.1	4.1	3.9	3.1	4.9	8.4	14.2	16.9	19.3	23.1	30.4	28.9	22.3	14.7	10.8	8.5	7.7	7.3	6.6	5.3	4.1	3.4	3.2	3.3
19	3.2	3.7	3.6	3.5	3.2	3.9	5.6	8.6	9.4	9.2	11.8	20.0	23.8	20.9	15.4	10.2	6.2	4.3	3.7	3.5	3.2	2.8	2.7	2.8	2.9
18	3.2	3.4	3.3	3.3	3.1	3.0	3.6	4.4	4.8	5.0	7.4	14.3	19.4	17.7	14.5	11.1	6.9	3.8	2.7	2.4	2.4	2.4	2.5	2.8	3.0
17	3.4	3.3	3.6	3.6	3.1	2.5	2.6	2.6	3.3	6.2	13.6	17.9	16.2	13.7	11.7	8.6	5.6	4.0	3.3	2.8	2.7	2.8	3.2	3.5	
16				4.7	3.5	2.8	2.1	1.9	1.9	2.8	6.4	14.2	17.7	15.4	12.3	9.9	8.3	7.6	6.9	5.4	4.1	3.4	3.2	3.6	4.2
15					5.1	3.7	2.0	1.4	1.6	2.7	6.9	14.5	17.1	13.9	9.6	7.0	6.2	7.8	9.4	8.5	6.4	4.8	4.2	4.3	4.9
14					4.5	1.9	1.2	1.4	2.8	6.9	12.8	13.9	10.6	6.5	4.4	4.4	6.6	10.4	11.1	8.9	6.6	5.3	5.1	5.6	
13					4.7	1.7	1.3	1.4	2.9	6.3	9.6	10.0	7.6	4.7	3.0	3.0	6.0	11.0	12.6	10.7	8.1	6.6	6.0	6.1	
12						2.0	1.4	1.4	2.9	5.2	6.0	6.0	5.4	3.4	2.2	2.1	5.3	11.0	13.2	11.5	9.2	7.6	6.7	6.2	
11						5.0	1.5	1.5	2.9	4.0	3.2	3.4	4.1	3.1	1.7	1.7	3.9	9.2	11.4	10.4	9.1	8.0	6.9	6.0	
10						5.3	3.1	2.0	3.6	3.1	1.8	2.1	3.2	2.9	1.3	1.3	2.9	6.6	8.5	8.5	8.2	7.4	6.1	5.9	
9						5.3	4.1	3.5	3.6	2.8	1.1	1.6	2.6	2.7	1.1	1.3	2.9	4.1	5.7	7.6	7.0	6.3	5.1	5.3	
8						5.1	4.3	3.7	3.4	2.8	1.6	2.4	3.1	3.5	1.1	2.1	3.7	3.1	3.2	4.9	5.1	4.6	4.2	5.0	
7						5.2	4.8	4.5	4.1	4.0	4.0	4.0	4.8	4.6	3.8	4.9	4.8	3.3	2.5	3.0	4.2	4.0	4.0	4.9	
6						5.5	5.4	5.2	4.9	5.1	5.3	5.3	6.8	5.3	5.9	5.1	5.1	3.8	2.5	2.4	3.5	4.4	4.4	4.5	
5																	4.2	4.7	3.9	2.4	2.7	3.9	4.6	4.8	4.3
4																									
3																									
2																									
1																									
					</																				

FIGURE 4. TYPICAL COMPUTER DISPLAY OF THE HOURLY-AVERAGED GROUND LEVEL CONCENTRATIONS

AVERAGE GROUND LEVEL CONCENTRATIONS (PPHM) OF O3 BETWEEN THE HOURS OF 1000. AND 1100. PST																									
1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	
25	4	4	4	3	3	3	4	9	11	8	4														
24	4	3	3	3	3	4	8	20	22	16	8														
23	3	3	3	3	3	6	12	23	30	29	20	10	6												
22	2	2	2	2	3	5	9	15	23	33	34	21	10	7	7	9									
21	2	2	2	2	2	5	8	12	17	24	37	32	18	11	9	10	13	14	13	10	8	6	5	4	4
20	4	4	4	3	2	4	8	12	16	18	26	33	25	16	11	11	11	11	10	7	5	4	3	3	3
19	4	4	4	3	3	3	5	9	11	10	14	24	24	17	11	9	7	7	6	4	3	3	3	3	3
18	3	3	3	3	3	3	4	5	6	6	8	16	18	14	9	6	5	4	3	3	2	2	3	3	3
17	3	3	3	3	3	2	3	3	3	3	6	13	14	11	10	7	4	3	3	3	2	3	3	3	3
16				4	3	3	2	2	2	3	6	13	13	10	10	8	5	4	4	3	3	3	3	3	4
15				4	3	2	1	1	2	7	13	13	10	8	7	5	6	6	5	4	3	3	4	5	
14					3	1	1	1	2	6	11	12	9	7	5	5	7	8	7	5	4	4	5	5	
13					3	1	1	1	3	5	8	9	7	4	3	4	7	10	9	7	5	5	5	6	
12							1	1	1	3	4	5	6	5	3	2	3	7	10	11	8	6	6	6	6
11							4	1	1	3	3	3	4	3	2	1	3	6	9	10	8	7	6	6	5
10							4	2	2	3	2	2	3	3	2	1	2	5	7	8	7	7	6	5	5
9							4	3	3	3	2	1	2	2	1	2	4	4	6	6	6	5	4	5	
8							4	4	3	3	2	1	2	3	2	1	2	3	2	4	5	4	4	4	4
7							4	4	4	3	3	3	3	4	3	3	4	3	2	2	3	4	3	3	4
6							4	4	4	4	3	3	4	5	4	5	6	4	2	2	3	3	3	4	4
5																	5	5	3	2	2	3	4	4	4
4																		5	3	2	3	4	4	4	4
3																			3	5	5	5	4	4	4
2																				6	6	5	4	3	4
1																					6	4	3	4	4

Considering the number and types of parameters involved, it is convenient to treat the input of emissions and meteorological data separately. This enables the user to concentrate fully on the task of establishing the emissions and meteorological data files. Thus, the EDF and the MDF are created and checked for accuracy and correctness before an airshed simulation is attempted. The contents of the EDF and the MDF are listed in the program output of the EDPP and the MDPP respectively.

This concludes our discussion of the general system considerations. In the next section we examine each of the four programs in sufficient detail to give the user a basic understanding of individual program structure and capabilities.

II. DESCRIPTION OF THE PROGRAMS

A. The Emissions Data Preparation Program

1. Program Objective and Capability

Pollutant emissions from automobiles, aircraft, and distributed fixed sources are combined in the Emissions Data Preparation Program to produce a total flux of each pollutant species into every ground level grid cell. The fluxes are stored in the Emissions Data File for future use by the APSP. Calculation of the fluxes requires an emissions model and inventory. The emissions model forms the basis for the algorithms in the code, while the emissions inventory serves as the input data to the program. To fully appreciate the scope of a comprehensive emissions model and inventory for a large urban area, the user is encouraged to read Appendix A of Roth et al. (1971), and Appendix A in Volume I of this report.

Since most source emissions rates undergo diurnal variations, fluxes are calculated at a sufficient number of times throughout the day to represent the characteristic temporal changes. In the present study, we calculate emissions at five minute intervals between 0500* and 1000 hours, and hourly thereafter. For convenience, all times used in this study are Pacific Standard Time (PST). The emissions inventory, however, is based on "local time". We note that when daylight savings time is in effect, local time and standard time differ by one hour. Therefore, we include the appropriate logic in the EDPP to make a one hour shift in the emissions for use on those days when local time and standard time do not correspond.

An important point must be made regarding the treatment of sources. Emissions from large point sources, such as power plants, are treated separately in the APSP. Thus, two fixed source inventories are required. The first contains all distributed, ground-based fixed source emissions, such as those from petroleum marketing operations. These sources are processed by the EDPP. The second fixed source inventory includes the remaining point sources, which only emit pollutants from a relatively few locations. Typically, these sources inject pollutants into the atmosphere from high stacks, which makes it inappropriate to treat them with the other ground-based sources. The point source inventory is input to the APSP on punched cards, while the ground-based emissions are input to the APSP using the EDF.

We wish to note that the EDPP is presently structured to make computations of emissions between 0500 and 1655 hours. However, the program can easily be modified to compute emissions to 2355 hours. Further alterations to the code will be required to compute emissions prior to 0500 hours, or after 2400 hours (i.e., into the next day). In Section III, we include instructions for extending the computation of emissions from 1655 to 2355 hours.

*0500 hours corresponds to 5 A.M.

The EDPP is primarily used to create the EDF. This file contains the information needed by the APSP to calculate ground level emissions fluxes. In the following discussion we explain the structure of the EDF. The discussion is illustrated in Figures 5 and 6.

First, emissions fluxes are calculated for all species at the starting time, 0500 hours, and written on the EDF. Then emissions fluxes are calculated at 0505 hours. If we assume that the flux varies linearly between 0500 and 0505 hours, the time rate of change of the emissions flux is given by

$$\frac{dQ_{l,i,j}}{dt} = \frac{Q_{l,i,j}(0505) - Q_{l,i,j}(0500)}{5 \text{ minutes}} \quad \text{for } 0500 \leq t \leq 0505,$$

where $Q_{l,i,j}(t)$ is the flux of species l from grid square (i,j) at time t .

Note that we can calculate any value of $Q_{l,i,j}(t)$, where $0500 \leq t \leq 0505$, if we know $Q_{l,i,j}(0500)$, since

$$Q_{l,i,j}(t) = Q_{l,i,j}(0500) + \frac{dQ_{l,i,j}}{dt} (t-0500)$$

The two times, 0500 and 0505, are written on the EDF followed by values of the time rate of change of the emissions fluxes.

Next, we compute the emissions fluxes at 0510 hours and again assume linear time behavior. We calculate the time rate of change of the fluxes, as before, applicable between 0505 and 0510 hours. The two times, 0505 and 0510 are written on the EDF followed by values of the time rate of change of the emissions fluxes. To obtain the values of the emissions fluxes at any time t , we simply reconstruct the connected line segment curves (see Figures 5 and 6) using the initial fluxes, the time intervals, and the slopes of the lines (i.e., $dQ_{l,i,j}/dt$). This is essentially the way in which emissions fluxes are calculated by the APSP from the information contained in the EDF.

2. Program Structure

The EDPP consists of a MAIN program and one subprogram, TIME.

MAIN

Structurally, the MAIN program is divided into four sections. The first section is devoted to program initialization, which involves the input of the emissions inventory. In the second section, emissions are calculated every five minutes between 0500 and 0955 hours. The time rate of change of the emissions fluxes (ppm-ft/min²) are computed and written in the EDF. The third section is very similar to the second, except emissions fluxes are calculated hourly from 1000 to 1655 hours. Since the temporal distribution

FIGURE 5
 ASSUMED TEMPORAL VARIATION OF THE EMISSIONS FLUX AT A
 PARTICULAR LOCATION BETWEEN 0500 AND 0955 HOURS

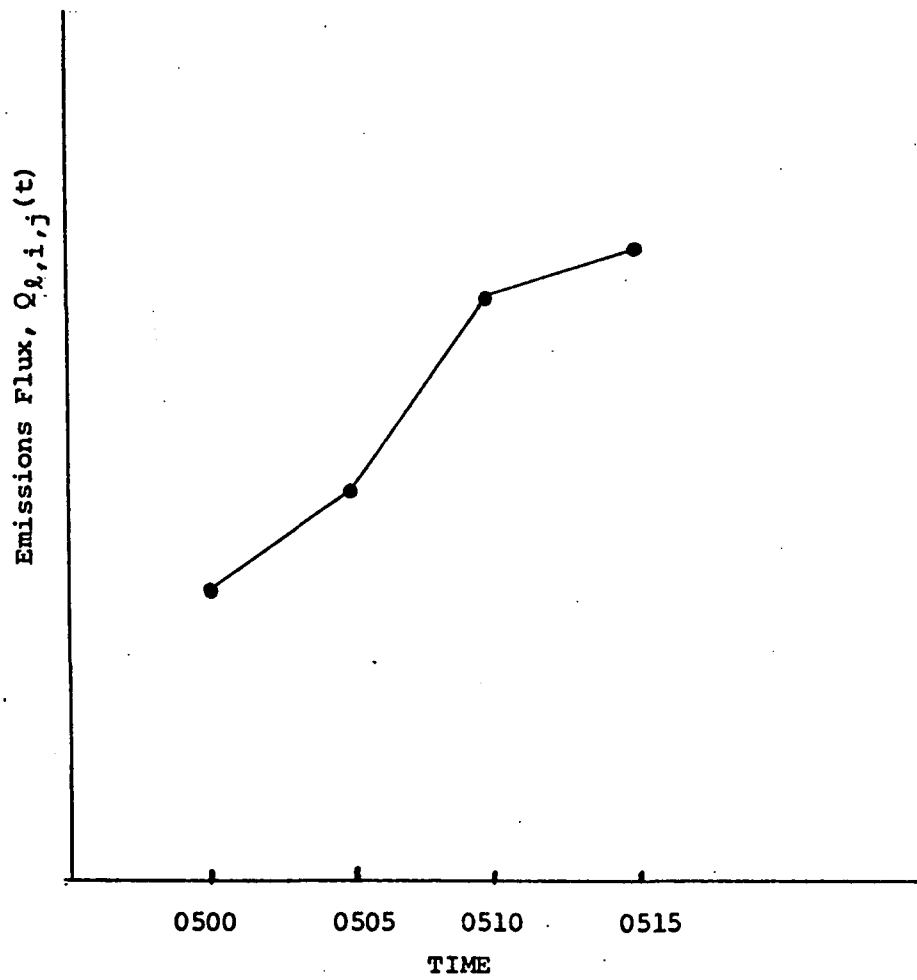
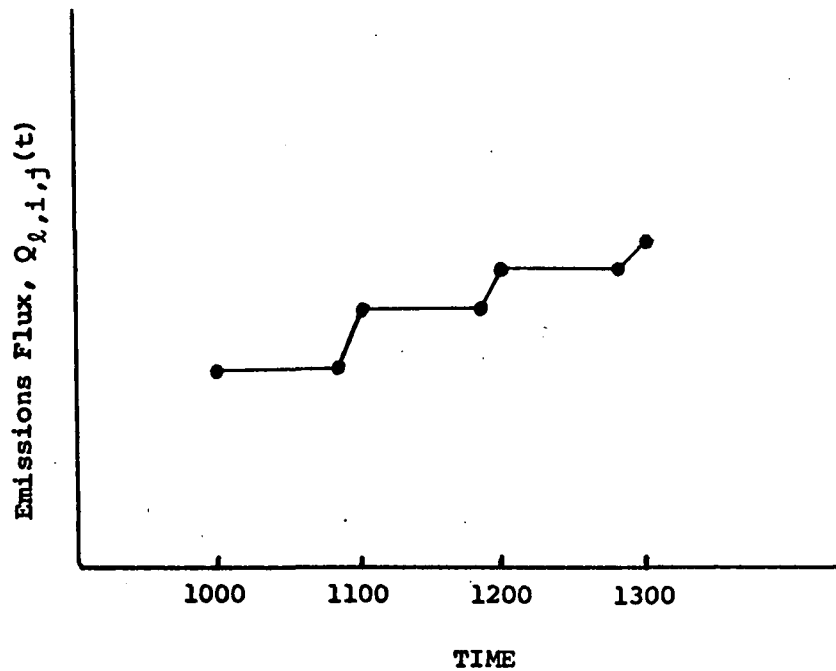


FIGURE 6
 ASSUMED TEMPORAL VARIATION OF THE EMISSIONS FLUX AT A
 PARTICULAR LOCATION AFTER 1000 HOURS



of automobile emissions is constant over hourly periods but discontinuous from one hour to the next, the computation for each hour takes place in two steps. Emissions rates are assumed constant over the first 55 minutes of the hour. Then from the 55 minute point to the beginning of the next hour, the emissions vary linearly in time between the two hourly values (see Figure 6).

In the last section of the EDPP, emissions fluxes are calculated using the newly created EDF. The fluxes applicable at the beginning of each hour are printed on the program output to provide a partial record of the contents of the EDF.

TIME (T1, T2, M)

Three types of arithmetic operations involving times in minutes and times based on a 2400 hour clock are performed in function subprogram TIME.

If M=1, add T2 to T1 and return the sum, where T1 is 2400 hour time, and T2 has the units of minutes. For example, if T1=0530 and T2=40, the result is 0610 (add 40 minutes to 5:30 A.M. to obtain 6:10 A.M. = 0610 hours).

If M=2, subtract T2 from T1, where T1 and T2 are 2400 hour times. The result is expressed in minutes. For example, if T1=0610 and T2=0530, the result is 40 minutes.

If M=3, the operation is analogous to that with M=1, except a subtraction is performed. If T1=0610 and T2=40, the result is 0530 (subtract 40 minutes from 6:10 A.M. to obtain 5:30 A.M.=0530 hours).

3. Input Data Requirements

The following outline lists the general types of information that must be provided as inputs to the EDPP. See Table 2 for a complete summary of the input data required by the program.

a. Automotive Emissions

- daily miles driven on all streets (excluding freeways) in each grid square
- daily miles driven on freeways in each grid square
- hot and cold start emissions factors
- fraction of vehicles cold started
- correction factor (β) for the nonuniform distribution of trip starts
- freeway driving speeds in the fast and slow directions
- emissions - driving speed correlation factors
- ratio of freeway vehicle miles driven in the slow direction to the number driven in the fast direction
- temporal distributions of freeway and non-freeway traffic activity

b. Aircraft Emissions (Ground Operations)

- number of daily aircraft flights at each airport
- temporal distribution of aircraft activity
- emissions/aircraft engine
- number of aircraft engines/aircraft

c. Fixed Source Emissions (Ground-Based)

- total distributed fixed source emissions from each grid square

4. Program Output

The output of the EDPP consists of the EDF and the printed listing of hourly values of the emissions fluxes. The units of the fluxes displayed on the printed output are ppm-ft/minute. Examples of the printed output are included in Section IV.

B. The Meteorological Data Preparation Program

1. Program Objective and Capabilities

Digitized wind speed, wind direction, and mixing depth maps are converted in the MDPP to a format suitable for input to the APSP. The meteorological data is then placed in the Meteorological Data File, where it can be accessed at a later time. Thus, the operation performed by this program is basically that of transferring information from cards to tape or disc.

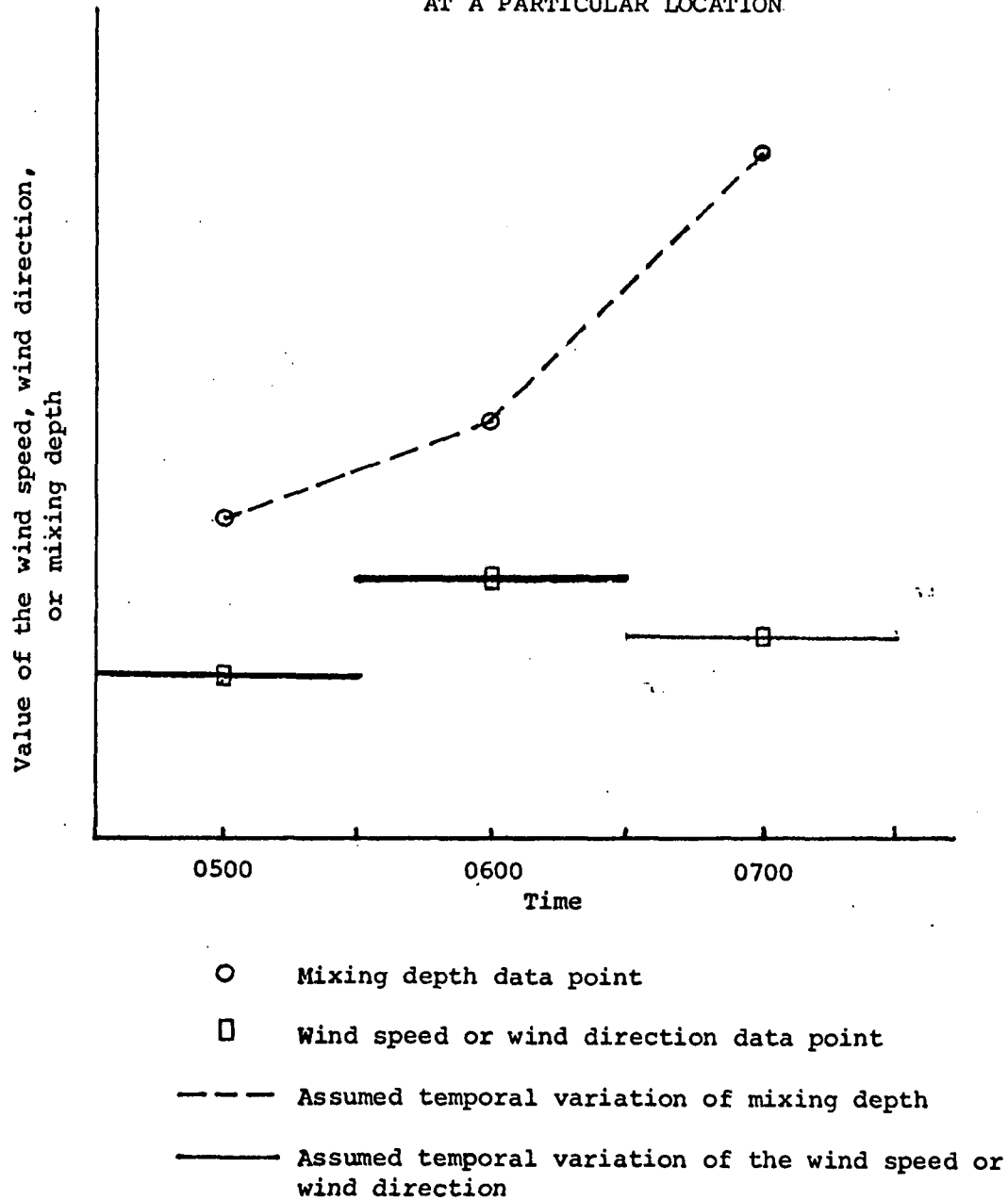
Hourly-averaged wind speed and wind direction maps must be prepared for each hour to be simulated. The time averaging is assumed to extend from the half hour to the half hour. Thus, wind speeds applicable at 0500 hours, for example, are obtained from the 0430 - 0530 wind speed map. Mixing depth maps are also prepared hourly, applicable at the beginning of each hour (i.e., at 0500 PST, 0600 PST, and etc.). Mixing depths are assumed to vary linearly in time between the values prescribed at two consecutive hours. In Figure 7, we represent the assumed temporal changes of the wind speed, wind direction, and the mixing depth.

In the following discussion, we describe the structure and content of the MDF. Initial values of the mixing depth at 0500 hours are read from the data-deck and placed directly in the MDF. Next, wind speeds, wind directions, and the time rate of change of the mixing depths are determined, applicable between 0500 and 0530 hours. The wind data are obtained from the data-deck, as are the values of the mixing depths at 0600 hours. The time rate of change of the mixing depths are calculated in the following manner. Assuming linear temporal behavior, the rate of change for the mixing depth at grid square (i,j) is given by:

$$\frac{d\Delta H_{i,j}}{dt} = \frac{\Delta H_{i,j}(0600) - \Delta H_{i,j}(0500)}{60 \text{ minutes}}$$

for $0500 \leq t < 0600$

FIGURE 7
TREATMENT OF THE TEMPORAL CHANGES
IN WIND SPEED, WIND DIRECTION, AND MIXING DEPTH
AT A PARTICULAR LOCATION



The time interval, designated by 0500 and 0530, is written on the MDF followed by values of the wind speed (feet/minute), wind direction (radians), and time rate of change of the mixing depth (feet/minute). We summarize below the order in which the first hour of meteorological data is arranged in the MDF.

- . Mixing depths at 0500 PST
- . Time interval, designated by 0500 and 0530, over which the following data are applicable
- . Wind speeds
- . Wind directions
- . Time rate of change of the mixing depths
- . Next time interval, designated by 0530 and 0600, over which the following data are applicable
- . Wind speeds
- . Wind directions
- . Time rate of change of the mixing depths

Succeeding blocks of meteorological data are arranged as follows:

- . Time interval, designated by t_1 and t_2 , over which the following data are applicable
- . Wind speeds
- . Wind directions
- . Time rate of change of the mixing depths

2. Program Structure

The MDPP is composed of a MAIN program and one subprogram, TIME.

MAIN

The MAIN program is used to perform two basic functions. First, meteorological input data supplied on punched cards is converted into a format suitable for input to the APSP and written on tape or disc. Wind speeds are converted from miles/hour to feet/minute, and wind directions are converted from degrees to radians. After all meteorological data is written in the MDF, hourly printed maps of wind speed, wind direction, and mixing depth are produced. These maps provide a complete summary of all meteorological data contained in the MDF.

TIME (T1, T2, M)

See the description given in the discussion of the EDPP.

3. Input Data Requirements

The following information must be supplied on punched cards for each hour

- Wind speeds
- Wind directions
- Mixing depths

A complete description of the order and format of the input data is given in Table 3.

4. Program Output

The primary output of the MDPP is the MDF. In addition, printed hourly maps of wind speed (m.p.h. x 10), wind direction (degrees), and mixing depth (feet) are also produced. Typical examples of the printed output are included in Section IV.

C. The Atmospheric Pollution Simulation Program

1. Program Objective and Capabilities

The actual airshed simulation is performed by the APSP. Meteorological inputs consisting of wind speed, wind direction, and mixing depth are obtained from the data in the MDF, while ground level emission inputs are calculated from information in the EDF. The simulation involves the numerical integration of the governing model equations by the finite-difference techniques described in Appendix D of Volume I of this report. The primary objective of the APSP is the prediction of ground level pollutant concentrations of both inert and photochemical species on a grid such as that illustrated in Figure 1.

Several useful features have been incorporated in the APSP. At present, the program is capable of simulating up to six chemical species. Each species is designated by a number, and we have adopted the following convention for this study:

Species Number	Species Name
1	Reactive Hydrocarbon
2	Nitric Oxide
3	Ozone
4	Nitrogen Dioxide
5	Carbon Monoxide
6	Unreactive Hydrocarbon

This numbering convention is consistent with that used in the EDPP. A full photochemical simulation involves all six species, but it is possible to operate the program simulating fewer species. The following list contains all the possible combinations of species that can be simulated simultaneously:

- a. species 1, 2, 3, 4, 5, and 6
- b. species 1, 2, 3, 4, and 5
- c. species 5 and 6
- d. species 5 or 6

The user specifies which species are to be simulated as part of the input data to the APSP. During photochemical validation studies, we use this feature as follows. First, CO is simulated to test the meteorological and automotive source inputs. If the results indicate that these parameters are specified correctly, then a full photochemical simulation is carried out involving all six chemical species. We also note that other inert species can be substituted for CO and/or unreactive hydrocarbon simply by changing a few input parameters in the data-deck of the program.

Another important feature designed into the program is the capability of performing the numerical integration on an irregularly shaped grid. We note in Figure 1, that many grid squares are located over the Pacific Ocean and the San Gabriel Mountains. It is computationally advantageous to eliminate these low population areas since a 30% reduction in the total computing can be realized. To generalize this procedure, the shape of the modeling region is specified as part of the input data to the program. In Figure 1, we illustrate that portion of the original 25x25 ground level grid layout actually used in the Los Angeles simulation study.

The chemical kinetic mechanism is an important component of this simulation model. The mechanism is also subject to change as further studies of atmospheric chemistry are carried out. Since rate constants are treated as input data to the program, they can easily be changed at any time. The mechanism currently employed in the APSP is described in Appendix B of Volume I of this report. To alter the formulation of the mechanism in the program, minor changes in the code are required. In Section III, we include a detailed discussion of these changes.

Before closing this section, we wish to mention that the coding of the APSP has been formulated very carefully. We note that a major portion of the total computing time is spent solving the governing model equations. Therefore, computational efficiency is stressed in the coding of the numerical integration procedure. In other sections of the code, general utility is considered more important. In the next section, we discuss in more detail the structural and computational aspects of the APSP.

2. Program Structure

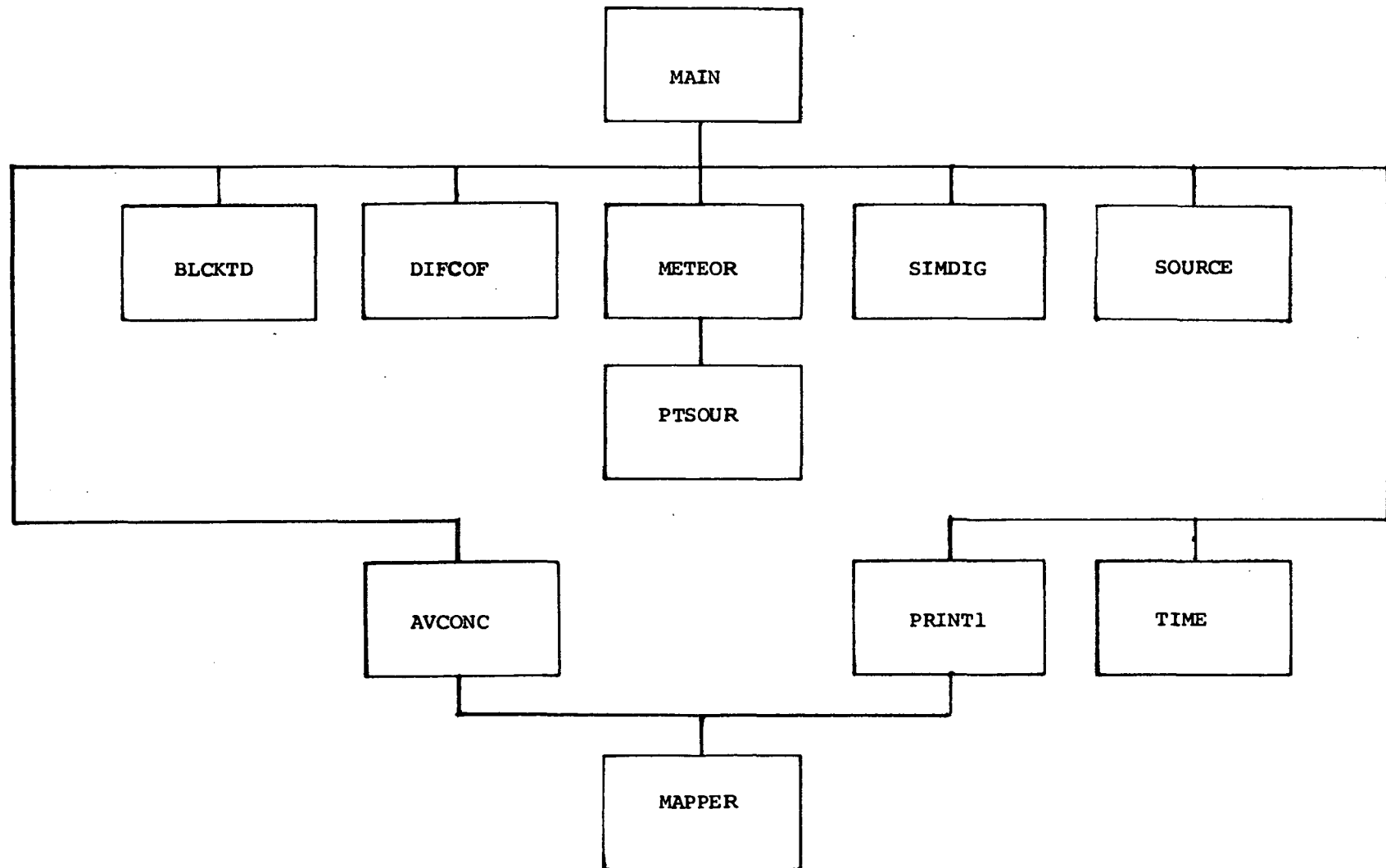
The APSP consists of a MAIN program and several subroutines. In Figure 8 we show a schematic diagram of the structure of the APSP.

MAIN

Two tasks are performed by the MAIN program:

- (1) the control of model initialization
- (2) the numerical integration of the governing airshed equations

FIGURE 8
STRUCTURE OF THE APSP



Model initialization consists of the following procedures that must be performed before the numerical integration can be initiated:

- input of program operating parameters specified on punched cards
- open the EDF and initialize the ground level pollutant flux array (subroutine SOURCE)
- open the MDF and initialize all meteorological variables (subroutine METEOR)
- establish the initial concentration distribution (subroutine ICCONC)

After all parameters in the model have been initialized, the airshed simulation may proceed. Predicted concentrations are obtained by integrating the governing equations in discrete steps over time. The operations involved in advancing from one instant in time to the next, over a discrete time interval, are as follows:

- establish the size of the integration time step
- update meteorological variables (subroutine METEOR) and the distribution of elevated point source emissions (subroutine PTSOUR)
- update ground level emissions fluxes (subroutine SOURCE)
- increment the time-integrated ground level concentration array and the time-integrated station prediction array (entry point CALIVC in subroutine AVCONC)
- update boundary concentrations on the horizontal boundaries (subroutine BCCONC)
- perform Steps I and II of the numerical integration procedure - integration in the x and y directions
- perform Step III of the numerical integration procedure - integration in the z direction; the following calculations are involved:
 - 1. compute turbulent diffusivities (subroutine DIFCOF)
 - 2. solve the finite-difference equations for inert species (subroutine SIMDIG)
 - 3. solve the finite-difference equations for reactive species (subroutine BLCKTD)
- increment the time-integrated ground level concentration array and the time-integrated station prediction array (entry point CALIVC in subroutine AVCONC)
- print hourly-averaged ground level concentrations and station predictions if one hour has elapsed since the last hourly-averaged concentrations were printed (subroutines AVCONC and MAPPER)

When the simulation has been completed, the user may specify that the entire concentration field be dumped onto a save disc/tape area. These concentrations may be used at a later time as initial conditions in a program restart. The restart procedure is discussed further in Section III.

AVCONC

All tasks related to the calculation and printing of the hourly-averaged predicted concentrations are performed in subroutine AVCONC. Hourly-averaged concentrations are calculated at every ground level cell on the grid, and at each air quality monitoring station. We define the hourly-averaged concentration as follows:

$$\bar{c} = \frac{\int_{t_0}^{t_0+60} c(t) dt}{60 \text{ minutes}} \quad (1)$$

where

$c(t)$ is the concentration predicted at time t ,
 \bar{c} is the hourly-averaged concentration, and
 t_0 is the beginning of the time interval over which the concentrations are averaged.

The integration is approximated numerically by the trapezoidal rule. Since monitoring stations are not, in general, located at the center of a ground level grid cell, we interpolate for the predicted concentration at the station using the concentrations predicted in the four nearest ground level grid cells. The interpolation procedure is illustrated in Figure 9.

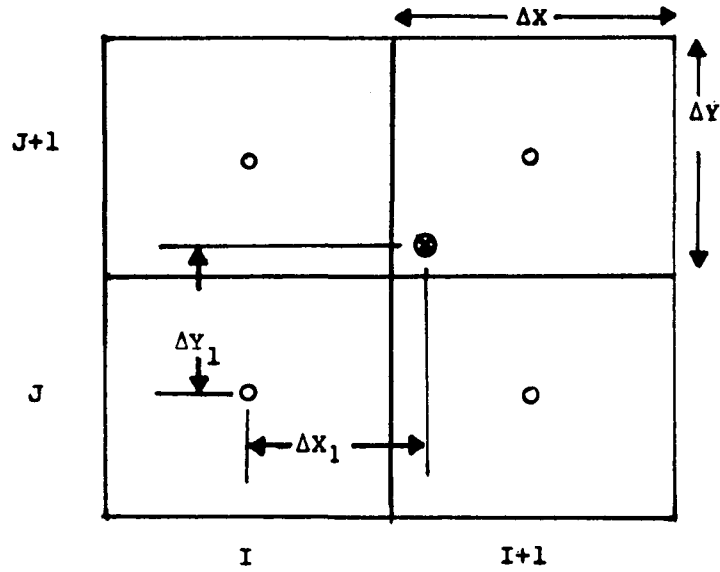
There are two entry points in subroutine AVCONC, and we now discuss the calculations performed in each.

1. Entry Point AVINIT

When AVINIT is entered from MAIN, the arrays which contain the numerical approximations of the integrals are all set to zero. This is an initialization procedure.

FIGURE 9

INTERPOLATION PROCEDURE FOR CALCULATING
THE PREDICTED CONCENTRATION AT A MONITORING STATION



⊗ - monitoring station location

$$C_{\text{station}} = \left[C_{I,J}(1-\xi) + C_{I+1,J} \xi \right] (1-\eta) + \left[C_{I,J+1}(1-\xi) + C_{I+1,J+1} \xi \right] \eta$$

where $\xi = \frac{\Delta X_1}{\Delta X}$

$\eta = \frac{\Delta Y_1}{\Delta Y}$

2. Entry Point CALIVC

The numerical evaluation of the integration defined in Equation (1) is performed in CALIVC. The trapezoidal rule is employed and may be written as follows:

$$\int_{t_0}^{t_n} c(t) dt \approx \frac{1}{2} \sum_{i=0}^{n-1} [c(t_{i+1}) + c(t_i)] (t_{i+1} - t_i) \quad (2)$$

where

$$t_n = t_0 + 60 \text{ minutes}$$

and t_i designates a discrete point in time at which the governing equations of the model are solved.

Before the governing equations are integrated from t_i to t_{i+1} , CALIVC is entered, and the following values of A are calculated for each ground level grid cell and monitoring station.

$$A = \frac{1}{2} c(t_i) (t_{i+1} - t_i) \quad (3)$$

Arrays that will eventually contain the complete expression on the right hand side of Equation (2) for all ground level cells and stations are incremented by the appropriate value of A given in Equation (3).

After the governing equations have been integrated from t_i to t_{i+1} , CALIVC is again entered from MAIN, and the following values of B are calculated for each ground level cell and station.

$$B = \frac{1}{2} c(t_{i+1}) (t_{i+1} - t_i) \quad (4)$$

The arrays that will contain the expression in Equation (2) are this time incremented by the appropriate values of B given in Equation (4). If A and B are summed, we obtain:

$$A + B = \frac{1}{2} [c(t_{i+1}) + c(t_i)] (t_{i+1} - t_i)$$

which is one of the terms in Equation (2). When the governing equations have been integrated to t_n , the complete expression on the right hand side of Equation (2) is available for all ground level grid cells and monitoring stations. This completes our discussion of CALIVC.

AVCONC is called from MAIN once each hour, and the expression for each ground level grid cell and monitoring station given in Equation (2) is divided by 60 minutes to yield the hourly-averaged concentrations. Then the following output is produced by this subroutine:

- . printed hourly-averaged ground level concentration maps for each species (see Figure 4 and Section IV)
- . printed summary of the hourly-averaged concentrations predicted at the monitoring stations (see Section IV)
- . punched cards containing the hourly-averaged concentrations predicted at the monitoring stations

AVINIT

An entry point in subroutine AVCONC (see AVCONC).

BCCONC

In Steps I and II of the numerical integration procedure (integration in the x and y directions), pollutant concentrations are required at points of horizontal inflow to the model. During the simulation, subroutine BCCONC is called from MAIN to update the values of the boundary concentrations. These concentrations are inputs to the model and included in the data-deck of the APSP. A concentration specified at a particular point on the boundary is assumed to apply at all levels between the ground and the inversion base.

To account for temporal changes, the boundary concentrations are allowed to vary in time in a stepwise manner. The user defines a time interval (designated by two times) and a set of boundary concentrations that are to apply during that time interval. For example, to specify a set of boundary concentrations that are to apply between 0500 and 0600 hours, the time interval is designated by the two times, 0500 and 0600.

The operational characteristics of BCCONC are best illustrated by an example. Suppose we wish to perform a two hour simulation from 0500 to 0700 hours, and also suppose that the boundary concentrations are to change hourly. Thus, we specify a set of boundary concentrations that apply from 0500 to 0600 hours, and another set that apply from 0600 to 0700 hours. The cards in the data-deck are arranged in the following order (see Card No. 18-19 in Table 4):

- . time interval, designated by 0500 and 0600, and boundary concentrations that apply between 0500 and 0600 hours
- . time interval, designated by 0600 and 0700, and boundary concentrations that apply between 0600 and 0700 hours.

The first time BCCONC is called from MAIN, the time interval and boundary concentrations are determined from the first set of data cards. Thus, a set of boundary concentrations are established and applied between 0500 and 0600 hours. Each time BCCONC is called to update the boundary concentrations, the current simulation time is checked against the time interval. In the present example, when the simulation time finally becomes greater than 0600 hours, the next time interval and boundary concentrations are read from the data-deck. These concentrations that apply from 0600 to 0700 hours are then used for the remainder of the simulation.

When photochemical simulations are performed, ozone concentrations at the boundary are determined by assuming that the rate of reaction of ozone is equal to zero. Upon making this assumption and utilizing the reaction rate expression given in Appendix B of Volume I, we obtain the following algebraic relation for the boundary concentration of ozone:

$$[O_3] = \frac{k_2 [O]}{k_3 [NO] + k_4 [NO_2] + k_{13} [HC]}$$

where

$$[O] = \frac{k_1 [NO_2]}{k_2 + k_{11} [HC]}$$

and $[NO]$, $[NO_2]$, and $[HC]$ are the boundary concentrations of NO , NO_2 , and reactive hydrocarbon respectively.

BLCKTD (N,M)

Subroutine BLCKTD is used to solve a block-tridiagonal system of N·M linear equations. Each block is an M x M matrix, and all off-diagonal matrices are assumed to be diagonal. A discussion of the algorithm is presented in Appendix D of Volume I. The solution of a system of equations in this form is required as part of the numerical integration procedure.

CALIVC

An entry point in subroutine AVCONC (see AVCONC).

DIFCOF (I,J,KZ)

In Step III of the numerical integration procedure, vertical turbulent diffusivities must be determined to compute the vertical diffusion of pollutants. Vertical diffusivities are specified in the array KZ applicable in grid cells above grid square (I,J). KZ(K) is the value of the diffusivity at the interface between grid cells (I,J,K-1) and (I,J,K). See Appendix C of Roth et al. (1971) for a discussion of the algorithm.

ICCONC

The initial concentration distribution is established in subroutine ICCONC. Two modes of initial concentration input are possible. In the first mode, the initial ground level concentrations are read from cards included in the data-deck. The values in the ground cells are extended vertically to the inversion to complete the definition of the initial concentration field. The second mode of input arises when a simulation begins at a point in time at which a previous simulation terminated. Recall from our discussion of the MAIN program that at the end of a simulation, the entire concentration field may be "dumped" onto a save disc area. Thus, the second mode of initial concentration input simply consists of a READ statement to read these "dumped" values.

Initial ozone concentrations are determined by making the assumption that the rate of reaction of ozone is equal to zero at the starting time of the simulation. Using the reaction rate expression for ozone given in Appendix B of Volume I, we obtain

$$[O_3] = \frac{k_2 [O]}{k_3 [NO] + k_4 [NO_2] + k_{13} [HC]}$$

where

$$[O] = \frac{k_1 [NO_2]}{k_2 + k_{11} [HC]}$$

and $[O_3]$, $[NO]$, $[NO_2]$, and $[HC]$ are the initial concentrations of O_3 , NO , NO_2 , and reactive hydrocarbon respectively.

MAPPER (I, IHOLD, ISTART, ISTOP, APRINT)

This subroutine is used during the printing of the ground level concentration maps to produce "blanks" in those locations on the map which are outside the computational grid. For example, cells over the Pacific Ocean are not included in the current simulation study of Los Angeles. Note that in Figures 3 and 4, no concentrations are printed in areas of the grid over the Pacific Ocean. The blanks printed in this area are a direct result of the use of subroutine MAPPER.

The subroutine operates as follows. Before a particular row of ground level predictions are printed in subroutines AVCONC or PRINT1, the concentrations in that row are stored in the array IHOLD. Next, the values in IHOLD which represent predictions within the computational grid are determined. These values are stored in IHOLD between IHOLD (ISTART) and IHOLD (ISTOP). This information is used in subroutine MAPPER to produce the array APRINT, which is returned to the calling program. This alphanumeric array is then printed (128 printing columns) in the calling program, and only numbers within the computational grid appear on the printed map. If $I = 0$, integers are produced on the printed output. To obtain numbers with one decimal digit, we set $I = 1$. We note that this subroutine is written in Assembly Language.

METEOR

The processing of all meteorological data is done in subroutine METEOR. During model initialization, the MDF is opened, and initial values of the meteorological variables are calculated. As the simulation progresses, the meteorological variables are updated as necessary by reading the file. See Appendix C of Roth et al. (1971) for a further discussion of the meteorological data. Subroutine PTSOUR is called from METEOR every time the wind changes speed or direction to establish the spatial distribution of emissions from elevated point sources.

PRINT1

Instantaneous concentrations are printed on the program output by subroutine PRINT1. Vertical concentration profiles above monitoring stations and ground level concentration maps are printed at regular

time intervals. We have found that an interval of 60 minutes between printouts gives a good indication of hourly trends and does not result in endless pages of unused computer output. A typical example of a ground level concentration map printed by this subroutine is illustrated in Figure 3. Other examples are included in Section IV. Subroutine MAPPER is used in the preparation of the ground level maps.

PTSOUR

Emissions from elevated point sources are distributed among several downwind grid cells in subroutine PTSOUR. The algorithm employed is described fully in Appendix A of Volume I. This subroutine is called from METEOR each time the wind changes speed or direction since the downwind distribution of the emissions is directly affected by a change in either of these parameters.

SIMDIG(N)

Subroutine SIMDIG is employed in the solution of a tridiagonal system of N linear equations. The computational algorithm is given in Appendix D of Volume I.

SOURCE

Ground level pollutant fluxes are calculated in subroutine SOURCE using the data contained in the EDF. During model initialization, the EDF is opened, and initial values of the fluxes are computed. SOURCE is called from MAIN throughout the course of a simulation to update the ground level fluxes.

TIME (T1, T2, M)

This subprogram is discussed as part of the EDPP.

3. Input Data Requirements

The following outline lists the types of input information needed to run the APSP. The detailed listing of all parameters is given in Table 4.

- . grid characteristics, including number of vertical strata, horizontal grid spacing, and shape of the region
- . starting and stopping time of the simulation
- . time interval between instantaneous concentration printouts
- . location of monitoring stations
- . rate, location, and temporal variation of major elevated point source emissions
- . integration parameters, including minimum and maximum time step size, relative error tolerance to be satisfied in the iterative solution of the nonlinear finite-difference equations, maximum number of iterations to be allowed in the iterative solution, and the initial size of the integration time step
- . rate constants, temporal variation of the photolysis rate constants, and values of the generalized coefficients
- . initial conditions
- . concentrations aloft
- . boundary concentrations at points of horizontal inflow

4. Program Output

Three types of output are provided by the APSP

- . printed hourly-averaged ground level concentration maps and a printed summary of the hourly-averaged concentrations predicted at each monitoring station
- . printed instantaneous ground level concentration maps and a printed summary of the instantaneous vertical concentration distribution above each monitoring station
- . punched cards for input to the DPP containing the hourly-averaged concentrations predicted at each monitoring station

See Section IV for examples of the printed output from the APSP.

D. The Data Plotting Program

1. Program Objective and Capabilities

The evaluation procedure adopted for the simulation study reported in Volume I requires that model predictions be compared with actual

measurements of pollutant concentrations. These comparisons are best made by displaying the temporal variation of the measured and predicted concentrations together on one plot. In this manner, similarities and differences in the two concentrations at any particular time are readily apparent. Thus, the primary objective of the DPP is the automatic preparation of plots of predicted and measured concentrations at each air quality monitoring station.

Available measurements of particular interest are those of total hydrocarbon (as parts per million carbon), NO, NO₂, CO, and oxidant. Before the air quality measurements can be plotted, however, they must be corrected to account for interferences caused by the presence of other pollutants. These interferences are discussed in Appendix E of Roth et al. (1971). The following corrections are made to the NO and oxidant measurements:

$$\text{NO}_{\text{plotted}} = 1.25 \text{ NO}_{\text{measured}}$$

$$\text{OX}_{\text{plotted}} = \text{OX}_{\text{measured}} - 0.15 \text{ NO}_{2\text{measured}} + \text{SO}_{2\text{measured}}$$

A useful feature of the DPP is that the user may specify, as part of the program input data, which species are to be plotted at each station. If measurements are not available for a particular species at a station, the DPP may be used to plot only the predicted results at that station. In fact, the user may wish to completely suppress the plotting since no comparisons can be made. As an example, total hydrocarbon is measured at six stations in the Los Angeles area. Thus, for evaluation purposes, we only prepare plots of the hydrocarbon concentrations at these six stations.

In Appendix C of Volume I, we describe a technique to account for the effects of near-by sources on the field measurements. These effects are especially important to include when a monitoring station is located adjacent to a heavily-traveled street. The local concentration elevations are calculated using the algorithms in the Appendix cited and included on punched cards in the data-deck of the DPP. These concentration elevations are then added to the model predictions to obtain an "improved prediction" at the station. We wish to note that, as of this writing, local corrections may be calculated only for inert species, such as CO, due to the nonlinear effects of chemical reactions.

2. Program Structure

The DPP consists of a MAIN program and three subroutines, each of which performs a specific task in the drawing of the plots. The creation of a plot may be described by the following four step process:

1. draw and label the axes; print the title block
2. plot the predicted concentrations
3. plot the station measurements
4. plot the locally corrected predicted concentrations

We now discuss the function of the MAIN program and each subroutine. The structure of the DPP is illustrated in Figure 10.

MAIN

In the first section of code in MAIN, all input cards are read, and the NO and oxidant measurements are corrected for interferences. Having accomplished this, the program is ready to make all plots specified by the user. The plots are drawn in the following order:

1. CO plots for each station
2. total hydrocarbon plots for each station
3. NO, NO₂, and O₃ plots for each station

We describe the operations performed in the MAIN program by discussing the manner in which a CO plot is made. First, the maximum CO concentration to be plotted is found, and the scale of the concentration axis is calculated accordingly. Then the data points are examined to be certain that none will be plotted in the title block located in the upper right hand corner of the plot (See Figure 11). If a data point does fall in the title block, then the concentration axis is scaled in such a manner that no data points will be plotted in this area.

FIGURE 10
THE STRUCTURE OF THE DPP

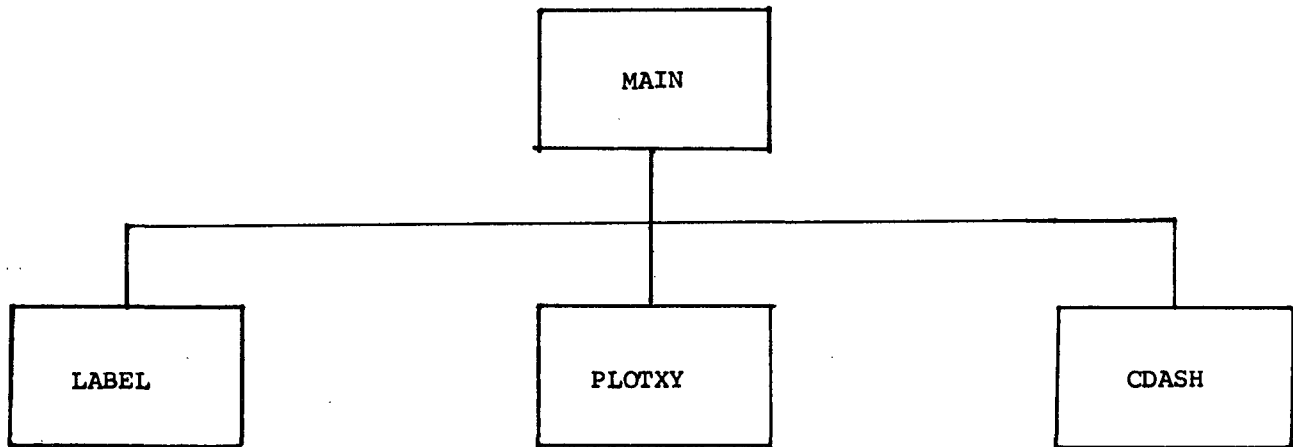
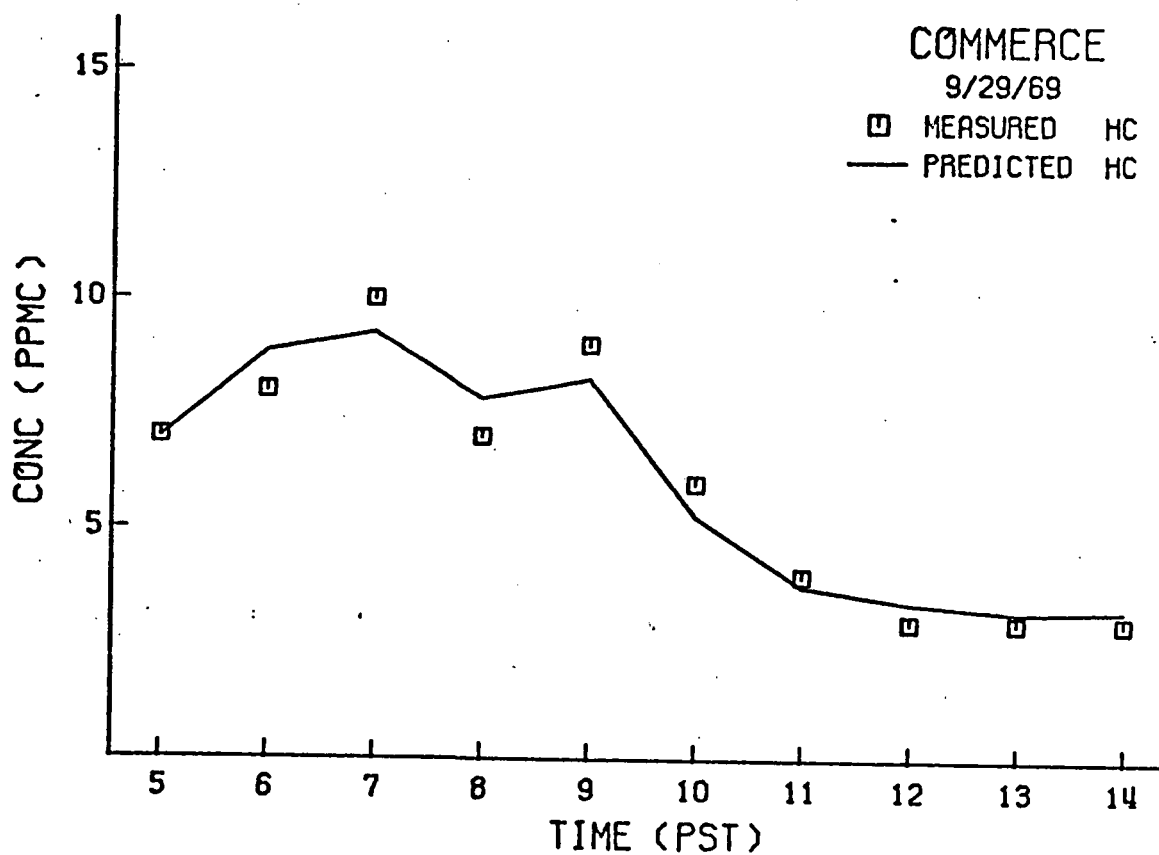
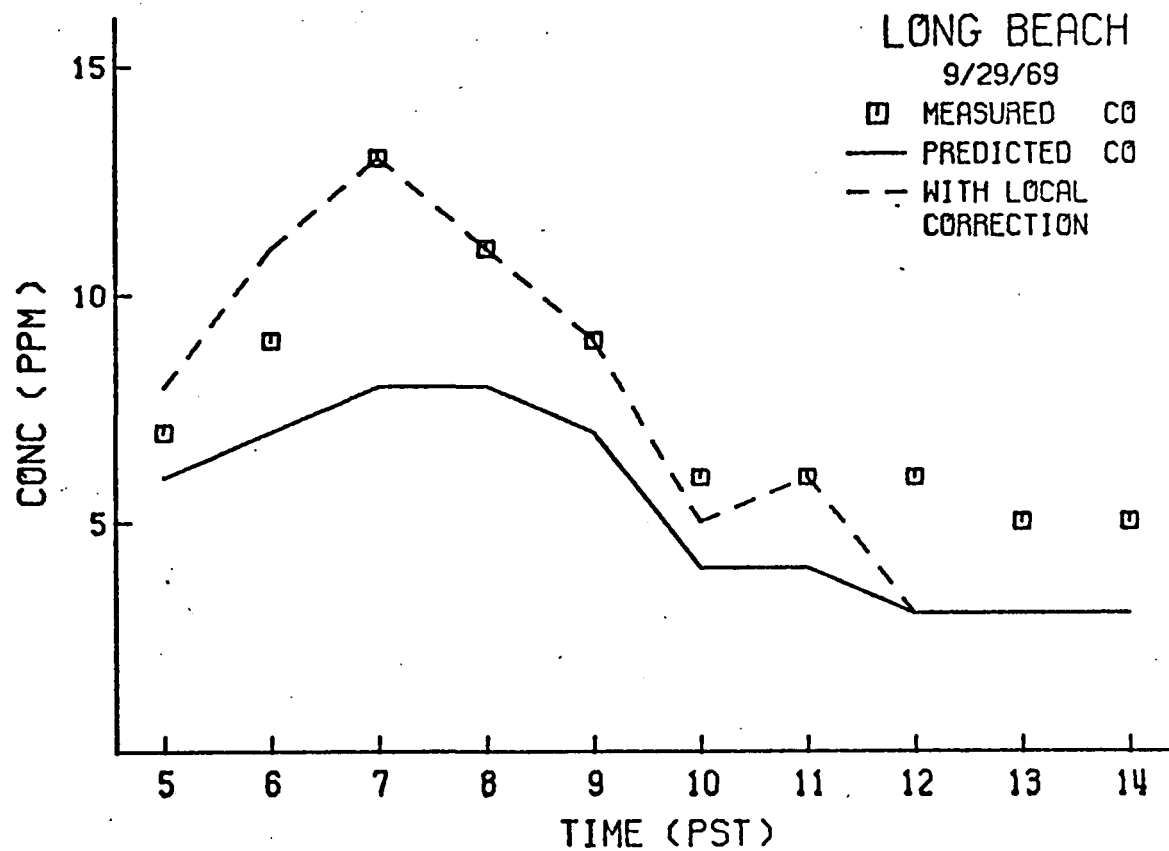


FIGURE 11
EXAMPLE OF PLOTS FOR CO AND TOTAL HYDROCARBON



After determining the scale of the concentration axis, subroutine LABEL is called to draw and label the two axes representing concentration and time. Then subroutine PLOTXY is called to plot the model predictions. This plot consists of solid line segments connecting the discrete hourly-averaged predictions. After the predictions have been plotted, subroutine PLOTXY is called again, this time to produce a symbol plot representing the measured concentrations. We note that the solid lines have no other meaning than to correct the predicted concentration data points and to provide a contrast to the discrete symbol plot.

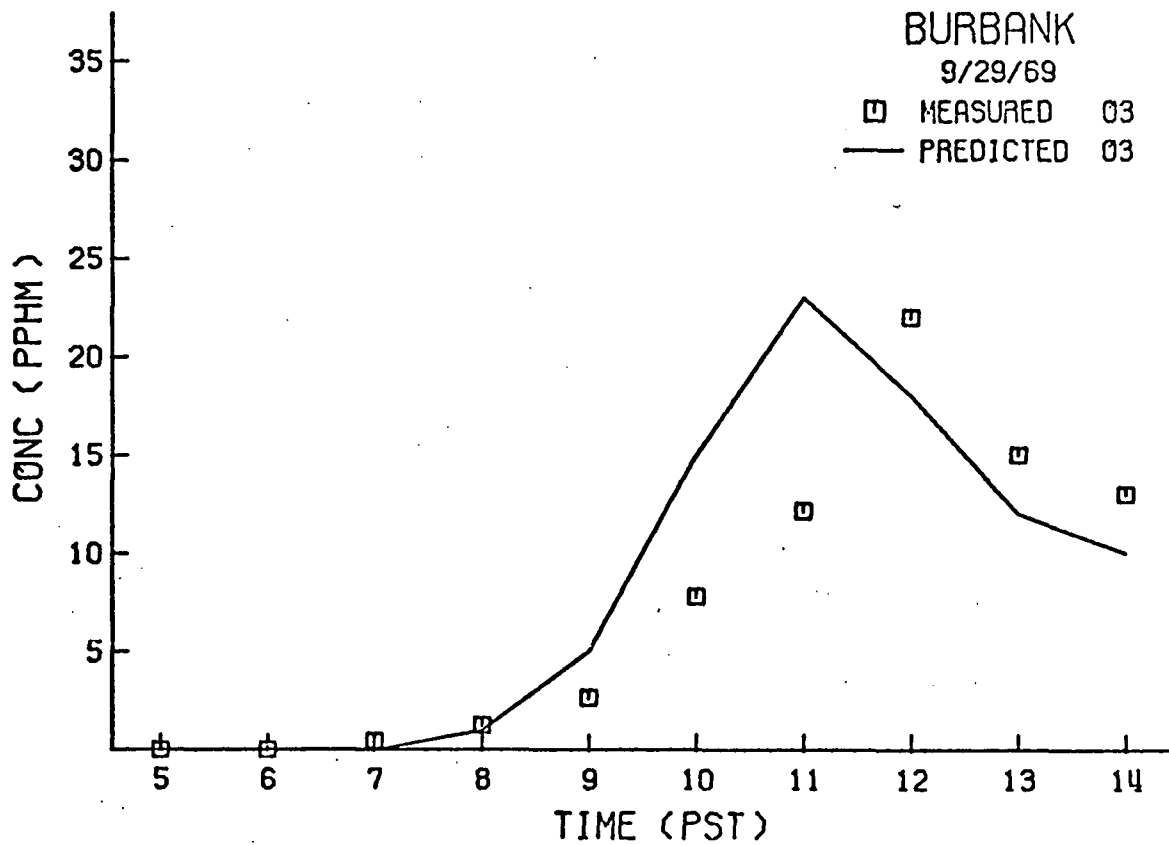
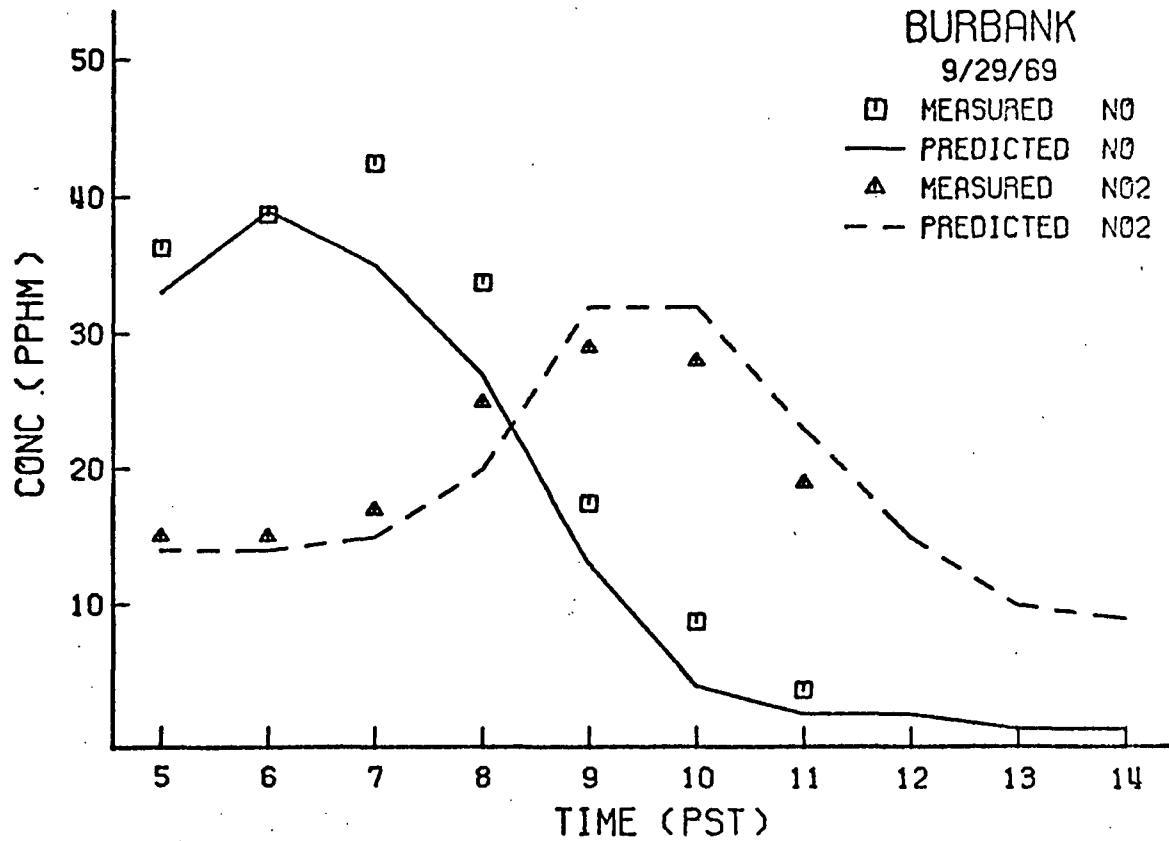
If local corrections are required, the predictions at the station and the corresponding local corrections are transferred to subroutine CDASH. An array is defined by CDASH consisting of model predictions augmented by the local corrections. This array is then plotted by PLOTXY as a dashed line. In Figure 11, we illustrate a typical CO plot drawn by the DPP.

The basic operations described above are repeated for each succeeding plot. All CO and total hydrocarbon plots are drawn, displaying two sets of results on each page. The format is somewhat different, however, for the display of the NO, NO₂, and O₃ results. In this case, the predictions and measurements for all three species at a particular station are presented on the same page. A typical plot involving these three species is given in Figure 12.

CDASH (NOHOUR, T, C, B, NOCORR, TCORR, CCORR)

Before the local corrections to the model predictions are plotted, the MAIN program supplies subroutine CDASH with the number of data points, NOHOUR, and three arrays T, C, and B, containing the times, model predictions, and local corrections respectively at the particular station. An array of times, TCORR, and an array of model predicted concentrations plus local corrections, CCORR, are calculated in subroutine CDASH. The number of data points in these arrays is equal to NOCORR. The MAIN program passes NOCORR, TCORR, and CCORR to subroutine PLOTXY, which then produces the dashed line plot representing the locally corrected model predictions.

FIGURE 12
EXAMPLE OF PLOTS FOR NO, NO₂ and O₃



LABEL (X,Y,N, XDATA, NY, YMAX, UNIT, DATE, STN, NONAME, NAME, CORECT)

Subroutine LABEL is used to 1) draw and label the axes, and 2) print the title block for each plot. The axes intersect at the point (X,Y) on the plotting area, where X and Y are measured in inches. N tick marks are drawn on the X axis, representing the N data points that will eventually be plotted. XDATA is an array of hours (or abscissa), and the subroutine uses this array to write the hours under the X-axis. NY is the number of increments into which the Y-axis is to be subdivided, and YMAX is the largest value to be represented on the axis. The Y-axis is labeled to reflect that it represents concentration, and the units (PPM, PPTM, or PPHM) are also written according to the alphameric information contained in the variable UNIT. For example, if the concentration units are to be pphm (parts per hundred million), then UNIT = 'PPHM'. DATE and STN are alphameric designations of the date and monitoring station name respectively, which appear in the title block. NONAME is the number of species to be plotted on the plot, and NAME is an alphameric array containing the abbreviation of each species' name. For example, an abbreviation for hydrocarbon is 'HC'. CORECT is a logical variable passed by MAIN to inform LABEL whether or not local corrections will be plotted on the current plot. If CORECT = .TRUE., then the local corrections will appear, and LABEL will make a comment to that effect in the title block.

PLOTXY (N,X,Y,XMN, XMX, YMN, YMX, IP, ISYS, SUPRES)

Subroutine PLOTXY is a general data plotting routine which is capable of making point, solid line, or dashed line plots. The program operates in a conventional manner, in which the user designates N points of an array of abscissa and ordinates, X and Y, to be plotted. The values of the abscissa on the left and right hand borders of the plotting area are specified by XMN and XMX. Similarly, the values of the ordinate on the bottom and top of the plotting area are YMN and YMX. The pen is moved from one data point to the next, where the location of the pen is determined by linear interpolation using the particular values of X and Y to be plotted, and the values of the abscissa and ordinate along the plotting area borders.

The type of plot produced by PLOTXY is controlled by the parameter IP, where

$$IP = \begin{Bmatrix} 0 \\ 1 \\ 2 \end{Bmatrix} \text{ produces a } \begin{Bmatrix} \text{symbol plot} \\ \text{solid line plot} \\ \text{dashed line plot} \end{Bmatrix}$$

The value of ISYS determines which symbol is plotted when IP = 0.

A symbol will not be plotted for any value of Y which is equal to SUPRES. This feature is used to denote a missing data point, and hence, no symbol should be plotted. For the simulation study reported in Volume I, we set all missing values of the measured concentrations equal to minus one. To correspond with this convention, we also set SUPRES equal to minus one.

The subroutine normally uses a 15 x 10 inch plotting area, but the user can alter this specification by including a BLOCK DATA subprogram as follows:

```
BLOCK DATA
COMMON/COMPXY/
DATA ITEST, XLNGTH, YLNGTH/1,...,.../
END
```

where XLNGTH and YLNGTH are the altered X-length and Y-length of the plotting area, in inches, respectively. XLNGTH must be specified at least 8-1/2 inches, and YLNGTH must be specified at least 10 inches.

3. Input Data Requirements

The DPP requires the following types of input data:

- . number of carbon atoms per molecule of reactive and unreactive hydrocarbon
- . air quality measurements
- . model predictions
- . corrections due to local effects

The complete data-deck setup for the DPP is given in Table 5.

4. Program Output

The only output from the DPP are the plots, such as those illustrated in Figures 11 and 12.

III. OPERATING PROCEDURES

This section of the User's Guide is divided into two parts. In the first part, we give general instructions regarding the use of all programs. Included is a four or five step procedure outlining the manner in which each program is to be operated. The second part of this section is devoted to a presentation of the specific operating characteristics of each program. The following topics are discussed:

- limitations in the use of the programs
- instructions for making important changes in the codes
- instructions for assembling the input data-deck
- computing system information

Before discussing these specific details, however, we first consider the general operating procedures for the use of airshed simulation package.

A. General Information and Instructions

The main tasks involved in exercising the airshed simulation package are those of establishing the meteorological and emissions input data files, and then running the APSP. All programs, except the APSP, operate solely from punched card input data; the APSP requires inputs from both punched cards and the two data files. Consequently, we work primarily with the input data-deck to each program and are not required to make substantial coding changes in any of the programs. There are some model parameters that have been specified in the programs, however, and in the next section we discuss which parameters these are and where they are located in the code.

Assembling the input data-deck for each program is one of the most important aspects of operating the model. The data-decks for the EDPP, MDPP, and APSP consist of hundreds of cards, all of which must be specified correctly. As an aid in defining the contents and format of the data-decks, we have prepared, for all programs, tables listing the parameters appearing on each input card. The units of the parameter and the card format are included in the table.

Since the number of input data cards may vary from one simulation to the next, a generalized means of denoting the card order is employed in the data-deck tables. To illustrate this convention, we refer the reader to Table 4. We find that Card No. 1 actually consists of two physical cards on which the array NOTE is stored. Card No. 2, however, is only one physical card on which several input parameters are specified. The number of cards required to input arrays can be determined from the format information given in the table. For example, the format of Card No. 1 is 2(20A4). The "two" outside the parentheses denotes the number of physical cards.

The next topic we wish to discuss deals with making coding changes in the programs. In Section III-B, we discuss several alterations that

the user may wish to make in the codes. It is conceivable, however, that a change may be required that we have not discussed. If this is the case, the user should first determine which subroutine contains the algorithm of interest. The discussion in Section II will be helpful in this respect. The comments in the program can then be used to further pinpoint the location of the algorithm, and with the aid of the appropriate symbol glossary, minor code alterations can be made. Major alterations in any code will, of course, require that the user understand the basic computational structure of the program.

Another important consideration involves the use of subscripts in the codes. This is especially important since several multidimensional arrays are employed in the programs. We note that any grid cell may be addressed by the integer triple (I,J,K). The numbering convention for I and J is illustrated in Figure 1. K designates the vertical level in which the cell is located, where K = 1 corresponds to the ground level cells. Those variables which are independent of height are designated by the ordered pair (I,J). For example, since the wind direction is invariant with height above grid square (I,J), it is denoted as WINDAN(I,J). The pollutant concentration array, CONC(L,I,J,K), denotes the concentration of species L in grid cell (I,J,K), where

$$L = \begin{cases} 1 - \text{Reactive Hydrocarbon} \\ 2 - \text{NO} \\ 3 - \text{O}_3 \\ 4 - \text{NO}_2 \\ 5 - \text{CO} \\ 6 - \text{Unreactive Hydrocarbon} \end{cases}$$

Having discussed several topics related to the operation of the programs, we now present a set of instructions for the use of the airshed simulation package. These instructions are included in Table 1. Since the instructions are formulated in a general manner, they apply to all simulations performed by the programs given in this Guide. The user will find information pertaining to computing time, program size, pages of printed output, and hardware requirements for each program in the next section.

B. Program Operating Characteristics

1. The Emissions Data Preparation Program

The following parameters are specified in the code of the EDPP:

<u>Parameter</u>	<u>Card ID</u>	<u>Description</u>
XMOL	EDPP 0330	molecular weights of auto emissions species
WTFS	EDPP 0370	molecular weights of fixed source emissions species
DX	EDPP 0410	grid spacing in x-direction (feet)
DY	EDPP 0420	grid spacing in y-direction (feet)

TABLE 1
OPERATING INSTRUCTIONS

- A. EDPP - use this program to create the EDF
 - 1. Make any required coding changes
 - 2. Prepare the data-deck (use Table 2)
 - 3. Specify the JCL
 - 4. Run the program

- B. MDPP - use this program to create the MDF
 - 1. Make any required coding changes
 - 2. Prepare the data-deck (use Table 3)
 - 3. Specify the JCL
 - 4. Run the program

- C. APSP - use this program to perform the airshed simulation
 - 1. Create the EDF and the MDF (see A and B above)
 - 2. Make any required coding changes
 - 3. Prepare the data-deck (use Table 4)
 - 4. Specify the JCL
 - 5. Run the program

- D. DPP - use this program to plot the results obtained from the APSP
 - 1. Obtain model predictions from the APSP (see C above)
 - 2. Make any required coding changes
 - 3. Prepare the data-deck (use Table 5)
 - 4. Specify the JCL
 - 5. Run the program

<u>Parameter</u>	<u>Card ID</u>	<u>Description</u>
FAIRNO	EDPP 0470	mole fraction of NO in aircraft NO _x emissions
FCARHC	EDPP 0480	mole fraction of reactive hydrocarbon in auto hydrocarbon emissions
FCARNO	EDPP 0490	mole fraction of NO in auto NO _x emissions
FFSNO	EDPP 0500	mole fraction of NO in fixed source NO _x emissions
HCEVAP	EDPP 0590	molecular weight of evaporative hydrocarbon emissions from autos

These parameters must be checked for correctness before the EDPP is used.

We list below two alterations that may be required in the code.

- The temporal distribution for traffic activity is delayed by one hour in the Downtown Los Angeles area - grid squares (11,17), (12,17) and (12,16). See cards EDPP 1890, EDPP 1900, EDPP 1910 and EDPP 3060, EDPP 3070, EDPP 3080.
- Emissions are not calculated after 1655 hours. To compute emissions to a later time, the upper bound on the range of the DO loop at card EDPP 2940 should be increased, but specified no larger than 19.

We wish to note the following limitations on the use of the EDPP. These limitations can be overcome, however, with further program development.

- The calculation of emissions after 2355 hours should not be attempted.
- Emissions cannot be computed prior to 0500 hours.

Computing System Information

Hardware:

1 - disc area/tape drive	FT04F001
1 - card reader	FT05F001
1 - printer	FT06F001

Program Size: 130K bytes

CPU Time (IBM 370/155): 1 minute

Printed Output: 144 pages

In Table 2 which follows, we give a detailed specification of the data-deck setup for the EDPP.

TABLE 2
DATA-DECK SETUP FOR THE EMISSIONS DATA PREPARATION PROGRAM

<u>Card No.</u>	<u>Column No.</u>	<u>Variable</u>	<u>Format</u>	<u>Units</u>	<u>Note</u>
1	1-80	YCS(I)	3(8F10.0)	--	Fraction of cars "cold-started" during hourly period I (I=1 corresponds to the period midnight to 1 A.M.); input sequence: (YCS(I), I 1, 24)
2	1-30	EC(L)	3F10.0	grams/mile	Cold-start emissions from automobiles for species L, where $L = \begin{cases} 1 & \text{CO} \\ 2 & \text{HC} \\ 3 & \text{NO}_x \end{cases}$ input sequence: (EC(L), L=1, 3)
2	31	PDT	L1	--	If daylight savings time is in effect, PDT=.TRUE.; if standard time is in effect, PDT=.FALSE.
3	1-30	EH(L)	3F10.0	grams/mile	Hot start emissions from automobiles for species L; input sequence: (EH(L), L=1, 3)
4	1-30	XA(L)	3F10.0	--	The parameter "a" in the automotive speed-emissions correlation for species L, input sequence: (XA(L), L=1, 3)

TABLE 2 (Cont'd)
DATA-DECK SETUP FOR THE EMISSIONS DATA PREPARATION PROGRAM

<u>Card No.</u>	<u>Column No.</u>	<u>Variable</u>	<u>Format</u>	<u>Units</u>	<u>Note</u>
5	1-30	XB(L)	3F10.0	--	The parameter "b" in the automotive speed-emissions correlation for species L; input sequence: (XB(L), L=1,3)
6	1-80	TSURF(I)	3(8F10.0)	minute ⁻¹	Temporal distribution of non-freeway traffic; fraction of total daily miles driven in each grid square each minute during hourly period I; on input, this array is to be specified 10 ⁴ times larger than its true value; input sequence: (TSURF(I), I=1,24)
7	1-80	TFREE(I)	3(8F10.0)	minute ⁻¹	Temporal distribution of freeway traffic; fraction of total daily miles driven on freeways in each grid square each minute during hourly period I; on input, this array is to be specified 10 ⁴ times larger than its true value; input sequence: (TFREE(I), I=1,24)
8	1-75	SURMLG(I,J)	25(25F3.0)	10 ³ miles	Total daily non-freeway mileage driven in grid square (I,J); input sequence: ((SURMLG(I,J), I=1,25), J=1,25)

TABLE 2 (Cont'd)
DATA-DECK SETUP FOR THE EMISSIONS DATA PREPARATION PROGRAM

<u>Card No.</u>	<u>Column No.</u>	<u>Variable</u>	<u>Format</u>	<u>Units</u>	<u>Note</u>
9	1-75	FWYMLG(I,J)	25(25F3.0)	10 ³ miles	Total daily freeway mileage driven in grid square (I,J); input sequence: ((FWYMLG(I,J),I=1,25), J=1,25)
10	1-72	BETA(M,L,K)	15(12F6.3)	--	The "beta" correction curve for species M accounting for the nonuniform distribution of vehicle starts, where $M = \begin{cases} 1 & \text{CO} \\ 2 & \text{HC} \\ 3 & \text{NO}_x \end{cases}$ <p>and L designates the hour (L=1,5), where L=1,2,...,5 corresponds to 5 A.M., 6 A.M., ..., 9 A.M. K designates each 5 minutes of hour L, (K=1,12); input sequence: ((BETA(M,L,K),K=1,12), L=1,5),M=1,3)</p>
11	1-65/1-60	VS1(I,J)	25(13F5.0 /12F5.0)	mph	Average automobile speed in the slow freeway direction in grid square (I,J) at 5 A.M. local time; input sequence: ((VS1(I,J),I=1,25),J=1,25)
12	1-65/1-60	VF1(I,J)	25(13F5.0 /12F5.0)	mph	Average automobile speed in the fast freeway direction in grid square (I,J) at 5 A.M. local time; input sequence: ((VF1(I,J),I=1,25),J=1,25)

TABLE 2 (Cont'd)
DATA-DECK SETUP FOR THE EMISSIONS DATA PREPARATION PROGRAM

<u>Card No.</u>	<u>Column No.</u>	<u>Variable</u>	<u>Format</u>	<u>Units</u>	<u>Note</u>
13	1-65/1-60	FXSOUR(I,J,L)	150(13F5.0 /12F5.0)	Kgm./hr	Fixed source emissions for species L in grid square (I,J); input sequence: (((FXSOUR(I,J,L),I=1,25), J=1,25),L=1,6) where $\left\{ \begin{array}{l} 1 \text{ reactive HC} \\ 2 \text{ NO} \\ 3 \text{ O}_3 \\ 4 \text{ NO}_2 \\ 5 \text{ CO} \\ 6 \text{ unreactive HC} \end{array} \right.$ L =
14	1-5	NOARPT	15	--	Number of airports
If NOARPT=0, then do <u>NOT</u> include Card No. 15-23.					
15	1-70	AIREMS(M,L,I)	18(7F10.1)	lb./min	Emissions rate of species L from class I aircraft in operating mode M, where $\left\{ \begin{array}{l} 1 \text{ long range jet} \\ \text{transport} \\ 2 \text{ medium range jet} \\ \text{transport} \\ 3 \text{ business jet} \\ \text{transport} \\ 4 \text{ turboprop trans-} \\ \text{port} \\ 5 \text{ piston engine} \\ \text{transport} \\ 6 \text{ piston engine} \\ \text{utility} \\ 7 \text{ turbine engine} \\ \text{helicopter} \end{array} \right.$ I =

TABLE 2 (Cont'd)
DATA-DECK SETUP FOR THE EMISSIONS DATA PREPARATION PROGRAM

<u>Card No.</u>	<u>Column No.</u>	<u>Variable</u>	<u>Format</u>	<u>Units</u>	<u>Note</u>
					$M = \begin{cases} 1 & \text{taxi} \\ 2 & \text{landing} \\ 3 & \text{take-off} \end{cases}$ <p>L - see Card No. 13 input sequence: (((AIREMS(M,L,I),I=1,7), I=1,6),M=1,3)</p>
16	1-70	TMODE(M,I)	3(7F10.0)	minute	<p>The amount of time class I aircraft spend in opera- ting mode M; see Card No. 15 for description of I and M; input sequence: ((TMODE(M,I),I=1,7),M=1,3)</p>
Include a complete set of Card No. 17-23 for each airport (J=1,NOARPT)					
17	1-4	AIRPRT	A4	--	<p>Alphameric designation of the airport initials (such as 'LAX','BUR', and etc.)</p>
17	5-6	NCORT(J)	I2	--	<p>Number of grid squares which receive emissions from airport J</p>
18	1-30	IXORT(J,I)	6I5	--	<p>Column numbers of the grid squares that receive emis- sions from airport J; input sequence: (IXORT(J,I),I=1,NCORT(J))</p>

TABLE 2 (Cont'd)
DATA-DECK SETUP FOR THE EMISSIONS DATA PREPARATION PROGRAM

<u>Card No.</u>	<u>Column No.</u>	<u>Variable</u>	<u>Format</u>	<u>Units</u>	<u>Note</u>
19	1-30	IYORT(J,I)	6I5	--	Row numbers of the grid squares that receive emissions from airport J; input sequence: (IYORT(J,I),I=1,NCORT(J))
20	1-60	DIST(J,I)	2(12F5.3)	hour ⁻¹	Fraction of total daily aircraft operations occurring at airport J during hour I (I=1 corresponds to the period midnight - 1 A.M.); input sequence: (DIST(J,I),I=1,24)
21	1-78	PCT(J,I)	13F6.2	--	Fraction of emissions from airport J that are apportioned to grid square (IXORT(J,I),IYORT(J,I)); input sequence: (PCT(J,I),I=1,NCORT(J))
22	1-42	ACFT(J,I)	7F6.2	aircraft/ day	Number of daily flights of class I aircraft at airport J; input sequence: (ACFT(J,I),I=1,7) See Card No. 15 for a detailed description of I.
23	1-42	EMIX(J,I)	7F6.2	engines/ aircraft	Number of engines on class I aircraft operating at airport J; input sequence: (EMIX(J,I),I=1,7)

TABLE 2 (Cont'd)
DATA-DECK SETUP FOR THE EMISSIONS DATA PREPARATION PROGRAM

<u>Card No.</u>	<u>Column No.</u>	<u>Variable</u>	<u>Format</u>	<u>Units</u>	<u>Note</u>
24	1-65/1-60	X(I,J)	25(13F5.0/ 12F5.0)	--	Ratio of the number of miles traveled in the slow direction to the number traveled in the fast direction in grid square (I,J) between 5 and 6 A.M. local time; input sequence: ((X(I,J),I=1,25),J=1,25)
25	1-65/1-60	VS1(I,J)	25(13F5.0 /12F5.0)	mph	Average speed traveled by automobiles in the slow direction on freeways in grid square (I,J) at 6 A.M. local time; input sequence: ((VS(I,J),I=1,25),J=1,25)
26	1-65/1-60	VF1(I,J)	25(13F5.0 /12F5.0)	mph	Average speed traveled by automobiles in the fast direction on freeways in grid square (I,J) at 6 A.M. local time; input sequence: ((VF(I,J),I=1,25),J=1,25)

Include four additional sets of Card No. 24-26 to cover the time period
6 A.M. - 10 A.M.

2. The Meteorological Data Preparation Program

The MDPP is a general program, and the only limitations on its use are:

- mixing depths must be specified on the hour
- wind speed and wind direction are constant over hourly periods measured from the half hour to the half hour
- the initial mixing depths are to be applicable at the same time the airshed simulation is to start. That is, if a simulation is to start at 0500 hours, then the first mixing depth data should be applicable at 0500 hours. This is a limitation imposed by the APSP.

Computing System Information

Hardware:

1 - disc area/tape drive	FT04F001
1 - card reader	FT05F001
1 - printer	FT06F001

Program Size: 60K bytes

CPU Time (IBM 370/155):

time required to process 10 hours of meteorological data - 25 seconds

Printed Output:

number of pages of printed output from 10 hours of meteorological input data

10 hours x 3 pages/hour = 30 pages

The complete data-deck setup for the MDPP is described in Table 3.

3. The Atmospheric Pollution Simulation Program

We list below four operating parameters which are specified in the code of the APSP. They are all located in the MAIN program.

<u>Parameter</u>	<u>Card ID</u>	<u>Description</u>
KXY	APS 00850	horizontal turbulent diffusivity
NOSPEC	APS 00860	maximum number of chemical species
NORATE	APS 00870	number of chemical reactions
DTAVEC	APS 00910	time period (in minutes) over which the predicted concentrations are time averaged

TABLE 3
DATA-DECK SETUP FOR THE METEOROLOGICAL DATA PREPARATION PROGRAM

<u>Card No.</u>	<u>Column No.</u>	<u>Variable</u>	<u>Format</u>	<u>Units</u>	<u>Note</u>
1	1-5	NX	I5	--	Number of grid squares in the x-direction
1	6-10	NY	I5	--	Number of grid squares in the y-direction
1	11-20	TSTART	F10.0	2400 time	Starting time
1	21-30	TSTOP	F10.0	2400 time	Terminating time
1	31-38	DATE(I)	2A4	--	Alphameric designation of the date; input sequence: (DATE(I), I=1,2)
2	1-65/1-60	H(I,J,1)	25(13F5.0/ 12F5.0)	feet	Mixing depths applicable at TSTART; input sequence: ((H(I,J,1), I=1,NX), J=1,NY)
3	1-65/1-60	W(I,J)	25(13F5.1/ 12F5.1)	mph	Wind speed applicable at TSTART; input sequence: ((W(I,J), I=1,25), J=1,25)
4	1-65/1-60	A(I,J)	25(13F5.1/ 12F5.1)	degrees	Wind direction measured clockwise from north,* applicable at TSTART; input sequence: ((A(I,J), I=1,25), J=1,25)
5	1-65/1-60	H(I,J,2)	25(13F5.1/ 12F5.1)	feet	Mixing depths applicable at the next hour; input sequence: ((H(I,J,2), I=1,NX), J=1,NY)
6	1-65/1-60	W(I,J)	25(13F5.1/ 12F5.1)	mph	Wind speeds applicable at the next hour; input sequence: ((W(I,J), I=1,25), J=1,25)

* The direction in which the wind is flowing.

TABLE 3 (Cont'd)
DATA-DECK SETUP FOR THE METEOROLOGICAL DATA PREPARATION PROGRAM

<u>Card No.</u>	<u>Column No.</u>	<u>Variable</u>	<u>Format</u>	<u>Units</u>	<u>Note</u>
7	1-65/1-60	A(I,J)	25(13F5.1/ 12F5.1)	degrees	Wind directions applicable at the next hour; input sequence: ((A(I,J),I=1,25),J=1,25)

Include a complete set of Card No. 5-7 for each hour of meteorological data.

Note: Mixing depths are assigned on the hour (0500, 0600, and etc.), and wind speeds and wind directions are applicable from the half hour to the half hour (0430-0530, 0530-0630, and etc.). TSTART must be assigned an even hour, such as 0500 hours.

An important change the user may wish to make in the APSP involves the formulation of the chemical kinetic mechanism. Rate constants and certain stoichiometric coefficients are input via punched cards, which allows these parameters to be altered without changing the code. We summarize below those sections of the code which are directly affected by the formulation of the kinetic mechanism.

<u>Routine</u>	<u>Card ID</u>	<u>Description</u>
MAIN	APS 06560-06630	Expressions relating the concentrations of the "steady state" species to the concentrations of HC, NO, NO ₂ , and O ₃
MAIN	APS 00920-00950 APS 06710-06890	RATE(L) = rate of reaction of species L $R(I,J) = - \frac{\partial(\text{rate expression for species I})}{\partial(\text{concentration of species J})}$
MAIN BCCONC ICCONC	APS 05520-05530 APS 11490-11540 APS 13200-13250	Initial and boundary concentrations of ozone are determined by assuming that the rate of reaction of ozone, both initially and at the boundary, is equal to zero. Thus, we can write an algebraic expression relating the initial and boundary concentrations of ozone to the initial and boundary concentrations of HC, NO, and NO ₂ .
MAIN ICCONC	APS 04980-05010 APS 02790-02810 APS 13150	Calculations involving the temporal variation of photolysis rate constants.

In order to establish the boundary concentrations aloft correctly, the first set of mixing depths in the MDF must be applicable at the starting time of the airshed simulation.

During the evaluation phase of model development, we found it advantageous to perform a 10 hour simulation in two 5 hour segments. Thus, a simulation for 0500-1500 hours is carried out in two sequential steps: 0500-1000 and 1000-1500 hours. To do this, we have made provisions for restarting the program using the results obtained at the end of a previous simulation as initial conditions. The parameter PUNCH, specified on Card No. 2 of the data-deck (see Table 4), determines whether or not the concentration array, CONC(L,I,J,K), is "dumped" onto a save disc area or tape at the time the program terminates. A program restart is controlled by the parameter RESTR (see Card No. 2 in Table 4). During the restart procedure the initial concentrations on the grid are established by reading the file containing the last concentrations predicted in the previous run. We note that the restart option should only be used when it is of interest to closely monitor the outcome of a particular simulation.

One of the important features of the APSP is that the user can easily modify the computational grid - both horizontally and vertically. The number of vertical cells (or strata) employed must be at least three,

and up to six can be specified in the present code. Only available storage restrictions limit the present code to a maximum of six levels. As far as the horizontal extent of the grid is concerned, the user defines, as part of the program input, the shape of the modeling area. In Figure 1, we illustrate that portion of the original 25x25 grid actually used during the simulation studies of the Los Angeles airshed.

To obtain the shape of the computational grid, we eliminate a series of consecutive grid squares starting from the left and/or right hand borders. Consider the region illustrated in Figure 1. In row 1, 20 consecutive grid squares, starting from the left hand border, are eliminated from the original 25x25 grid. As another example, 14 consecutive grid squares, starting from the right hand border, are eliminated from row 25. The region designation is made by specifying two arrays, ILEFT(J) and IRIGHT(J), containing the column numbers of the left and right-most cells in row J. The following values of ILEFT and IRIGHT are obtained from Figure 1:

ILEFT(1) = 21	IRIGHT(1) = 25
ILEFT(2) = 20	IRIGHT(2) = 25
ILEFT(25) = 1	IRIGHT(25) = 11

Instantaneous and time-averaged ground level concentrations can be predicted at up to 16 user-selected sites. The x and y-coordinates of each site are input to the program on punched cards, where the center of grid square (I,J) has an x-coordinate of I and a y-coordinate of J. In addition, the name of each station is printed on the ground level concentration maps near its location on the grid (see Figures 3 and 4). The user can also specify up to 8 landmarks. The name of each landmark is printed on the ground level concentration maps as an aid in identifying the location of a particular area of the grid. Four landmarks are illustrated in Figures 3 and 4, including the Pacific Ocean, the Santa Monica Mountains, the San Gabriel Mountains, and Palos Verdes.

Computing System Information

Hardware:

5 - disc areas/tape drives

- | | |
|---|----------|
| a. EDF (required) | FT02F001 |
| b. MDF (required) | FT04F001 |
| c. Scratch-Area (required) | FT08F001 |
| d. Save area where concentrations can be written at the end of a simulation for use as initial conditions in a program restart (optional) | FT03F001 |
| e. Save area where concentrations are located to be used as initial conditions in a program restart (optional). | FT09F001 |

- | | |
|-----------------|----------|
| 1 - card reader | FT05F001 |
| 1 - printer | FT06F001 |
| 1 - card punch | FT07F001 |

Program Size: 304K bytes

CPU time (IBM 370/155):

10 hour CO simulation - 4 minutes

10 hour photochemical simulation involving RHC, URHC, NO, NO₂, O₃,
and CO - 73 minutes

Printed Output:

10 hour CO simulation with instantaneous concentration values
printed once an hour.

- hourly-averaged ground level concentration maps
1 species x 10 hours x 1 page/species hour = 10 pages
- hourly-averaged predictions at monitoring stations
10 hours x 1 page/hour = 10 pages
- instantaneous ground level concentration maps
1 species x 10 hours x 1 page/species hour = 10 pages
- instantaneous concentration profiles above each
station (15 stations)
10 hours x 2 pages/hour = 20 pages
- miscellaneous, including grid specifications, rate
constants, and initial conditions = 4 pages

Total Printed Output = 54 pages

10 hour photochemical simulation (6 species) with instantaneous
concentration values printed once an hour.

- hourly-averaged ground level concentration maps
6 species x 10 hours x 1 page/species hour = 60 pages
- hourly-averaged predictions at monitoring stations
10 hours x 1 page/hour = 10 pages
- instantaneous ground-level concentration maps
6 species x 10 hours x 1 page/species hour = 60 pages
- instantaneous concentration profiles above each
station (15 stations)
10 hours x 3 pages/hour = 30 pages
- miscellaneous, including grid specifications,
rate constants, and initial conditions = 10 pages

Total Printed Output = 170 pages

In Table 4 which follows, we describe in detail the data-deck
setup for the APSP.

TABLE 4
DATA-DECK SETUP FOR THE ATMOSPHERIC POLLUTION SIMULATION PROGRAM

<u>Card No.</u>	<u>Column No.</u>	<u>Variable</u>	<u>Format</u>	<u>Units</u>	<u>Note</u>
1	1-80	NOTE(I)	2(20A4)	--	Two cards of user-supplied alphameric information to be printed on program output; input sequence: (NOTE(I), I=1,40)
2	1	PUNCH	L1	--	If PUNCH=.TRUE., then the entire concentration array (CONC) will be dumped onto a peripheral storage area at the end of the simulation. These concentrations can be used for a program restart.
2	2	RESTRT	L1	--	If RESTRT=.TRUE., then the program restarts using the results obtained in a previous simulation for initial conditions
2	6-10	NOX	I5	--	Number of grid points in x-direction
2	11-15	NOY	I5	--	Number of grid points in y-direction
2	16-20	NOZ	I5	--	Number of grid points in z-direction
2	21-30	DT	F10.0	minute	Initial time step size for the numerical integration

TABLE 4 (Cont'd)
DATA-DECK SETUP FOR THE ATMOSPHERIC POLLUTION SIMULATION PROGRAM

<u>Card No.</u>	<u>Column No.</u>	<u>Variable</u>	<u>Format</u>	<u>Units</u>	<u>Note</u>
2	31-40	DELTAX	F10.0	feet	Grid spacing in x-direction
2	41-50	DELTAY	F10.0	feet	Grid spacing in y-direction
2	51-60	PRTDT	F10.0	minute	Time interval between instantaneous concentration print-outs
2	61-70	TSTART	F10.0	2400 time	Simulation starting time
2	71-80	TSTOP	F10.0	2400 time	Simulation stopping time
3	1-6	ISPEC(L)	6L1	--	<p>If ISPEC(L)=.TRUE., then species L will be simulated</p> <div style="display: flex; align-items: center;"> <div style="margin-right: 10px;">L=</div> <div style="border-left: 1px solid black; padding-left: 10px;"> <p>1 reactive hydrocarbon</p> <p>2 nitric oxide</p> <p>3 ozone</p> <p>4 nitrogen dioxide</p> <p>5 carbon monoxide</p> <p>6 unreactive hydrocarbon</p> </div> </div> <p>Species 1-5 must <u>all</u> be simulated when performing photochemical calculations; species 5 and/or 6 can be simulated independently; input sequence: (ISPEC(L), L=1,6)</p>
3	7-30	UNIT(L)	6A4	--	<p>Alphameric designation of the units to be used on input/output for the concentration of species L. For the above species</p>

TABLE 4 (Cont'd)
DATA-DECK SETUP FOR THE ATMOSPHERIC POLLUTION SIMULATION PROGRAM

<u>Card No.</u>	<u>Column No.</u>	<u>Variable</u>	<u>Format</u>	<u>Units</u>	<u>Note</u>
					$\text{UNIT}(L) \begin{cases} L=1, 'PPHM' \\ L=2, 'PPHM' \\ L=3, 'PPHM' \\ L=4, 'PPHM' \\ L=5, 'PPM' \\ L=6, 'PPTM' \end{cases}$
					input sequence: (UNIT(L), L=1,6)
3	31-60	FACTOR(L)	6F5.1	--	Conversion factor; must be consistant with UNIT(L)
					If $\text{UNIT}(L) = \begin{cases} 'PPHM' \\ 'PPTM' \\ 'PPM' \end{cases},$
					then $\text{FACTOR}(L) = \begin{cases} 100. \\ 10. \\ 1. \end{cases}.$
					input sequence: (FACTOR(L), L=1,6)
3	61-64	TIMEZN	A4	--	Alphameric designation of the time zone (for Los Angeles, use 'PST ')
4	1-80	REGION(I)	20A4	--	Alphameric designation of the geographical location to be modeled (for example, 'LOS ANGELES AND VICINITY'); input sequence: (REGION(I), I=1,20)

TABLE 4 (Cont'd)
DATA-DECK SETUP FOR THE ATMOSPHERIC POLLUTION SIMULATION PROGRAM

<u>Card No.</u>	<u>Column No.</u>	<u>Variable</u>	<u>Format</u>	<u>Units</u>	<u>Note</u>
5	1-75	ILEFT(J)	25I3	--	ILEFT defines the left (western) border of the model. ILEFT(J) is the column number of the left-most cell in row J; input sequence: (ILEFT(J),J=1,NOY)
6	1-75	IRIGHT(J)	25I3	--	IRIGHT defines the right (eastern) border of the model. IRIGHT(J) is the column number of the right-most cell in row J; input sequence: (IRIGHT(J),J=1,NOY)
7	1-3	NOSTN	I3	--	Number of stations for which vertical concentration distributions and hourly-averaged ground level concentrations will be calculated and printed
7	4-6	NOLAND	I3	--	Number of landmarks that will be printed on the program output
7	7-9	NOPTS	I3	--	Number of point sources

If NOSTN = 0, do NOT include Card No. 8.

If NOSTN>0, include one Card No. 8 for each station (I=1,NOSTN). Sort all Card No. 8 until YSTN(1)> YSTN(2)>...> YSTN(NOSTN).

TABLE 4 (Cont'd)
DATA-DECK SETUP FOR THE ATMOSPHERIC POLLUTION SIMULATION PROGRAM

<u>Card No.</u>	<u>Column No.</u>	<u>Variable</u>	<u>Format</u>	<u>Units</u>	<u>Note</u>
8	1-20	STNAME(I,J)	5A4	--	Alphameric designation of station I (for example 'DOWNTOWN LA'); input sequence: (STNAME(I,J),J=1,5)
8	21-30	XSTN(I)	F10.0	--	x-coordinate of station I.
8	31-40	YSTN(I)	F10.0	--	y-coordinate of station I.

If NOLAND = , do NOT include Card No. 9.

If NOLAND>0, include one Card No. 9 for each landmark (I = 1, NOLAND).
Sort all Card No. 9 until YLAND(1)>YLAND(2)>...>YLAND(NOLAND).

9
0

9	1-20	LANDMK(I,J)	5A4	--	Alphameric designation of landmark I (for example 'PACIFIC OCEAN'); input sequence: (LANDMK(I,J),J=1,5)
9	21-30	XLAND(I)	F10.0	--	x-coordinate of landmark I
9	31-40	YLAND(I)	F10.0	--	y-coordinate of landmark I

If NOPTS = 0, do NOT include Card No. 10-11.

If NOPTS>0, include a set of Card No. 10-11 for each point source (I = 1, NOPTS).

10	1-5	XPTS(I)	F5.0	--	x-coordinate of point source I
10	6-10	YPTS(I)	F5.0	--	y-coordinate of point source I

TABLE 4 (Cont'd)
DATA-DECK SETUP FOR THE ATMOSPHERIC POLLUTION SIMULATION PROGRAM

<u>Card No.</u>	<u>Column No.</u>	<u>Variable</u>	<u>Format</u>	<u>Units</u>	<u>Note</u>
10	11-20	HEMIS(I)	F10.0	feet	Height at which point source I emits pollutants
10	21-80	PTEMIS(L,I)	6F10.0	pound-mole /hour	Nominal emissions rate of species L from point source I; input sequence: (PTEMIS(L,I), L=1,6)
11	1-80	TEMPTS(I,J)	3(8F10.0)	--	Temporal distribution for point source I; fraction of nominal emissions rate, PTEMIS(L,I), during hourly period J. PTEMIS(L,I) * TEMPTS(I,J) = emissions rate of species L from point source I during hourly period J; input sequence: (TEMPTS(I,J), J=1,24)
12	1-5	MAXITR	I5	--	Maximum number of iterations allowed in the Newton solution of the non-linear difference equations
12	6-10	ERROR	F5.0	--	Relative error tolerance that must be satisfied before the Newton iteration is considered finished
12	11-15	DTMIN	F5.0	Minute	Minimum allowable integration time step. If the program must take a smaller step, it terminates.
12	16-20	DTMAX	F5.0	Minute	Maximum allowable integration time step

TABLE 4 (Cont'd)
DATA-DECK SETUP FOR THE ATMOSPHERIC POLLUTION SIMULATION PROGRAM

<u>Card No.</u>	<u>Column No.</u>	<u>Variable</u>	<u>Format</u>	<u>Units</u>	<u>Note</u>
12	21-25	ALPHA	F5.0	--	Chemical kinetics parameter
12	26-30	BETA	F5.0	--	Chemical kinetics parameter
12	31-35	GAMMA	F5.0	--	Chemical kinetics parameter
12	36-40	EPS	F5.0	--	Chemical kinetics parameter
12	41-45	HTOP	F5.0	feet	Height above which the ambient concentration above the inversion base is CALOFT (see Card No. 16)
13	1-80	RKO(I)	(8F10.0)	ppm-min	Nominal chemical reaction rate constant for reaction I; input sequence: (RKO(I), I=1, NORATE) NORATE = number of chemical reactions (this parameter is defined in the MAIN program)
14	1-80	FACTRK(J)	3(8F10.0)	--	Light intensity curve; fraction of nominal photo- lysis rate constant (k_1, k_7) at hour J (J=1 corresponds to mid- night) $k_1 = \text{RKO}(1) * \text{FACTRK}(J)$ at hour J; input sequence: (FACTRK(J), J=1, 24)

TABLE 4 (Cont'd)
DATA-DECK SETUP FOR THE ATMOSPHERIC POLLUTION SIMULATION PROGRAM

<u>Card No.</u>	<u>Column No.</u>	<u>Variable</u>	<u>Format</u>	<u>Units</u>	<u>Note</u>
15	1-24	NAME(L)	6A4	--	<p>Alphameric designation of the name of species L</p> <p>NAME(L) = $\begin{cases} L=1, & \text{' HC ' } \\ L=2, & \text{' NO ' } \\ L=3, & \text{' O3 ' } \\ L=4, & \text{' NO2 ' } \\ L=5, & \text{' CO ' } \\ L=6, & \text{' URHC ' } \end{cases}$</p> <p>input sequence: (NAME(L), L=1,6)</p>
16	1-75	CALOFT(L,I,J)	(25F3.0) (see note)	see note	<p>Ambient concentration aloft of species L above grid square (I,J). These concentrations apply when the mixing depth above grid square (I,J) is greater than HTOP (see Card No. 12).</p> <p>The concentration units are the same as those designated by UNIT(L) (see Card No. 3). The input sequence is governed by the following logic:</p> <pre> DO 3 L=1,NOSPEC IF(.NOT.ISPEC(L)) GO TO 3 DO 1 J=1,NOY 1 READ(5,2) (CALOFT(L,I,J), 1I=1,NOX) 2 FORMAT(25F3.0) 3 CONTINUE </pre> <p>Note that input cards are included only for those species simulated.</p>

TABLE 4 (Cont'd)
DATA-DECK SETUP FOR THE ATMOSPHERIC POLLUTION SIMULATION PROGRAM

<u>Card No.</u>	<u>Column No.</u>	<u>Variable</u>	<u>Format</u>	<u>Units</u>	<u>Note</u>
17	1-75	CONCI(L,I,J)	25F3.0 (see note)	see note	Initial ground level concentration of species L in grid cell (I,J,1). The concentration units are the same as those designated by UNIT(L) (see Card No. 3). The input sequence is governed by the same logic as that used for the input of CALOFT(L,I,J) (see Card No. 16). No cards are included for those species not being simulated.

Include a sufficient number of sets of Card No. 18-19 to cover the entire time period to be simulated (i.e., TSTART to TSTOP-see Card No. 2). The sets of Card No. 18-19 should be arranged sequentially, according to the time interval designated by TDATA and TNEXT. For example, consider the following sequence:

Set #1	{	Card No. 18 - TDATA = 0500, TNEXT = 0600.
		Card No. 19 - Boundary conditions that apply between 0500 and 0600.
Set #2	{	Card No. 18 - TDATA = 0600, TNEXT = 0700.
		Card No. 19 - Boundary conditions that apply between 0600 and 0700

18	1-10	TDATA	F10.0	2400 time	Beginning of the time interval over which the following boundary conditions hold.
18	11-20	TNEXT	F10.0	2400 time	End of the time interval over which the following boundary conditions hold.

TABLE 4 (Cont'd)
DATA-DECK SETUP FOR THE ATMOSPHERIC POLLUTION SIMULATION PROGRAM

<u>Card No.</u>	<u>Column No.</u>	<u>Variable</u>	<u>Format</u>	<u>Units</u>	<u>Note</u>
19	1-75	BC(L,I,J)	25F3.0 (see note)	see note	Boundary concentrations for species L at points of horizontal inflow to the model. I denotes the row (east or west border) or column (north or south border) number of the boundary cell on border J.

$J = \begin{pmatrix} 1 \\ 2 \\ 3 \\ 4 \end{pmatrix}$ refers to the

$\begin{pmatrix} \text{top} & (\text{north}) \\ \text{bottom} & (\text{south}) \\ \text{right} & (\text{east}) \\ \text{left} & (\text{west}) \end{pmatrix}$ border

The concentration units are the same as those designated by UNIT(L) (see Card No. 3). The input sequence is governed by the following logic:

```
DO 3 L=1,NOSPEC
IF(.NOT.ISPEC(L))GO TO 3
ISTOP=NOX
DO 1 J=1,4
IF(J.GT.2) ISTOP=NOY
```

```
1 READ(5,2) (BC(L,I,J),I=1,
1 ISTOP)
2 FORMAT(25F3.0)
3 CONTINUE
```

Note that input cards are included only for those species simulated.

4. The Data Plotting Program

We summarize below the changes that may be required in the code of the DPP.

- The NO measurements at stations 5 and 9 (El Monte and Commerce) are not corrected. To make corrections at these stations, remove card DPP 1920.
- Oxidant measurements are not corrected at stations 5 and 9 (El Monte and Commerce). To make oxidant corrections at these stations, remove card DPP 2000.
- Oxidant measurements are not corrected at station number 13 (Long Beach). To correct oxidant measurements at this station, remove card DPP 1990.

The following limitations are placed on the use of the DPP:

- Only local corrections to CO predictions will be plotted
- No more than 12 hours of data can be plotted

Computing System Information

Hardware:

1 - card reader	FT05F001
1 - printer	FT06F001
1 - Calcomp Plotter	

Program Size: 68K bytes

CPU Time (IBM 370/155): 30 seconds

Printed Output: 1 page

Software:

The following Calcomp routines are used in the DPP. All coordinates and heights are measured in inches.

SYSPLT(X,Y,IPN)

This routine moves the pen from its present location to (X,Y) with the pen up (IPN=3) or down (IPN=2).

SYSSYM(X,Y,H,SYMBOL,N,DEG)

This routine plots the alphanumeric information contained in SYMBOL at the point (X,Y). The height of the plotting is H, and the plot is produced at an angle of DEG with respect to the x-axis. The number of symbols to be plotted is N.

SYSEND(LAB,FLAG)

This routine is used to terminate a plot with or without plotting the page number at the lower-right corner of the paper.

LAB	{	= 0, the pen will return to the current origin without plotting a page number.
		> 0, the page number is plotted. Then the pen is moved to the next origin.
		< 0, the pen is moved to the next origin without plotting the page number.
FLAG	{	≠ 0, the statements "ONE SHEET PLOTTED" and "ENDING PLOT LABELED..." will be printed on user's output.
		= 0, the above printing will be suppressed.

The data-deck setup for the DPP is described in Table 5.

TABLE 5
DATA-DECK SETUP FOR THE DATA PLOTTING PROGRAM

<u>Card No.</u>	<u>Column No.</u>	<u>Variable</u>	<u>Format</u>	<u>Units</u>	<u>Note</u>
1	1-5	NOSTN	I5	--	Number of monitoring stations
1	6-10	NOHOUR	I5	--	Number of hours simulated
1	11-20	TSTART	F10.0	2400 time	Simulation starting time
1	21-30	CARRHC	F10.0	--	Number of carbon atoms per molecule of reactive hydrocarbon
1	31-40	CARUHC	F10.0	--	Number of carbon atoms per molecule of unreactive hydrocarbon
1	41-48	DATE (I)	2A4	--	Alphameric designation of the date - for example, '9/29/69'; input sequence: (DATE(I),I=1,2)
<p>Include a Card No. 2 for each monitoring station (K=1,NOSTN); be certain station K corresponds to station number K in the Atmospheric Pollution Simulation Program.</p>					
2	1-20	STNAME (L,K)	5A4	--	20 columns of alphameric information designating the name or location of monitoring station K; input sequence: (STNAME (L,K) ,L=1,5)
2	21-26	PLSPEC (K,L)	6L1	--	If PLSPEC(K,L)=.TRUE., then plot species L at monitoring station K; input sequence: (PLSPEC(K,L) ,L=1,6)

TABLE 5 (Cont'd)
DATA-DECK SETUP FOR THE DATA PLOTTING PROGRAM

<u>Card No.</u>	<u>Column No.</u>	<u>Variable</u>	<u>Format</u>	<u>Units</u>	<u>Note</u>
Include a Card No. 3 for each monitoring station reporting and each chemical species measured. The cards may be in any order; columns 7-9 should be left blank on all cards EXCEPT the last one, on which a "T" must be punched somewhere in columns 7-9.					
3	7-9	LAST	L3	--	If LAST=.TRUE., then the present card is the last Card No. 3 in the data-deck
3	10-11	ISTN	I2	--	Monitoring station number
3	12-13	ISPEC	I2	--	Chemical species number ISPEC= { 1 SO ₂ (pphm) 2 NO (pphm) 3 O ₃ (pphm) 4 NO ₂ (pphm) 5 CO (ppm) 6 total HC (ppmC)
3	33-80	DATA(I)	24F2.0	--	Measured hourly-averaged pollutant concentrations starting at midnight (see ISPEC above for units); input sequence: (DATA(I), I=1,24)
Include a Card No. 4 for each station and each chemical species for which a local correction is to be made; columns 1-3 should be left blank on all cards EXCEPT the last one, on which a "T" must be punched somewhere in columns 1-3.					
4	1-3	LAST	L3	--	If LAST=.TRUE., then the present card is the last Card No. 4 in the data-deck

TABLE 5 (Cont'd)
DATA-DECK SETUP FOR THE DATA PLOTTING PROGRAM

<u>Card No.</u>	<u>Column No.</u>	<u>Variable</u>	<u>Format</u>	<u>Units</u>	<u>Note</u>
4	4-6	ISTN	I3	--	Monitoring station number
4	7-9	ISPEC	I3	--	Chemical species number ISPEC= { 1 reactive hydrocarbon (pphm) 2 NO (pphm) 3 O ₃ (pphm) 4 NO ₂ (pphm) 5 CO (ppm) 6 unreactive hydrocarbon (pptm)
4	10-45	STCORR(ISTN,ISPEC,I)	12F3.0	--	Local correction to be applied to the model prediction at station ISTN for species ISPEC at hour I; I=1 corresponds to the hourly average starting at TSTART (see Card No. 1); see ISPEC above for the concentration units; input sequence: (STCORR(ISTN,ISPEC,I),I=1,NOHOUR)

Include a Card No. 5 for each chemical species and each hour simulated. The cards may be in any order. These cards are punched by the Atmospheric Pollution Simulation Program.

5	5-10	ISPEC	I6	--	Chemical species number
5	11-16	T1	F6.0	2400 time	Hour the model predictions were averaged over
5	17-80	A(I)	16F4.0	--	Concentration of species ISPEC predicted at monitoring site I over hour T1; input sequence: (A(I),I=1,NOSTN)

IV. LISTINGS, SYMBOL GLOSSARIES, AND SAMPLE OUTPUT

In this section we include the listing, symbol glossary, and sample output for each computer program.


```

C*****EODPP0010
C*EDPP0020
C*THE EMISSIONS DATA PREPARATION PROGRAMEDPP0030
C*EDPP0040
C*EDPP0050
C*WRITTEN BY: STEVEN D. REYNOLDSEDPP0060
C*EDPP0070
C*FOREDPP0080
C*EDPP0090
C*SYSTEMS APPLICATIONS, INC.,EDPP0100
C*9418 WILSHIRE BLVD.,EDPP0110
C*BEVERLY HILLS, CALIFORNIA 90212EDPP0120
C*EDPP0130
C*EDPP0140
C*JCL INFORMATIONEDPP0150
C*EDPP0160
C*FT04F001 EMISSIONS DATA FILEEDPP0170
C*FT05F001 CARD READEREDPP0180
C*FT06F001 PRINTEREDPP0190
C*EDPP0200
C*THE EMISSIONS DATA FILE IS DEFINED AS FOLLOWS (USING A 9EDPP0210
C*TRACK, 1600 BPI TAPE) :EDPP0220
C*EDPP0230
C*FT04F001 DD UNIT=(TAPE16,,DEFER),LABEL=(1,BLP),DISP=(OLD,KEEP),EDPP0240
C*VOL=SER=EDF001,DCB=(RECFM=VS,LRECL=2504,BLKSIZE=2508)EDPP0250
C*EDPP0260
C*****EODPP0270
C*DIMENSION EC(3),EH(3),XA(3),TSURF(24),TPFREE(24),SURMLG(25,25),FWYMEODPP0280
C*1LG(25,25),BETA(6,5,12),VS(25,25),VF(25,25),VS1(25,25),VF1(25,25),EDPP0290
C*1 SMILES(25,25),FMILES(25,25),E(3,25,25),X(25,25),Q1(6,25,25),EDPP0300
C*1 Q2(6,25,25),QSLOPE(25,25),XMOL(6),XB(3)EDPP0310
C*DIMENSION FXSDUR(25,25,6),FACTFS(6),AIRFLX(6,60),YCS(24)EDPP0320
C*DATA XMOL/47.8,30.,48.,46.,28.,21.1 /EDPP0330
C*COMMON/AIRCFT/NOARPT,NCORT(15),EMIX(15,7),ACFT(15,7),PCT(15,4),EDPP0340
C*1 DIST(15,24),IXORT(15,4),IYORT(15,4),TMODE(3,7),AIREMS(3,6,7)EDPP0350
C*REAL NAME(6),WTF8(6)EDPP0360
C*DATA WTF8/60.,30.,48.,46.,28.,18./EDPP0370
C*DATA NAME/4H HC ,4H NO ,4H O3 ,4H NO2,4H CO ,4HURHC/EDPP0380
C*LOGICAL KFLAG,PDTEDPP0390
C*KFLAG=.FALSE.,EDPP0400
C*DX=10560.,EDPP0410
C*DY=10560.,EDPP0420
C*EDPP0430
C*EDPP0440
C*** DEFINE MOLE FRACTIONS OF NO AND REACTIVE HYDROCARBON INEDPP0450
C*TOTAL NOX AND HYDROCARBON EMISSIONS
C*EDPP0460
C*FAIRNO=0.99EDPP0470
C*FCARHC=0.674EDPP0480
C*FCARNO=0.99EDPP0490
C*FFSNO=0.98EDPP0500
C*EDPP0510
C*** COMPUTE THE MASS FRACTION OF NO AND REACTIVE HYDROCARBONEDPP0520
C*IN TOTAL NOX AND HYDROCARBON EMISSIONS
C*EDPP0530
C*EDPP0540
C*XCARHC=FCARHC*XMOL(1)/(FCARHC*XMOL(1) + (1.-FCARHC)*XMOL(6))EDPP0550
C*XAIRNO=FAIRNO*XMOL(2)/(FAIRNO*XMOL(2) + (1.-FAIRNO)*XMOL(4))EDPP0560
C*XCARNO=FCARNO*XMOL(2)/(FCARNO*XMOL(2) + (1.-FCARNO)*XMOL(4))EDPP0570
C*XFSNO=FFSNO*WTF8(2)/(FFSNO*WTF8(2) + (1.-FFSNO)*WTF8(4))EDPP0580
C*HCEVAP=67.6EDPP0590
C*DENCAR=46./30. + (1.-XCARNO)/XCARNOEDPP0600

```

	DENAIR=XAIRND*46./30. + 1.=XAIRND	EDPP0610
	DENFS=46./30. + (1.=XFSND)/XFSND	EDPP0620
	FACTEV=0.343*8.68E5/(60.*HCEVAP*DX*DY)	EDPP0630
C		EDPP0640
C	*** INPUT CARD NO. 1-7	EDPP0650
C		EDPP0660
	READ(5,900) YCS	EDPP0670
	READ(5,901) EC,PDT	EDPP0680
	READ(5,900) EH	EDPP0690
	READ(5,900) XA	EDPP0700
	READ(5,900) XB	EDPP0710
	READ(5,900) TSURF	EDPP0720
	READ(5,900) TFREE	EDPP0730
900	FORMAT(8F10.0)	EDPP0740
901	FORMAT(3F10.0,L1)	EDPP0750
C		EDPP0760
C	*** ESTABLISH STARTING TIME	EDPP0770
C		EDPP0780
	TDATA=455.	EDPP0790
	TNEXT=500.	EDPP0800
	IF(.NOT.PDT) GO TO 902	EDPP0810
	TDATA=355.	EDPP0820
	TNEXT=400.	EDPP0830
902	CONTINUE	EDPP0840
	DO 699 L=1,24	EDPP0850
	TSURF(L)=TSURF(L)*1.0E-4	EDPP0860
699	TFREE(L)=TFREE(L)*1.0E-4	EDPP0870
C		EDPP0880
C	*** INPUT CARD NO. 8 AND 9	EDPP0890
C		EDPP0900
	READ(5,100) SURMLG,FWYMLG	EDPP0910
100	FORMAT(25F3.0)	EDPP0920
C		EDPP0930
C	*** CONVERT FROM THOUSANDS OF MILES TO MILES	EDPP0940
C		EDPP0950
	DO 101 I=1,25	EDPP0960
	DO 101 J=1,25	EDPP0970
	SURMLG(I,J)=SURMLG(I,J)*1000	EDPP0980
101	FWYMLG(I,J)=FWYMLG(I,J)*1000	EDPP0990
C		EDPP1000
C	*** INPUT CARD NO. 10-14	EDPP1010
C		EDPP1020
	READ(5,400) (((BETA(M,L,K),K=1,12),L=1,5),M=1,3)	EDPP1030
400	FORMAT(12F6.3)	EDPP1040
	READ(5,300) V81,VF1	EDPP1050
300	FORMAT(13F5.0/12F5.0)	EDPP1060
	READ(5,300) FX8OUR	EDPP1070
	READ(5,11) NOARPT	EDPP1080
	IF(NOARPT.LE.0) GO TO 13	EDPP1090
C		EDPP1100
C	*** INPUT CARD NO. 15-16	EDPP1110
C		EDPP1120
	READ(5,10) (((AIREMS(M,L,I),I=1,7),L=1,6),M=1,3)	EDPP1130
	READ(5,10) ((THODE(M,I),I=1,7),M=1,3)	EDPP1140
10	FORMAT(7F10.1)	EDPP1150
11	FORMAT(I5)	EDPP1160
C		EDPP1170
C	*** INPUT CARD NO. 17-23 FOR EACH AIRPORT	EDPP1180
C		EDPP1190
	DO 12 J=1,NOARPT	EDPP1200

	READ(5,17) AIRPRT,NCORT(J)	EDPP1210
	M=NCORT(J)	EDPP1220
	READ(5,16) (IXORT(J,I),I=1,M)	EDPP1230
	READ(5,16) (IYORT(J,I),I=1,M)	EDPP1240
	READ(5,19) (DIST(J,I),I=1,24)	EDPP1250
	READ(5,15) (PCT(J,I),I=1,M)	EDPP1260
	READ(5,15) (ACFT(J,I),I=1,7)	EDPP1270
	READ(5,15) (EMIX(J,I),I=1,7)	EDPP1280
15	FORMAT(13F6,2)	EDPP1290
16	FORMAT(6I5)	EDPP1300
19	FORMAT(12F5,3)	EDPP1310
17	FORMAT(A4,I2)	EDPP1320
12	CONTINUE	EDPP1330
13	CONTINUE	EDPP1340
C		EDPP1350
C	*** CONVERT FIXED SOURCE EMISSIONS INTO A SURFACE FLUX WITH	EDPP1360
C	THE UNITS PPM*FEET/MINUTE	EDPP1370
C		EDPP1380
	DO 14 L=1,6	EDPP1390
14	FACTFS(L)=1000,*8.680E5/(WTFS(L)*60,*DX*DY)	EDPP1400
	FACTFS(2)=FACTFS(2)/DENFS	EDPP1410
	FACTFS(4)=FACTFS(4)*((1.0-XFSNO)/(XFSNO*DENFS))	EDPP1420
	DO 105 L=1,6	EDPP1430
	DO 105 I=1,25	EDPP1440
	DO 105 J=1,25	EDPP1450
105	FXSOUR(I,J,L)=FXSOUR(I,J,L)*FACTFS(L)	EDPP1460
C		EDPP1470
C	*** CALCULATE TOTAL POLLUTANT FLUX EMITTED FROM EACH AIRPORT	EDPP1480
C		EDPP1490
	IF(NOARPT,LE,0) GO TO 50	EDPP1500
	DO 36 L=1,6	EDPP1510
	DO 35 J=1,NOARPT	EDPP1520
	FLUX=0.	EDPP1530
	DO 37 I=1,7	EDPP1540
37	FLUX=FLUX + ACFT(J,I)*EMIX(J,I)*(AIREMS(1,L,I)*TMODE(1,I) + AIREMS	EDPP1550
	1(2,L,I)*TMODE(2,I) + AIREMS(3,L,I)*TMODE(3,I))	EDPP1560
	AIRFLX(L,J)=FLUX*1.0E-3*394.0*1.0E6/(60,*XMOL(L)*DX*DY)	EDPP1570
	IF(L,EQ,2.OR,L,EQ,4)AIRFLX(L,J)=AIRFLX(L,J)/DENAIR	EDPP1580
35	CONTINUE	EDPP1590
36	CONTINUE	EDPP1600
C		EDPP1610
C	*** IN THE NEXT SECTION OF CODE, EMISSIONS ARE CALCULATED FOR	EDPP1620
C	EACH FIVE MINUTE INTERVAL BETWEEN 0500 AND 0955 HOURS	EDPP1630
C	LOCAL TIME	EDPP1640
C		EDPP1650
50	DO 1 LL=1,5	EDPP1660
C		EDPP1670
C	*** SET PARAMETERS CONTROLLING THE TEMPORAL DISTRIBUTION OF	EDPP1680
C	FIXED SOURCE EMISSIONS AND EVAPORATIVE EMISSIONS FROM	EDPP1690
C	AUTOMOBILES	EDPP1700
C		EDPP1710
	LM=0	EDPP1720
	LN=0	EDPP1730
	IF(LL,GT,1) LM=1	EDPP1740
	IF(LL,GT,2) LN=1	EDPP1750
C		EDPP1760
C	*** CALCULATE THE NUMBER OF MILES DRIVEN ON SURFACE STREETS	EDPP1770
C	AND FREEWAYS	EDPP1780
C		EDPP1790
	DO 450 I=1,25	EDPP1800

DO 450 J=1,25	EDPP1810
V8(I,J)=V81(I,J)	EDPP1820
VF(I,J)=VF1(I,J)	EDPP1830
LO=LL	EDPP1840
C	EDPP1850
C *** SHIFT THE TEMPORAL DISTRIBUTION OF TRAFFIC ACTIVITY IN THE	EDPP1860
C DOWNTOWN LOS ANGELES AREA BACK BY ONE HOUR	EDPP1870
C	EDPP1880
IF(I,EQ,11,AND,J,EQ,17) LO=LL-1	EDPP1890
IF(I,EQ,12,AND,J,EQ,17) LO=LL-1	EDPP1900
IF(I,EQ,12,AND,J,EQ,16) LO=LL-1	EDPP1910
SMILES(I,J)=SURMLG(I,J)*TSURF(LO+5)	EDPP1920
450 FMILES(I,J)=FWYMLG(I,J)*TFREE(LO+5)	EDPP1930
C	EDPP1940
C *** INPUT CARD NO. 24=26	EDPP1950
C	EDPP1960
READ (5,300)((X (I,J),I=1,25),J=1,25)	EDPP1970
READ (5,300)((V81(I,J),I=1,25),J=1,25),((VF1(I,J),I=1,25),J=1,25)	EDPP1980
C	EDPP1990
C *** DO LOOP FOR EACH FIVE MINUTES IN THE HOUR	EDPP2000
C	EDPP2010
DO 111 K=1,12	EDPP2020
XK=FLOAT(K-1)/12.	EDPP2030
C	EDPP2040
C *** CALCULATE TOTAL EMISSIONS FROM AUTOMOBILES IN EACH GRID	EDPP2050
C SQUARE	EDPP2060
C	EDPP2070
DO 120 I=1,25	EDPP2080
DO 120 J=1,25	EDPP2090
VSS=V8(I,J)+(V81(I,J)-V8(I,J))*XK	EDPP2100
VFF=VF(I,J)+(VF1(I,J)-VF(I,J))*XK	EDPP2110
DO 120 M=1,3	EDPP2120
IF(VSS,EQ,0.) GO TO 550	EDPP2130
ALS=VSS**XB(M)	EDPP2140
ALF=VFF**XB(M)	EDPP2150
GO TO 551	EDPP2160
550 ALS=0.	EDPP2170
ALF=0.	EDPP2180
551 CONTINUE	EDPP2190
E(M ,I,J)=XA(M)*FMILES(I,J)*(ALF+X(I,J)*ALS)/(1.+X(I,J))+	EDPP2200
1 BETA(M,LL,K)*(YCS(LL+5)*EC(M)+(1.-YCS(LL+5))*EH(M))*SMILES(I,J)	EDPP2210
120 CONTINUE	EDPP2220
C	EDPP2230
C *** CONVERT AUTOMOTIVE EMISSIONS (MASS/TIME) TO A FLUX BASED	EDPP2240
C ON THE AREA OF A GRID SQUARE. THIS IS A PARTIAL CONVERSION	EDPP2250
C OF THE UNITS TO PPM=FEET/MINUTE. THE REMAINDER OF THE	EDPP2260
C CONVERSION TAKES PLACE IN THE NEXT SECTION OF CODE.	EDPP2270
C	EDPP2280
DO 330 L=1,3	EDPP2290
DO 330 I=1,25	EDPP2300
DO 330 J=1,25	EDPP2310
330 E(L,I,J)=E(L,I,J) *8.680E5/(DX*DY)	EDPP2320
C	EDPP2330
C *** COMPLETE THE CONVERSION OF THE AUTOMOTIVE FLUX TO PPM=	EDPP2340
C FEET/MINUTE AND COMBINE WITH THE FIXED SOURCE FLUX	EDPP2350
C	EDPP2360
DO 331 I=1,25	EDPP2370
DO 331 J=1,25	EDPP2380
G2(1,I,J)=E(2,I,J)*XCARNC/XMOL(1)+FXSOUR(I,J,1)*LM+LN*FACTEV*SURML	EDPP2390
1G(I,J)	EDPP2400

	Q2(2,I,J)=E(3,I,J)/(XMOL(2)*DENCAR) + FXSOUR(I,J,2)*LM	EDPP2410
	Q2(3,I,J)=0,	EDPP2420
	Q2(4,I,J)=E(3,I,J)*(1,-XCARN0)/(XMOL(4)*XCARN0*DENCAR) +	EDPP2430
	1 FXSOUR(I,J,4)*LM	EDPP2440
	Q2(5,I,J)=E(1,I,J)/XMOL(5) + FXSOUR(I,J,5)*LM	EDPP2450
331	Q2(6,I,J)=E(2,I,J)*(1,-XCARHC)/XMOL(6) + FXSOUR(I,J,6)*LM	EDPP2460
C		EDPP2470
C	*** ADD EMISSIONS FLUXES FROM AIRPORTS	EDPP2480
C		EDPP2490
	IF(N0ARPT,LE,0) GO TO 55	EDPP2500
	DO 40 J=1,N0ARPT	EDPP2510
	M=NCORT(J)	EDPP2520
	DO 41 II=1,M	EDPP2530
	DO 336 L=1,6	EDPP2540
336	Q2(L,IXORT(J,II),IYORT(J,II))=Q2(L,IXORT(J,II),IYORT(J,II)) + PCT(EDPP2550
	1J, II)*DIST(J,LL+5)*AIRFLX(L,J)	EDPP2560
41	CONTINUE	EDPP2570
40	CONTINUE	EDPP2580
55	CONTINUE	EDPP2590
	IF(KFLAG) GO TO 88	EDPP2600
C		EDPP2610
C	*** WRITE THE INITIAL EMISSIONS FLUXES ON THE FILE	EDPP2620
C		EDPP2630
	KFLAG=.TRUE.	EDPP2640
	DO 86 L=1,6	EDPP2650
	WRITE(4) ((Q2(L,I,J),I=1,25),J=1,25)	EDPP2660
86	CONTINUE	EDPP2670
	GO TO 92	EDPP2680
C		EDPP2690
C	*** DEFINE AND WRITE THE TIME INTERVAL ON THE FILE	EDPP2700
C		EDPP2710
88	TDATA=TIME(TDATA,5,,1)	EDPP2720
	TNEXT=TIME(TNEXT,5,,1)	EDPP2730
	WRITE(4) TDATA,TNEXT	EDPP2740
C		EDPP2750
C	*** CALCULATE THE TIME RATE OF CHANGE OF THE EMISSIONS FLUXES	EDPP2760
C	AND WRITE THEM ON THE FILE	EDPP2770
C		EDPP2780
	DO 91 L=1,6	EDPP2790
	DO 90 J=1,25	EDPP2800
	DO 90 I=1,25	EDPP2810
90	Q8LOPE(I,J)=(Q2(L,I,J)-Q1(L,I,J))/5,	EDPP2820
91	WRITE(4) Q8LOPE	EDPP2830
92	DO 554 L=1,6	EDPP2840
	DO 554 I=1,25	EDPP2850
	DO 554 J=1,25	EDPP2860
554	Q1(L,I,J)=Q2(L,I,J)	EDPP2870
111	CONTINUE	EDPP2880
1	CONTINUE	EDPP2890
C		EDPP2900
C	*** IN THE NEXT SECTION OF THE CODE, EMISSIONS ARE CALCULATED	EDPP2910
C	HOURLY	EDPP2920
C		EDPP2930
	DO 3 LL=6,12	EDPP2940
C		EDPP2950
C	*** COMPUTE AUTOMOTIVE EMISSIONS FLUXES	EDPP2960
C		EDPP2970
	DO 2 M=1,3	EDPP2980
	DO 2 I=1,25	EDPP2990
	DO 2 J=1,25	EDPP3000

	LO=LL	EDPP3010
C		EDPP3020
C	*** SHIFT TEMPORAL DISTRIBUTION OF AUTOMOBILE TRAFFIC ACTIVITY	EDPP3030
C	IN THE DOWNTOWN LOS ANGELES AREA BACK BY ONE HOUR	EDPP3040
C		EDPP3050
	IF(I,EQ,11,AND,J,EQ,17) LO=LL-1	EDPP3060
	IF(I,EQ,12,AND,J,EQ,17) LO=LL-1	EDPP3070
	IF(I,EQ,12,AND,J,EQ,16) LO=LL-1	EDPP3080
	SMILES(I,J)=SURMLG(I,J)*TSURF(LO+5)	EDPP3090
	FMILES(I,J)=FWYMLG(I,J)*TFREE(LO+5)	EDPP3100
	E(M,I,J)= SMILES(I,J)*(YCS(LL+5)*EC(M)+(1.-YCS(LL+5))*EH(M)) + FMILES(I,J)*XA(M)*(60,**XB(M))	EDPP3110
1	LL+5))	EDPP3120
2	E(M,I,J)=E(M,I,J)*8.680E5/(DX*DY)	EDPP3130
C		EDPP3140
C	*** ADD FIXED SOURCE EMISSIONS FLUXES TO AUTOMOTIVE FLUXES	EDPP3150
C		EDPP3160
	DO 631 I=1,25	EDPP3170
	DO 631 J=1,25	EDPP3180
	Q2(1,I,J)=E(2,I,J)*XCARCH/XMOL(1)+FXSOUR(I,J,1)+FACTEV*SURMLG(I,J)	EDPP3190
	Q2(2,I,J)=E(3,I,J)/(XMOL(2)*DENCAR) + FXSOUR(I,J,2)*LM	EDPP3200
	Q2(3,I,J)=0,	EDPP3210
	Q2(4,I,J)=E(3,I,J)*(1.-XCARNQ)/(XMOL(4)*XCARNQ*DENCAR) +	EDPP3220
1	FXSOUR(I,J,4)*LM	EDPP3230
	Q2(5,I,J)=E(1,I,J)/XMOL(5) + FXSOUR(I,J,5)	EDPP3240
631	Q2(6,I,J)=E(2,I,J)*(1.-XCARCH)/XMOL(6) + FXSOUR(I,J,6)	EDPP3250
C		EDPP3260
C	*** ADD FLUXES FROM AIRPORTS	EDPP3270
C		EDPP3280
	IF(NOARPT,LE,0) GO TO 655	EDPP3290
	DO 640 J=1,NOARPT	EDPP3300
	M=NCORT(J)	EDPP3310
	DO 641 L=1,6	EDPP3320
	DO 641 II=1,M	EDPP3330
641	Q2(L,IXORT(J,II),IYORT(J,II))=Q2(L,IXORT(J,II),IYORT(J,II)) + PCT(EDPP3340
1J, II)*DIST(J,LL+5)*AIRFLX(L,J)		EDPP3350
640	CONTINUE	EDPP3360
655	CONTINUE	EDPP3370
C		EDPP3380
C	*** DEFINE AND WRITE ON THE FILE THE TIME INTERVAL CORRESPONDING	EDPP3390
C	TO THE LAST FIVE MINUTES OF THE HOUR (I.E., 0955-1000	EDPP3400
C	HOURS, 1055-1100 HOURS, AND ETC.,)	EDPP3410
C		EDPP3420
	TDATA=TNEXT	EDPP3430
	TNEXT=TIME(TDATA,5,,1)	EDPP3440
	WRITE(4) TDATA,TNEXT	EDPP3450
C		EDPP3460
C	*** CALCULATE THE TIME RATE OF CHANGE OF THE EMISSIONS FLUXES	EDPP3470
C	OVER THE LAST FIVE MINUTES OF THE HOUR, AND WRITE THEM ON	EDPP3480
C	THE FILE	EDPP3490
C		EDPP3500
	DO 691 L=1,6	EDPP3510
	DO 690 I=1,25	EDPP3520
	DO 690 J=1,25	EDPP3530
690	QSLOPE(I,J)=(Q2(L,I,J)-Q1(L,I,J))/5,	EDPP3540
691	WRITE(4) QSLOPE	EDPP3550
C		EDPP3560
C	*** DEFINE AND WRITE ON THE FILE THE TIME INTERVAL CORRESPONDING	EDPP3570
C	TO THE FIRST 55 MINUTES OF THE HOUR (I.E., 1000-1055 HOURS,	EDPP3580
C	1100-1155 HOURS, AND ETC.,)	EDPP3590
C		EDPP3600

	TDATA=TNEXT	EDPP3610
	TNEXT=TIME(TDATA,55,,1)	EDPP3620
	WRITE(4) TDATA,TNEXT	EDPP3630
C		EDPP3640
C	*** SET THE TIME RATE OF CHANGE OF THE EMISSIONS FLUXES TO	EDPP3650
C	ZERO SINCE EMISSIONS ARE ASSUMED TO BE CONSTANT OVER THE	EDPP3660
C	FIRST 55 MINUTES OF THE HOUR	EDPP3670
C		EDPP3680
	DO 692 I=1,25	EDPP3690
	DO 692 J=1,25	EDPP3700
692	QSLOPE(I,J)=0,	EDPP3710
C		EDPP3720
C	*** WRITE THE TIME RATE OF CHANGE OF THE EMISSIONS FLUXES ON	EDPP3730
C	THE FILE	EDPP3740
C		EDPP3750
	DO 693 L=1,6	EDPP3760
693	WRITE(4) QSLOPE	EDPP3770
	DO 664 L=1,6	EDPP3780
	DO 664 I=1,25	EDPP3790
	DO 664 J=1,25	EDPP3800
664	Q1(L,I,J)=Q2(L,I,J)	EDPP3810
3	CONTINUE	EDPP3820
C		EDPP3830
C	*** IN THE NEXT SECTION OF CODE, HOURLY MAPS OF EMISSIONS	EDPP3840
C	FLUXES ARE PRINTED	EDPP3850
C		EDPP3860
2000	REWIND 4	EDPP3870
	TWRITE=500,	EDPP3880
	DO 1000 L=1,6	EDPP3890
1000	READ(4) ((Q1(L,I,J),I=1,25),J=1,25)	EDPP3900
1011	READ(4,END=1010) TDATA,TNEXT	EDPP3910
	IF(TDATA,LT,TWRITE) GO TO 1001	EDPP3920
	TWRITE=TWRITE + 100,	EDPP3930
	DO 1002 L=1,6	EDPP3940
	WRITE(6,1003) NAME(L),TDATA,(I,I=1,13)	EDPP3950
1003	FORMAT(1H1,47X,'SOURCE STRENGTHS OF ',A4,' AT ',F6.1,' PST'///5X,	EDPP3960
	113I9//)	EDPP3970
	DO 1004 JJ=1,25	EDPP3980
	J=26=JJ	EDPP3990
1004	WRITE(6,1005) J,(Q1(L,I,J),I=1,13)	EDPP4000
1005	FORMAT(/1X,I2,4X,1P13E9,1)	EDPP4010
	WRITE(6,1007) (I,I=14,25)	EDPP4020
1007	FORMAT(////////5X,12I9//)	EDPP4030
	DO 1006 JJ=1,25	EDPP4040
	J=26=JJ	EDPP4050
1006	WRITE(6,1005) J,(Q1(L,I,J),I=14,25)	EDPP4060
1002	CONTINUE	EDPP4070
1001	DT=TIME(TNEXT,TDATA,2)	EDPP4080
	DO 1008 L=1,6	EDPP4090
	READ(4) QSLOPE	EDPP4100
	DO 1008 I=1,25	EDPP4110
	DO 1008 J=1,25	EDPP4120
1008	Q1(L,I,J)=Q1(L,I,J) + DT*QSLOPE(I,J)	EDPP4130
	GO TO 1011	EDPP4140
1010	STOP	EDPP4150
	END	EDPP4160

	REAL FUNCTION TIME(T1,T2,M)	EDPP4170
	GO TO (1,2,3),M	EDPP4180
C		EDPP4190
C	*** ADD A TIME IN MINUTES TO A 2400 HOUR TIME AND RETURN A 2400	EDPP4200
C	HOUR TIME	EDPP4210
C		EDPP4220
1	I100=T1/100	EDPP4230
	T3=T1 - 100.0*I100 + T2	EDPP4240
	I100=I100 + INT(T3/60)	EDPP4250
	TIME=I100*100.0 + T3 - 60.0*INT(T3/60)	EDPP4260
	RETURN	EDPP4270
C		EDPP4280
C	*** SUBTRACT TWO 2400 HOUR TIMES AND RETURN THE RESULT IN MINUTES	EDPP4290
C		EDPP4300
2	I100=T1/100	EDPP4310
	TIME=T1 - I100*40.0	EDPP4320
	I100=T2/100	EDPP4330
	TIME=TIME - T2 + I100*40.0	EDPP4340
	RETURN	EDPP4350
C		EDPP4360
C	*** SUBTRACT A TIME IN MINUTES FROM A 2400 HOUR TIME AND RETURN	EDPP4370
C	A 2400 HOUR TIME	EDPP4380
C		EDPP4390
3	IF(T1-T2-INT(T1/100.)*100.0,LT.0.0) GO TO 4	EDPP4400
	TIME=T1-T2	EDPP4410
	RETURN	EDPP4420
4	T3=T1 - INT(T1/100.)*100.	EDPP4430
	TIME=INT(T1/100.)*100. - 40. + T3-T2	EDPP4440
	RETURN	EDPP4450
	END	EDPP4460

SYMBOL GLOSSARY
EMISSIONS DATA PREPARATION PROGRAM

<u>Variable</u>	<u>Units</u>	<u>Dimension</u>	<u>Description</u>
ACFT(J,I)	aircraft/day	15x7	Number of flights per day of class I aircraft at airport J
AIREMS (M,L,I)	lb/min	3x6x7	<p>Aircraft emissions from class I aircraft operating in mode M</p> $L = \begin{cases} 1 & \text{reactive hydrocarbon} \\ 2 & \text{NO} \\ 3 & \text{O}_3 \\ 4 & \text{NO}_2 \\ 5 & \text{CO} \\ 6 & \text{unreacting hydrocarbon} \end{cases}$
AIRFLX(L,J)	ppm-ft/min	6x60	Total flux of species L from airport J
AIRPRT	--	Scalar	Name of the airport
BETA(M,K,L)	--	6x5x12	<p>The "β" correction factor that accounts for the nonuniform distribution of trip starts. M denotes the chemical species</p> $M = \begin{cases} 1 & \text{CO} \\ 2 & \text{HC} \\ 3 & \text{NO}_x \end{cases}$
DIST(J,I)	--	15x24	Fraction of daily aircraft flights at airport J assigned to hourly period I (I=1 corresponds to the time period midnight - 1 A.M.)
DT	minute	Scalar	Time interval
DX	feet	Scalar	Grid spacing in x-direction
DY	feet	Scalar	Grid spacing in y-direction
E(M,I,J)	gm/min	3x25x25	<p>Total emissions of species M from automobiles driven in grid square (I,J)</p> $M = \begin{cases} 1 & \text{CO} \\ 2 & \text{HC} \\ 3 & \text{NO}_x \end{cases}$

SYMBOL GLOSSARY (Cont'd)
EMISSIONS DATA PREPARATION PROGRAM

<u>Variable</u>	<u>Units</u>	<u>Dimension</u>	<u>Description</u>
EC(I)	grams/mile	3	Automotive cold-start emissions rates $I = \begin{cases} 1 & \text{CO} \\ 2 & \text{HC} \\ 3 & \text{NO}_x \end{cases}$
EH(I)	grams/mile	3	Automotive hot-start emissions rates $I = \begin{cases} 1 & \text{CO} \\ 2 & \text{HC} \\ 3 & \text{NO}_x \end{cases}$
EMIX(J,I)	engines/ aircraft	15x7	Number of engines on class I aircraft operating at airport J
FAIRHC	--	Scalar	Mole fraction of reactive hydrocarbon in total hydrocarbon emissions from aircraft
FAIRNO	--	Scalar	Mole fraction of NO in total NO _x emissions from aircraft
FCARHC	--	Scalar	Mole fraction of reactive hydrocarbon in total hydrocarbon emissions from automobiles
FCARNO	--	Scalar	Mole fraction of NO in total NO _x emissions from automobiles
FFSNO	--	Scalar	Mole fraction of NO in total NO _x emissions from fixed sources
FMIJES(I,J)	miles/min	25x25	Number of miles driven each minute on freeways in grid square (I,J)

SYMBOL GLOSSARY (Cont'd)
EMISSIONS DATA PREPARATION PROGRAM

<u>Variable</u>	<u>Units</u>	<u>Dimension</u>	<u>Description</u>
FWYMLG(I,J)	mile/day	25x25	Total freeway mileage driven each day in grid square (I,J)
FXSOUR(I,J,L)	Kgm/hr	25x25x6	Fixed source emissions assigned to grid square (I,J) <div style="margin-left: 150px;"> $L = \begin{cases} 1 & \text{reactive hydrocarbon} \\ 2 & \text{NO} \\ 3 & \text{O}_3 \\ 4 & \text{NO}_2 \\ 5 & \text{CO} \\ 6 & \text{unreactive hydrocarbon} \end{cases}$ </div>
HCEVAP	gm/gm mole	Scalar	Molecular weight of evaporative hydrocarbon
IXORT(J,I)	--	15x4	x-coordinates of the grid squares receiving emissions from airport J
IYORT(J,I)	--	15x4	y-coordinates of the grid squares receiving emissions from airport J
LM	--	Scalar	Controls temporal distribution of fixed sources $LM = \begin{cases} 0 & \text{before 0600 (local time)} \\ 1 & \text{after 0600} \end{cases}$
LN	--	Scalar	Controls the temporal distribution of evaporative hydrocarbon emissions from automobiles $LN = \begin{cases} 0 & \text{before 0700 (local time)} \\ 1 & \text{after 0700} \end{cases}$
NAME(L)	--	6	Alphameric designation of the name of species L