United States
Environmental Protection
Agency

Environmental Sciences Research
Laboratory
Research Triangle Park NC 27711

EPA-600/8-78-014a
July 1978

Research and Development

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User's Manual for Kinetics Model and Ozone Isopleth Plotting Package

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July 1978

USER'S MANUAL FOR KINETICS MODEL AND OZONE ISOPLETH PLOTTING PACKAGE

by

Gary Z. Whitten
H. Hogo

Systems Applications, Incorporated
950 Northgate Drive
San Rafael, California 94903

Contract 68-02-2428

Project Officer

Marcia C. Dodge

Atmospheric Chemistry and Physics Division
Environmental Sciences Research Laboratory
Research Triangle Park, North Carolina 27711

This study was conducted in cooperation with
Monitoring and Data Analysis Division
Office of Air Quality Planning and Standards

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PREFACE

This publication contains information on and the computer programs for the Kinetics Model and Ozone Isopleth Plotting Package (OZIPP). OZIPP can be used to estimate maximum ozone concentrations as a function of initial precursor concentrations, transported ozone/precursors, post-0800 emissions and meteorological conditions which are appropriate for a specific city. From these estimates, the program can generate ozone isopleths which are specific to a city under review. These isopleths can then be applied in the Empirical Kinetic Modeling Approach (EKMA) as described in EPA-450/2-77-021a and EPA-450/2-77-021b. EKMA is useful for (1) estimating NMHC and/or NO_x reductions required to attain the NAAQS for ozone and (2) estimating the change in peak daytime ozone concentrations downwind of cities accompanying a specified change in NMHC and/or NO_x.

Although the computer program has been checked thoroughly on Univac and CDC computing systems, incompatibilities on other systems may be found. In case there is a need to update this model, revisions will be distributed in the same manner as this report. Revisions may be obtained as they are issued by completing and mailing the form at the front of the manual.

The computer program described in this manual is available on magnetic tape as EPA-600/8-78-014b and can be acquired in either of two ways:

(1) Government and non-profit agencies may obtain a copy of the program by writing:

Chief, Modeling Support Section (MD-14)
Source Receptor Analysis Branch/MDAD
U.S. Enviornmental Protection Agency
Research Triangle Park, North Carolina 27711

(2) Others wishing a copy of the program may purchase it from the National Technical Information Service, Springfield, Virginia 22161, Telephone (703) 557-4650.

ABSTRACT

The Kinetics Model and Ozone Isopleth Plotting Package (OZIPP) is a computerized model that simulates ozone formation in urban atmospheres. OZIPP calculates maximum one-hour average ozone concentrations given a set of input assumptions about initial precursor concentrations, light intensity, dilution, diurnal and spatial emission patterns, transported pollutant concentrations, and reactivity of the precursor mix. The results of multiple simulations are used to produce an ozone isopleth diagram tailored to particular cities. Such a diagram relates maximum ozone concentrations to concentrations of non-methane hydrocarbons and oxides of nitrogen, and can be used in the Empirical Kinetic Modeling Approach (EKMA) to calculate emissions reductions necessary to achieve air quality standards for photochemical oxidants. This user's manual describes the technical basis, necessary and optional input data, computer code and the use of OZIPP.

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ACKNOWLEDGEMENTS

The authors are pleased to acknowledge the valuable contributions of the Environmental Protection Agency Project Officer, Dr. Marcia Dodge, of the Chemistry and Physics Division, Environmental Sciences Research Laboratory, and Dr. Edwin L. Meyer, John E. Summerhays, and Gerald L. Gipson of the Monitoring and Data Analysis Division, Office of Air Quality Planning and Standards. Whitmel M. Joyner (OAQPS) provided valuable assistance in editing the manual, and special thanks are due to Carole J. Mask (OAQPS) for help in typing and assembling the document.

1.0 MODEL OVERVIEW

1.1 BACKGROUND AND PURPOSE

The Empirical Kinetic Modeling Approach (EKMA) has been developed as a procedure for relating photochemical oxidants (expressed as ozone) to organic compounds and oxides of nitrogen.[1] The EKMA utilizes a set of ozone isopleths (lines of equal concentration) which depict maximum afternoon concentrations of ozone downwind from a city as a function of the following parameters:

- Morning concentrations of non-methane hydrocarbons (NMHC) and oxides of nitrogen (NO_x)
- Emissions of NMHC and NO_x occurring during the day
- Meteorological conditions
- Reactivity of the NMHC mix
- Concentrations of ozone and precursors transported from upwind areas.

The isopleths are developed by performing computer simulations of atmospheric photochemical reactions with various assumed levels of initial NMHC and NO_x concentrations. The ozone isopleths are then plotted as a function of initial precursor concentrations. (An example diagram is shown in Figure 1-1).

A computer program has been developed to provide users of EKMA with an easy, reliable, efficient and versatile means of constructing ozone isopleth diagrams. This program is called the Ozone Isopleth Plotting Package, or OZIPP. OZIPP allows explicit consideration of transport, different emission patterns, etc. The purpose of this manual is to describe the computer program, the associated input requirements, the information generated and the procedures for executing the program.

1.2 SCOPE AND USE

1.2.1 Applications

EKMA is a technique for relating changes in the maximum one-hour average ozone concentrations observed within or downwind of an urban area to changes

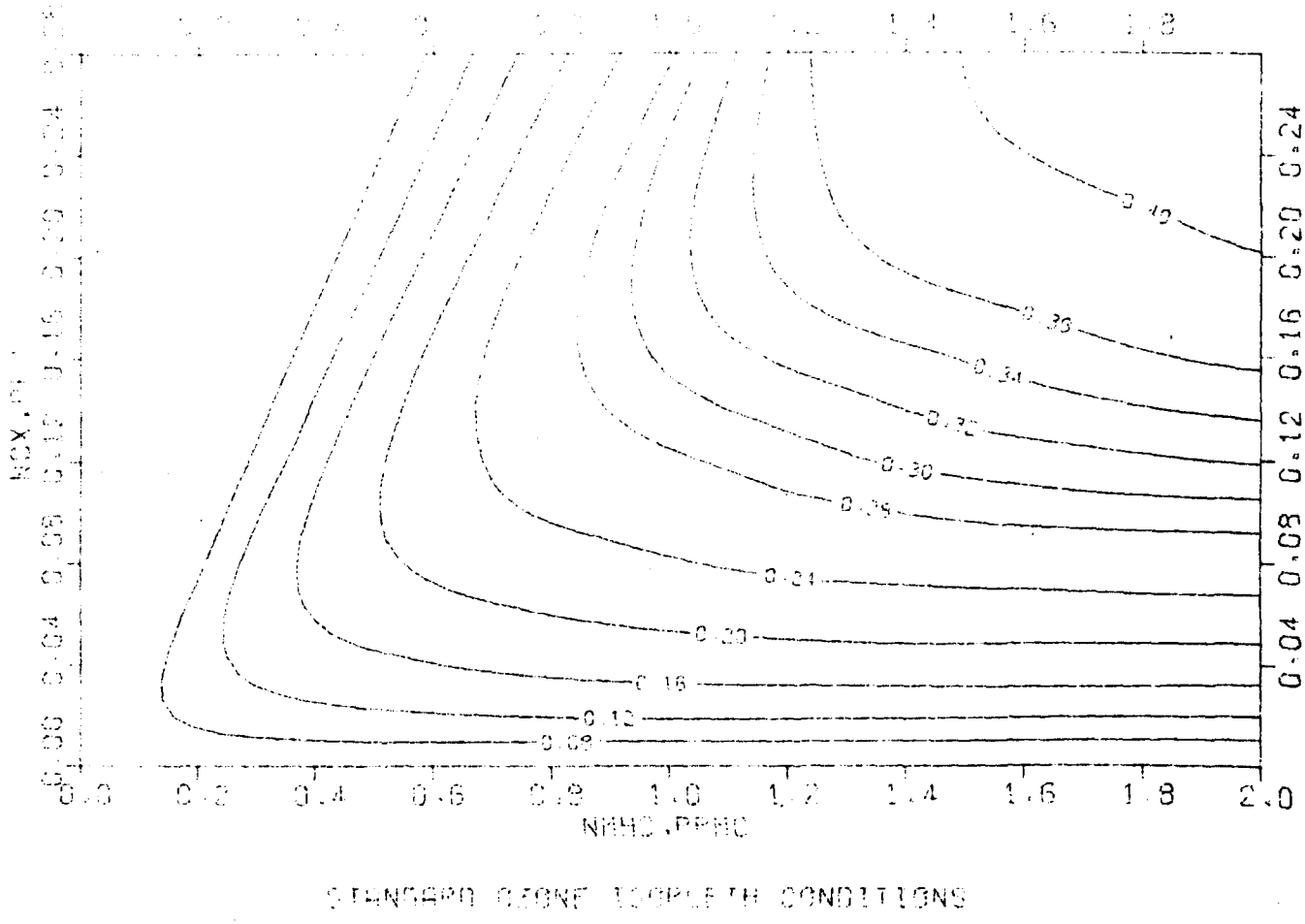

Figure 1-1. Example Ozone Isopleth Diagram

in the ambient concentrations of NMHC and NO_x in that urban area. It is intended primarily for estimating the emissions controls required in urban areas as part of the State Implementation Plans (SIP) to meet national ambient air quality standards. Thus, EKMA is used to address questions such as:

- What percentage reduction in the ambient concentration of NMHC or NO_x, or both, would be needed to attain compliance with the federal air quality standard for photochemical oxidants (ozone)?
- What reduction in the maximum one-hour-average ozone concentration is likely to accompany a given reduction in the ambient concentration of NMHC or NO_x?

Procedures for applying the EKMA technique are described in Reference 1. This reference also discusses the derivation of the information which is used in OZIPP.

The primary function of OZIPP is to generate ozone isopleth diagrams that are representative of conditions in a particular city. These types of diagrams, termed city-specific diagrams, are generated by OZIPP using city-specific information on the location and time of year (thereby defining sunlight intensity), local atmospheric dilution rate and local diurnal patterns of NMHC and NO_x emissions. OZIPP can also be used to regenerate the Standard Ozone Isopleth Diagram presented in Reference 1. In this situation, the diagram is based on fixed assumptions regarding sunlight intensity, atmospheric dilution rate and the diurnal pattern of emissions. OZIPP can also be used to simulate ozone formation for a set of city-specific assumptions and specified initial NMHC and NO_x concentrations. When operating in this mode, OZIPP has the capability of displaying the time rate of change of pollutant concentrations, chemical reaction rates, etc.

1.2.2 Limitations

EKMA, and therefore OZIPP, is limited in applicability to ozone problems within or immediately downwind of large urban areas. Thus, the OZIPP is not applicable to the following situations:

- The rural ozone problem.
- Situations in which transported ozone and/or precursors are clearly dominant (i.e., a rural area downwind of a city).
- Cases in which the maximum ozone concentration occurs at night or in the early morning.
- Development of control strategies for single or small groups of emissions sources.

The validity of an ozone isopleth diagram generated by OZIPP for a particular city may be limited by the following properties:

- The kinetic mechanism used to describe the transformations of NMHC and NO_x.
- The physical assumptions used to formulate the model underlying the isopleths generated by OZIPP.
- The meteorological data and assumptions for specifying the parameters required to apply OZIPP.
- The availability and reliability of current NMHC, NO_x and ozone data.
- The mathematical assumptions needed to solve the differential equations formulated within OZIPP.
- The interpolations necessary to generate isopleths from the results of a number of computer simulations.

Because these factors are part of the basic definitions and concepts that constitute OZIPP and EKMA, they are explained more fully in the following sections.

1.3 BASIC DEFINITIONS AND CONCEPTS

1.3.1 Basic Definitions

- Kinetic Mechanism -- A kinetic mechanism is a set of chemical reactions and rate constants that is intended to describe some chemical process. From a kinetic mechanism, one can derive coupled, first-order, non-linear differential equations that describe the rates of change of pollutant concentrations with time. These equations can be solved using a computer to simulate the changing pollutant concentrations in a smog

chamber or in the atmosphere. The kinetic mechanism used in OZIPP was developed by Dodge[2] and is shown in Appendix A.

- Precursors of Ozone -- Precursors of ozone are the emitted chemical species that react to form ozone. The primary precursors are non-methane hydrocarbons and oxides of nitrogen. In OZIPP, non-methane hydrocarbons are represented by butane and propylene. Methane is not considered a precursor because it reacts very slowly. NO_x, as used in this report, signifies the sum of the concentrations of nitric oxide (NO) and nitrogen dioxide (NO_2).

- Simulation -- A computer simulation involves the calculation of the concentrations of pollutants included in the kinetic mechanism. Concentrations are calculated at various times beginning at 0800 Local Daylight Time (LDT) and ending at 1800 LDT. The calculations involve the integration of a set of coupled, first-order, non-linear, differential equations that describe the kinetic mechanism and the physical processes underlying the model. User specified assumptions about initial precursor concentrations, emission patterns, dilution, transported pollutants, reactivity and light intensity are incorporated in each simulation.

- Ozone Isopleth Diagram -- An ozone isopleth diagram as generated by OZIPP is illustrated in Figure 1-1. Each curved line in the diagram represents a constant maximum one-hour average ozone concentration. Thus, the NMHC and NO_x coordinates associated with any point on a single, curved line produce the same maximum concentration of ozone. In OZIPP, about 60 simulations are normally performed to produce such a diagram.

- Reactivity -- This is a property of the precursors that governs the rate of ozone production. The kinetic mechanism contained in OZIPP uses a mixture of propylene, which is very reactive, and n-butane, which is only marginally reactive, to represent the reactivity of the NMHC in an urban area.[2] Thus, propylene and n-butane are surrogates for the urban mixture of NMHC, with 100 percent propylene defining the highest possible reactivity and 100 percent n-butane the lowest.

- Default Values -- Certain parameters are necessary for running OZIPP. The default values are the values of these parameters that will be used unless other values are entered in the input data. For example, the default value for the highest initial NMHC concentration used in any simulation is 2.0 ppmC; if no number is entered in the input data for this parameter, OZIPP will use 2.0 ppmC by default. Running OZIPP with all of the default values will generate the standard isopleth diagram described in Reference 1.

- Diagram Point -- Any point on an ozone isopleth diagram generated by OZIPP has three parameters associated with it: an initial NMHC concentration, an initial NO_x concentration and a maximum one-hour average

ozone concentration corresponding to the initial NMHC and NO_x concentrations. A set of these three parameters is termed a diagram point. The ozone concentrations at some diagram points are determined from actual computer simulations (i.e., by solving the set of differential equations). The ozone concentrations at other diagram points are interpolated from the simulation diagram points. It is important to note that the NMHC and NO_x diagram points represent only the concentrations of these pollutants resulting from the city's emissions prior to the beginning of a simulation. The precursor concentrations associated with these diagram points do not include pollutant concentrations transported into the urban area, nor the pollutant concentrations resulting from emissions occurring after the beginning of the simulation. Thus, the diagram point precursor concentrations do not necessarily represent the absolute amounts of NMHC and NO_x that generated the ozone in a simulation. However, the ozone concentration associated with each diagram point includes the effects of all these factors.

- Spline Interpolation -- A spline interpolation is the use of a cubic polynomial or a hyperbolic function to interpolate ozone concentrations between diagram points for which ozone concentrations have been calculated by computer simulations. (Interpolation is used to reduce the number of computer simulations necessary to construct an isopleth diagram, and hence to reduce the cost of running OZIPP). Typically, the values of these spline functions and their first and second derivatives are matched at the calculated diagram points, resulting overall in one smooth line that passes through these points. A mechanical analogy of a spline function is a wire constrained to touch certain points. If the wire is pulled taut, it will bend at each point but be straight between points. If the tension is reduced, the wire will provide a smooth curve touching the points. The hyperbolic spline functions used to interpolate between calculated diagram points in OZIPP have an adjustable tension factor analogous to the tension on the wire. However, these interpolations are performed internally by the OZIPP, and normally there is no need for the user to be directly concerned with the spline functions.

1.3.2 Concepts

The physical model underlying the OZIPP is similar in concept to a trajectory-type photochemical model. A column of air consisting of initial concentrations of ozone and precursors is transported along an assumed trajectory. As the column moves, it can encounter fresh precursor emissions, which are assumed to be mixed uniformly within the column. The column is assumed to act like a large smog chamber in which the precursors react according to the kinetic mechanism in Appendix A to form ozone and other products. The column extends from the earth's surface to the base of an elevated inversion. The

diameter of the column is such that concentrations inside and just outside the column are similar, so that the horizontal exchange of air in and out of the column can be ignored. The volume of the column increases only as the inversion rises. Thus, the pollutants within the column are diluted as they are mixed with the air aloft. If the air aloft is polluted, the inversion rise also introduces ozone and precursors. The OZIPP mathematically simulates these physical and chemical processes.

As discussed in Section 1.2.1, the primary function of OZIPP is to generate an ozone isopleth diagram specific to a particular city. OZIPP operates in two stages. The first stage performs computer simulations to calculate maximum ozone concentrations as a function of initial NMHC and NO_x concentrations. The initial concentrations at which these simulations are performed are carefully selected in such a way as to favor accurate interpolation of the desired ozone isopleths. The first stage, which includes all of the computer simulations using the kinetic mechanism, is by far the most time-consuming part of OZIPP operations. In the second stage, interpolation schemes are used to determine the isopleth lines from the calculated diagram points and to draw the isopleth diagram that is OZIPP's major output.

1.4 SYSTEM DESCRIPTION

A schematic diagram of the OZIPP system is presented in Figure 1-2. Note that the off-line plotter is optional. The two major sections of the OZIPP program (i.e., the simulation section and the interpolation and plotting section) are described below.

1.4.1 Simulation Section

A schematic diagram of the simulation section is given in Figure 1-3. The input deck activates or suppresses various options in OZIPP and supplies city-specific input data to replace default values. The processor passes the data on sunlight intensity, dilution rate, reactivity of precursors, diurnal pattern of precursor emissions, and data on transported pollutants to the differential equation intergrator for use in the simulations. The information

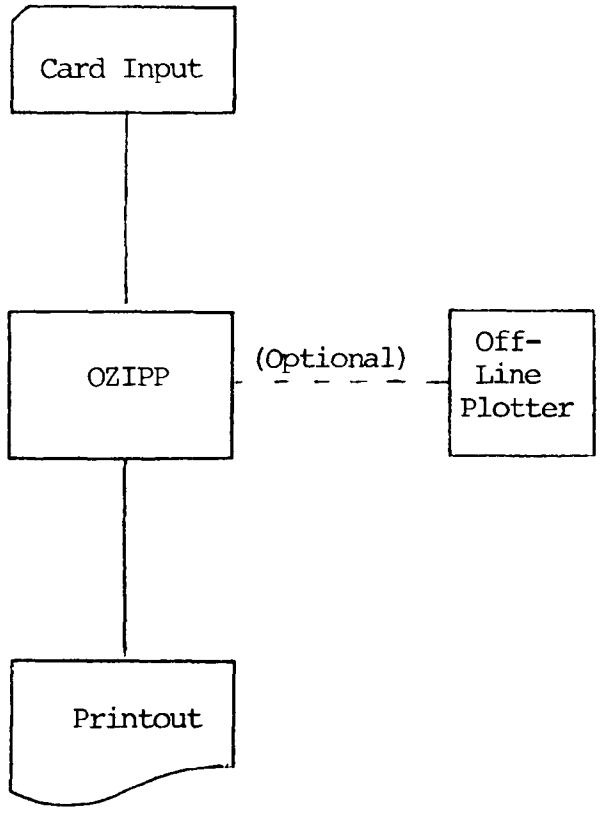

Figure 1-2. Schematic of OZIPP System

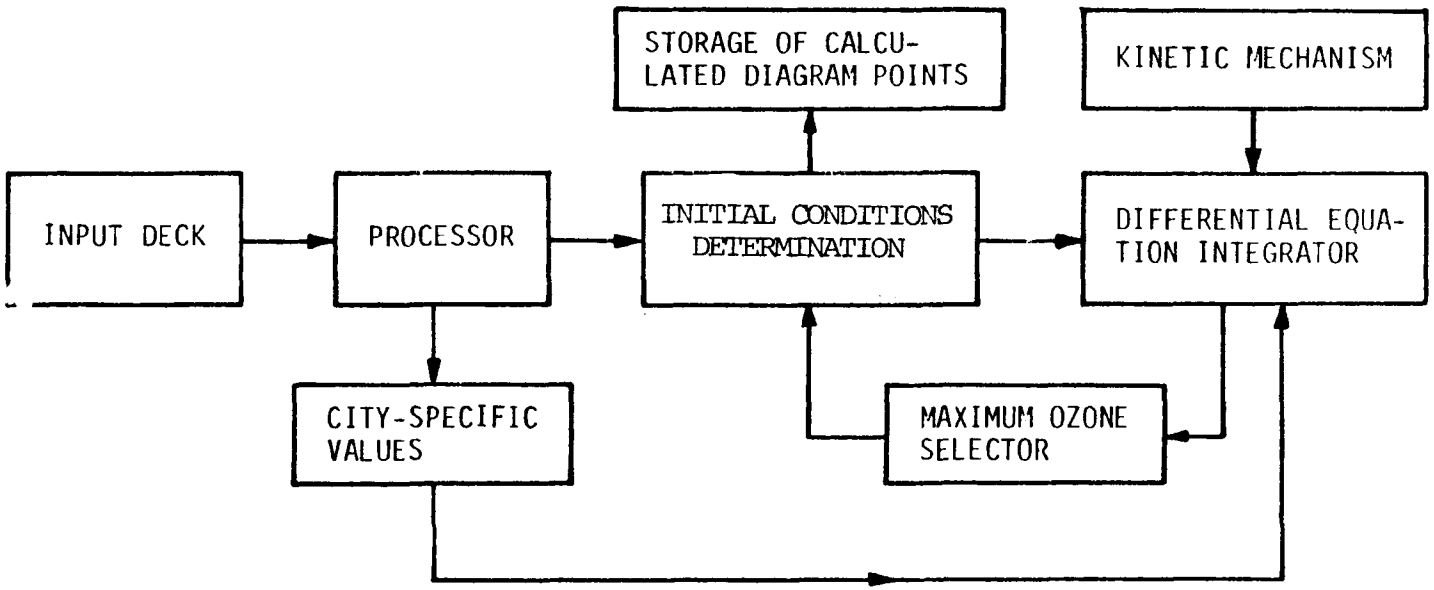

Figure 1-3. Schematic of Simulation Section

on OZIPP options (described in Chapter 3) is passed to the initial conditions determination subsection.

The initial conditions determination subsection directs the performance of the computer simulations used to construct an ozone isopleth diagram. More simulations may produce a more accurate isopleth diagram, but they increase the cost of running OZIPP. (The number of simulations performed can be varied by the user). The initial conditions determination subsection attempts to select simulations which will permit the optimal interpolation accuracy. It includes a feedback scheme, so that calculated diagram points can be used to determine NMHC and NO_x concentrations for subsequent simulations. For example, if the lowest ozone concentration for which an isopleth is to be drawn is 0.08 ppm, a diagram point with a maximum one-hour average ozone concentration of 0.04 ppm is not as valuable as a 0.08 ppm diagram point. The feedback scheme ensures that few simulations will be performed at NMHC and NO_x concentrations similar to those of a previously calculated diagram point, or at concentrations for which the calculated maximum one-hour average ozone concentration is likely to be very low.

After the selection of the NMHC and NO_x concentrations at which simulations are to be performed, the simulations are actually performed by the differential equation integrator. The set of first-order, differential equations is solved numerically. The differential equation integrator calculates the concentrations of 32 chemical species in the kinetic mechanism as a function of time during the simulation period. (The period from 0800 to 1800 LDT is simulated). The ozone concentrations are passed from the differential equation integrator to the maximum ozone selector, which determines the maximum one-hour average ozone concentration. This value is passed to the initial conditions determination subsection, which uses it and its associated NMHC and NO_x concentrations in choosing new NMHC and NO_x concentrations for the next simulation.

1.4.2 Interpolation and Plotting Section

After all simulations have been performed, the calculated diagram points are passed to the interpolation and plotting section (represented schematically

in Figure 1-4). In the first interpolation stage, spline interpolation is performed between the calculated diagram points to determine specific NMHC and NO_x concentrations corresponding to a specified ozone concentration (i.e., a level for which an isopleth is to be drawn). Unless the user directs otherwise, there are 11 specified ozone levels ranging from 0.08 to 0.40 ppm. The diagram points for the isopleths are then passed to the second interpolation stage, which uses the spline interpolation scheme to determine the final coordinates for the isopleth points. All coordinates are then passed to the plotting software for generation of the final ozone isopleth diagram.

1.5 SUMMARY OF INPUT DATA

For generation of the standard ozone isopleth diagram, city-specific values are not necessary. The default values in OZIPP will produce the standard diagram. (The default values are given in Section 3.1). The more city-specific values the user substitutes for default values, the more city-specific the ozone isopleth diagram produced by OZIPP will be. Values of the city-specific parameters that can be input to OZIPP include the following:

- Latitude
- Longitude
- Time Zone
- Date
- Morning and afternoon inversion heights (also called mixing depths)
- Times at which the inversion starts and stops rising
- Concentrations of NMHC, NO_x and ozone in the air above the inversion layer due to transport aloft
- Concentrations of NMHC, NO_x and ozone transported in the surface layer from upwind of the city
- NMHC and NO_x emissions after 0800 LDT
- NMHC reactivity
- Initial ratio of aldehydes to NMHC
- NO_x reactivity (initial fraction of NO_x that is NO_2).

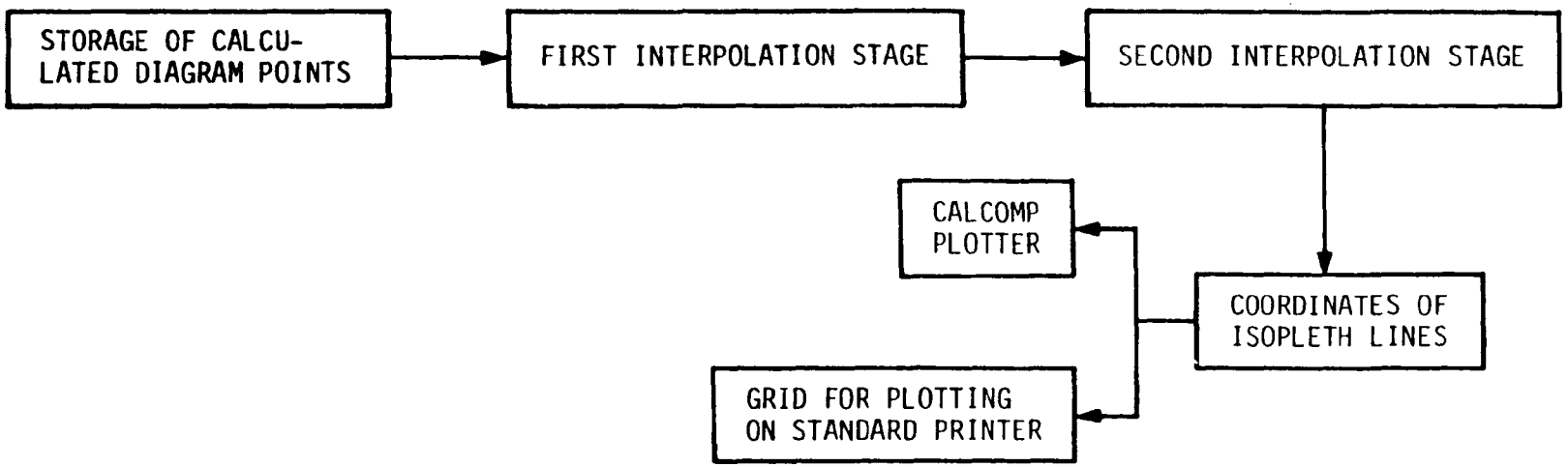

Figure 1-4. Schematic of Interpolation and Plotting Section

The sources of values for the parameters in this list and the uses of those parameters in OZIPP are discussed in Chapter 3 and 5.

In addition to city-specific values, OZIPP provides the options of changing several parameters to control its operation. For example, the user can select the number of simulations performed in each OZIPP run, the error tolerance in the differential equation integrator and the form of the output. These input data and options are also described in Chapter 3.

1.6 OUTPUT

As previously described, the major function of OZIPP is to produce a city-specific ozone isopleth diagram. The output includes a table summarizing the simulation conditions, a table summarizing the results of each simulation performed, and a line-printer plot of the isopleth diagram. A diagram produced by an off-line plotter (such as CALCOMP) is optional. Under another OZIPP option, a single simulation is performed and the results of that simulation alone are presented. The user also has the option to obtain detailed information for the simulation (e.g., concentrations of all species, rates of reactions, etc.). Examples of OZIPP output are presented in Chapter 5.

2.0 TECHNICAL DISCUSSION

OZIPP is designed to simulate ozone formation in urban atmospheres. As discussed in Chapter 1, it consists of two distinct parts. The first part, a kinetics model, mathematically simulates the physical and chemical processes taking place in the atmosphere. The second part, the ozone isopleth plotting package, uses the simulation results to construct an ozone isopleth diagram. This chapter describes the conceptual basis for the kinetics model, the mathematical techniques used in performing a simulation, and the procedures used to generate an ozone isopleth diagram from simulation results.

The descriptions in this chapter are very detailed. Potential users of OZIPP may wish to read the remaining chapters and perhaps run OZIPP once, before reading this chapter.

2.1 CONCEPTUAL BASIS FOR THE OZIPP KINETICS MODEL

As previously described, the physical model underlying the kinetics model in OZIPP is similar in concept to a trajectory-type photochemical model. In the kinetics model, a column of air transported along an assumed trajectory is modeled. The column is assumed to extend from the earth's surface to the base of a temperature inversion. The horizontal dimensions of this column are such that the concentration gradients are small. This makes it unnecessary to consider horizontal exchange of air between the column and its surroundings. The air within the column is assumed to be uniformly mixed at all times.

At the beginning of a simulation, the column is assumed to contain some specified initial concentrations of NMHC and NO_x due to prior emissions. The column may also contain NMHC and NO_x that were transported with the column from areas upwind of the city being considered. These pollutants, sometimes called background, are in this report termed pollutants "transported in the surface layer." As the column moves along the assumed trajectory, the height of the column can change because of temporal and spatial variations in mixing height. The height of the column is assumed to change exponentially with time during a user selected period, and to be constant before and after that period.

As the height of the column increases, its volume increases, and air above the inversion layer is mixed in. Pollutants in the inversion layer are described as "transported above the surface layer" or "transported aloft" in this report. Any ozone or ozone precursors from the inversion layer that are mixed into the column as it expands are assumed to be immediately mixed uniformly throughout the column.

The kinetics model in OZIPP can also consider emissions of NMHC and NO_x into the column as it moves along its trajectory. The concentrations of the species within the column are physically decreased by dilution due to the inversion rise, and physically increased by entrainment of pollutants transported aloft and by fresh emissions. All species react chemically according to the kinetic mechanism shown in Appendix A. Certain photolysis rates within that mechanism are functions of the intensity and spectral distribution of sunlight, and they vary diurnally according to time of year and location.

The assumptions and specifications that describe the kinetics model are:

- The air mass of interest is an imaginary air parcel (column) of fixed horizontal area at a constant temperature, within which pollutants are well mixed.
- There is sufficient homogeneity that horizontal diffusion does not affect pollutant concentrations within the column.
- The height of the column varies exponentially with time during a specified period and is constant at other times (an exponential variation is equivalent to a constant percentage dilution per unit time).
- The column contains specified initial concentrations of NMHC and NO_x due to emissions prior to the simulation starting time within the urban area of interest. (These concentrations are shown on the NMHC and NO_x scales of the resulting ozone isopleth diagram). The NMHC is assumed to be 25 percent propylene and 75 percent n-butane, unless changed by the user. Five percent of the initial NMHC concentration is added as aldehydes, unless changed by the user.
- Pollutants transported within the surface layer from outside the urban area of interest (sometimes called background) may be present in the column at the start of each simulation (0800 LDT). The pollutant concentrations due to transport in

the surface layer are normally assumed to be zero, but the user may specify other values for the NMHC, NO_x and ozone concentrations transported within this layer. The NMHC transported within the surface layer is assumed to be 10 percent propylene and 90 percent butane (as carbon). The NO_x transported in the surface layer is assumed to be 100 percent NO_2.

- The initial concentrations in the column are thus the sum of the contributions from emissions occurring prior to 0800 LDT plus concentrations transported in the surface layer from upwind locations. Emitted species include propylene, n-butane, NO, NO_2, acetaldehyde and formaldehyde. Transported species include propylene, n-butane, NO_2 and ozone.

- The changes in pollutant concentrations within the column are calculated, by computer simulation, from 0800 to 1800 LDT. The chemical reactions involving these pollutants are listed in Appendix A.

- Entrainment of pollutants transported aloft is possible during the rise of the inversion layer. OZIPP only permits entrainment of constant concentrations of NMHC, NO_x and ozone. NMHC in pollutants transported aloft is assumed to be 10 percent propylene and 90 percent n-butane (as carbon). No acetaldehyde or formaldehyde is added. NO_x transported aloft is assumed to be 100 percent NO_2.

- Pollutants emitted into the column after 0800 LDT can be represented by specifying additions of NMHC and NO_x each hour. The assumptions about the propylene/n-butane and the aldehyde additions are the same as for the initial condition assumptions. The fraction of NO_x that is NO_2, however, is 10 percent for post-0800 emissions.

- The rate constants of all chemical reactions in the kinetic mechanism are as shown in Appendix A, except for the photolysis reactions. Photolytic rate constants vary according to the time of day, date and location being simulated. (Default photolysis rate constants are intended to represent the period from 0800 to 1800 PDT on the summer solstice in Los Angeles).

- Zero cloud cover is assumed.

Other assumptions relating to the use of EKMA to predict control requirements or changes in urban ozone concentrations as a result of changes in precursor emissions are discussed elsewhere.[1,3,4]

2.2 DESCRIPTION OF A SINGLE SIMULATION

This section describes in considerable detail the mathematical procedures used in OZIPP to calculate the maximum one-hour average ozone concentration that results from given initial concentrations of NMHC and NO_x. The procedures are based on the physical and chemical processes described in the last section. Before the beginning of a simulation, data preparation steps are performed. A simulation is conducted by first determining concentrations at 0800 LDT and then numerically integrating the equations that form the basis of the model. The numerical solution yields species concentration as a function of time between 0800 and 1800 LDT. The following discussion describes the data preparation steps, the calculation of initial concentrations, model formulation and the numerical integration technique.

2.2.1 Data Preparation Steps

Because all simulations performed by OZIPP in generating an ozone isopleth diagram have identical conditions except for the initial NMHC and NO_x concentrations, a data preparation step is performed before a simulation is commenced. The purpose of this step is to eliminate abrupt changes in photolytic rate constants and post-0800 emission rates. Elimination of these abrupt changes (i.e., discontinuities) is desirable for three reasons:

- The integration scheme requires less computer time (discontinuities require the use of small time steps).
- The results are more accurate numerically (stepping past discontinuities can lead to error).
- The atmosphere does not normally have discontinuities. (The simulation of intermittent cloud cover or sudden changes in emissions is outside the scope of OZIPP).

The photolytic rate constants are evaluated every hour using an algorithm developed by Schere and Demerjian.[5] The algorithm uses input data of latitude, longitude, time zone and date to calculate photolytic constants. A set of third-order polynomial spline functions is then generated so that photolytic constants can be easily calculated from a smooth curve for any time of the

day. A set of four coefficients for each of the eight photolytic rate constants in the kinetic mechanism shown in Appendix A is prepared for each hour of the ten-hour simulation period. Thus, at any time during the simulation period, the photolytic rate constants can be calculated from a simple third-order polynomial equation.

If post-0800 emissions are to be considered, it is necessary to specify the emission rate(s) of NMHC and/or NO_x injected into the column each hour after the 0800 simulation start time. These emission rates are expressed as fractions of the initial NMHC and/or NO_x concentrations. They represent the ratio of emissions injected into the column during the specified hour after 0800 to the emissions injected into the air column prior to the beginning of the simulation. A set of cubic spline coefficients is determined each hour so that the instantaneous emission rate(s) can be evaluated for any time during the simulation period. For the first hour, a straight line is used, and for each subsequent hour a simple cubic (or lower order) polynomial is used subject to the following limitations:

- The total, or integrated, emissions for each hour must equal the input value.
- The spline functions at each hour must match in value, slope and curvature unless lower order functions are used.
- At the end of the last hour of post-0800 emissions, the emissions must be zero with zero curvature.
- If cubic splines lead to any minima (points of zero slope) which are less than zero, then a lower order spline function is used for that hour.

2.2.2 Determination of Initial Concentrations

Before a simulation can begin, the concentrations of all pollutant species at 0800 LDT must be determined. These initial concentrations are based on assumed initial concentrations of NMHC and NO_x and on the concentrations of pollutants transported in the surface layer. The concentrations of transported pollutants are assumed to be zero unless otherwise specified. If only a single simulation is being performed, the initial concentrations of

NMHC and NO_x must be input to OZIPP. However, if an ozone isopleth diagram is being generated, the initial NMHC and NO_x concentrations are determined internally by OZIPP. This procedure is discussed in Section 2.3.

The concentrations of all but seven species in the kinetic mechanism are initially zero. The concentrations of the other seven species (NO_2, NO, O_3, propylene, n-butane, formaldehyde and acetaldehyde) are calculated as described below.

1. NO_2 is set to the initial NO_x concentration times the NO_2/NO_x fraction (default is 0.25), plus any NO_2 transported in the surface layer.

2. NO is set to the initial NO_x concentration times the quantity one minus the NO_2/NO_x fraction. The NO_x transported in the surface layer is assumed to have zero NO.

3. O_3 is set to the concentration transported in the surface layer (default is zero).

4. The concentration of propylene is determined from the assumed initial NMHC concentration, the assumed reactivity fraction and the NMHC transported in the surface layer. Mathematically,

$$[C_3H_6]_o = \frac{1}{3}\left\{[NMHC]_o\,(R_1)+[NMHC]_{ts}(0.1)\right\} \qquad (1)$$

where

$[C_3H_6]_o$ = initial propylene concentration, ppm

$[NMHC]_o$ = initial NMHC concentration, ppmC

R_1 = fraction of initial NMHC that is assumed to be propylene (Default = 0.25)

$[NMHC]_{ts}$ = NMHC concentration transported in the surface layer, ppmC

In equation (1), NMHC transported in the surface layer is assumed to be 10 percent propylene. Multiplication by the fraction $\frac{1}{3}$ converts ppmC to ppm (i.e., there are three carbon atoms per molecule of propylene).

5. The initial concentration of n-butane is determined in a manner similar to the initial propylene fraction.

$$[n\text{-}C_4H_{10}]_o = \frac{1}{4}\left\{[NMHC]_o\ (1-R_1)+[NMHC]_{ts}(0.9)\right\} \qquad (2)$$

where

$[n\text{-}C_4H_{10}]_o$ = initial concentration of n-butane, ppm

$(1-R_1)$ = fraction of initial NMHC concentration assumed to be n-butane (Default = 0.75)

and $[NMHC]_o$ and $[NMHC]_{ts}$ have the same meaning as in Equation (1).

Note that 90 percent of the NMHC transported in the surface layer is assumed to be n-butane. Once again the multiplication by the fraction $\frac{1}{4}$ is necessary to convert from ppmC to ppm.

6. Formaldehyde is initialized according to the initial NMHC concentration and an aldehyde addition factor.

$$[HCHO]_o = [NMHC]_o\ (0.4)\ (R_2) \qquad (3)$$

where

$[HCHO]_o$ = initial formaldehyde concentration, ppm

$[NMHC]_o$ = initial NMHC concentration, ppmC

R_2 = fraction of initial NMHC concentration that is to be added as aldehyde (Default = .05)

The fraction of aldehydes assumed to be formaldehyde is fixed at 0.4.

7. Acetaldehyde is initialized similarly to formaldehyde:

$$[CH_3CHO]_o = \frac{1}{2}\ [NMHC]_o\ (0.6)\ (R_2) \qquad (4)$$

where

$[CH_3CHO]_o$ = initial acetaldehyde concentration, ppm

$[NMHC]_o$ = initial NMHC concentration, ppmC

R_2 = fraction of initial NMHC concentration to be added as aldehydes

Note that the fraction of aldehyde assumed to be acetaldehyde is fixed at 0.6. Multiplication by $\frac{1}{2}$ converts ppmC to ppm.

2.2.3 Mathematical Formulation of Kinetics Model

The kinetics model in OZIPP mathematically simulates physical and chemical processes taking place in the atmosphere. This is accomplished by solving numerically a system of ordinary, non-linear differential equations that describe the effects of these processes on pollutant concentrations. The solution gives the concentration of pollutants as a function of time. The mathematical formulation of the system of differential equations is described in this section.

In OZIPP, there are four processes that are assumed to effect pollutant concentrations:

1) Chemical Reactions
2) Dilution
3) Entrainment of Pollutants Transported Aloft
4) Post-0800 Emissions

Differential equations have been formulated to describe the time rate of change of pollutant concentrations due to each process, and these are presented below. The total time rate of change of each pollutant's concentration is then simply equal to the sum of all these effects. Thus, the system of equations consists of one equation for each species in the kinetic mechanism shown in Appendix A. In OZIPP, however, all equations for species that appear only as products of chemical reactions have been eliminated because of computational considerations. Consequently, the set of equations solved in OZIPP is made up of 32 equations, one for each pollutant appearing as a reactant in any of the 76 reactions in the mechanism.

A. Chemical Reaction Effects

The change in pollutant concentration due to chemical reaction is a function of the rates of the chemical reactions in Appendix A. The rate of each reaction is the product of a rate constant and a concentration term. The rate constants for the non-photolytic reactions are shown in Appendix A. The photolytic rate constants are calculated by the procedures described in Section 2.2.1. The concentration term for unimolecular or psuedo-first-order

reactions (such as photolytic reactions) is simply the concentration of the reactant. Bi-molecular reaction rates are calculated similarly, except the concentration term is the product of the two reactant concentrations. For example, the reaction rate (RT) for the first reaction in Appendix A would be expressed as follows:

$$(RT)_1 = k_1 C_{NO_2} \quad (5)$$

where

$(RT)_1$ = rate of reaction (1), ppm min^{-1}

k_1 = photolytic rate constant for reaction (1)

C_{NO_2} = concentration of NO_2, ppm

The time rate of change of a species due to chemical reaction is simply equal to the sum of all rates for those reactions in which the species is a product minus the sum of the rates for those reactions in which the species is a reactant. Thus,

$$\left(\frac{\Delta C_i}{\Delta t}\right)_R = \Sigma\ (RT)_{PROD} - \Sigma\ (RT)_{REAC} \quad (6)$$

where

$\left(\frac{\Delta C_i}{\Delta t}\right)_R$ = reaction rate contribution to the time rate of change of species i

$\Sigma(RT)_{PROD}$ = the sum of all reaction rates in which species i appears as a product

$\Sigma(RT)_{REAC}$ = the sum of all reaction rates in which species i appears as a reactant

B. Dilution Effects

The mathematical representation for simple dilution due to inversion rise is a first-order decay process. The rate of change due to this effect can be represented as follows:

$$\left(\frac{\Delta C_i}{\Delta t}\right)_D = -DC_i \qquad (7)$$

where

$\left(\frac{\Delta C_i}{\Delta t}\right)_D$ = dilution effect contribution to the time rate of change of pollutant species i, ppm min^{-1}

D = dilution factor, min^{-1}

C_i = concentration of species i, ppm

The dilution factor is calculated from the following equation:

$$D = \frac{\ln(Z_2/Z_1)}{\Delta t} \qquad (8)$$

where

D = dilution factor, min^{-1}

Z_2 = afternoon mixing height

Z_1 = morning mixing height

Δt = total time during which the inversion rise takes place, minutes

Note that, before and after the inversion rise period, the dilution factor is zero since there are no dilution effects for those periods.

C. Entrainment Effects

There are only four species subject to being entrained from pollutants transported aloft: propylene, n-butane, ozone and NO_2. The mathematical treatment of entrainment assumes that the concentrations aloft do not change with time and extend uniformly to at least the height of afternoon mixed layer. The pollutants entrained are assumed to be instantaneously mixed within the enlarged surface layer. The mathematical expressions for the rates of change for the four pollutants are shown below:

$$\left(\frac{\Delta C_{O_3}}{\Delta t}\right)_{AL} = D(C_{O_3})_{AL} \quad (9)$$

$$\left(\frac{\Delta C_{NO_2}}{\Delta t}\right)_{AL} = D(C_{NO_2})_{AL} \quad (10)$$

$$\left(\frac{\Delta C_{C_3H_6}}{\Delta t}\right)_{AL} = \frac{1}{3} D(0.1)(C_{NMHC})_{AL} \quad (11)$$

$$\left(\frac{\Delta C_{n\text{-}C_4H_{10}}}{\Delta t}\right)_{AL} = \frac{1}{4} D(0.9)(C_{NMHC})_{AL} \quad (12)$$

where

$\left(\frac{\Delta C_{O_3}}{\Delta t}\right)_{AL}$, $\left(\frac{\Delta C_{NO_2}}{\Delta t}\right)_{AL}$, $\left(\frac{\Delta C_{C_3H_6}}{\Delta t}\right)_{AL}$, $\left(\frac{\Delta C_{n\text{-}C_4H_{10}}}{\Delta t}\right)_{AL}$ =

entrainment effect contribution to the time rates of change of ozone, nitrogen dioxide, propylene, and n-butane concentrations, respectively ppm min^{-1}

D = dilution factor (i.e., the rate constant for the mixing height rise), min^{-1}

$(C_{O_3})_{AL}$ = concentration of ozone trapped aloft, ppm

$(C_{NO_2})_{AL}$ = concentration of NO_2 trapped aloft, ppm

$(C_{NMHC})_{AL}$ = concentration of total non-methane hydrocarbon trapped aloft, ppmC

C_{O_3}, C_{NO_2}, $C_{C_3H_6}$, $C_{n\text{-}C_4H_{10}}$ =

concentrations of ozone, nitrogen dioxide, propylene, and n-butane, respectively, in the mixed layer, ppm

The numerical constants (i.e., 0.1, $\frac{1}{3}$, 0.9, and $\frac{1}{4}$) in Equations 11 and 12 result from the fixed assumptions about the reactivity of the hydrocarbon mix trapped aloft (i.e., 10 percent of the NMHC is assumed propylene) and from the conversion of ppmC to ppm. It should be noted that the effect of the change in mixing height is the sum of the dilution and the entrainment effects.

E. Post-0800 Emissions Effect

The fourth factor affecting the rate of change of pollutant concentration is post-0800 emissions. The rates of change due to post-0800 emissions are equal to the additional concentrations produced by the emissions. However, recall that the post-0800 emissions are expressed relative to the pre-0800 emissions. For example, for a simulation in which the initial concentration of NO_x due to pre-0800 emissions is 1.0 ppm, and the emissions that occur between 0800 and 0900 are 20% of the pre-0800 emissions, an addition of 0.20 ppm NO_x will occur over the first hour.

Because equivalent emissions into different volumes will produce different concentrations, it is necessary to adjust the relative emissions to reflect the change in the column volumes due to the inversion rise. This is done internally by OZIPP by first calculating the ratio of the 0800 LDT inversion height to the current inversion height. (This is equivalent to the ratio of initial volume to the current volume). Before the inversion rise begins, this ratio is simply one. After the inversion rise has ceased, the ratio is the 0800 mixing height divided by the final mixing height. For the period during which the inversion rises, the ratio (f_t) is calculated as follows:

$$f_t = \exp[-(D)(\Delta t)] \qquad (13)$$

where

f_t = ratio of the 0800 LDT mixing height to the mixing height at time t

D = dilution factor (i.e., the rate constant for the mixing height rise, min^{-1})

Δt = elapsed time between the start of the mixing height rise and the current time, minutes.

The rates of change due to the post-0800 emissions are calculated from the values of the emission rates (calculated using the polynomial spline functions described earlier), the f_t ratio described above, the initial pollutant concentrations and the reactivity assumptions. The equations for the

rates of change due to post-0800 emissions for each of the six affected species are shown below:

$$\left(\frac{\Delta C_{NO_2}}{\Delta t}\right)_E = 0.1\ f_t\ (E_{NO_x})_t\ [NO_x]_o \quad (14)$$

$$\left(\frac{\Delta C_{NO}}{\Delta t}\right)_E = 0.9\ f_t\ (E_{NO_x})_t\ [NO_x]_o \quad (15)$$

$$\left(\frac{\Delta C_{C_3H_6}}{\Delta t}\right)_E = \frac{1}{3}\ f_t\ (E_{NMHC})_t\ (R_1)\ [NMHC]_o \quad (16)$$

$$\left(\frac{\Delta C_{n\text{-}C_4H_{10}}}{\Delta t}\right)_E = \frac{1}{4}\ f_t\ (E_{NMHC})_t\ (1\text{-}R_1)\ [NMHC]_o \quad (17)$$

$$\left(\frac{\Delta C_{HCHO}}{\Delta t}\right)_E = 0.4\ f_t\ (E_{NMHC})_t\ (R_2)\ [NMHC]_o \quad (18)$$

$$\left(\frac{\Delta C_{CH_3CHO}}{\Delta t}\right)_E = \frac{1}{2}\ (0.6)\ f_t\ (E_{NMHC})_t\ (R_2)\ [NMHC]_o \quad (19)$$

where

$(\quad)_E$ = post-0800 emissions contribution to the rates of change of NO_2, NO, propylene, n-butane, formaldehyde and acetaldehyde, ppm min^{-1}

f_t = defined above (Eq. 13)

$(E_{NO_x})_t$ = value of post-0800 relative NO_x emission rate, fraction per minute

$(E_{NMHC})_t$ = same as above except for NMHC emissions

$[NO_x]_o$ = initial NO_x concentration due to pre-0800 emissions, ppm

$[NMHC]_o$ = initial NMHC concentration due to pre-0800 emissions, ppmC

R_1 = fraction of initial NMHC (in ppmC) assumed to be propylene

R_2 = fraction of initial NMHC (in ppmC) concentration to be added as aldehydes

Note that, in the above formulations, a conversion from ppmC to ppm is performed and that the aldehydes are assumed to be 40 % formaldehyde and 60 % acetaldehyde.

2.2.4 Description of Numerical Integration

The kinetics model in OZIPP employs a Gear-type integration scheme to numerically solve the set of differential equations described in the previous section. A detailed description is not given here because the method is not unique to OZIPP, and the procedure has been described elsewhere.[6,7,8] The integration scheme initially uses a time step of 1×10^{-10} minutes (i.e., pollutant concentrations are to be calculated 1×10^{-10} minutes after the 0800 LDT start time). Subsequent time steps are computed by the Gear-type integration scheme according to the estimated error at each step. However, since the onset and cessation of dilution represent changing conditions, it is necessary for maximal numerical accuracy to begin or end a time step at precisely these points (i.e., the times at which onset and cessation of dilution take place). The pollutant concentrations are calculated at each time step throughout the ten-hour simulation period. (Once the time reaches ten hours, there is no restriction on precisely matching the final time step, since the concentrations can be interpolated back to exactly the tenth hour). A typical simulation in OZIPP takes between 150 and 200 time steps, with about one half of these used in simulating the first minute.

The total rate of change of any species is the sum of the rates of change due to dilution, entrainment, post-0800 emission and chemical reaction described above. At each time step, the concentrations of all species are calculated along with the current rates of change for each species. The Gear method utilizes a Taylor series polynomial for each species to predict the species concentration at the end of the time step. The order of the polynomial is varied internally for optimum efficiency and is based on the values at the beginning of the time step. A corrector scheme then "corrects" the new concentration values, updates the Taylor polynomials and estimates the average error. The corrector is a set of linear equations based on a matrix whose elements are the set of partial derivatives of the rate of change of concentrations of each species with respect to all other species. OZIPP utilizes a

linear system solving package for sparse matrices (i.e., those matrices in which most elements are equal to zero). The integration method used in this step has been modified somewhat from the version published in Reference 7. In particular, the error estimation is done relative to the current concentration of a species rather than to its maximum concentration. The method utilizes the error estimate to determine the optimum step size and order, so that the allowable error specified by the user is met with the minimum number of integration steps. For a more detailed discussion of the numerical integration scheme, the user is referred to References 6, 7 and 8.

The final task performed by the differential equations integrator is the calculation of the maximum one-hour average ozone concentration. Ozone concentrations are calculated for precisely every minute of the 10-hour simulation. This calculation is performed by interpolation between the time step solutions to the differential equations. Running one-hour average concentrations are calculated using Simpson's rule. The largest one-hour average concentration is then selected as the maximum.

2.3 SELECTION OF SIMULATIONS FOR GENERATION OF ISOPLETH DIAGRAMS

When generating an ozone isopleth diagram, the initial NMHC and NO_x concentrations for each simulation performed by OZIPP are selected in the initial conditions determination subsection (see Figure 1-3). The function of this subsection is to control the selection of initial NMHC and NO_x concentrations in order to obtain as accurate an isopleth diagram as possible from the number of simulations specified. This is accomplished by:

- Performing few simulations for which the maximum one-hour average ozone concentration is below the lowest isopleth to be plotted.

- Minimizing the interpolation error between simulation points when constructing the ozone diagram.

Simulations are first performed at six individual points along the edges of the diagram. Based on these results, simulations are then performed

at points along lines of constant NMHC/NO_x ratio (i.e., a radial line emanating from the origin). The user can control the number of radial lines to be considered and the number of points on each radial line. Normally (i.e., under default conditions), simulations are performed at five points along each of 11 radials. Finally, two more simulations are performed for individual points on the edges of the diagram to aid in plotting the lowest valued isopleth. In all, 62 simulations are performed under default conditions.

2.3.1 Selection of Individual Points

The first step in the initial conditions determination subsection is to call for four simulations at initial NMHC and NO_x concentrations corresponding to the four corners of the isopleth diagram as shown by points 1 through 4 in Figure 2-1. (Note that the user specifies the maximum NMHC and NO_x concentrations to be used). Next, two simulations (at points 5 and 6) are performed to estimate where the lowest valued ozone isopleth will intersect the diagram edges. The initial conditions for point 5 are determined by using the maximum NO_x value and an NMHC concentration calculated by the following equation:

$$(C_{NMHC})_5 = \frac{(C_{O_3})_{LL} - (C_{O_3})_2}{(C_{O_3})_3 - (C_{O_3})_2} (C_{NMHC})_{MAX} \quad (20)$$

where

$(C_{NMHC})_5$ = NMHC concentration at point 5

$(C_{O_3})_2$ = O_3 concentration at point 2

$(C_{O_3})_3$ = O_3 concentration at point 3

$(C_{O_3})_{LL}$ = The lowest ozone value to be plotted as an isopleth

$(C_{NMHC})_{MAX}$ = Maximum NMHC concentration on the diagram

Thus, the coordinates of point 5 are calculated according to the assumption that, at constant initial NO_x concentration, the maximum one-hour average ozone concentration is proportional to the initial NMHC concentration. This

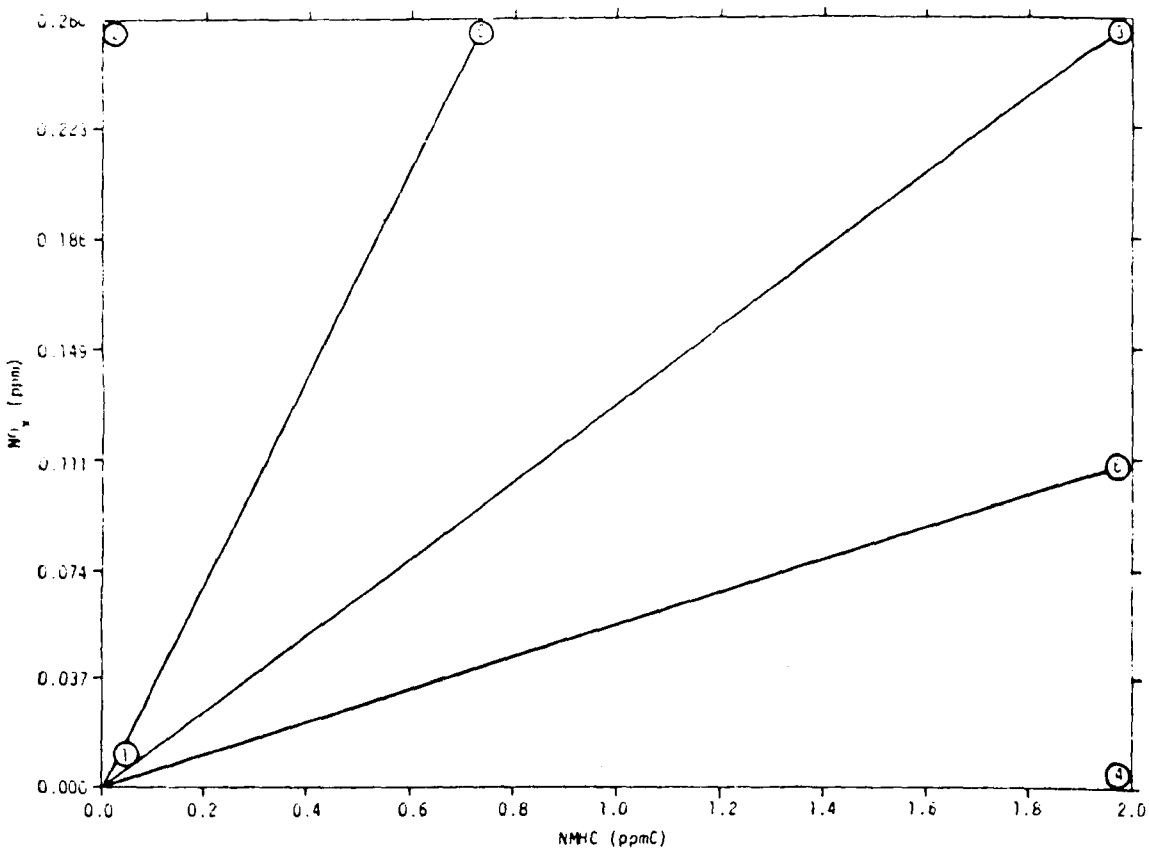

Figure 2-1. Initial Simulation Points

assumption of linearity is generally not true, but the results are used in the next to last simulation in order to calculate a more accurate location. An analogous procedure is performed for the right side of the diagram.

2.3.2 Selection of Radials and Points Along Radials

After the simulations are completed for points 1-6, the initial conditions determination subsection directs the simulations at various points along selected radial lines (i.e., lines of constant NMHC to NO_x ratio). The radial lines are used for the following reasons:

- Because most isopleths are roughly L-shaped, simulations at points on radial lines provide the highest density of simulation results near the region of highest curvature.
- Simplified theoretical considerations and empirical evidence show that along any radial line, it is easy to interpolate the maximum one-hour average ozone concentrations as a function of distance from the origin of the isopleth diagram. Typically, these functions are nearly linear at low to intermediate ozone concentrations (e.g., 0.04 to 0.2 ppm ozone) and second order at high concentrations ($\geq$0.5 ppm ozone). At the very lowest concentrations, various effects can lead to non-linear behavior, but the functions needed to interpolate along the main part of the radial lines have few inflection points, and therefore the interpolations should have high accuracy.

The first ratio determined corresponds to the diagonal line from the origin of the diagram to the opposite corner (i.e., the point of maximum NMHC and NO_x concentration). Simulations are then performed at various points along that diagonal (the user controls the number of points). The points on the radial are determined by estimating the locations of ozone concentrations along the line. The procedure begins with finding the ozone concentrations that form a geometric progression from the lowest ozone concentration to be plotted (e.g., 0.08 ppm) to the maximum ozone concentration at the terminal point of the radial. A geometric progression gives the minimum relative change in ozone concentration from one point to another. The algorithm is built on the general assumption that the accuracy of the interpolation will be optimized if the relative change in ozone concentration between interpolation points is minimized.

To illustrate the procedure, assume that five simulations are to be performed along the diagonal radial. (Recall that the user can change the actual number of simulation points along the radial). Further, assume that the lowest ozone isopleth to be plotted is 0.08 ppm and that the concentrations of NMHC, NO_x and ozone at the terminal point of the radial are 2.0 ppmC, 0.28 ppm and 0.449 ppm, respectively. In general, the expression for the nth term of a geometric progression is:

$$a_n = a_1 r^{n-1} \qquad (21)$$

where

a_1 = the first term

r = the common factor

n = the number of terms

For the example problem, the geometric progression would be:

0.08, 0.12, 0.19, 0.29, 0.449

The common factor (r) was calculated as shown below:

$$r = (0.449/0.08)^{1/4} = 1.54$$

After determining the progression, the next step in the procedure is to estimate the NMHC and NO_x concentrations corresponding to the second highest ozone concentration in the progression (i.e., the first point along the radial below the terminal point). Linear interpolation is used in the following equation to estimate the NMHC concentration associated with this point.

$$(C_{NMHC})_P = (C_{NMHC})_{MAX} \frac{(C_{O_3})_P - (C_{O_3})_1}{(C_{O_3})_{MAX} - (C_{O_3})_1} \qquad (22)$$

where

$(C_{NMHC})_P$ = the NMHC concentration associated with the point

$(C_{O_3})_P$ = the projected ozone concentration associated with the point

$(C_{O_3})_{MAX}$ = the highest ozone concentration in the progression

$(C_{O_3})_1$ = the ozone concentration at point 1

For the example, the NMHC concentration corresponding to the projected 0.29 ppm ozone concentration is 1.30 ppmC. Because the NMHC/NO_x ratio is constant at 7.14 along the line, the associated NO_x concentration is 0.18 ppm. Thus, a simulation is performed with NMHC and NO_x initial conditions of 1.30 ppmC and 0.18 ppm, respectively.

The procedure for determining the locations of subsequent points along the radial is slightly different from the one described above. First, the original geometric progression is updated, using the latest actual simulation result. In the example, the simulation result for the projected 0.29 point was actually 0.34 ppm, so the new progression becomes

.08, .13, 0.21, 0.34

with a new constant factor equal to 1.62. The problem is now one of estimating the location of the 0.21 ozone concentration on the radial. Once again, Equation 22 is used to predict the NMHC concentration associated with the projected 0.21 ozone concentration. However, because two interpolations fairly near each other have been completed (i.e., those giving ozone concentrations of 0.449 and 0.34), a linear extrapolation using these two points is performed to obtain a second estimate. These two estimates are then averaged to obtain the final NMHC value for simulation. This procedure (i.e., new progression, estimation by linear interpolation, estimation by extrapolation, and averaging of the two estimations) is repeated for each point except the last (i.e., the 0.08 point in the example). For this final estimation, a hyperbolic spline interpolation algorithm is employed.

Once all the simulations have been performed for all points on a radial, a new radial is chosen and the procedure repeated. New radials are selected by estimating the location of the terminal points along the top or right edge of the diagram. The scheme for locating the terminal points is essentially identical to the one used in determining the points along the radial. An even distribution of the radial lines is important for obtaining accurate isopleth diagrams. Points too close to each other can introduce erroneous, high-frequency oscillations in the spline interpolations because of errors in the integration scheme. Points too far apart on the isopleth diagram itself leave

large areas on the diagram in which no simulations have been performed. The initial conditions subsection contains internal tests on the termination points of the radial lines to avoid these difficulties.

2.4 INTERPOLATION AND PLOTTING OF ISOPLETH DIAGRAM

The interpolation and plotting section directs the construction of the ozone isopleth diagram using the results of previous simulations. Interpolation is done with hyperbolic splines rather than with classical polynomial types, because kinetic systems lead to curves resembling exponential functions. A noteworthy feature of the spline functions employed in this algorithm is the tension factor.[9] The highest tension produces straight lines between points, while the lowest value produces roughly cubic fits.

Two stages of interpolation are used to generate the isopleths. In the first stage, the NMHC and NO_x coordinates of the ozone levels to be plotted are determined along each of the radials described in the preceeding section. The second stage draws a smooth curve for each ozone level through the points determined in the first stage. The curves are then plotted using the line printer and, if desired, an off-line plotter such as CALCOMP.

3.0 OZIPP OPTIONS AND DATA REQUIREMENTS

As noted earlier, OZIPP contains a complete set of default values which can generate the standard ozone isopleth diagram. The user can obtain other isopleth diagrams by selecting one or more options. This chapter presents the options in OZIPP and their input data requirements. The type of information required for each option is discussed as well as its source, limitations, restrictions and form. Specific information on the format of input data, however, is given in Chapter 4. The use of the options is illustrated with example problems in Chapter 5.

3.1 CATEGORIES OF OPTIONS

Data are input to OZIPP by means of option cards with special code words. The options fall into four categories:

- Incorporation of city-specific data.
- Diagram definition (e.g., the number of isopleths to be drawn and the NMHC and NO_x concentration ranges to be considered).
- Methods for reducing computer time.
- Accuracy Tests.

The first two categories are the most important. The last two are available for users who require a means to reduce computing costs or who desire further assurance that the isopleth lines are accurately placed in the diagram.

3.1.1 Summary of Code Words and Input Data

The 12 options used to enter data in OZIPP are presented below. Each of these options is identified by a special code word. The input parameters and associated default values for each option are briefly described below. Each of the options and the input data are described in more detail in Section 3.2 and again in Chapter 4.

- ISOPLETH -- This option calls for an isopleth diagram to be constructed according to all specified input parameters. The parameters associated with this option include specification of the maximum NMHC and NO_x concentrations to be considered and selection of the ozone isopleth levels to be drawn. Default values are as follows: maximum NMHC is 2.0 ppmC; maximum NO_x is 0.28 ppm; and 11 ozone levels to be plotted - 0.08, 0.12, 0.16, 0.20, 0.24, 0.28, 0.30, 0.32, 0.34, 0.36 and 0.40 ppm. An additional parameter activates printing solar noon and the time of the center of the maximum one-hour average ozone concentration for each simulation. This information will not be printed under default conditions.

- CALCULATE -- With this option, only one simulation is performed (i.e., only one diagram point calculated) according to the specified input parameters. No isopleth diagram is produced. Initial NMHC and NO_x concentrations must be input with this option. An additional parameter activates the printing of the following: reaction rates, species concentrations, net rates of change in concentrations of all species, and photolytic rate constants for user specified times during the simulation. This information will not be printed under default conditions.

- PLOT -- This option activates the drawing of the isopleth diagram on an offline plotter. Standard CALCOMP routines are used. Input parameters associated with this option control the physical dimensions of the offline plot. Parameters to be specified and their associated default values are as follows: length of abscissa (8.5 inches), length of ordinate (5.95 inches), character and number size (0.10 inches) and label size (0.07 inches). An additional parameter activates the overlaying of a grid of different color on the diagram. Under default conditions, the grid is not drawn.

- TITLE -- This option allows the user to title the program output. Under default conditions, all output is titled "Standard Ozone Isopleth Conditions."

- PLACE -- This option allows determination of the photolysis constants in the kinetic mechanism according to geographical location and time of year. Input parameters associated with this option include the geographic location of the urban area (latitude and longitude), the time zone in which the urban area is located and the time of the simulation. Default values are for a simulation for Los Angeles, California, on June 21, 1975.

- REACTIVITY -- This option allows the user to specify three factors that affect reactivity: the initial fraction of NMHC that is propylene, the initial NO_2/NO_x ratio and the initial fraction of NMHC to be added as aldehydes. Default values for these parameters are 0.25, 0.25 and 0.05, respectively.

- EMISSIONS -- This option permits the consideration of post-0800 emissions. Under default conditions, post-0800 emissions are assumed zero. To override this assumption, the user must specify the fractions of the initial NMHC and/or NO_x concentrations that are to be added each hour to represent the effect of post-0800 emissions.

- TRANSPORT -- This option allows the consideration of transported pollutants. Pollutants can be transported in both the surface layer and aloft. Input parameters include the initial surface layer transported concentrations of NMHC, NO_x and ozone and the concentrations of these pollutants in the air above the base of the inversion layer. All of these concentrations are assumed zero under default conditions.

- DILUTION -- This option allows for the consideration of dilution due to the rise of the inversion layer. Input parameters include the height of the inversion layer in the morning, the final height of the inversion after the rise, the time at which the rise begins, and the time at which the inversion reaches its final height. Under default conditions, the inversion height is assumed to rise from 510 meters at 0800 LDT to 630 meters at 1500 LDT. This represents a 3%/hr dilution rate for the 7 hours between 0800 and 1500.

- ALREADY -- This option permits the use of results from a previous simulation. Input parameters include the initial NMHC concentration, the initial NO_x concentration and the maximum one-hour ozone concentration from each previous simulation. Under default conditions, this option is not exercised.

- ACCURACY -- This option controls the number of simulations, the accuracy of each simultion and the accuracy of the interpolations. Input parameters and their associated default values are as follows: the number of constant NMHC/NO_x radials to be included in the simulations (11), the number of simulations per radial line (5), the error tolerance in the numerical integration scheme (0.01), the tension factor for the first stage of interpolation (1.0) and the tension factor for the hyperbolic spline functions used in plotting isopleths (1.0).

- bbbb (blanks) -- This card terminates the program, and is a required item of input.

3.1.2 Structure of Option Cards

To activate an option described in the previous section, a computer card with the appropriate code word must be included with the input deck. Each code must begin in Column 1; however, only the first four characters of each code word are read. Each code word card contains up to six numeric fields, each 10 spaces wide, beginning in Column 11. With some options, one or more subsequent card(s) may be required. These following cards are read either as seven fields of 10 columns each (beginning with Column 1), or as a string of alphanumeric characters. The format for each option card is described in detail in Chapter 4.

3.2 DETAILED DESCRIPTION OF OPTIONS

This section describes the options available in OZIPP, the input necessary for each option, and the proper form, card and field for each input value. Chapter 4 presents much the same information from a different point of view, namely, an index of the input data corresponding to each card. The options are described by category below, but note that this order is not the typical order of cards in a deck, CALCULATE and ISOPLETH usually being the next-to-last cards (see Section 5.2).

3.2.1 Incorporation of City-Specific Information

Five options are used to input information that is specific to the city under consideration. The input data fix the simulation assumptions about light intensity, dilution, post-0800 emissions, transport and reactivity.

A. Place and Date

In all OZIPP runs, the rate constants of the photolysis reactions in the kinetic mechanism are varied in accordance with the diurnal change in sunlight intensity from 0800 to 1800 LDT. This diurnal variation is calculated using a computer code written by Schere and Demerjian[5] which is incorporated in OZIPP. The user can adjust the photolysis rate constants to the area of interest by

changing the date or location, or both, from the default values of 21 June 1975 at Los Angeles, California. The option is activated by the code word PLACE. The first three numeric fields of the PLACE card (Columns 11 through 40) contain the latitude (decimal degrees North), longitude (decimal degrees West) and time zone (hours from Greenwich Mean Time). The next three fields are used to specify the year, month and day in Columns 41-50, 51-60 and 61-70, respectively. An additional card may be required to follow the PLACE card. On this card, the name of the city of interest is entered between Columns 1 and 24. This card is necessary only if a non-zero value for the latitude or the longitude is entered on the PLACE card. Therefore, even if the default values of 34.058 and 118.250 are entered, a second card is required with the name of the place. Users interested in the default location need not specify the latitude and longitude.

The correct set of numerical time zones for the continental United States is as follows:

Numerical time zone	Common name
5.0	Eastern Daylight Time
6.0	Central Daylight Time
7.0	Mountain Daylight Time
8.0	Pacific Daylight Time

To produce standard time simulations, even though the output will show daylight time units, a false time zone of one unit (hour) more can be used. Thus, Pacific Standard Time photolysis constants would be generated if a 9.0 was entered instead of the correct 8.0 time zone. The output should then show that solar noon occurs near 1200 hours when the printing of solar noon is activated.

B. Dilution Rate

The only form of dispersion incorporated in OZIPP is dilution resulting from the rise in the early morning inversion. Under default conditions, the inversion is assumed to rise from 510 meters to 630 meters over a 7 hour period, starting at 0800 LDT. It is assumed that the rise is exponential in

nature. This corresponds to an exponential decay in concentration where the decay constant is calculated as follows:

$$D = \frac{\ln (Z_2/Z_1)}{\Delta t}$$

where

D = dilution factor, min^{-1}

Z_1, Z_2 = the morning and afternoon mixing heights, respectively (any consistent units)

Δt = the length of time over which the change in mixing height occurs (minutes)

For the default values, the value of the dilution factor is 5.00×10^{-4} min^{-1}. This corresponds to a dilution rate of about 3 percent per hour.

City-specific values for determining the dilution rate are entered using the word DILUTE. The values of the morning mixing height, afternoon mixing height, inversion rise starting time and inversion rise stopping time are entered in the first four numeric fields of the DILUTE card (i.e., Columns 11-20, 21-30, 31-40 and 41-50, respectively). The starting and stopping time should be in 24-hour time format, LDT. For both default and specific conditions, dilution is assumed not to occur outside the starting and stopping times.

C. Post-0800 Emissions

OZIPP has the capability of treating emissions of NMHC and NO_x that occur after 0800 LDT. (Recall that under default conditions, these emissions are assumed to be insignificant and, thus, zero). The post-0800 emissions are meant to reflect only those emissions injected into the imaginary column of air after the beginning of the simulation. They are expressed relative to the emissions injected into the column of air prior to the 0800 LDT simulation starting time. The pre-0800 emissions are represented by the initial NMHC and NO_x concentrations. The post-0800 emissions are represented by hourly additions to these concentrations. Thus, the post-0800 emission input values are actually the fractions of initial NMHC and NO_x concentrations to be added each hour after the simulation starts. For example, if 20% of the pre-0800 NO_x emissions occur during the first hour, 20% of the initial NO_x concentration

(excluding transported pollutant concentrations) would be added to the column concentration between 0800 and 0900 LDT.

The reactivity of organic emissions is assumed to be the same as for the initial concentrations [i.e., the same propylene-butane split (ordinarily 75% - 25%) and the same aldehyde to NMHC ratio (ordinarily .05) are used for post-0800 emissions as for pre-0800 emissions]. However, the post-0800 NO_x emissions are assumed to be 90 % NO and only 10 % NO_2. This cannot be altered using the OZIPP options.

The fractions of initial NMHC and NO_x to be added each hour are modified within OZIPP to account for the volume change associated with dilution. For example, assuming default dilution conditions, an emissions fraction of 1.0 in the eighth hour of the simulation would be multiplied actually by 510/630 (or 0.81) to account for the larger volume in the air column, because the inversion rose to 630 meters from the original 510 meters. Additional modifications to the input data are performed by OZIPP to smooth out abrupt changes in the emissions.

In developing the input data, three pieces of information are required. The number of hours during which the post-0800 emissions continue must be specified. Then, for each of these hours, the fractions of both NMHC and NO_x initial concentrations to be added must be specified. If the fractions for both pollutants are essentially the same, then only one set of fractions need be input. This single set will be applicable to both pollutants. Reference 1 includes guidelines for estimating post-0800 emissions. These guidelines are also briefly discussed in Section 5.2.

If post-0800 emissions are to be included, a card with the code word EMISSIONS should be used. The second numeric field (Columns 11-20) must contain the number of hours for which post-0800 emissions are to be specified (the maximum is 10). If only one set of emission fractions will be input, and that set will apply to both NMHC and NO_x emissions, the number of hours should be coded as a positive number. Then the emission fractions should be coded in the next five numeric fields and, if necessary, coded on an additional card

starting in the first 10 column field (i.e., Columns 1-10). For example, if 10 hours of emissions were to be input, the EMISSIONS cards would contain the first five fractions in fields 3 through 7, i.e., Columns 21-30, 31-40, 41-50, 51-60 and 61-70 (recall that only the first seven fields are normally used in OZIPP option cards). The next card would contain the fraction for the sixth through the tenth hours, with the fractions for the sixth hour coded in Columns 1-10, the fractions for the seventh hour coded in Columns 11-20, etc.

If different fractions for NMHC and NO_x are to be used, the number of hours for which post-0800 emissions are to be input should be coded as a negative number in the second field of the EMISSIONS card. The NMHC fractions are coded exactly as described above. The first NO_x fraction is then entered in the first field (Columns 1-10) on a card immediately following the NMHC fractions. The remaining NO_x fractions are coded in the following fields on this card and additional cards, if necessary.

If it is desired to input emissions for only one pollutant, it is not necessary to code zeros for the other pollutant's emission fractions. Any negative number coded for the first hour's fraction will indicate to OZIPP that no fractions are to be input for that pollutant. Thus, if no NMHC emissions are to be added, a negative number coded for the first NMHC fraction will cause OZIPP to skip immediately to the next card and to process NO_x fractions. Likewise, a negative number for the first NO_x field will cause OZIPP to skip the next card and to begin processing the next option.

D. Transported Concentrations

OZIPP's default conditions do not include any pollutants transported from upwind areas. However, the TRANSPORT option is available to include the effects of ozone and precursors transported from areas upwind of the city of interest. Two types of transport can be included. The first type results from the transport of pollutants into the urban area within the surface layer. The second type results from pollutants being transported within air masses trapped above the mixing height at night. As the mixing height rises during the day, the transported pollutants trapped aloft are entrained into the

mixing layer. For both types of transport, the following assumptions about precursor reactivity are made:

1) 10% of the transported NMHC concentration is propylene, 90% n-butane
2) No aldehydes are transported into the area
3) All transported NO_x is NO_2.

These assumptions cannot be changed by the user.

Concentrations of O_3, NMHC and NO_x transported in the surface layer are entered in the first, third and fifth numeric fields of the TRANSPORT card (Columns 11-20, 31-40 and 51-60, respectively). The appropriate units for O_3 and NO_x are ppm, and for NMHC the units are ppmC. Subsequent simulations will have these concentrations added to the initial concentrations. Thus, the actual initial NMHC and NO_x concentrations simulated will be the sum of the diagram point values and the values transported in the surface layer.

The treatment of pollutants being entrained from aloft is also activated with the same TRANSPORT card. The concentrations of O_3 (ppm), NMHC (ppmC) and NO_x (ppm) in the air aloft are entered in the second, fourth and sixth numeric fields of the card (Columns 21-30, 41-50 and 61-70, respectively).

E. Reactivity Changes

The reactivity of the ozone precursors can be modified by changing any of three factors: the hydrocarbon mix* (i.e., the fraction of NMHC assumed to be propylene), the fraction of the initial NO_x concentration that is NO_2, and the fraction of the initial NMHC concentration that is added as aldehyde. Any one or all of these factors can be changed by using a card with the code word REACTIVITY before the ISOPLETH or CALCULATE cards. A number entered in the first numeric field (Columns 11-20) of REACTIVITY will replace the default value of 0.25 for the fraction of initial carbon atoms in the form of propylene. A number in the next field (Columns 21-30) replaces the default initial

* Although this capability exists, at the present time it is uncertain how to characterize reactivity of mixtures differing greatly from automobile exhaust in terms of propylene to NMHC ratios.

NO_2/NO_x ratio of 0.25, and a number in the third field (Columns 31-40) replaces the default value of 0.05 for the fraction of initial carbon atoms added as aldehydes. (The initial aldehyde concentration is assumed to be 40 % formaldehyde and 60 % acetaldehyde as ppmC).

3.2.2 Diagram Definition Options

The possible modifications to the form of the isopleth diagram constructed by OZIPP are described below.

A. NMHC and NO_x Concentration Ranges

In all OZIPP isopleth diagrams, the origin represents 0.0 ppmC NMHC and 0.0 ppm NO_x. The maximum NMHC and NO_x concentrations represented on the abscissa and the ordinate can be changed from their respective default values of 2.0 ppmC NMHC and 0.28 ppm NO_x by putting the desired maxima in the first two numeric fields of the ISOPLETH card. The desired maximum NMHC concentration (in units of ppmC) should be punched in the field of Columns 11 through 20. The desired maximum NO_x concentration (in units of ppm) should be punched in the field of Columns 21 through 30.

Any number may be used for the desired maximum NMHC or NO_x concentrations, but because the scales on the abscissa and the ordinate are divided into ten and seven divisions, respectively, only certain values of the maxima will produce even markers. Thus, to produce an easy-to-use diagram, the NO_x maxima should be evenly divisable by seven (e.g., .07 ppm, .14 ppm, .21 ppm, .28 ppm, etc). Similar considerations should be given to selecting a NMHC maximum.

B. Number and Spacing of Isopleths

The desired number of isopleths in the diagram should be inserted (followed by a decimal point) in the field of Columns 31 through 40 of the ISOPLETH card. Up to 20 isopleths can be drawn (the default value is 11). OZIPP then reads the proper number of fields from the succeeding card or cards to find the ozone concentrations (in units of ppm) for which isopleths are to be drawn. For example, inserting 10.0 in Columns 31-34 of ISOPLETH causes OZIPP

to read the seven 10-space numeric fields on the next card and three on the succeeding card. (As noted earlier, OZIPP does not read past Column 70 on any card except the program title card).

C. Title

The title can be changed by inserting a card with the code word TITLE followed by a card with the desired title. Everything in Columns 1 through 72 of this title card will be printed on the output and isopleth diagrams in place of the default title, "Standard Ozone Isopleth Conditions." As with all options, these cards must precede the ISOPLETH or CALCULATE cards.

D. CALCOMP Plotting

Any plotting package that can be called using standard CALCOMP subroutines can be used. Calls to these routines are activated by a card with the code word PLOT. This card must precede the ISOPLETH card. The actual CALCOMP routines called are PLOTS, PLOT, NUMBER, SYMBOL and NEWPEN (if necessary). The use of the CALCOMP routines is discussed in Section 4.3.2.

The user also has the option to specify the actual size of the plot by defining the lengths (in inches) of the sides of the diagram. Columns 31-40 are used for the abscissa of the diagram. Columns 41-50 are used for the ordinate of the diagram. The size of title characters and axes numbers and the size of the isopleth labels can also be set by the user in Columns 51-60 and 61-70, respectively. The default values were given in Section 3.1.1. If the user wishes to reset any of these values, it is recommended that all values change proportionally.

Another option on the CALCOMP plots is the overlay of gridded lines on the isopleth diagram. This is done by declaring any non-zero positive value in Columns 21-30. If this option is exercised, a grid of different color will be overlayed onto the diagram. If the user does not have access to the choice of different pen colors, it is not recommended to use this option. For users with access to a matrix plotter (such as the VERSATEC plotter), and the choice

of lines consists of thickness and patterns (i.e., dot-dash, on solid patterns) then the user may enter a negative non-zero value in Columns 21-30. The absolute value of the number entered represents the user's choice of pattern and thickness. This number varies with different computer systems.

3.2.3 Methods for Reducing Computer Time

Most of the computing time of an OZIPP run is expended in performing simulations. OZIPP performs simulations at diagram points located along straight lines radiating from the origin of the isopleth diagram. In other words, OZIPP performs several simulations on each of a number of lines of constant NMHC/NO_x ratio. The number of radial lines (i.e., lines of constant NMHC/NO_x ratio) and the number of simulations per line can be varied by the user. (OZIPP also performs simulations at the corners of the isopleth diagram and elsewhere that cannot be controlled by the user).

A means of reducing computer costs is often necessary, so several options are available in OZIPP to allow such savings. For example, fewer radial lines and fewer simulations per line in OZIPP can produce an isopleth diagram at lower cost. However, the isopleths will have been interpolated from fewer points. For control strategy usage, the default values of eleven radial lines and five simulations per line are recommended. Much computer time can be wasted by a poor choice of maximum initial NMHC and NO_x concentrations on the abscissa and the ordinate of the isopleth diagram. When city-specific options are activated, some of the isopleth lines desired by the user may be off the diagram specified or may be cramped into a small part of the diagram. In addition, CALCOMP plotting may require extra time or added expense. In such cases, trial OZIPP runs without the CALCOMP option can be made with the number of simulations reduced. Then, the maximum NMHC and NO_x values that produce the best display of the ozone isopleth lines can be determined. This is discussed further in Section 5.2.

A. Radial Line Control

The number of radial lines used in construction of the isopleth

diagram can be controlled by specifying the desired number of lines (any odd number from 1 to 19) in the first numeric field (Columns 11-20) of the ACCURACY card. Leaving this field blank produces the default value of 11.

B. Number of Simulations Per Radial

This number is controlled using the second field of the ACCURACY card (Columns 21-30). The possible values are 1 through 8 and the default value is 5. Thus, the isopleth diagram requiring the least computer time would result from a 1.0 in both of the first two numeric fields on the ACCURACY card. Essentially, only the diagram points at the corners of the diagram would be simulated. These results would be useful in estimating the NMHC and NO_x concentrations that define the limits of an isopleth diagram.

C. The Use of Previous Simulation Results

The results from previous simulations can be utilized with the card coded with ALREADY. In order to incorporate results from a previous run, the following conditions must be identical in both runs: the NMHC and NO_x scales, the city-specific options, number of radial lines and the number of simulations per line. Such a situation could occur when:

- An initial run may have terminated because of time restriction
- The user may wish to repeat the run with PLOT option in order to obtain a CALCOMP generated plot
- The user may wish to alter the tension factors used in the interpolation schemes.

To input the results of previous runs, the number of completed simulations is entered in the first numeric field (Columns 11-20) of the ALREADY card. The results of those simulations must be entered on the following cards in the same order in which they are calculated. Each card contains the results of one simulation. Field 1 (Columns 1-10) contains the initial NMHC concentration, Field 2 (Columns 11-20) initial NO_x concentration and Field 3 (Columns 21-30) the resulting maximum one-hour average O_3 concentration.

D. First Ozone Peak

A considerable amount of computer time is wasted when the maximum one-hour average O_3 concentration in a simulation occurs early but the simulation is continued for the full ten hours. The default condition in OZIPP forces this continuation because two ozone peaks often occur in simulations, and the second may be the larger. Nevertheless, a sizeable reduction in computer costs is possible for simulations with single ozone peaks if the simulations are stopped after their peaks are reached. This can be done in OZIPP by placing any number in the sixth numeric field (Columns 61-70) of the ACCURACY card. However, the reasons for two ozone peaks are not well understood, so the full 10 hours must be used to generate isopleth diagrams intended for control strategy usage.

E. Multiple Isopleths or Calculations

Any number of isopleth diagrams or individual calculations can be performed in one run of OZIPP. The user merely needs to insert the desired number of ISOPLETH and CALCULATE cards. One set of simulations and an associated ozone isopleth diagram will be produced for each ISOPLETH card. Likewise, a single simulation will be performed for each occurrence of the CALCULATE card. Except for options that cannot be deactivated, all options activated will remain in effect until respecified. Likewise, all input data will be fixed until redefined. Thus, if the default value for a parameter is desired in place of a value specified earlier, the default value must be respecified.

Once activated, the following two options cannot be turned off: PLOT, and the first ozone peak option of ACCURACY. If the ALREADY option has been activated, it also will remain activated until turned off (i.e., previous simulation results will be used with all subsequent ISOPLETH options). To deactivate the ALREADY option, another ALREADY card must be entered with a zero or blanks in the first numeric field (Columns 11-20).

To illustrate the procedure for obtaining multiple diagrams, assume that it is desired to produce two ozone isopleth diagrams. One diagram is to

reflect default dilution conditions, and the second diagram different assumptions about dilution. The option cards might then be ordered as follows:

1) a set of cards specifying all options and input values other than dilution (thereby invoking default dilution conditions)

2) an ISOPLETH card causing an ozone isopleth diagram with default dilution condition to be produced

3) a DILUTION card specifying the new dilution condition

4) an ISOPLETH card causing an ozone isopleth diagram with the new dilution conditions to be produced.

Note that two sets of simulations are performed, and that the same results could be accomplished with two separate runs.

3.2.4 Accuracy Tests of the Isopleth Diagram

Options have been incorporated into OZIPP to allow users to test the accuracy of the diagram. In this manual, the term "accuracy" is always used in reference to the numerical solution of an implied initial value problem in ordinary differential equations. Thus, accuracy does not refer to the degree of correspondence between an isopleth diagram and atmospheric data.

Although the extensive experience gained in the development of OZIPP suggests that the default radial lines, number of simulations per line, tension factor, and so on, will generate sufficiently accurate isopleth diagrams, this experience does not guarantee sufficient accuracy. The recommended procedures to check many of the factors that affect accuracy are similar. They merely answer the following question: Do somewhat higher or somewhat lower values of the factor significantly affect the resulting isopleth diagram? OZIPP has been designed to respond properly to these factors. For instance, an increase in simulation density (more radial lines or more simulations per line) should produce a more accurate isopleth diagram. The procedures in OZIPP to check accuracy and to generate additional information are discussed below.

A. The Density of Simulations

As described above, the number of radial lines and the number of simulations per line can be decreased to reduce computer time using the ACCURACY card. These numbers can also be increased to check accuracy. The first numeric field (Columns 11-20) on ACCURACY specifies the number of radial lines, and the second field (Columns 21-30) the number of simulations per radial line. The limits of acceptable input are odd numbers from 1 to 19 for the former and any number from 1 to 8 for the latter.

The accuracy of the points at which isopleths touch the edges of the diagram can be checked (with minimal computer cost) by specifying 19 lines and 1 calculation per line. The accuracy of the isopleth lines along the diagonal of the isopleth diagrams can be checked by specifying 1 radial line and 8 simulations per line. The spacing and values along any one radial line can be checked by adjusting the diagram to make that line the diagonal (using the ISOPLETH card) and using the ACCURACY card with 1 radial line and 8 calculations on that line. (The ISOPLETH card must follow the ACCURACY card).

B. Calculation at Specified Points

Individual simulations can be performed at specified initial NMHC and NO_x concentrations using the CALCULATE card. This option might be required to check an interpolated point or to gain more information about a simulation actually performed on a previous isopleth diagram. The first two numeric fields on the CALCULATE card (Columns 11-20 and 21-30) must specify the desired initial NMHC and NO_x concentrations. The initial conditions and hourly ozone concentrations will be printed to show the change of ozone in the simulation with time. Any number entered in the third numeric field (Columns 31-40) will activate an information option that will print:

- The rate constants used in the kinetic mecahnism.
- The concentrations of all species in the kinetic mechanism.
- The net rate of change of all species.
- The reaction rates for each reaction.
- The photolysis constants for all photolysis reactions.

If the information option is activated, the user may specify the simulation time (in minutes) for which concentrations of all species, current reaction rates, etc., will be printed. The number of minutes after the simulation starting time at which the initial printing is made (Default value = 60 minutes after start) is entered in Columns 41-50. The integral time step for which subsequent printings are made (Default value = 60 minutes) is entered in Columns 51-60. Under default values, hourly concentrations of species, net rates of change, etc., are printed.

After the simulation has ended, a concentration versus time profile is printed for ozone. An example of output from this option is given in Chapter 5.

C. Accuracy of Simulations

The numerical integration scheme employed in OZIPP estimates the error at every step of the integration. The size of the time step taken by the computer is adjusted to keep the estimated error in the range specified. The error is conveniently controlled by a single parameter with a default value of 0.01. Smaller values of this parameter increase both the accuracy and computer time. Larger values do the opposite. By entering numbers smaller than 0.01 in the third numeric field of the ACCURACY card (Columns 31-40), one can estimate the accuracy of the simulations. For example, if several CALCULATE and ACCURACY cards are used, several simulations can be performed with the same initial NMHC and NO_x concentrations but with different time steps in the numerical integration. This procedure can be used to demonstrate how the simulation results vary with increased error tolerance. Table 3-1 shows the results of such a test using the default conditions.

D. Spline Interpolation Accuracy

There are two parameters that can be used to control the spline interpolation schemes. Normally, the default values are perfectly adequate. The parameters should only have to be modified under rare circumstances. Consequently, the following discussion is included primarily for thoroughness.

TABLE 3-1. MAXIMUM OZONE CONCENTRATIONS IN SIMULATIONS AT VARIOUS ERROR TOLERANCES IN THE NUMERICAL INTEGRATION

Maximum Ozone Concentration (ppm)	Error Tolerance
0.28624	0.00001
0.28617	0.0001
0.28581	0.001
0.28602	0.01 (default)
0.28158	0.1
0.28158	0.2
0.27957	0.5

NOTE: In all simulations, the initial NMHC concentration was 1.0 ppmC, the initial NO_x concentration was 0.13 ppm and the default values were used for all other variables.

Unfortunately, the spline functions used to interpolate between simulation results do not have a parameter as relevant to accuracy as does the numerical integration scheme used for the simulations. The spline functions can be controlled to a limited extent by a simple factor analogous to tension. The lowest values (e.g., 0.001) cause the hyperbolic spline function to resemble cubic splines, and high values (e.g., 50.0) result in virtually straight lines between points or linear interpolation. Since two stages of interpolation are used in OZIPP, there are two parameters available to control tension. Default values for both are 1.0, and control is obtainable by entering the desired number in the fourth and/or fifth numeric fields of the ACCURACY card (Columns 41-50 and 51-60). The first factor controls the first stage, namely interpolation between diagram points along the top edge of the isopleth diagram, along the right edge and along each radial line. This interpolation stage estimates the coordinates of ozone concentrations for which isopleths are to be constructed. The second stage interpolates between diagram points calculated in the first stage to generate the coordinates of the isopleths themselves. Thus, a value of 50.0 in the fourth numeric field of the ACCURACY card would cause nearly linear interpolation to be used to locate the diagram points on the radial lines and edges that correspond to the ozone concentrations at which isopleths are to be drawn. A value of 50.0 in the fifth field would result in nearly straight lines between diagram points calculated in the first stage.

To a limited extent, the tension factor for the first stage of interpolation controls the selection of initial NMHC and NO_x concentrations for some simulations because the same interpolation scheme is used in selecting the initial concentrations for the simulations. Therefore, using the results of a set of simulations (via the ALREADY option) with different first stage tension factors may produce slightly different isopleth diagrams.

3.3 LIMITATIONS ON ISOPLETH SHAPES

In general, most of the parameters used in OZIPP have a limited range of acceptable values. These have been described in this chapter and the next.

In addition to these limits, there are certain types of isopleths that cannot be plotted by OZIPP. But the designers of OZIPP are not aware of any conditions that would result in isopleths of these types. Among the types of isopleths OZIPP cannot plot are:

- Lines that touch the lower edge.*
- Lines that are closed or that loop in any way.
- Lines that touch the left edge in two places.
- Two or more separate lines at the same O_3 concentration (only the line closest to the left edge will be plotted).

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* As shown in Figure 1, the lower edge of an OZIPP ozone isopleth diagram is at 0.0 initial NO_x. The left edge is 0.0 initial NMHC, the top edge the maximum initial NO_x and the right edge the maximum initial NMHC concentration.

4.0 USER'S GUIDE

This chapter describes the format of the input data, types of error and warning messages that can occur, and some special problems to consider in installing the program on any one facility. In addition, example job control language is presented for illustration.

4.1 FORMAT OF INPUT DATA

The twelve options in OZIPP, which were discussed in Chapter 3, are listed in Table 4-1. For each option, the locations of the different parameters on the appropriate cards are shown. The order of the OZIPP options in the input deck is not important except for the ISOPLETH and CALCULATE options. Any options to be activated for simulations must precede these two options. Consequently, the order shown in Table 4-1 is recommended. This ordering has the TITLE option listed first, followed by the options used to input city-specific information (PLACE, DILUTION, EMISSIONS, REACTIVITY and TRANSPORT). The next group of options affect some of the operational aspects of OZIPP (ACCURACY, ALREADY and PLOT). The two options that actually initiate simulations follow (CALCULATE, and ISOPLETH). The last card of any input set must be a blank card.

As shown in Table 4-1, all 4-letter code words (e.g., TITL, PLAC, etc.) which activate an option must begin in Column 1. Each card with such a code word has up to six numeric fields, each ten spaces wide, beginning in Column 11. An entry can be made anywhere in a field, but a decimal point must always be used, even with integral values. Some options have additional data cards associated with them. These cards must follow the option card in the order specified in Table 4-1. For example, the card containing the title must immediately follow the card with the code word TITL. Data cards that do not begin with code words contain 7 ten-column fields beginning in Column 1. Like the numeric fields on cards with code words, entries may be made anywhere in the field provided a decimal is used.

As previously described, most parameters have default values associated with them. These are indicated by DF in Table 4-1. If no entry is

made in a numeric field, the default value will be assumed. For example, if the only entry made on the PLACE card is in the first numeric field, the default value of 118.25 will be assumed for the second numeric field, 8.0 for the third, etc.

TABLE 4-1.

INPUT FORMAT FOR OZIPP OPTIONS

OPTION	DESCRIPTION		
	Card No.	Columns	Contents
TITLE		Input a new title. If this option is not activated, the default title is "Standard Ozone Isopleth Conditions."	
	1	1-4	TITL
	2	1-72	The title can be placed anywhere in card columns (cc) 1-72
PLACE		Input city-specific information on light intensity. Default values correspond to Los Angeles on June 21, 1975.	
	1	1-4	PLAC
		11-20	Latitude, in decimal degrees north of the equator; DF = 34.058.
		21-30	Longitude, in decimal degrees west of Greenwich meridian; DF = 118.250.
		31-40	The time zone, in hours from Greenwich mean time; DF = 8.0.
		41-50	The year; DF = 1975.
		51-60	The month of year; DF = 6.
		61-70	The numerical day of month; DF = 21.
	2 (optional)	1-24	The name of the place can be entered anywhere in cc 1-24. Include this card only if a new value is entered for the latitude or longitude on the previous card.

TABLE 4-1. (Cont'd)

INPUT FORMAT FOR OZIPP OPTIONS

OPTION	DESCRIPTION		
	Card No.	Columns	Contents
DILUTION		Input city-specific information on inversion rise.	
	1	1-4	DILU
		11-20	Initial inversion height, Z1, in any units; DF = 510.
		21-30	Final inversion height, Z2, in same units as initial inversion height; DF = 630.
		31-40	Starting time of inversion rise (24 hour daylight time); DF = 0800.
		41-50	Ending time of inversion rise (24 hour daylight time); DF = 1500.
EMISSIONS		Input city-specific information on post-0800 emissions.	
	1	1-4	EMIS
		11-20	The number of hours for which emission fractions are to be input, from 1.0 to 10.0; DF = 0. This number should be coded as positive if the same fractions for NMHC and NO_x are to be used. It should be coded as negative if different fractions are to be used.
		21-30	NMHC or NMHC and NO_x emission fraction for hour 1; DF = 0. If all NMHC fractions are to be set to zero, enter any negative number and skip to card 3.
		31-40	NMHC or NMHC and NO_x emission fraction for hour 2; DF = 0.
		41-50	NMHC or NMHC and NO_x emission fraction for hour 3; DF = 0.

TABLE 4-1. (Cont'd)

INPUT FORMAT FOR OZIPP OPTIONS

OPTION	DESCRIPTION	
	Card No.	Columns	Contents
EMISSIONS (Cont'd)		51-60	NMHC or NMHC and NO_x emission fraction for hour 4; DF = 0.
		61-70	NMHC or NMHC and NO_x emission fraction for hour 5; DF = 0.
	2* (optional)	1-10	NMHC or NMHC and NO_x emission fraction for hour 6; DF = 0.
		11-20	NMHC or NMHC and NO_x emission fraction for hour 7; DF = 0.
		21-30	NMHC or NMHC and NO_x emission fraction for hour 8; DF = 0.
		31-40	NMHC or NMHC and NO_x emission fraction for hour 9; DF = 0.
		41-50	NMHC or NMHC and NO_x emission fraction for hour 10; DF = 0.
	3* (optional)	1-10	NO_x emission fraction for hour 1; DF^X = 0. If all NO_x fractions are to be set to zero, enter any negative number in cc 1-10, skip card 4 and proceed to the next option.
		11-20	NO_x emission fraction for hour 2; DF^X = 0.
		21-30	NO_x emission fraction for hour 3; DF^X = 0.
		31-40	NO_x emission fraction for hour 4; DF^X = 0.
		41-50	NO_x emission fraction for hour 5; DF^X = 0.
		51-60	NO_x emission fraction for hour 6; DF^X = 0.
		61-70	NO_x emission fraction for hour 7; DF^X = 0.

* See footnote on next page.

TABLE 4-1 (Cont'd)

INPUT FORMAT FOR OZIPP OPTIONS

OPTION	DESCRIPTION		
	Card No.	Columns	Contents
EMISSIONS (Cont'd)			
	4*	1-10	NO_x emission fraction for hour 8; DF^x= 0.
	(optional)	11-20	NO_x emission fraction for hour 9; DF^x= 0.
		21-30	NO_x emission fraction for hour 10; DF^x= 0.

* Card 2 is not included if there are less than 5 hours of emissions or if all individual NMHC fractions were set to zero by entering a negative number in cc 21-30 of Card 1. Cards 3 and 4 are not included if combined NMHC and NO_x fractions were entered in Cards 1 and 2. Card 4 is not included if all individual NO_x fractions were set to zero by entering a negative number in cc 1-10 of Card 3, or if there are less than 8 hours of NO_x emissions.

TABLE 4-1 (Cont'd)

INPUT FORMAT FOR OZIPP OPTIONS

OPTION	DESCRIPTION		
	Card No.	Columns	Contents
REACTIVITY		Input city-specific information on reactivity.	
	1	1-4	REAC
		11-20	Initial fraction of carbon atoms in the form of propylene; DF = 0.25.
		21-30	Initial NO_2/NO_x ratio; DF = 0.25.
		31-40	Fraction of initial NMHC concentration (in ppmC) added as aldehyde: DF = 0.05.
TRANSPORT		Input city-specific information on transported pollutants.	
	1	1-4	TRAN
		11-20	Concentration of O_3 transported in the surface layer, in ppm; DF = 0.
		21-30	Concentration of O_3 transported aloft, in ppm; DF = 0.
		31-40	Concentration of NMHC transported in the surface layer, in ppmC; DF = 0.
		41-50	Concentration of NMHC transported aloft, in ppmC; DF = 0.
		51-60	Concentration of NO_x transported in the surface layer, in ppm; DF = 0.
		61-70	Concentration of NO_x transported aloft, in ppm; DF = 0.

TABLE 4-1 (Cont'd)

INPUT FORMAT FOR OZIPP OPTIONS

OPTION	DESCRIPTION		
	Card No.	Columns	Contents
ACCURACY		Increase or reduce the mathematical accuracy of the isopleth diagram by using more or fewer simulations, more or less accurate interpolation, etc.	
	1	1-4	ACCU
		11-20	Number of constant initial NMHC/NO_x ratios (radial lines from the origin of the isopleth diagram) on which simulations are to be performed, any odd number from 1. to 19.; DF = 11.
		21-30	Number of simulations per radial line, from 1. to 8.; DF = 5.
		31-40	Error tolerance in the numerical integration routine, from 0.1 to 0.00001; DF = 0.01.
		41-50	Tension factor for hyperbolic spline functions used in first stage of interpolation from .001 to 50.; DF = 1.
		51-60	Tension factor for hyperbolic spline functions used in plotting isopleth lines (high tensions lead to straight lines drawn between the points obtained from the first stage), from .001 to 50.; DF = 1.
		61-70	If any non-zero value is entered in this field, simulations will terminate after any ozone maximum; no entry produces full 10-hour simulations.

TABLE 4-1 (Cont'd)

INPUT FORMAT FOR OZIPP OPTIONS

OPTION	DESCRIPTION		
	Card No.	Columns	Contents
ALREADY		Include results from a previous run.	
	1	1-4	ALRE
		11-20	Number of previous simulations to be input.
	2*	1-10	Initial NMHC concentration, ppmC
		11-20	Initial NO_x concentration, ppm.
		21-30	Maximum one-hour average ozone concentration, ppm.

* One card is included for each simulation result. Thus, the number of these cards must be equal to the value coded in cc 11-20 of Card 1. Also, the cards must be put in the same order in which the simulations were performed.

TABLE 4-1 (Cont'd)

INPUT FORMAT FOR OZIPP OPTIONS

OPTION	DESCRIPTION		
	Card No.	Columns	Contents
PLOT		Activates the drawing of the isopleth diagram on an offline plotter	
	1	1-4	PLOT
		11-20	Scaling factor for the location of labels for each ozone isopleth. The value should be between 0.1 and 0.8.; DF = 0.6.
		21-30	If non-zero, a grid is overlaid on the diagram. If the value is positive and non-zero, a grid is overlaid on the diagram using a different color pen (if available). If the value is negative, a grid with lines of different patterns (e.g., dot-dash) is overlaid on the plot. The absolute value of this number corresponds to different patterns and texture.
		31-40	Length (in inches) of the abscissa (NMHC scale) of the isopleth diagram; DF = 8.5.
		41-50	Length (in inches) of the ordinate (NO_x scale) of the isopleth diagram; DF $\triangleq$ 5.95.
		51-60	Sizes (in inches) of the numbers to be printed on the axes and of the characters in the title; DF = 0.10.
		61-70	The sizes (in inches) of the labels on the ozone isopleths and the division marks on the axis; DF = 0.07.

TABLE 4-1 (Cont'd)

INPUT FORMAT FOR OZIPP OPTIONS

OPTION	DESCRIPTION		
	Card No.	Columns	Contents
CALCULATE		Perform a single simulation with the initial NMHC and NO_x concentrations specified on this card.	
	1	1-4	CALC
		11-20	Initial NMHC concentration in ppmC.
		21-30	Initial NO_x concentration in ppm.
		31-40	Information option; entry of any positive value will result in printing of the computed concentrations of all species, the rates of change of all species, reaction rates, etc. Photolysis constants are also printed.
		41-50	Time (in minutes) from the beginning of the simulation at which computed concentrations of all species in the kinetic mechanism are to be printed; DF = 60.
		51-60	Time step (in minutes) for subsequent printing of concentrations; DF = 60.

TABLE 4-1 (Cont'd)

INPUT FORMAT FOR OZIPP OPTIONS

OPTION	DESCRIPTION		
	Card No.	Columns	Contents
ISOPLETH		Construct an ozone isopleth diagram according to the input parameters. Default isopleths are 0.08, 0.12, 0.16, 0.20, 0.24, 0.28, 0.30, 0.32, 0.34, 0.36 and 0.40 ppm.	
	1	1-4	ISOP
		11-20	Maximum NMHC concentration (in ppmC) on abscissa of isopleth diagram; DF = 2.0.
		21-30	Maximum NO_x concentration (in ppm) on ordinate of isopleth diagram; DF = 0.28.
		31-40	Number of ozone isopleths to be drawn, from 1. to 20.; DF = 11.
		41-50	Any non-zero value will activate the printing of solar noon and the time of the center of the maximum one-hour average ozone concentration for each simulation.
	2* (optional)	1-10	Ozone concentration of 1st isopleth, ppm;
		11-20	Ozone concentration of 2nd isopleth, ppm;
		21-30	Ozone concentration of 3rd isopleth, ppm;
		31-40	Ozone concentration of 4th isopleth, ppm;
		41-50	Ozone concentration of 5th isopleth, ppm;
		51-60	Ozone concentration of 6th isopleth, ppm;
		61-70	Ozone concentration of 7th isopleth, ppm.

* See footnote on next page.

TABLE 4-1 (Cont'd)

INPUT FORMAT FOR OZIPP OPTIONS

OPTION	DESCRIPTION		
	Card No.	Columns	Contents
	3* (optional)	1-10	Ozone concentration of 8th isopleth, ppm.
		.	.
		.	.
		.	.
		61-70	Ozone concentration of 14th isopleth, ppm.
	4* (optional)	1-10	Ozone concentration of 15th isopleth, ppm.
		.	.
		.	.
		.	.
		.	.
		51-60	Ozone concentration of 20th isopleth, ppm.
bbbb		A blank card must follow all input cards to terminate the program.	
	1	1-4	Blanks.

* Optional cards 2,3, and 4 are input only if the number of isopleths to be drawn is specified on Card 1. The number of entries, and thus the number of optional cards, must correspond to the number of isopleths to be drawn. For example, if 10 isopleths are specified, entries are made in the first 7 fields of Card 2 and the first 3 fields of Card 3. Card 4 would not be included with the input. Note that the default scheme does not apply when an entry is made in Columns 31-40 of the first card (i.e., the ISOP card).

4.2 PROGRAM GENERATED ERROR MESSAGES

This section discusses potential output error messages produced by OZIPP. Two types or error messages are generated:

- Fatal error messages -- messages caused by problems that immediately halt any further computation.
- Non-Fatal error messages--messages caused by problems that do not cause an immediate halt in computation.

These types of messages are discussed below.

4.2.1 Fatal Error Messages

There are seven fatal error messages that may occur during OZIPP runs. Five of these occur because the integration scheme cannot proceed further. Descriptions of each message are included below:

- THE LOWEST OZONE LINE CANNOT BE PLOTTED
  INCREASE THE MAXIMUM HC AND NO_x VALUES

  If the concentration of ozone predicted from the maximum initial NMHC and NO_x concentrations (listed on the ISOPLETH card, or NMHC = 2.0 ppmC, NO_x = 0.28 ppm by default) is less than the lowest ozone isopleth line to be plotted, the program will stop. The user may fix this problem by either increasing the maximum NMHC or NO_x concentrations or reducing the concentrations at which ozone isopleths are to be plotted.

- NO LINES CAN BE PLOTTED
  BACKGROUND ONLY PRODUCES TOO MUCH OZONE ____ PPM

  This message is the opposite of the previous message. If the amount of ozone predicted at NMHC and NO_x concentrations of 0.0 is greater than the highest ozone isopleth line desired, the program will stop.

The following error messages all stem from problems encountered in the integration scheme routines:

- PROBLEM APPEARS UNSOLVABLE WITH GIVEN INPUT
- INTEGRATION HALTED BY DRIVER AT T = ____
  EPS TOO SMALL TO BE ATTAINED FOR THE MACHINE PRECISION

- KFLAG = -2 FROM INTEGRATOR AT T = ____, H = _____
  THE REQUESTED ERROR IS SMALLER THAN CAN BE HANDLED

- KFLAG = -3 FROM INTEGRATOR AT T = _____
  CORRECTOR CONVERGENCE COULD NOT BE ACHIEVED

- ILLEGAL INPUT..EPS.LE.0.

If any of these messages occur, the user should try the following:

- Check input to be sure all data are correct (e.g., check hydrocarbon and NO_x values on a CALCULATE option, check for negative error tolerance, and so on).

- Raise the value of the error tolerance, if necessary.

- Redefine the density of simulations (e.g., change the number of radials, number of simulations per line, maximum initial NMHC or NO_x concentrations, etc.)

- As a last resort, alter the simulation conditions slightly (e.g., change post-0800 emissions, dilution, etc.)

4.2.2 Non-fatal Error Messages

Two non-fatal error messages may occur in OZIPP runs. The user may wish to redefine the situation (i.e., the limits of the diagram) or to check the input data.

- THE OPTIONS INSTRUCTION__CANNOT BE PROCESSED

  If this message occurs, the user should check for an error in the input data.

- DUE TO HIGH BACKGROUND CONDITIONS
  THE LOWEST OZONE PLOTTED WILL BE ____PPM

  This message indicates that some of the ozone isopleths desired lie outside the limits of the diagram. For example, if the maximum ozone concentration associated with zero initial conditions were greater than 0.08 ppm, a 0.08 ppm isopleth could not be drawn. However, isopleths greater than 0.08 ppm could possibly be drawn.

4.3 COMPUTER CONSIDERATIONS

The OZIPP program consists of one main program and 39 subprograms. It requires about 41K, 36-BIT words of core in a UNIVAC-1110 computer system. Run times on the system average 5-7 minutes. Complete listings, along with flow diagrams of selected subroutines, are shown in Appendices B and C, respectively. Also included are five calls to CALCOMP subroutines. Discussed below are special language considerations, use of CALCOMP routines and computer control language.

4.3.1 Language Considerations

Although OZIPP has been written to conform with ANSI standard FORTRAN language, there are certain types of language usage in OZIPP that are not compatible on all computer systems. Areas to check include the following multiple-entry points:

```
*Subroutine DIFFUN          card(L.1)
 entry point:
     ENTRY DIFSET(...)        card(L.71)

*Subroutine ISOPLT          card(V.1)
 2 entry points:
     ENTRY SAVLIN(...)        card(V.77)
     ENTRY LINPRT(...)        card(V.93)

*Subroutine VVLBLF          card(AL.1)
 2 entry points:
     ENTRY VVLBLC(...)        card(AL.60)
     ENTRY VVLBLL(...)        card(AL.165)
```

These entry points may or may not require the argument list after the ENTRY statement.

The variable UROUND in subroutine DRIVES should be set to the round-off error associated with each computer system. Currently, UROUND is set to the round-off error of 7.5×10^{-9} associated with a UNIVAC 1110 computer system. To reset UROUND, the card (J.12) in subroutine DRIVES should be changed:

```
*DATA     UROUND/user's round-off error/     (card J.12)
```

UROUND is calculated from the number of significant digits (N) used for the mantissa of a floating point constant:

$$UROUND = 2^{-N}$$

For the UNIVAC 1110 computer, each word contains 36-BITs of which 27 are used for the mantissa. Thus, 2^{-27} is equal to approximately 7.5×10^{-9}. This is the value currently set in OZIPP.

Another variable in OZIPP which is machine dependent is the variable EXPMAX found in subroutines CURV1 and KURV1. This variable represents the maximum possible value for the exponent of e. For the UNIVAC 1110 computer, the range of the real constants is from 10^{-38} to 10^{38}. Hence, the maximum value for the exponent of e:

$$e^{EXPMAX} = 10^{38}$$

or EXPMAX is 87.5 for the UNIVAC 1110 computer. The value currently set in OZIPP is 87.4, which is slightly lower than the actual maximum value to ensure that the actual maximum is never reached. To reset EXPMAX, the user must change the cards (W.43 and Y.45A) accordingly:

```
          DATA EXPMAX/user's maximum exponent/          W.43
and       DATA EXPMAX/user's maximum exponent/          Y.45A
```

4.3.2 Use of CALCOMP Routines

The CALCOMP routines required by OZIPP are:

```
*Subroutine PLOT (XX,YY,IX)
     "      PLOTS (XX,YY,IX)
     "      SYMBOL (XX,YY,HT,ITX,ANG,NCH)
     "      NUMBER (XX,YY,HT,FPN,ANG,NDEC)
     "      NEWPEN (IPEN)
```

For users without access to these CALCOMP routines, dummy routines may be needed in order to run OZIPP. To generate the dummy routines, the user must have the following cards for each of the above routines:

```
'SUBROUTINE_____(argument list)
'RETURN
'END
```

For users with standard CALCOMP routines, no modifications to OZIPP are required. The user should check that the five routines have the same names in their system as given above.

4.3.3 Control Language

The following runstream illustrates the Executive Control Language (ECL) necessary to execute the OZIPP program on a UNIVAC 1110 computer system:

```
@RUN,   priority, job, account, userid, time
@ASG,A  prog-file
@PLOT   plotfile.
@XQT    prog-file.abselement
card input deck
@FREE   PLOTFILE.
@SYM    PLOTFILE.,,PLOT
@FIN
```

where:

priority	=	job priority
jobid	=	six-character job identification
account	=	user account number
userid	=	user identification code
time	=	time requirement for executing the job
prog-file	=	name of program file containing the OZIPP absolute element
plotfile	=	a CALCOMP-produced file that contains the controls for constructing the plot on an off-line plotter
card input deck	=	the input option cards

Note that the job control language will be different for most computer systems, but the basic requirements for running OZIPP are the same.

5.0 EXAMPLE OZIPP RUNS

In this chapter, examples demonstrating the routine functioning of OZIPP are presented. The procedures for obtaining both the standard ozone isopleth diagram and city-specific diagram are illustrated. Input and output data for each type of run are described. These examples can be used as installation test cases. Because of the internal precision associated with various computer systems, comparisons between results obtained using two different computing systems may show slight numerical differences. However, these differences should not exceed one percent.

One important application of the city-specific OZIPP is to estimate control requirements for the case in which transported pollutant concentrations in the future are expected to be reduced. An example of how OZIPP is used with the EKMA technique for this situation is presented in Section 5.3.

OZIPP was designed to handle a wide variety of isopleth diagrams, but there may be some sets of conditions that cause unusual plots (e.g., wavy isopleths, uneven spacing of isopleths, etc.) In some cases, such plots can be modified by altering the tension factor. This is illustrated in Section 5.4.

5.1 THE STANDARD OZONE ISOPLETH DIAGRAM

The standard ozone isopleth diagram is produced by using all default values as input. Sixty-two simulations are performed in all, with 5 simulations performed on each of eleven radials. Seven additional simulations are performed as described in Section 2.3.

5.1.1 Input Data For Standard Diagram Example

Because all input data are set to default conditions to produce the standard ozone isopleth diagram, only one option needs to be activated - the ISOPLETH option. However, in this example, it is assumed that a CALCOMP plot of the standard diagram is also to be produced, with a grid system overlaid on the diagram. Figure 5-1 shows the input data necessary to produce such a standard diagram.

FIGURE 5-1. INPUT DATA FOR STANDARD OZONE ISOPLETH DIAGRAM EXAMPLE

```
PLOT                1.0       5.1       3.6       0.06      .042
ISOP
blank card
```

The PLOT option activates the off-line plotting software. The "1.0" is entered in the second numeric field on that card (i.e., Columns 21-30). This parameter causes gridded lines of different color to be overlaid on the diagram. If no overlay is desired, the "1.0" should not be entered on the card. The remaining parameters on the PLOT card set the lengths of the abscissa and ordinate, the size of the characters, and the size of the labels. (The size of the plot produced with these parameters is roughly 60 percent of the size produced with default values). If only a line-printer plot is desired, the PLOT option card should be removed from the input data.

The ISOPLETH card causes OZIPP to perform the sixty-two simulations with default simulation conditions (since no default conditions were overridden except for the PLOT option) and to produce the standard ozone isopleth diagram. The blank card at the end of the input deck is required for all runs. It terminates the program after processing all options.

5.1.2 Program Output For Standard Diagram Example

The output for the standard diagram run is presented in Appendix D. The output from this run consists of three parts. The first part contains a header page describing the conditions used for the simulations. Assumptions about location, time of year, dilution and reactivity are all summarized.

The second part of the output presents the simulation results. For each simulation, the initial NMHC and NO_x concentration, the initial NMHC/NO_x ratio and the calculated maximum one-hour average ozone concentration are printed. In some simulations, the ozone concentration rises throughout the 10-hour simulation period. If this condition is encountered in a simulation, "NOT MAX" is printed next to the ozone value.

The final part of the output is the ozone isopleth diagram. A line-printer plot is always produced. The off-line diagram produced as a result of activating the PLOT option is also shown in Appendix D.

5.2 EXAMPLE CITY-SPECIFIC DIAGRAM

In developing a city-specific isopleth diagram, there are two important factors to consider. The first involves estimating city-specific parameters (such as emissions, dilution and transport conditions) that are representative of the city of interest. The second involves setting the other OZIPP input parameters so that a diagram is obtained which is suitable for use with the EKMA method. In this section, procedures for addressing both of these problems are illustrated through the use of an example problem.

5.2.1 Determination of City-Specific Parameters

The assumptions made for the city-specific parameters used in the example problem are described below. The primary guide to be used in formulating these parameters for any particular city is Appendix B of Reference 1. Some of the information presented in Reference 1 has been repeated here to illustrate the procedures to be used in developing city-specific information.

A. Light Intensity Data

The OZIPP model requires information on city location and day of the year to calculate the diurnal variation of photolytic rate constants. Latitude and longitude for city center are used to specify the city location. The date used should be the day on which the design ozone concentration occurs. (The design value of ozone is normally defined as the highest second-high hourly ozone concentration measured in or near a city. The reader is referred to Reference 1 for more details.) For the example problem, a latitude of 39.0 and a longitude of 77.0 were selected. Because this latitude and longitude fall in the Eastern Time Zone, the Numerical Time Zone of 5.0 corresponding to Eastern Daylight Time was chosen (see Section 3.2.1). The design ozone concentration was assumed to have been measured on August 1, 1977.

B. Dilution Data

To account for dilution effects, the OZIPP model requires data on a minimum mixing height, a maximum mixing height, the time at which the mixing

height rise begins and the time at which it ends. Ideally, these data should be based on observations taken on the day being modeled. However, it is usually necessary to use some other indicators of these data. For example, a suitable surrogate for the design day data is median data based on days with high ozone levels. Often, the only data available are seasonal mean morning and afternoon mixing heights as provided in Reference 10. If no local information is available on the time of day during which the mixing height is increasing, it may be assumed that increases in mixing height typically occur between 0800 and 1500 LDT. For the example problem, data from Reference 10 for the Washington, D. C. area were used. The morning mixing height was assumed to be 425 meters, and the afternoon height 1900 meters. The mixing height rise was assumed to take place over a seven hour period beginning at 0800 LDT.

C. Post-0800 Emissions Data

If it is desired to include the effects of post-0800 emissions, information on relative emission rates must be input. Relative emission rates express the rate of emissions injected into the imaginary column of air for each hour of simulation relative to emissions into the air column prior to the 0800 LDT simulation starting time. The emissions prior to 0800 are represented by the initial NMHC and NO_x concentrations. Post-0800 emissions are represented by additions to these precursor concentrations.

Relative emission rates are required for each hour of simulation. A rigorous calculation would require a precise specification of: (1) the location of the column, (2) the spatial variation in emissions and (3) the temporal variation in emissions. Unfortunately, these data are not often available and the task then becomes one of deriving reasonable approximations with the data that are available. The most practical approach is then to roughly approximate the spatial and temporal variations in emissions along a hypothetical column trajectory. One such approach is described below. However, the assumptions and values discussed below are included primarily for illustrative purposes. City-specific information should be used wherever possible.

An estimation of relative emission rates may be made assuming column trajectories that move from the center of the city to the urban limit. As the column moves away from the center of the city, emissions into it typically decrease. One formulation that can be used to depict the decrease of emissions with distance from the center of the city is:

$$e_s = Q_0 \exp(-ax^2)$$

where

e_s = emissions at location s

Q_0 = the emissions in the center of the city

a = constant (may relate to the wind speed or speed at which the column is moving)

x = the distance the column has moved from the center of the city

This spatial pattern is in the form of a Gaussian distribution as discussed in Reference 1. (Other types of distributions may be postulated.) For the example problem, the spatial distribution of emissions was determined using the same assumptions as used in Reference 1: (1) the column leaves the center of the city at 0800 LDT and moves at constant velocity until it leaves the urban area three hours later; and (2) the emissions at the edge of the urban area are e^{-2} (approximately 0.14) of the emissions in the center of the city. An estimate of the average emissions for each hour was made by calculating the emissions at the mid-point of each hour (e.g., 0830 for the hour from 0800 to 0900). The second column of Table 5-1 shows the results of these calculations. These spatial adjustment factors are the hourly factors expressing the emissions at the location of the column relative to the emissions in the center city.

After the spatial distribution of emissions has been determined, the temporal distribution is required. In the absence of site-specific information, a city-wide average may be used. This distribution may be calculated as

TABLE 5-1. EXAMPLE OF ESTIMATION OF EMISSIONS FRACTIONS FOR OZIPP

Time (LDT)	Spatial Adjustment		Percent of Day's Emissions		Composite Relative Emission Rate (percent)	Normalized Relative Emission fraction*
12 - 8 a.m.	1.0	x	16.9	=	16.9	1.0
8 - 9 a.m.	0.95	x	6.4	=	6.1	.36
9 - 10 a.m.	0.61	x	4.4	=	2.7	.16
10 - 11 a.m.	0.25	x	4.8	=	1.2	.07
after 11 a.m.	negligible		---		negligible	negligible

* The composite relative emission rate normalized relative to the 0800 composite rate. These are the input values for OZIPP.

Source: Reference 1.

the average of the temporal distribution of mobile and stationary sources. In some cases, the temporal distribution of automotive emissions may be an adequate representation of the temporal distribution of the total emissions. The distribution used for the example problem was taken from Reference 1, and is shown in the third column of Table 5-1.

To obtain the relative emissions for input to OZIPP, the spatial and temporal factors are multiplied and then normalized to the initial emissions. These processes are presented in Columns 4 and 5 in Table 5-1. The fractions in the last column were used as input for the example problem.

D. Transported Pollutant Data

For a detailed discussion of pollutant transport as it relates to EKMA, the reader is referred to Reference 1. Normally, estimates of pollutants transported into the area of interest are based on measurements taken upwind of the city. Recall that transport of three types of pollutants (NMHC, NO_x and ozone) can be considered in two layers - the surface layer and the air above the base of a nocturnal inversion layer. For the example problem, it was assumed that ozone was transported aloft with a concentration of 0.10 ppm. The concentrations of the other pollutants were assumed negligible.

E. Reactivity Data

In Reference 1, it is recommended that the default reactivity factors not be altered. This recommendation is based on two premises:

1) sensitivity studies have indicated that the maximum calculated ozone concentration is relatively insensitive to the NO_2/NO_x mix, and

2) limited knowledge exists about the mix of organic species in urban areas and it is very difficult to estimate the equivalent combination of propylene and n-butane.

For the example run, all reactivity factors, consequently, were left at the default values.

5.2.2 Diagram Definition

The basic data needed to use an ozone isopleth diagram with EKMA are an NMHC/NO_x ratio and an observed one-hour average ozone concentration. The optimal diagram arrangement is one in which the observed NMHC/NO_x ratio is near the diagonal of the diagram and the ozone isopleth corresponding to the observed ozone design value is in the upper right quadrant of the diagram. The isopleth lines should be fairly evenly spaced and spread across the diagram, rather than in one corner or along an edge. Even spacing and coverage provides optimal utilization of the OZIPP algorithm.

The basic procedure recommended for determining the appropriate maximum NMHC and NO_x initial concentrations and the isopleth levels for the diagram is one of trial and error. It should be remembered that all isopleth diagrams in OZIPP are plotted with 10 horizontal scale divisions and 7 vertical ones. Consequently, it may be advisable to choose an NO_x maximum evenly divisable by 7. One way to test for the appropriate scale is to use the CALCULATE option to calculate the maximum ozone concentrations associated with potential NMHC and NO_x diagram maxima. The combination of NMHC and NO_x maxima to use in the run creating the diagram is one which will result in the ozone design value being located in the upper right quadrant of the diagram. The concentrations for the isopleths may be altered from the default values, depending on the calculated maximum ozone concentration. For example, if the calculated maximum ozone concentration were 0.20 ppm, isopleth values much greater than this could be replaced with lower values in order to obtain better diagram resolution.

The above procedure can be illustrated with the example problem. Assume that the design NMHC/NO_x ratio is 5.0 and the design ozone concentration is 0.16 ppm. A single OZIPP run was made using multiple CALCULATE options to test possible NMHC and NO_x maxima. Because the NO_x scale is divided into seven equal increments, the NO_x values selected were all even multiples of 0.07. (Using one of these values will produce a graph that is easy to read.) The NMHC value corresponding to each of the potential NO_x maxima was chosen

such that the NMHC/NO_x ratio was approximately equal to the design value and the NMHC scale would be easy to read. The results of the simulations performed to test the maxima are summarized below:

NO_x	NMHC	NMHC/NO_x	Maximum Ozone
.42	2.0	4.8	.30
.35	1.8	5.1	.28
.28	1.5	5.4	.25
.21	1.0	4.8	.21
.14	0.7	5.0	.17

The maxima selected for use in producing the isopleth diagram were 0.21 and 1.0 for NO_x and NMHC, respectively. These values will result in the design ozone concentration being located in the upper right quadrant of the diagram.

5.2.3 Input Data For City-specific Example

The input data for the example city-specific run are shown in Figure 5-2. Several options have been included for illustrative purposes. The input data are set up to perform two single simulations and then to construct an isopleth diagram using the ISOPLETH option.

The first option causes the default title to be replaced by the title on the next card, i.e., "CITY-SPECIFIC EXAMPLE". All output is labeled with this title.

The PLACE option is used to override the default location and day of year. The first two numeric fields contain the latitude and longitude for the example city. The next numeric field contains the time zone indicator. The city is assumed to be in the Eastern Time Zone, so 5.0 is entered as the numerical time zone (see Section 3.2.1). The next three fields contain the year, month and day - August 1, 1977. The card following the PLACE option contains the name of the example city.

FIGURE 5-2. INPUT DATA FOR CITY-SPECIFIC DIAGRAM EXAMPLE

```
TITL
CITY-SPECIFIC EXAMPLE
PLAC          39.0        77.0        5.          1977.          8.          .1.
TEST RUN CITY
DILU          425.0       1900.0
EMIS          3.0         0.36        0.16        0.07
TRAN                      0.10
ALRE          4.
0.0           0.0          .06229
0.0           0.14         .04664
0.7           0.14         .17315
0.7           0.0          .06774
PLOT                                  5.1         3.6         0.08        0.06
CALC          1.0         0.21
CALC          1.0         0.21        1.0
ISOP          0.7         0.14        6.0         1.0
.06            .08         .10        0.12        0.14        0.16
blank card
```

The data on dilution is entered by using the DILUTION option card. The morning and afternoon mixing heights are entered in the first two numeric fields. Because no other entries are made on this card, the starting time and ending time of the inversion rise will remain at default values, namely 0800 and 1500 LDT, respectively.

The emissions data are entered via the EMISSIONS option card. The first numeric field indicates that emissions data are input for the first three hours of the simulation. The next three numeric fields contain the relative emission fractions. Note that, because the number of hours coded in the second numeric field is positive, the relative emission fractions apply to both NMHC and NO_x.

The TRANSPORT option card is used to enter the data on transported pollutant concentrations. The concentration of ozone transported aloft (0.10 ppm) is input in the second numeric field. Because all other fields are left blank, the concentrations of all other transported pollutants remain at default levels (i.e., zero).

The ALREADY option has been included simply to illustrate its use. The 4.0 entered in the first numeric field indicates that the results of 4 simulations are to be input. Note that these simulations must be input in the order that they would normally occur in the run, starting with the first. (In other words, if there are 10 input simulations, they must be the 1st through the 10th). The 4 cards following the ALREADY option contain the previous simulation results. On each card, the first field (i.e., Columns 1-10) contains the initial NMHC concentration, the second field the initial NO_x concentration, and the third field the maximum-one-hour ozone concentration.

The PLOT option activates the off-line plotting software. The lengths of the abscissas and ordinate of the diagram are set to 5.0 inches and 3.6 inches by the entries in the third and fourth numeric fields of this card. The other parameters control the size of the characters and labels on the graph.

The first CALCULATE option results in one particular simulation being performed with initial NMHC and NO_x concentrations of 1.0 ppmC and 0.21 ppm, respectively. The second CALCULATE option produces the same simulation. In this case, however, the information option is activated by entering "1.0" in the third numeric field. The detailed information is to be printed for hourly intervals because the fourth and fifth numeric fields have been left blank and the default values are used (see Table 4-1).

The final option, ISOPLETH, causes an ozone isopleth diagram to be produced. The first two numeric fields contain the maximum NMHC and NO_x initial concentrations for the diagram (0.7 ppmC and 0.14 ppm, respectively). The 6.0 coded in the third numeric field indicates that 6 isopleths are to be drawn on the diagram. The isopleth levels themselves are entered on the next two cards. The positive number coded in the fourth numeric field activates the printing of solar noon and the time of the center of the maximum one-hour average ozone concentration.

Again, note that the ordering of the option cards is unimportant, except that the ISOPLETH and CALCULATE cards must come after all other options have been activated. Data cards (i.e., those without a code word in the first field) must be in the order specified in Table 4-1. Also, default values will be assumed for any numeric field left blank.

5.2.4 Program Output For City-specific Example

Anpendix E contains all the program output for the city-specific example. First, the ALREADY option causes the input simulation results to be reprinted in tabular form. The first CALCULATE option produces three pages of output. The first page is a tabular summary of the simulation conditions. The second table gives instantaneous pollutant concentrations at hourly intervals. The maximum one-hour average ozone concentration is printed at the bottom of the table. The last page of output produced by this option is a graph of instantaneous ozone concentration versus time.

The second CALCULATE card has the informtion option activated and thus produces much more output. First, the table summarizing the simulation conditions is produced. A table is then printed giving the rate constants for each of the 76 reactions. Thirdly, a set of tables produces information on the instantaneous concentrations of all reactant species, their net rates of change, and the rates of all 76 reactions. For the example problem, such a table is produced at each hour of the simulation. Finally, a graph of ozone versus time is printed.

The ISOPLETH option produces three types of output. As with the CALCULATE option, a table summarizing the simulation conditions is first produced. Next, the results of each simulation are presented in tabular form. Note that the first simulation called for by the ISOPLETH option begins at the point where the simulations from the previous run ended (i.e., those entered using the ALREADY option). Finally, a line-printed plot of the ozone isopleth diagram is printed. Activation of the PLOT option along with the ISOPLETH option results in the off-line plot reproduced in Appendix E.

The conditions that produced this isopleth diagram led to some wiggles in the isopleth lines. The explanation for these wiggles is that these conditions produce two ozone peaks in the simulations. The first typically occurs after about 400 minutes of simulation, and the second near the termination of the simulation at 600 minutes. For low NMHC/NO_x ratios (the upper part of the isopleth diagram), the first maximum is always smaller than the second. But for high NMHC/NO_x ratios, the first maximum is larger. Near the diagonal, the two maxima are nearly equal. Thus, the isopleth diagram is really two diagrams superimposed. The area just above the diagonal is where the "first-peak" diagram is joined to the "second-peak" diagram.

This conclusion was reached after performing several simulations near the wiggles to ensure that these wiggles are not artifacts of interpolation. Another diagram for the same conditions, but with more calculations using the ACCURACY option, showed the same wiggles.

5.3 EXAMPLE TRANSPORT PROBLEM

An important application of the city-specific OZIPP is to estimate emission control requirements for the case in which future transported pollutant concentrations will be significantly different from current levels. Such a situation might occur as a result of the imposition of control measures upwind of the city of interest. The procedure of using OZIPP with the EKMA technique for this case is explained fully in Reference 1. An example transport problem is presented below to illustrate the technique.

For the example problem presented in Section 5.2, it was assumed that the concentration of ozone transported aloft was 0.10 ppm. It was also assumed that the design ozone value was 0.16 ppm and the design NMHC/NO_x ratio was 5.0. For the example transport problem, the following additional assumptions will be made:

1) NO_x concentrations will remain unchanged
2) ozone transported aloft will be reduced from 0.10 to 0.04 ppm
3) the air quality goal is 0.08 ppm.

The problem is then to estimate the reduction in NMHC concentrations required to meet the air quality goal.

The first step in the EKMA procedure is to generate the ozone isopleth diagram for the existing situation (i.e., 0.10 ppm ozone transported aloft). This is demonstrated in Section 5.2, and the diagram is shown in Figure E-3. The next step is to generate the isopleth for the air quality goal (i.e., 0.08 ppm) incorporating the assumption about future transported concentrations. This is accomplished by modifying only the TRANSPORT and ISOPLETH options of the input data that were used in the example problem in Section 5.2. The ozone transported aloft is changed from 0.10 to 0.04 ppm. The ISOPLETH option is modified to plot only the 0.08 ppm isopleth. The diagram generated by OZIPP with these modifications is shown in Figure 5-3.

The EKMA technique can now be applied to the problem. (For details of this procedure, see Reference 1.) The base initial NMHC and NO_x concentrations are determined by using the base case diagram (Figure E-3), the design ozone

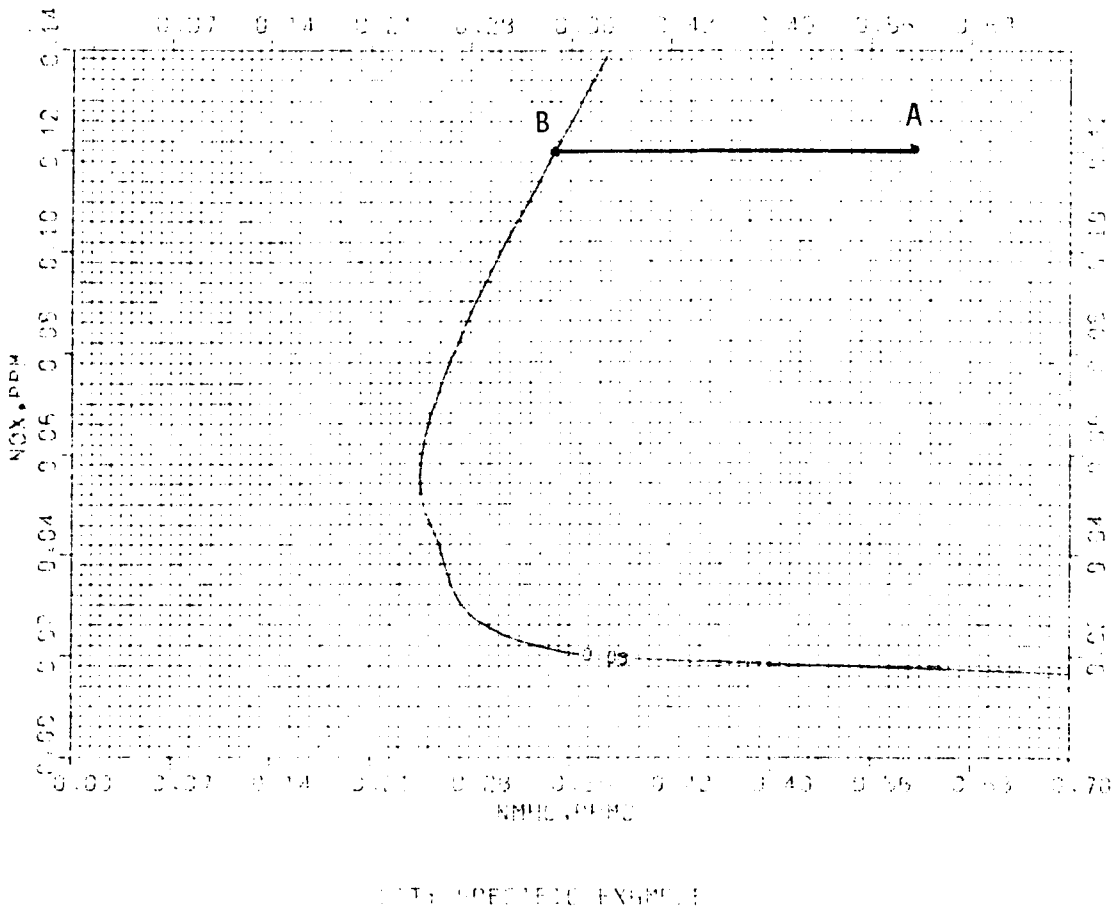

FIGURE 5-3. Example City-specific Diagram for Reduced Transport Case.

value and the NMHC/NO_x ratio. For this problem, the base initial NMHC concentration is .60 ppmC, and the base initial NO_x concentration is 0.12 ppm. This coordinate is then plotted on the new diagram (Point A on Figure 5-3). The NMHC reduction necessary to achieve the air quality goal is then represented by the line AB on Figure 5-3 (i.e., NMHC concentrations must be reduced from 0.6 ppmC to 0.34 ppmC, amounting to a NMHC reduction of 43 %).

5.4 USE OF THE TENSION FACTORS

In certain instances the user may have to plot ozone isopleths relatively close together on a large diagram. For example, a user may wish to plot isopleths at 0.10, 0.11 and 0.12 ppm on an isopleth diagram that has large maximum initial NMHC and NO_x concentrations. This may cause the isopleths to be squeezed close together. An example of such an isopleth is shown in Figure 5-4. Note in this figure that the 0.06 and 0.08 ozone isopleths almost touch.

To rectify this situation, the user can increase the second stage tension factor on the ACCURACY card. This causes partial straightening of the curve between the points used to draw the isopleths. For example, a second run was done (with the ALREADY option to save computing time) using a tension factor of 10.0 (see Figure 5-5). Note that the isopleths are now more evenly spaced in Figure 5-5 than in Figure 5-4. The input deck for the run with the default tension factor was:

```
EMIS    8.0     0.22    0.22    0.21    0.22    0.22
0.22    0.23    0.25
PLOT
ISOP                    12.0    1.0
0.06    0.08    0.12    0.16    0.20    0.24    0.28
0.30    0.32    0.34    0.36    0.40
blank card
```

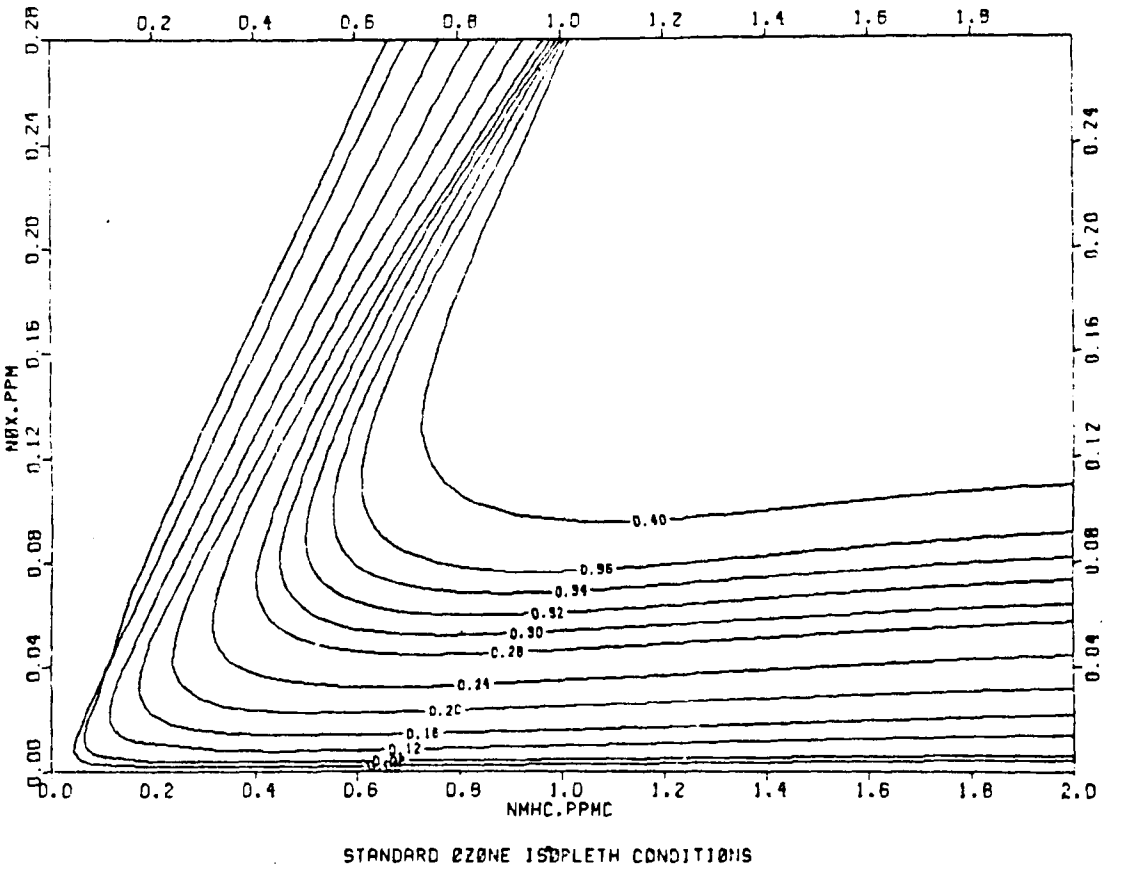

FIGURE 5-4. Isopleth Diagram with Default Tension Factor Showing Touching Isopleths

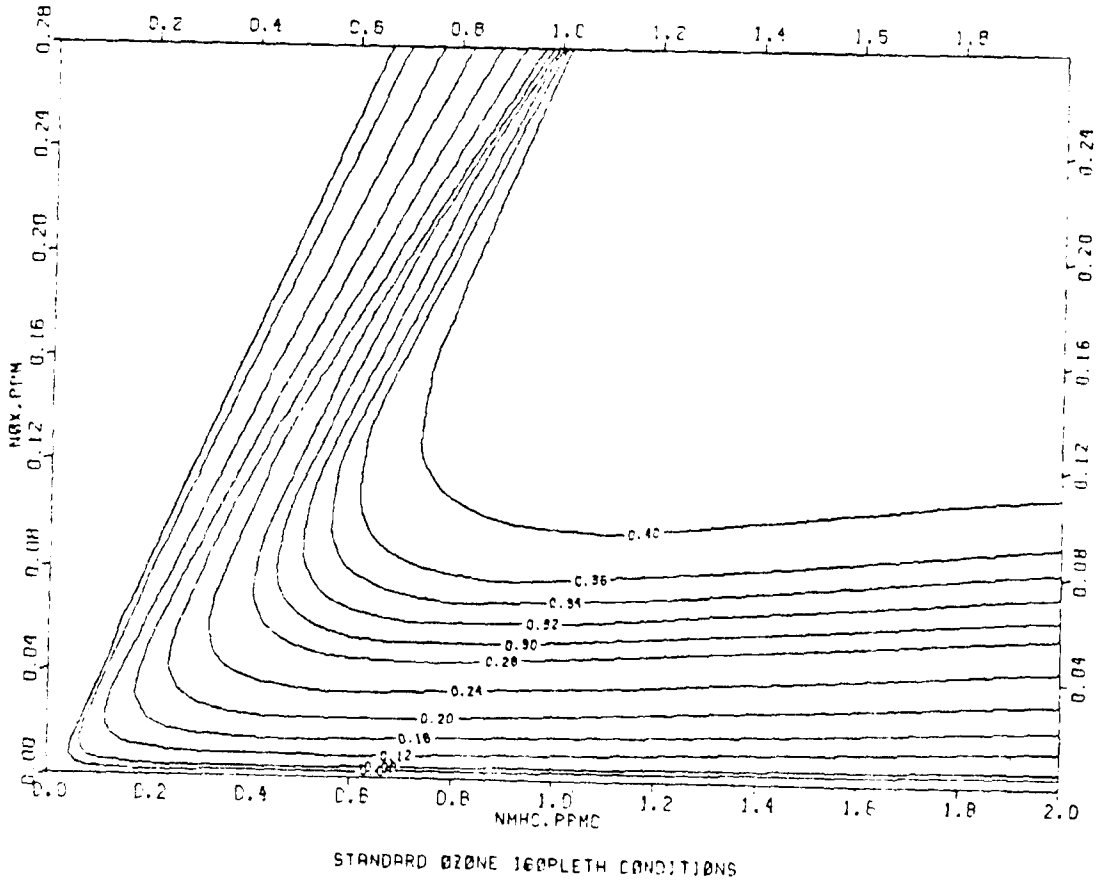

FIGURE 5-5. Isopleth Diagram with Increased Tension Factor To Eliminate Touching Isopleths

The input deck for the run with the tension factor of 10.0 was:

```
EMIS      8.0       0.22      0.22      0.21      0.22      0.22
0.22      0.23      0.25
ACCU                                                        10.0
ALRE     61.0
0.        0.        0.
 .
 .
 .
2.0        .00635    .07837
PLOT
ISOP                          12.0      1.0
0.06      0.08      0.12      0.16      0.20      0.24      0.28
0.30      0.32      0.34      0.36      0.40
blank card
```

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APPENDIX A

KINETIC MECHANISM USED IN OZIPP

APPENDIX A

KINETIC MECHANISM USED IN OZIPP

Number	Reaction	Rate Constant*
1	$NO_2 + h\nu \rightarrow NO + O(^3P)$	k_{vary}
2	$O(^3P) + O_2 + M \rightarrow O_3 + M$	2.0×10^{-5} $ppm^{-2}min^{-1}$
3	$O_3 + NO \rightarrow NO_2 + O_2$	25.0
4	$NO_2 + O_3 \rightarrow NO_3 + O_2$	0.045
5	$NO_2 + O(^3P) \rightarrow NO + O_2$	1.3×10^4
6	$NO_3 + NO \rightarrow 2NO_2$	1.3×10^4
7	$NO_2 + NO_3 \rightarrow N_2O_5$	5.6×10^3
8	$N_2O_5 \rightarrow NO_2 + NO_3$	$22.0\ min^{-1}$
9	$N_2O_5 + H_2O \rightarrow 2HNO_3$	2.5×10^{-6}
10	$NO + NO_2 + H_2O \rightarrow 2HONO$	1.0×10^{-9} $ppm^{-2}min^{-1}$
11	$2HONO \rightarrow NO + NO_2 + H_2O$	1.0×10^{-3}
12	$HONO + h\nu \rightarrow OH + NO$	k_{vary}
13	$OH + NO_2 \xrightarrow{M} HNO_3$	8.0×10^3
14	$OH + NO \xrightarrow{M} HONO$	3.0×10^3
15	$HO_2 + NO \rightarrow NO_2 + OH$	1.2×10^3
16	$HO_2 + HO_2 \rightarrow HOOH + O_2$	8.4×10^3
17	$HOOH + h\nu \rightarrow 2OH$	k_{vary}
18	$O_3 + h\nu \rightarrow O(^1D)$	k_{vary}
19	$O_3 + h\nu \rightarrow O(^3P)$	k_{vary}
20	$O(^1D) + M \rightarrow O(^3P) + M$	8.7×10^4
21	$O(^1D) + H_2O \rightarrow 2OH$	5.1×10^5

Number	Reaction	Rate Constant*
22	$OH + O_3 \rightarrow HO_2 + O_2$	84.0
23	$O_3 + HO_2 \rightarrow OH + 2O_2$	2.4
24	$PROP + OH \rightarrow ADD$	2.5×10^4
25	$ADD + NO \rightarrow X + NO_2$	1.0×10^3
26	$ADD + ADD \rightarrow 2X$	1.2×10^4
27	$ADD + MeO_2 \rightarrow X + MeO$	1.0×10^3
28	$ADD + C_2O_2 \rightarrow X + C_2O$	1.0×10^3
29	$ADD + C_3O_2 \rightarrow X + C_3O$	1.0×10^3
30	$X \rightarrow HCHO + ALD2 + HO_2$	1.0×10^5 min^{-1}
31	$PROP + O_3 \rightarrow OH + HO_2 + ALD2$	8.0×10^{-3}
32	$PROP + O_3 \rightarrow OH + C_2O_3 + HCHO$	8.0×10^{-3}
33	$BUT + OH \rightarrow ScO_2$	1.8×10^3
34	$BUT + OH \rightarrow C_4O_2$	1.8×10^3
35	$NO + C_4O_2 \rightarrow NO_2 + C_4O$	1.8×10^3
36	$NO + ScO_2 \rightarrow NO_2 + ScO$	1.8×10^3
37	$NO + C_3O_2 \rightarrow NO_2 + C_3O$	1.8×10^3
38	$NO + C_2O_2 \rightarrow NO_2 + C_2O$	1.8×10^3
39	$NO + MeO_2 \rightarrow NO_2 + MeO$	1.8×10^3
40	$C_4O \rightarrow HCHO + C_3O_2$	7.5×10^4 min^{-1}
41	$ScO \rightarrow ALD2 + C_2O_2$	1.0×10^5 min^{-1}
42	$C_3O \rightarrow HCHO + C_2O_2$	8.0×10^3 min^{-1}
43	$C_2O \rightarrow HCHO + MeO_2$	4.0×10^3 min^{-1}
44	$C_4O + O_2 \rightarrow ALD4 + HO_2$	0.7
45	$ScO + O_2 \rightarrow MEK + HO_2$	1.4

Number	Reaction	Rate Constant*
46	$C_3O + O_2 \rightarrow$ ALD3 + HO_2	0.5
47	$C_2O + O_2 \rightarrow$ ALD2 + HO_2	0.4
48	MeO + $O_2 \rightarrow$ HCHO + HO_2	0.4
49	HCHO + hν → Stable Products	k_{vary}
50	HCHO + hν → $2HO_2$	k_{vary}
51	HCHO + OH → HO_2	1.5×10^4
52	ALD2 + hν → Stable Products	4.2×10^{-6} min^{-1}
53	ALD2 + hν → MeO_2 + HO_2	k_{vary}
54	ALD2 + OH → C_2O_3	1.5×10^4
55	ALD3 + hν → Stable Products	6.0×10^{-5} min^{-1}
56	ALD3 + hν → C_2O_2 + HO_2	2.5×10^{-3} min^{-1}
57	ALD3 + OH → C_3O_3	4.5×10^4
58	ALD4 + hν → Stable Products	6.0×10^{-5} min^{-1}
59	ALD4 + hν → C_3O_2 + HO_2	1.9×10^{-3} min^{-1}
60	ALD4 + OH → C_4O_3	4.5×10^4
61	ADD + C_4O_2 → X + C_4O	1.0×10^3
62	ADD + ScO_2 → X + ScO	1.0×10^3
63	C_4O_3 + NO → C_3O_2 + NO_2	8.0×10^2
64	C_3O_3 + NO → C_2O_3 + NO_2	8.0×10^2
65	C_2O_3 + NO → MeO_2 + NO_2	8.0×10^2
66	C_4O_3 + NO_2 → PAN	1.0×10^2
67	C_3O_3 + NO_2 → PAN	1.0×10^2
68	C_2O_3 + NO_2 → PAN	1.0×10^2

Number	Reaction	Rate Constant*
69	$C_4O_2 + HO_2 \rightarrow$ Stable Products	4.0×10^3
70	$C_3O_2 + HO_2 \rightarrow$ Stable Products	4.0×10^3
71	$ScO_2 + HO_2 \rightarrow$ Stable Products	4.0×10^3
72	$C_2O_2 + HO_2 \rightarrow$ Stable Products	4.0×10^3
73	$MeO_2 + HO_2 \rightarrow$ Stable Products	4.0×10^3
74	$C_4O_3 + HO_2 \rightarrow$ Stable Products	4.0×10^3
75	$C_3O_3 + HO_2 \rightarrow$ Stable Products	4.0×10^3
76	$C_2O_3 + HO_2 \rightarrow$ Stable Products	4.0×10^3

* Units of $ppm^{-1}min^{-1}$ unless otherwise indicated

Source: Dodge (1977).

Symbol	Definition
k_{vary}	Diurnal 1-hour average photolytic rate constant
PROP	C_3H_6
BUT	$n\text{-}C_4H_{10}$
ADD	$CH_3CH(OH)CH_2OO$
X	$CH_3CH(OH)CH_2O$
MeO_2	CH_3O_2
C_2O_2	$CH_3CH_2O_2$
C_3O_2	$CH_3CH_2CH_2O_2$
C_4O_2	$CH_3CH_2CH_2CH_2O_2$
ScO_2	$CH_3CH(O_2)CH_2CH_3$
ALD2	CH_3CHO
ALD3	CH_3CH_2CHO

Symbol	Definition
ALD4	$CH_3CH_2CH_2CHO$
C_2O_3	CH_3CO_3
C_3O_3	$CH_3CH_2CO_3$
C_4O_3	$CH_3CH_2CH_2CO_3$

APPENDIX B

PROGRAM SOURCE LISTINGS

APPENDIX B

PROGRAM SOURCE LISTINGS

```
      COMMON /CALC/ NR,KR(77,3),A(77),S(77),R(77),ITYPE(77),IA(34),JA(21 A     2
     18),DILUT,TEMP,ERR,START,STOPP,SPECIS(34),TPRNT,TSTEP              A     3
      COMMON /CNTRL/ SIG,SIGMA,INFO,NPTO,XNF,RCTY,ALDX,OZIN,OZAL,HCIN,HC A     4
     1AL,XNIN,XNAL,TSRT,DTIM,Z1,Z2,DCON,EHC,EXN,FLST,TLST               A     5
      COMMON /EMIS/ NEM,EM(11),EMHC(11),EMNOX(11),ESTRT(2),ESTOP,ESLP,EH A     6
     1SLP,ENSLP,EC(38),ECHC(38),ECXN(38)                                A     7
      COMMON /INOUT/ IN,IOUT,ITAPE                                      A     8
      COMMON /TITL/ ITTL(18)                                            A     9
      COMMON /PLTVEC/ HCT(20),OT(20),NT,OHC,HCG,PLTGRD,OXN,XNG,HC1,XN1,T A    10
     1ICZ,DIGZ,CHRZ                                                     A    11
      COMMON /VVLBL/ FCTR,DIST,CHRSIZ,NNCHR,OZBL                        A    12
      COMMON /NEED/ HC,XN,NL,NRTO,RTO(20),OZP(20),OZN(8,20),RHO(8,20),NR A    13
     1,OC(4),OS(2),HCS,XNS,LS,HCLL(8)                                   A    14
      COMMON /HOUR/ OZN,NGO,TM                                          A    15
      COMMON /SUNLIT/ XJ(47,10),SIGMO(31,10),PHI(31,10),Z(10),RTCON(10), A    16
     1LAMI,INC,SLA,SLO,TZ,IY,IM,ID,ISTRT,ISTOP,IINC,IEND,SPECIE,MAXZ,ITI A    17
     2ME(13),XZ(13),K(13),JSTRT,JSTOP,SPEC(11),MNLM(11),MXLM(11),MAXL,MA A    18
     3XJ                                                                A    19
      DIMENSION F(21), X(6), PLACE(6)                                   A    20
      DIMENSION NRTC(76), XRTC(76)                                      A    21
      DATA ISPD/4HISOP/,ICAL/4HCALC/,IACR/4HACCU/,IDIL/4HDILU/,IPLC/4HPL A    22
     1AC/,IEMS/4HEMIS/,IRDY/4HALRE/,IBLK/4H     /,IPLT/4HPLOT/,ITRN/4HTRA A    23
     2N/,ITIT/4HTITL/,IRCT/4HREAC/                                      A    24
C  SET DEFAULTS                                                        A    25
      DATA HC/2.0/,XN/0.28/,NL/11/,NC/11/,NR/5/                         A    26
      DATA ITTL/4HSTAN,4HDARD,4H OZO,4HNE I,4HSOPL,4HETH ,4HCOND,4HITIO, A    27
     14HNS  ,9*4H    /                                                  A    28
      DATA IOUT/6/,KALCMP/0/,INFO/0/,NPTO/0/,KS/1/,NGO/1/               A    29
      DATA OZP/.08,.12,.16,.20,.24,.28,.30,.32,.34,.36,.40,9*0./        A    30
      DATA TSRT/0.0/,DTIM/420./,Z1/510./,Z2/630./,DCON/0.0/             A    31
      DATA DSTRT/800./,DEND/1500./,PLTGRD/0./,OHC/0./,FCTR/0.6/,OXN/0./ A    32
      DATA CHRSIZ/0.07/,TICZ/0.07/,DIGZ/0.10/,CHRZ/0.10/,HC1/8.5/,XN1/5. A    33
     195/                                                               A    33A
      DATA SIG/1./,SIGMA/1./,RCTY/.25/,XNF/.25/,ALDX/.05/               A    34
      DATA OZIN/0./,OZAL/0./,HCIN/0./,HCAL/0./,XNIN/0./,XNAL/0./        A    35
      DATA ERR/0.01/,TEMP/303.0/,KSS/0/,KS1/0/,JS/0/                    A    36
      DATA F(21)/0.0/,ESTOP/0.0/,STOPP/600./,TPRNT/60./,TSTEP/60./      A    37
      DATA PLACE/4H LOS,4H ANG,4HELES,4H,  CA,4HLIF.,4H     /           A    38
      DATA SLA/34.058/,SLO/118.250/,TZ/8.0/,IY/1973/,IM/6/,ID/21/       A    39
      DATA IEM/0/,EMHC(1)/-3./,EMNOX(1)/-3./,NEM/0/                     A    40
      CALL PHOT (PLACE)                                                 A    41
C                                                                       A    42
C OPTIONS LOOP                                                          A    43
C                                                                       A    44
    5 READ 120, IOPT,(X(I),I=1,6)                                       A    45
      IF (IOPT.NE.ISPD) GO TO 10                                        A    46
      IF (ABS(X(1)).NE.0.) HC=X(1)                                      A    47
      IF (ABS(X(2)).NE.0.) XN=X(2)                                      A    48
      IF (ABS(X(4)).NE.0.) INFO=-1                                      A    49
      IF (ABS(X(3)).NE.0.) NL=IFIX(X(3)+0.1)                            A    51
      IF (ABS(X(3)).NE.0.) READ 130, (OZP(I),I=1,NL)                    A    52
      WRITE (IOUT,145) (ITTL(I),I=1,18)                                 A    53
      KSTOP=JSTOP-100                                                   A    54
      WRITE (IOUT,170) PLACE,SLA,SLO,TZ,IM,ID,IY,JSTRT,KSTOP            A    55
      NOON=SPECIE                                                       A    56
      IF (INFO.EQ.-1) WRITE (IOUT,175) NOON                             A    57
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      DDTRT=DSTRT                                                          A   58
      DDEND=DEND                                                           A   59
      WRITE (IOUT,180) Z1,Z2,DDTRT,DDEND                                   A   60
      WRITE (IOUT,185) RCTY,XNF,ALDX                                       A   61
      IF (OZIN+HCIN+XNIN.GT.0..OR.OZAL+HCAL+XNAL.GT.0.) WRITE (IOUT,225)   A   61A
      IF (OZIN+HCIN+XNIN.GT.0.) WRITE (IOUT,190) OZIN,HCIN,XNIN            A   62
      IF (OZAL+HCAL+XNAL.GT.0.) WRITE (IOUT,195) OZAL,HCAL,XNAL            A   63
      IF (NEM.GT.0) WRITE (IOUT,200) (I,I=1,NEM)                           A   64
      IF (NEM.GT.0) WRITE (IOUT,205) (EM(I),I=1,NEM)                       A   65
      IF (NEM.LE.-1.AND.EMHC(1).GE.-0.) WRITE (IOUT,210) (I,I=1,IEMD       A   66
      IF (NEM.LE.-1.AND.EMHC(1).GE.-0.0) WRITE (IOUT,215) (EMHC(I),I=1,I   A   67
     1EMD                                                                  A   68
      IF (NEM.LE.-1.AND.EMNOX(1).GE.-0.) WRITE (IOUT,220) (I,I=1,IEM)      A   69
      IF (NEM.LE.-1.AND.EMNOX(1).GE.-0.) WRITE (IOUT,215) (EMNOX(I),I=1,   A   70
     1IEMD                                                                 A   71
      CALL RLINE (NC,F,KS1,JS)                                             A   72
      CALL LINER (SIG,KALCMP,F)                                            A   73
      INFO=0                                                               A   74
      GO TO 5                                                              A   75
   10 IF (IOPT.NE.ICAL) GO TO 15                                           A   76
      NPTO=1                                                               A   77
      WRITE (IOUT,145) (ITTL(I),I=1,18)                                    A   78
      KSTOP=JSTOP-100                                                      A   79
      WRITE (IOUT,170) PLACE,SLA,SLO,TZ,IM,ID,IY,JSTRT,KSTOP               A   80
      NOON=SPECIE                                                          A   81
      WRITE (IOUT,175) NOON                                                A   82
      DDTRT=DSTRT                                                          A   83
      DDEND=DEND                                                           A   84
      WRITE (IOUT,180) Z1,Z2,DDTRT,DDEND                                   A   85
      WRITE (IOUT,185) RCTY,XNF,ALDX                                       A   86
      IF (OZIN+HCIN+XNIN.GT.0..OR.OZAL+HCAL+XNAL.GT.0.) WRITE (IOUT,225)   A   86A
      IF (OZIN+HCIN+XNIN.GT.0.) WRITE (IOUT,190) OZIN,HCIN,XNIN            A   87
      IF (OZAL+HCAL+XNAL.GT.0.) WRITE (IOUT,195) OZAL,HCAL,XNAL            A   88
      IF (NEM.GT.0) WRITE (IOUT,200) (I,I=1,NEM)                           A   89
      IF (NEM.GT.0) WRITE (IOUT,205) (EM(I),I=1,NEM)                       A   90
      IF (NEM.LE.-1.AND.EMHC(1).GE.-0.) WRITE (IOUT,210) (I,I=1,IEMD       A   91
      IF (NEM.LE.-1.AND.EMHC(1).GE.-0.0) WRITE (IOUT,215) (EMHC(I),I=1,I   A   92
     1EMD                                                                  A   93
      IF (NEM.LE.-1.AND.EMNOX(1).GE.-0.) WRITE (IOUT,220) (I,I=1,IEM)      A   94
      IF (NEM.LE.-1.AND.EMNOX(1).GE.-0.) WRITE (IOUT,215) (EMNOX(I),I=1,   A   95
     1IEMD                                                                 A   96
      IF (ABS(X(3)).NE.0.) INFO=1                                          A   97
      TPRNT=60.                                                            A   98
      TSTEP=60.                                                            A   99
      IF (ABS(X(4)).NE.0.) TPRNT=X(4)                                      A  100
      IF (ABS(X(5)).NE.0.) TSTEP=X(5)                                      A  101
      CALL SIM (X(1),X(2),ZN,1)                                            A  102
      IF (TM.GT.0.) WRITE (IOUT,140) ZN,TM                                 A  103
      IF (TM.LE.0.) WRITE (IOUT,165) ZN                                    A  104
      CALL LINPRT (X(1),X(2))                                              A  105
      NPTO=0                                                               A  106
      INFO=0                                                               A  107
      GO TO 5                                                              A  108
   15 IF (IOPT.NE.IACR) GO TO 20                                           A  109
      IF (ABS(X(1)).NE.0.) NC=IFIX(X(1)+0.1)                               A  110
      IF ((NC/2).EQ.((NC+1)/2)) NC=NC+1                                    A  111
      IF (ABS(X(2)).NE.0.) MR=IFIX(X(2)+0.1)                               A  112
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      IF (ABS(X(3)).NE.0.) ERR=X(3)                                          A  113
      IF (ABS(X(4)).NE.0.) SIG=X(4)                                          A  114
      IF (ABS(X(5)).NE.0.) SIGMA=X(5)                                        A  115
      IF (ABS(X(6)).NE.0.) NCO=0                                             A  116
      GO TO 5                                                                A  117
   20 IF (IOPT.NE.IPLC) GO TO 25                                             A  118
      IF (ABS(X(1)).NE.0.) SLA=X(1)                                          A  119
      IF (ABS(X(2)).NE.0.) SLO=X(2)                                          A  120
      IF (ABS(X(3)).NE.0.) TZ=X(3)                                           A  121
      IF (ABS(X(4)).NE.0.) IY=IFIX(X(4)+0.01)                                A  122
      IF (ABS(X(5)).NE.0.) IM=IFIX(X(5)+0.01)                                A  123
      IF (ABS(X(6)).NE.0.) ID=IFIX(X(6)+0.01)                                A  124
      IF (ABS(X(1)).NE.0..OR.ABS(X(2)).NE.0.) READ 160, (PLACE(I),I=1,6)     A  125
      CALL PHOT (PLACE)                                                      A  126
      GO TO 5                                                                A  127
   25 IF (IOPT.NE.IDIL) GO TO 30                                             A  128
      IF (ABS(X(1)).NE.0.) Z1=X(1)                                           A  129
      IF (ABS(X(2)).NE.0.) Z2=X(2)                                           A  130
      IF (ABS(X(3)).NE.0.) DSTRT=X(3)                                        A  131
      IF (ABS(X(4)).NE.0.) DEND=X(4)                                         A  132
      JMIN=IFIX(DSTRT)-((IFIX(DSTRT)/100)*100)                               A  133
      TMIN1=FLOAT((IFIX(DSTRT)/100)*60+JMIN)                                 A  134
      JMIN=IFIX(DEND)-((IFIX(DEND)/100)*100)                                 A  135
      TMIN2=FLOAT((IFIX(DEND)/100)*60+JMIN)                                  A  136
      DTIM=TMIN2-TMIN1                                                       A  137
      TSRT=TMIN1-480.                                                        A  138
      GO TO 5                                                                A  140
   30 IF (IOPT.NE.IEMS) GO TO 55                                             A  141
      NEM=IFIX(X(1)+0.1)                                                     A  142
      IEM=IFIX(ABS(X(1))+0.1)                                                A  143
      IF (X(1).LT.-0.999999999) GO TO 40                                     A  144
      DO 35 I=1,5                                                            A  145
   35 EM(I)=ABS(X(I+1))                                                      A  146
      IF (NEM-5.GT.0) READ 130, (EM(I),I=6,NEM)                              A  147
      CALL EMISS (NEM,EM,ESTRT(1),ESTOP,ESLP,EC)                             A  148
      EMHC(1)=-3.                                                            A  149
      EMNOX(1)=-3.                                                           A  150
      GO TO 5                                                                A  151
   40 DO 45 I=1,5                                                            A  152
   45 EMHC(I)=X(I+1)                                                         A  153
      IF (EMHC(1).LT.-0.0001) GO TO 50                                       A  154
      IF (IEM-5.GT.0) READ 130, (EMHC(I),I=6,IEM)                            A  155
      CALL EMISS (IEM,EMHC,ESTRT(1),ESTOP,EHSLP,ECHC)                        A  156
   50 READ 130, (EMNOX(I),I=1,7)                                             A  157
      IF (EMNOX(1).LT.-0.0001) GO TO 5                                       A  158
      IF (IEM-7.GT.0) READ 130, (EMNOX(I),I=8,IEM)                           A  159
      CALL EMISS (IEM,EMNOX,ESTRT(2),ESTOP,ENSLP,ECXN)                       A  160
      GO TO 5                                                                A  161
   55 IF (IOPT.NE.IPLT) GO TO 60                                             A  162
      KALCMP=1                                                               A  163
      FCTR=0.6                                                               A  164
      HC1=8.5                                                                A  165
      XN1=5.95                                                               A  166
      CHRZ=0.10                                                              A  167
      CHRSIZ=0.07                                                            A  168
      IF (ABS(X(1)).NE.0.) FCTR=X(1)                                         A  169
      PLTGRD=X(2)                                                            A  170
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      IF (ABS(X(3)).NE.0.) HC1=X(3)                                    A  171
      IF (ABS(X(4)).NE.0.) XN1=X(4)                                    A  172
      IF (ABS(X(5)).NE.0.) CHRZ=X(5)                                   A  173
      IF (ABS(X(6)).NE.0.) CHRSIZ=X(6)                                 A  174
      DIGZ=CHRZ                                                        A  174A
      TICZ=CHRSIZ                                                      A  174B
      GO TO 5                                                          A  175
   60 IF (IOPT.NE.IRCT) GO TO 65                                       A  176
      IF (ABS(X(1)).NE.0.) RCTY=X(1)                                   A  177
      IF (ABS(X(2)).NE.0.) XNF=X(2)                                    A  178
      IF (ABS(X(3)).NE.0.) ALDX=X(3)                                   A  179
      GO TO 5                                                          A  180
   65 IF (IOPT.NE.ITIT) GO TO 70                                       A  181
      READ 125, (ITTL(I),I=1,18)                                       A  182
      GO TO 5                                                          A  183
   70 IF (IOPT.NE.ITRN) GO TO 75                                       A  184
      OZIN=X(1)                                                        A  185
      OZAL=X(2)                                                        A  186
      HCIN=X(3)                                                        A  187
      HCAL=X(4)                                                        A  188
      XNIN=X(5)                                                        A  189
      XNAL=X(6)                                                        A  190
      GO TO 5                                                          A  191
   75 IF (IOPT.NE.IRDY) GO TO 115                                      A  192
      KS1=IFIX(X(1)+0.1)                                               A  193
      KK=0                                                             A  194
      JS=1                                                             A  195
      IF (KK.EQ.KS1) GO TO 5                                           A  196
      WRITE (IOUT,150)                                                 A  197
      DO 80 I=1,4                                                      A  198
      READ 130, HCC,XNN,OC(I)                                          A  199
      IF (XNN.NE.0.0) RTO1=HCC/XNN                                     A  200
      IF (XNN.EQ.0.0) RTO1=0.00000                                     A  201
      WRITE (IOUT,155) HCC,XNN,RTO1,OC(I)                              A  202
      KK=KK+1                                                          A  203
      IF (I.EQ.2) HCLL(MR)=XNN                                         A  204
      IF (I.NE.3) GO TO 80                                             A  205
      RTO(1)=RTO1                                                      A  206
      F(1)=SQRT(RTO1*RTO1+1.)                                          A  207
      RHO(MR,1)=F(1)*XNN                                               A  208
      OZN(MR,1)=OC(3)                                                  A  209
      HCE=0.98*HCC                                                     A  210
      NCE=1                                                            A  211
   80 IF (KK.EQ.KS1) GO TO 5                                           A  212
      IF (NC.EQ.1) GO TO 95                                            A  213
   85 DO 90 I=1,2                                                      A  214
      HCS=HCC                                                          A  215
      READ 130, HCC,XNS,OS(I)                                          A  216
      RTO2=HCC/XNS                                                     A  217
      WRITE (IOUT,155) HCC,XNS,RTO2,OS(I)                              A  218
      KK=KK+1                                                          A  219
      IF (KK.EQ.5) HCG=HCC                                             A  220
      IF (KK.EQ.5) OHC=OS(I)                                           A  221
      IF (KK.EQ.6) XNG=XNS                                             A  222
      IF (KK.EQ.6) OXN=OS(I)                                           A  223
   90 IF (KK.EQ.KS1) GO TO 5                                           A  224
   95 JK=MR-1                                                          A  225
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      NCR=(NC+1)/2                                                          A  226
      DO 110 I=1,NC                                                         A  227
      IF (JK+1.EQ.1) GO TO 110                                              A  228
  100 READ 130, HCC,XNN,ZN                                                  A  229
      IF (HCC.GT.HCE) NCE=NCE+1                                             A  230
      IF (JK.EQ.MR) RTO(I)=HCC/XNN                                          A  231
      IF (JK.EQ.MR) F(I)=SQRT(RTO(I)*RTO(I)+1.)                             A  232
      WRITE (IOUT,155) HCC,XNN,RTO(I),ZN                                    A  233
      IF (JK.LT.MR) GO TO 105                                               A  234
      IF (RTO(I).GT.1.02*RTO2.OR.RTO(I).LT.0.98*RTO2) GO TO 105             A  235
      RHO(MR,I)=SQRT(HCE*HCE*1.041232+XNS*XNS)                              A  236
      OZN(MR,I)=OS(2)                                                       A  237
      JK=MR-1                                                               A  238
      NCE=NCE+1                                                             A  239
      JS=JS+1                                                               A  240
  105 OZN(JK,I)=ZN                                                          A  241
      RHO(JK,I)=SQRT(HCC*HCC+XNN*XNN)                                       A  242
      IF (HCC.LE.0..AND.I.EQ.NCR) HCLL(JK)=XNN                              A  243
      KK=KK+1                                                               A  244
      IF (KK.EQ.KS1) GO TO 5                                                A  245
      JK=JK-1                                                               A  246
      IF (JK.GT.0) GO TO 100                                                A  247
      IF (NCE.EQ.(NC+1)/2) GO TO 85                                         A  248
  110 JK=MR                                                                 A  249
      GO TO 85                                                              A  250
  115 IF (IOPT.NE.IBLK) WRITE (IOUT,135) IOPT                               A  251
      IF (IOPT.EQ.IBLK) STOP                                                A  252
      GO TO 5                                                               A  253
C                                                                           A  254
C                                                                           A  255
  120 FORMAT (A4,6X,6F10.2)                                                 A  256
  125 FORMAT (18A4)                                                         A  257
  130 FORMAT (7F10.5)                                                       A  258
  135 FORMAT (1H1,24HTHE OPTIONS INSTRUCTION ,A4,21H CANNOT BE PROCESSED    A  259
     1.)                                                                    A  260
  140 FORMAT (1H0,30X,28HMAXIMUM ONE HOUR AVE OZONE =,F7.5,12H CENTERED     A  261
     1AT,F5.0,9H MINUTES.)                                                  A  262
  145 FORMAT (1H1,//,40X,18A4)                                              A  263
  150 FORMAT (1H1,//,14X,36HTHE FOLLOWING RESULTS WERE READ IN. ////1H ,    A  264
     116X,2HHC,18X,3HNOX,15X,5HRATIO,16X,5HOZONE)                           A  265
  155 FORMAT (1H0,4F20.5)                                                   A  266
  160 FORMAT (6A4)                                                          A  267
  165 FORMAT (1H0,30X,56HMAXIMUM OZONE NOT REACHED, THE LAST ONE HOUR AV    A  268
     1ERAGE WAS,F7.5,5H PPM.)                                               A  269
  170 FORMAT (1H0,//,40X,40HPHOTOLYTIC RATE CONSTANTS CALCULATED FOR,///    A  270
     1,49X,6A4,///,40X,9HLATITUDE ,F10.3,//,40X,10HLONGITUDE ,F10.3,//,4    A  271
     20X,9HTIME ZONE,F7.1,//,40X,5HDATE ,5X,3(I4,3X),//,40X,5HTIME ,7X,I    A  272
     34,3X,2HTO,3X,I4,5X,19HLOCAL DAYLIGHT TIME)                            A  273
  175 FORMAT (1H0,39X,10HSOLAR NOON,I7)                                     A  274
  180 FORMAT (1H0,//,40X,39HDILUTION DETERMINED FROM THE FOLLOWING ,//,4    A  275
     10X,17HINVERSION HEIGHTS,5X,7HINITIAL,F7.0,5X,5HFINAL,4X,F7.0,//,40    A  276
     2X,7HTIMING ,15X,5HSTART,F9.0,5X,4HSTOP,4X,F8.0)                       A  277
  185 FORMAT (1H0,//,40X,26HINITIAL PROPYLENE FRACTION,F9.3,6X,7HNO2/NOX    A  278
     1,F8.3,//,40X,25HINITIAL ALDEHYDE FRACTION,F10.3)                      A  279
  190 FORMAT (/,40X,13HSURFACE LAYER ,9X,5HOZONE,F8.3,6X,11HHYDROCARBON     A  280
     1,F7.3,4X,3HNOX,F7.3,4H PPM)                                           A  281
  195 FORMAT (/,40X,5HALOFT,17X,5HOZONE,F8.3,6X,11HHYDROCARBON,F7.3,4X,     A  282
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     13HNOX,F7.3,4H PPM)                                                    A  283
200  FORMAT (1H0,//,40X,50HCONTINUOUS EMISSIONS (EXPRESSED AS THE FRACT A  284
     1ION OF,//,40X,54HINITIAL NON-BACKGROUND CONCENTRATION EMITTED PER  A  285
     2HOUR),//,40X,4HHOUR,3X,10I6)                                       A  286
205  FORMAT (1H0,39X,8HFRACTION,10F6.3)                                  A  287
210  FORMAT (1H0,//,40X,58HCONTINUOUS EMISSIONS (EXPRESSED AS THE FRACT A  288
     1ON OF INITIAL,//,40X,58HNON-BACKGROUND HYDROCARBON CONCENTRATION E A  289
     2MITTED PER HOUR),//,40X,4HHOUR,3X,10I6)                            A  290
215  FORMAT (1H0,39X,8HFRACTION,10F6.3)                                  A  291
220  FORMAT (1H0,//,40X,58HCONTINUOUS EMISSIONS (EXPRESSED AS THE FRACT A  292
     1ION OF INITIAL,//,40X,50HNON-BACKGROUND NOX CONCENTRATION EMITTED  A  293
     2PER HOUR),//,40X,4HHOUR,3X,10I6)                                   A  294
225  FORMAT (1H0,//,40X,26HTRANSPORTED CONCENTRATIONS )                  A  295
     END                                                                 A  296-
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      SUBROUTINE PHOT (PLACE)                                                B     1
C                                                                            B     2
C     ****     RATE CONSTANT CALCULATIONS FOR FIRST ORDER PHOTOCHEMICAL RE    B     3
C                                                                            B     4
      REAL K                                                                 B     5
      COMMON /SUNLIT/ XJ(47,10),SIGMA(31,10),PHI(31,10),Z(10),RTCON(10),     B     6
     1LAM1,INC,SLA,SLO,TZ,IY,IM,ID,ISTRT,ISTOP,IINC,IEND,SPECIE,MAXZ,ITI     B     7
     2ME(015),XZ(015),K(015),JSTRT,JSTOP,SPEC(11),MNLM(11),MXLM(11),MAXL     B     8
     3,MAXJ                                                                  B     9
      COMMON /PHOTON/ CF(45,8),P(15,9),IPH(9)                                B    10
      DIMENSION D(2), C(27), W(45), V(5), TMS(16), PLACE(6)                  B    11
      DATA D/0.0,0.0/,JSTRT/0800/,JSTOP/1900/,IINC/60/                       B    12
C                                                                            B    13
      IEND=15                                                                B    14
      NTM=IEND                                                               B    15
      TIME=JSTRT                                                             B    16
      DO 5 II=1,IEND                                                         B    17
C                                                                            B    18
C     ****     CALL SUBROUTINE TO COMPUTE ZENITH ANGLES FROM TIME OF DAY     B    19
C                                                                            B    20
      XC=0.0                                                                 B    21
      TSTD=TIME-100.                                                         B    22
      IF (TSTD.LT.0.) TSTD=TSTD+2400.                                        B    23
      CALL SOLAR (SLA,SLO,TZ,IY,IM,ID,TSTD,XC,5)                             B    24
      ITIME(II)=TIME                                                         B    25
      XZ(II)=90.-XC                                                          B    26
      TIME=CLOCK(TIME,IINC)                                                  B    27
    5 CONTINUE                                                               B    28
C                                                                            B    29
      DO 20 L=1,MAXL                                                         B    30
      SPECIE=SPEC(L)                                                         B    31
      ISTRT=(MNLM(L)-LAM1)/INC+1                                             B    32
      ISTOP=(MXLM(L)-LAM1)/INC+1                                             B    33
      DO 10 M=1,MAXZ                                                         B    34
C                                                                            B    35
C     ****     CALL SUBROUTINE TO CALCULATE RATE CONSTANTS                   B    36
C                                                                            B    37
      CALL RATE (L,M,MNLM(L),MXLM(L),RTCON(M))                               B    38
   10 CONTINUE                                                               B    39
C                                                                            B    40
C     ****     CALL FIRST SUBROUTINE FOR SPLINE INTERPOLATION OF RATE CONS   B    41
C                                                                            B    42
      CALL SPLNA (MAXZ,Z,RTCON,2,D,C,W)                                      B    43
      DO 15 II=1,IEND                                                        B    44
      V(1)=XZ(II)                                                            B    45
      P(II,L)=0.                                                             B    46
      K(II)=P(II,L)                                                          B    47
      IF (V(1).GT.90.0) GO TO 15                                             B    48
C                                                                            B    49
C     ****     CALL SECOND SUBROUTINE IN SPLINE INTERPOLATION SCHEME         B    50
C                                                                            B    51
      CALL SPLNB (MAXZ,Z,RTCON,C,V)                                          B    52
      P(II,L)=AMAX1(0.0,V(2))                                                B    53
      K(II)=P(II,L)                                                          B    54
   15 CONTINUE                                                               B    55
C                                                                            B    56
   20 CONTINUE                                                               B    57
```

```
C     DETERMINE TIME OF SOLAR NOON                                    B   58
      DO 25 I=2,IEND                                                  B   59
   25 IF (XZ(I).GT.XZ(I-1)) GO TO 30                                  B   60
      I=IEND                                                          B   61
   30 TIME=ITIME(I-1)                                                 B   62
      XA=XZ(I-1)                                                      B   63
      DO 35 I=1,60                                                    B   64
      SPECIE=TIME                                                     B   65
      TIME=CLOCK(TIME,1)                                              B   66
      TSTD=TIME-100.                                                  B   67
      IF (TSTD.LT.0.) TSTD=TSTD+2400.                                 B   68
      XB=XA                                                           B   69
      CALL SOLAR (SLA,SLO,TZ,IY,IM,ID,TSTD,XC,5)                      B   70
      XA=90.-XC                                                       B   71
   35 IF (XA.GT.XB) GO TO 40                                          B   72
   40 DO 45 I=1,IEND                                                  B   73
      TMS(I)=60.*FLOAT(I-1)                                           B   74
   45 P(I,3)=P(I,3)+P(I,MAXL)                                         B   75
      DO 55 L=1,8                                                     B   76
      DO 50 I=2,IEND                                                  B   77
      NMM=IEND+2-I                                                    B   78
   50 IF (P(NMM-1,L).GT.0.) GO TO 55                                  B   79
   55 CALL SPLNA (NMM,TMS,P(1,L),2,D,CF(1,L),W)                       B   80
      RETURN                                                          B   81
      END                                                             B   82-
```

```
      SUBROUTINE RATE (L,NZ,MINLAM,MAXLAM,SUM)                          C     1
      REAL K                                                            C     2
      COMMON /SUNLIT/ XJ(47,10),SIGMA(31,10),PHI(31,10),Z(10),RTCON(10), C     3
     1LAM1,INC,SLA,SLO,TZ,IY,IM,ID,ISTRT,ISTOP,IINC,IEND,SPECIE,MAXZ,ITI C     4
     2ME(015),XZ(015),K(015),JSTRT,JSTOP,SPEC(11),MNLM(11),MXLM(11),MAXL C     5
     3,MAXJ                                                             C     6
C                                                                       C     7
C     ****     THIS SUBROUTINE CALCULATES A SINGLE RATE CONSTANT ACCORDING C     8
C     ****          THE GIVEN INPUTS                                    C     9
C                                                                       C    10
      SUM=0.0                                                           C    11
      DO 5 I=MINLAM,MAXLAM,INC                                          C    12
      II=(I-LAM1)/INC+1                                                 C    13
      IJ=II                                                             C    14
      IF (L.EQ.MAXL) IJ=II-16                                           C    15
      SUM=SUM+XJ(II,NZ)*1.0E+15*SIGMA(IJ,L)*PHI(IJ,L)                   C    16
    5 CONTINUE                                                          C    17
      SUM=SUM*60.                                                       C    18
      RETURN                                                            C    19
      END                                                               C    20-
```

```
      SUBROUTINE SOLAR (SLA,SLO,TZ,IY,IM,ID,TIME,D,NV)                    D     1
C***                                                                      D     2
C***     SLA...  LATITUDE (DEG)  SOUTH = MINUS                            D     3
C***     SLO...  LONGITUDE (DEG)  EAST = MINUS                            D     4
C***     TZ...  TIME ZONE                                                 D     5
C***             ALSO INCLUDES FRACTION IF LOCAL TIME IS NOT              D     6
C***              STANDARD MERIDIAN TIME.  E.G. POONA, INDIA 5.5          D     7
C***     IY..  YEAR                                                       D     8
C***     IM..  MONTH                                                      D     9
C***     ID..  DAY                                                        D    10
C***     TIME.. LOCAL STANDARD TIME IN HOURS AND MINUTES.                 D    11
C***             1 30 PM = 1330  ** STANDARD TIME **                      D    12
C***     D..  RETURNED VALUE                                              D    13
C***     NV..  VALUE TO BE RETURNED, SELECTED AS FOLLOWS....              D    14
C***           1...  DECLINATION (DEG.)                                   D    15
C***           2...  EQUATION OF TIME ADJUSTMENT (HRS.)                   D    16
C***           3...  TRUE SOLAR TIME (HRS.)                               D    17
C***           4...  HOUR ANGLE (DEG.)                                    D    18
C***           5...  SOLAR ELEVATION (DEG.)                              D    19
C***           6...  OPTICAL AIRMASS                                      D    20
C***     0 * NV * 7.  OTHERWISE, D = 9999.                                D    21
C***                                                                      D    22
      DIMENSION MD(11)                                                    D    23
      DATA MD/31,29,31,30,31,30,2*31,30,31,30/                            D    24
      DATA A,B,C,SIGA/0.15,3.885,1.253,279.9348/                          D    25
      RAD=572957.75913E-4                                                 D    26
      SDEC=39784.988432E-5                                                D    27
      RE=1.                                                               D    28
      IF (SLO.LT.0.) RE=-1.                                               D    29
      KZ=TZ                                                               D    30
      TC=(TZ-KZ)*RE                                                       D    31
      TZZ=KZ*RE                                                           D    32
      SLB=SLA/RAD                                                         D    33
      K=ID                                                                D    34
      TIMH=TIME/100.                                                      D    35
      I=TIMH                                                              D    36
      TIMLOC=(TIMH-I)/0.6+I+TC                                            D    37
      IMC=IM-1                                                            D    38
      IF (IMC.LT.1) GO TO 10                                              D    39
      DO 5 I=1,IMC                                                        D    40
    5 K=K+MD(I)                                                           D    41
   10 LEAP=1                                                              D    42
      NL=MOD(IY,4)                                                        D    43
      IF (NL.LT.1) LEAP=2                                                 D    44
      SMER=TZZ*15.                                                        D    45
      TK=((SMER-SLO)*4.)/60.                                              D    46
      KR=1                                                                D    47
      IF (K.GE.61.AND.LEAP.LT.2) KR=2                                     D    48
      DAD=(TIMLOC+TZZ)/24.                                                D    49
      DAD=DAD+K-KR                                                        D    50
      DF=DAD*360./365.242                                                 D    51
      DE=DF/RAD                                                           D    52
      DESIN=SIN(DE)                                                       D    53
      DECOS=COS(DE)                                                       D    54
      DESIN2=SIN(DE*2.)                                                   D    55
      DECOS2=COS(DE*2.)                                                   D    56
      SIG=SIGA+DF+1.914827*DESIN-0.079525*DECOS+0.019938*DESIN2-0.00162*  D    57
```

```
     1DECOS2                                                                    D   58
      SIG=SIG/RAD                                                               D   59
      DECSIN=SDEC*SIN(SIG)                                                      D   60
      EFFDEC=ASIN(DECSIN)                                                       D   61
      IF (NV.NE.1) GO TO 15                                                     D   62
      D=EFFDEC*RAD                                                              D   63
      RETURN                                                                    D   64
   15 EQT=0.12357*DESIN-0.004289*DECOS+0.153809*DESIN2+0.060783*DECOS2          D   65
      IF (NV.NE.2) GO TO 20                                                     D   66
      D=EQT                                                                     D   67
      RETURN                                                                    D   68
   20 TST=TK+TIMLOC-EQT                                                         D   69
      IF (NV.NE.3) GO TO 25                                                     D   70
      D=TST                                                                     D   71
      IF (D.LT.0.) D=D+24.                                                      D   72
      IF (D.GE.24.) D=D-24.                                                     D   73
      RETURN                                                                    D   74
   25 HRANGL=ABS(TST-12.)*15.                                                   D   75
      IF (NV.NE.4) GO TO 30                                                     D   76
      D=HRANGL                                                                  D   77
      RETURN                                                                    D   78
   30 HRANGL=HRANGL/RAD                                                         D   79
      SOLSIN=DECSIN*SIN(SLB)+COS(EFFDEC)*COS(SLB)*COS(HRANGL)                   D   80
      SOLEL=ASIN(SOLSIN)*RAD                                                    D   81
      IF (NV.NE.5) GO TO 35                                                     D   82
      D=SOLEL                                                                   D   83
      RETURN                                                                    D   84
   35 IF (NV.NE.6) GO TO 40                                                     D   85
      IF (SOLEL.LE.0.) GO TO 40                                                 D   86
      TK=SOLEL+B                                                                D   87
      E=1./TK**C                                                                D   88
      D=1./(A*E+SOLSIN)                                                         D   89
      RETURN                                                                    D   90
   40 D=9999.                                                                   D   91
      RETURN                                                                    D   92
      END                                                                       D   93-
```

```
      SUBROUTINE SPLNA (N,X,Y,J,D,C,W)                                  E    1
      DIMENSION X(10), Y(10), D(2), C(30), W(30)                        E    2
C     ------------------------------------------------------------------ E    3
C           OVER THE INTERVAL X(I) TO X(I+1), THE INTERPOLATING         E    4
C           POLYNOMIAL                                                  E    5
C                Y=Y(I)+A(I)*Z+B(I)*Z**2+E(I)*Z**3                      E    6
C           WHERE Z=(X-X(I))/(X(I+1)-X(I))                              E    7
C           IS USED. THE COEFFICIENTS A(I),B(I) AND E(I) ARE COMPUTED   E    8
C           BY SPLNA AND STORED IN LOCATIONS C(3*I-2),C(3*I-1) AND      E    9
C           C(3*I) RESPECTIVELY.                                        E   10
C           WHILE WORKING IN THE ITH INTERVAL,THE VARIABLE Q WILL       E   11
C           REPRESENT Q=X(I+1) - X(I), AND Y(I) WILL REPRESENT          E   12
C           Y(I+1)-Y(I)                                                 E   13
C     ------------------------------------------------------------------ E   14
C                                                                       E   15
      Q=X(2)-X(1)                                                       E   16
      YI=Y(2)-Y(1)                                                      E   17
      IF (J.EQ.2) GO TO 5                                               E   18
C     ------------------------------------------------------------------ E   19
C           IF THE FIRST DERIVATIVE AT THE END POINTS IS GIVEN,         E   20
C           A(1) IS KNOWN, AND THE SECOND EQUATION BECOMES              E   21
C           MERELY B(1)+E(1)=YI - Q*D(1).                               E   22
C     ------------------------------------------------------------------ E   23
      C(1)=Q*D(1)                                                       E   24
      C(2)=1.0                                                          E   25
      W(2)=YI-C(1)                                                      E   26
      GO TO 10                                                          E   27
C     ------------------------------------------------------------------ E   28
C           IF THE SECOND DERIVATIVE AT THE END POINTS IS GIVEN         E   29
C           B(1) IS KNOWN, THE SECOND EQUATION BECOMES                  E   30
C           A(1)+E(1)=YI-0.5*Q*Q*D(1). DURING THE SOLUTION OF           E   31
C           THE 3N-4 EQUATIONS,A1 WILL BE KEPT IN CELL C(2)             E   32
C           INSTEAD OF C(1) TO RETAIN THE TRIDIAGONAL FORM OF THE       E   33
C           COEFFICIENT MATRIX.                                         E   34
C     ------------------------------------------------------------------ E   35
    5 C(2)=0.0                                                          E   36
      W(2)=0.5*Q*Q*D(1)                                                 E   37
   10 M=N-2                                                             E   38
      IF (M.LE.0) GO TO 20                                              E   39
C     ------------------------------------------------------------------ E   40
C           UPPER TRIANGULARIZATION OF THE TRIDIAGONAL SYSTEM OF        E   41
C           EQUATIONS FOR THE COEFFICIENT MATRIX FOLLOWS--              E   42
C     ------------------------------------------------------------------ E   43
      DO 15 I=1,M                                                       E   44
      AI=Q                                                              E   45
      Q=X(I+2)-X(I+1)                                                   E   46
      H=AI/Q                                                            E   47
      C(3*I)=-H/(2.0-C(3*I-1))                                          E   48
      W(3*I)=(-YI-W(3*I-1))/(2.0-C(3*I-1))                              E   49
      C(3*I+1)=-H*H/(H-C(3*I))                                          E   50
      W(3*I+1)=(YI-W(3*I))/(H-C(3*I))                                   E   51
      YI=Y(I+2)-Y(I+1)                                                  E   52
      C(3*I+2)=1.0/(1.0-C(3*I+1))                                       E   53
   15 W(3*I+2)=(YI-W(3*I+1))/(1.0-C(3*I+1))                             E   54
C     ------------------------------------------------------------------ E   55
C           E(N-1) IS DETERMINED DIRECTLY FROM THE LAST EQUATION        E   56
C           OBTAINED ABOVE, AND THE FIRST OR SECOND DERIVATIVE          E   57
```

```
C               VALUE GIVEN AT THE END POINT.                                   E   58
C     ------------------------------------------------------------------------- E   59
   20 IF (J.EQ.1) GO TO 25                                                      E   60
      C(3*N-3)=(Q*Q*D(2)/2.0-W(3*N-4))/(3.0-C(3*N-4))                           E   61
      GO TO 30                                                                  E   62
   25 C(3*N-3)=(Q*D(2)-YI-W(3*N-4))/(2.0-C(3*N-4))                              E   63
   30 M=3*N-6                                                                   E   64
      IF (M.LE.0) GO TO 40                                                      E   65
C     ------------------------------------------------------------------------- E   66
C               BACK SOLUTION FOR ALL COEFFICENTS EXCEPT                        E   67
C               A(1) AND B(1) FOLLOWS--                                         E   68
C     ------------------------------------------------------------------------- E   69
      DO 35 II=1,M                                                              E   70
      I=M-II+3                                                                  E   71
   35 C(I)=W(I)-C(I)*C(I+1)                                                     E   72
   40 IF (J.EQ.1) GO TO 45                                                      E   73
C     ------------------------------------------------------------------------- E   74
C               IF THE SECOND DERIVATIVE IS GIVEN AT THE END POINTS,            E   75
C               A(1) CAN NOW BE COMPUTED FROM THE KNOWN VALUES OF               E   76
C               B(1) AND E(1). THEN A(1) AND B(1) ARE PUT INTO THEIR            E   77
C               PROPER PLACES IN THE C ARRAY.                                   E   78
C     ------------------------------------------------------------------------- E   79
      C(1)=Y(2)-Y(1)-W(2)-C(3)                                                  E   80
      C(2)=W(2)                                                                 E   81
      RETURN                                                                    E   82
   45 C(2)=W(2)-C(3)                                                            E   83
      RETURN                                                                    E   84
      END                                                                       E   85-
```

```
      SUBROUTINE SPLNB (N,X,Y,C,V)                                      F    1
      DIMENSION X(10), Y(10), C(30), V(5)                               F    2
      V(5)=2.0                                                          F    3
      LIM=N-1                                                           F    4
C     ------------------------------------------------------------      F    5
C                    DETERMINE IN WHICH INTERVAL THE INDEPENDENT       F    6
C                    VARIABLE,V(1),LIES.                               F    7
C     ------------------------------------------------------------      F    8
      DO 5 I=2,LIM                                                      F    9
    5 IF (V(1).LT.X(I)) GO TO 10                                        F   10
      I=N                                                               F   11
      IF (V(1).GT.X(N)) V(5)=3.0                                        F   12
      GO TO 15                                                          F   13
   10 IF (V(1).LT.X(1)) V(5)=1.0                                        F   14
C     ------------------------------------------------------------      F   15
C                    Q IS THE SIZE OF THE INTERVAL CONTAINING V(1).    F   16
C     ------------------------------------------------------------      F   17
C                    Z IS A LINEAR TRANSFORMATION OF THE INTERVAL      F   18
C                    ONTO (0,1) AND IS THE VARIABLE FOR WHICH          F   19
C                    THE COEFFICIENTS WERE COMPUTED BY SPLNA.          F   20
C     ------------------------------------------------------------      F   21
   15 Q=X(I)-X(I-1)                                                     F   22
      Z=(V(1)-X(I-1))/Q                                                 F   23
      V(2)=((Z*C(3*I-3)+C(3*I-4))*Z+C(3*I-5))*Z+Y(I-1)                  F   24
      V(3)=((3.*Z*C(3*I-3)+2.0*C(3*I-4))*Z+C(3*I-5))/Q                  F   25
      V(4)=(6.*Z*C(3*I-3)+2.0*C(3*I-4))/(Q*Q)                           F   26
      RETURN                                                            F   27
      END                                                               F   28-
```

```
      FUNCTION CLOCK (T1,IINC)                                                  C    1
C                                                                               C    2
C     ****     ADD A TIME IN MINUTES TO A 2400 HOUR TIME AND RETURN A 2400     C    3
C     ****     HOUR TIME                                                       C    4
C                                                                               C    5
      T2=IINC                                                                   C    6
      I100=T1/100                                                               C    7
      T3=T1-100.0*I100+T2                                                       C    8
      I100=I100+INT(T3/60)                                                      C    9
      CLOCK=I100*100.0+T3-60.0*INT(T3/60)                                       C   10
      RETURN                                                                    C   11
      END                                                                       C   12-
```

```
      SUBROUTINE RLINE (NC,F,KS1,JS)                                    H    1
      COMMON /NEED/ HC,XN,NL,NRTO,RTO(20),OZP(20),OZN(8,20),RHO(8,20),MR H    2
     1,OC(4),OS(2),HCS,XNS,LS,HCLL(8)                                   H    3
      COMMON /CNTRL/ SIG,SIGMA,INFO,NPTO,XNF,RCTY,ALDX,OZIN,OZAL,HCIN,HC H    4
     1AL,XNIN,XNAL,TSRT,DTIM,Z1,Z2,DCON,EHC,EXN,FLST,TLST               H    5
      COMMON /INOUT/ IN,IOUT,ITAPE                                      H    6
      COMMON /PLTVEC/ HCT(20),OT(20),NT,OHC,HCG,PLTGRD,OXN,XNG,HC1,XN1,T H    7
     1ICZ,DIGZ,CHRZ                                                     H    8
      DIMENSION R(20), F(21), YP(12), TMP(12), OE(20), XNE(20)          H    9
      EQUIVALENCE (NR,NRTO), (RTO,R)                                    H   10
      RLBK(A,B1,B2,B3)=A*(B1-B2)/(B3-B2)                                H   11
      KFACT=KS1-6+JS                                                    H   12
      IF (NC.EQ.1) KFACT=KFACT+2                                        H   13
      KS=MAX0(KFACT/MR,0)                                               H   14
      KS=MIN0(KS,NC)                                                    H   15
      KSS=MAX0(KFACT-KS*MR,0)                                           H   16
      KS=KS+1                                                           H   17
      IF (KS.GT.NC.AND.KSS.EQ.2) GO TO 5                                H   18
      IF (INFO.EQ.0) WRITE (IOUT,365)                                   H   19
      IF (INFO.LT.0) WRITE (IOUT,370)                                   H   20
    5 DO 15 J=1,NL                                                      H   21
      M=J.                                                              H   22
      DO 10 L=J,NL                                                      H   23
   10 IF (OZP(L).LT.OZP(M)) M=L                                         H   24
      IF (M.EQ.J) GO TO 15                                              H   25
      SV=OZP(J)                                                         H   26
      OZP(J)=OZP(M)                                                     H   27
      OZP(M)=SV                                                         H   28
   15 CONTINUE                                                          H   29
      NR=NC                                                             H   30
      NSHC=0                                                            H   31
      NSXN=0                                                            H   32
      KK=0                                                              H   33
      MR1=MR-1                                                          H   34
      INX=1                                                             H   35
      NCR=(NR+1)/2                                                      H   36
      TOL=1.0-(0.17/(SQRT(FLOAT(NR))))                                  H   37
      KSN=KS1+1                                                         H   38
      IF (KSN.GT.7) GO TO 40                                            H   39
      GO TO (20,25,30,35,40,40,40),KSN                                  H   40
C  DO CORNERS.                                                          H   41
   20 CALL SIM (0.,0.,OC(1),INX)                                        H   42
   25 CALL SIM (0.,XN,OC(2),INX)                                        H   43
   30 IF (KS.EQ.1) CALL SIM (HC,XN,OZN(MR,1),INX)                       H   44
      OC(3)=OZN(MR,1)                                                   H   45
   35 CALL SIM (HC,0.,OC(4),INX)                                        H   46
   40 DO 45 LS=1,NL                                                     H   47
   45 IF (OC(1).LT.OZP(LS)) GO TO 50                                    H   48
      WRITE (IOUT,355) OC(1)                                            H   49
      STOP                                                              H   50
   50 IF (LS.GT.1) WRITE (IOUT,360) OZP(LS)                             H   51
      IF (OZP(LS).GT.OC(3)) GO TO 345                                   H   52
      NCYC=0                                                            H   53
C  DO DOUBLE ROLLBACK ON EDGES                                          H   54
      IF (KSN.GE.7) GO TO 75                                            H   55
      HCG=RLBK(HC,OZP(LS),OC(2),OC(3))                                  H   56
      XNG=RLBK(XN,OZP(LS),OC(4),OC(3))                                  H   57
```

```
      IF (HCG.LE.0.) HCG=HC/20.                                          H   58
      IF (XNG.LE.0.) XNG=XN/10.                                          H   59
      IF (NCR.EQ.1) GO TO 90                                             H   60
      GO TO (55,55,55,55,55,65,75),KSN                                   H   61
   55 OS(1)=OZP(LS)                                                      H   62
      INX=-1                                                             H   63
   60 CALL SIM (HCG,XN,OS(1),INX)                                        H   64
      OHC=OS(1)                                                          H   65
      IF (INX.NE.-1) GO TO 65                                            H   66
      HCG1=RLBK(HCG,OZP(LS),OC(2),OS(1))                                 H   67
      IF (HCG1.GT.0.5*HC) HCG=HC/3.                                      H   68
      IF (HCG1.LE.0.5*HC) HCG=(RLBK(HC-HCG,OZP(LS),OS(1),OC(3))+HCG+HCG1 H   69
     1)/2.                                                               H   70
      INX=1                                                              H   71
      GO TO 60                                                           H   72
   65 OS(2)=OZP(LS)                                                      H   73
      INX=-1                                                             H   74
   70 CALL SIM (HC,XNG,OS(2),INX)                                        H   75
      OXN=OS(2)                                                          H   76
      IF (INX.NE.-1) GO TO 75                                            H   77
      XNG1=RLBK(XNG,OZP(LS),OC(4),OS(2))                                 H   78
      IF (XNG1.GT.0.5*XN) XNG=XN/3.                                      H   79
      IF (XNG1.LE.0.5*XN) XNG=(RLBK(XN-XNG,OZP(LS),OS(2),OC(3))+XNG+XNG1 H   80
     1)/2.                                                               H   81
      INX=1                                                              H   82
      GO TO 70                                                           H   83
   75 IF (KS.GT.NR.AND.KSS.EQ.2) GO TO 245                               H   84
      IF (KS.GT.NR.AND.KSS.EQ.1) GO TO 80                                H   85
      HCS=RLBK(HC-HCG,OZP(LS),OS(1),OC(3))+HCG                           H   86
      IF (HCS.LE.0.) HCS=HCG                                             H   87
   80 XNS=RLBK(XNG,OZP(LS),OC(4),OS(2))                                  H   88
      IF (XNS.GT.XNG) XNS=RLBK(XN-XNG,OZP(LS),OS(2),OC(3))+XNG           H   89
      IF (KS.GT.NR) GO TO 245                                            H   90
      IF (KS.GT.NCR) XSS=XNS                                             H   91
      IF (KS.GT.NCR) OSS=OS(2)                                           H   92
      IF (KS.LT.2) GO TO 90                                              H   93
      IF (KS.EQ.2) GO TO 85                                              H   94
      HTT1=RHO(MR,KS-2)*R(KS-2)/F(KS-2)                                  H   95
      XNN1=RHO(MR,KS-2)/F(KS-2)                                          H   96
   85 HTT=RHO(MR,KS-1)*R(KS-1)/F(KS-1)                                   H   97
      XNN=RHO(MR,KS-1)/F(KS-1)                                           H   98
      IF (KSS.EQ.0) GO TO 90                                             H   99
      HCC=RHO(MR,KS)*R(KS)/F(KS)                                         H  100
      XNX=RHO(MR,KS)/F(KS)                                               H  101
      GO TO 95                                                           H  102
   90 XNX=XN                                                             H  103
   95 XNX1=0.                                                            H  104
      ICNT=KS-1                                                          H  105
      DO 240 I=KS,NR                                                     H  106
      ICNT=ICNT+1                                                        H  107
      IF (I.GT.1) GO TO 100                                              H  108
      HTT=HC                                                             H  109
      XNN=XN                                                             H  110
      IF (KSS) 175,165,175                                               H  111
  100 IF (I-NCR-1) 105,125,130                                           H  112
  105 OZC=OZN(MR,I-1)*(OZP(LS)/OZN(MR,I-1))**(1./FLOAT(NCR+2-I))         H  113
      IF (KSS.NE.0) GO TO 120                                            H  114
```

```
      HSS=HCS                                                          H  115
      OSS=OS(1)                                                        H  116
      IF (OS(1).GT.OZC) HSS=0.                                         H  117
      IF (OS(1).GT.OZC) OSS=OC(2)                                      H  118
      IF (ICNT.GT.2) GO TO 110                                         H  119
      HCC=RLBK(HTT-HSS,OZC,OSS,OZN(MR,I-1))+HSS                        H  120
      IF (OC(3).GT.OZP(NL)) JJ=NCR-1                                   H  121
      IF (OC(3).LE.OZP(NL)) JJ=NCR                                     H  122
      HCC1=HC-(HC-HCS)/FLOAT(JJ)                                       H  123
      HCC=AMAX1(HCC,HCC1)                                              H  124
      GO TO 120                                                        H  125
  110 HCC=HTT1-RLBK(HTT1-HTT,OZC,OZN(MR,I-2),OZN(MR,I-1))              H  126
      A=RLBK(HTT-HSS,OZC,OSS,OZN(MR,I-1))+HSS                          H  127
      BX=HTT-HCC                                                       H  128
      AX=A-HCS                                                         H  129
      IF (OC(3)-OZN(MR,2).GT.0) GO TO 115                              H  130
      AX=0.                                                            H  131
      BX=1.                                                            H  132
  115 HCC=(HCC*AX+A*BX)/(AX+BX)                                        H  133
      HCC1=HTT-(HTT-HCS)/AMAX0(NCR+1-I,2)                              H  134
      HCC=AMAX1(HCC,HCC1)                                              H  135
  120 IF (HCC.GT.TOL*HTT) HCC=TOL*HTT                                  H  136
      HMR4=HC-(FLOAT(I-1)*HC/FLOAT(NCR))                               H  137
      IF (HCC.LT.HMR4) HCC=HMR4                                        H  138
      HTT1=HTT                                                         H  139
      HTT=HCC                                                          H  140
      XNN=XN                                                           H  141
      IF (KSS) 175,155,175                                             H  142
  125 OZC=OC(3)*(OZP(LS)/OC(3))**(1./FLOAT(NCR))                       H  143
      XNN=XN                                                           H  144
      OZL=OC(3)                                                        H  145
      OSS=OZP(LS)                                                      H  146
      XSS=XNS                                                          H  147
      ICNT=0                                                           H  148
      IF (KSS) 150,140,150                                             H  149
  130 OZC=OZN(MR,I-1)*(OZP(LS)/OZN(MR,I-1))**(1./FLOAT(NR+2-I))        H  150
      OZL=OZN(MR,I-1)                                                  H  151
      IF (KS.LE.NCR) GO TO 135                                         H  152
      ICNT=KS-NCR-1                                                    H  153
  135 ICNT=ICNT+1                                                      H  154
      IF (KSS.NE.0) GO TO 150                                          H  155
      IF (ICNT.LE.2) GO TO 140                                         H  156
      XNX1=XNN1-RLBK(XNN1-XNN,OZC,OZN(MR,I-2),OZN(MR,I-1))             H  157
  140 IF (XNN.GT.XSS) GO TO 145                                        H  158
      XSS=0.                                                           H  159
      OSS=OC(4)                                                        H  160
      XNS=XNS*0.5                                                      H  161
  145 XNX=RLBK(XNN-XSS,OZC,OSS,OZL)+XSS                                H  162
      IF (XNX1.GT.0.0.AND.XNX1.LT.XN) XNX=(XNX+XNX1)/2.0               H  163
      IF (OC(3).GT.OZP(NL)) L=1                                        H  164
      IF (OC(3).LE.OZP(NL)) L=2                                        H  165
      IF (NCR.GT.2) XNX=AMAX1(XNX,XNN-(XNN-XNS)/FLOAT(NR+L-I))         H  166
      IF (I.EQ.NR) XNX=(XNN+2.0*XNS)/3.0                               H  167
      IF (I.EQ.NR.AND.XNX.LE.0.) XNX=XNN/2.                            H  167A
      IF (NCR.LE.2) XNX=XN/3.0                                         H  168
      IF (XNX.LT.1.1*XNG.AND.XNX.GT.0.9*XNG) XNX=XNG                   H  169
  150 IF (XNX.GT.TOL*XNN) XNX=TOL*XNN                                  H  170
      XNN1=XNN                                                         H  171
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```
      XNN=XNX                                                                   H  172
      HTT=HC                                                                    H  173
      IF (KSS.NE.0) GO TO 175                                                   H  174
  155 IF (OZN(MR,I-1).GT.1.1*OZP(LS)) GO TO 165                                 H  175
      IF (IABS(NCR-I).LE.2) GO TO 165                                           H  176
      GAP=0.                                                                    H  177
      NCOUNT=I-2                                                                H  178
      IF (I.LE.(NR/2+1)) NSTART=1                                               H  179
      IF (I.GT.(NR/2+1)) NSTART=NR/2+1                                          H  180
      DO 160 JJ=NSTART,NCOUNT                                                   H  181
      GAP1=OZN(MR,JJ)-OZN(MR,JJ+1)                                              H  182
      IF (GAP1.LT.GAP) GO TO 160                                                H  183
      GAP=GAP1                                                                  H  184
      HTT=((R(JJ)*RHO(MR,JJ))/F(JJ)+(R(JJ+1)*RHO(MR,JJ+1))/F(JJ+1))/2.0        H  185
      XNN=HTT/((R(JJ)+R(JJ+1))/2.)                                              H  186
  160 CONTINUE                                                                  H  187
  165 R(I)=HTT/XNN                                                              H  188
      F(I)=SQRT(R(I)*R(I)+1.)                                                   H  189
      RHO(MR,I)=XNN*F(I)                                                        H  190
      IF (XNX.EQ.XNC) OZN(MR,I)=OS(2)                                           H  191
      IF (I.EQ.1.OR.XNX.EQ.XNC) GO TO 175                                       H  192
      IF (OZP(LS).GE.OC(2)) GO TO 170                                           H  193
      IF (I.NE.NCR) GO TO 170                                                   H  194
      R(I)=0.                                                                   H  195
      F(I)=1.                                                                   H  196
      RHO(MR,I)=XN                                                              H  197
      HTT=0.                                                                    H  198
      HCLL(MR)=XN                                                               H  199
      XNN=XN                                                                    H  200
  170 CALL SIM (HTT,XNN,OZN(MR,I),INX)                                          H  201
  175 IF (KSS.EQ.0) KSS1=2                                                      H  202
      IF (KSS.NE.0) KSS1=KSS+1                                                  H  203
      IF (MR1) 240,240,180                                                      H  204
  180 IF (MR.EQ.2) GO TO 200                                                    H  205
      IF (KSS1.GT.MR1) GO TO 195                                                H  206
      DO 190 J=KSS1,MR1                                                         H  207
      K=MR-J+1                                                                  H  208
      OZC=OZN(K+1,I)*(OZP(LS)/OZN(K+1,I))**(1./FLOAT(K))                        H  209
      IF (K.EQ.MR1) GO TO 185                                                   H  210
      RHO1=RHO(K+2,I)-RLBK(RHO(K+2,I)-RHO(K+1,I),OZC,OZN(K+2,I),OZN(K+1,        H  211
     1I))                                                                       H  212
  185 RHO(K,I)=RLBK(RHO(K+1,I),OZC,OC(1),OZN(K+1,I))                            H  213
      IF (K.EQ.MR1) RHO1=RHO(K,I)                                               H  214
      IF (RHO1.GT.0.) RHO(K,I)=(RHO1+RHO(K,I))/2.0                              H  215
      FK=AMAX0(K-2,2)                                                           H  216
      RHO(K,I)=AMAX1(RHO(K,I),RHO(K+1,I)-(RHO(K+1,I)/FK))                       H  217
      IF (RHO(K,I).GE.RHO(K+1,I)) RHO(K,I)=RHO(K+1,I)-(RHO(K+1,I)/FK)           H  218
      XNX=RHO(K,I)/F(I)                                                         H  219
      HCC=R(I)*XNX                                                              H  220
      IF (I.EQ.NCR.AND.OZP(LS).LT.OC(2)) HCLL(K)=XNX                            H  221
      CALL SIM (HCC,XNX,OZN(K,I),INX)                                           H  222
  190 CONTINUE                                                                  H  223
  195 IF (OZN(2,I).LT.OZP(LS)) RHO(1,I)=0.9*RHO(2,I)                            H  224
      IF (OZN(2,I).LT.OZP(LS)) GO TO 215                                        H  225
  200 OZN(1,I)=OC(1)                                                            H  226
      SX=-SIG*3.                                                                H  227
      IT=1                                                                      H  228
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      RHO(1,I)=0.                                                          H  229
      CALL EDGMX (RHO(1,I),OZN(1,I),MR,HMX,OZHX,LX)                        H  230
      MM=LX+1                                                              H  231
  205 RHO(1,I)=0.                                                          H  232
      CALL CURV1 (MM,OZN(1,I),RHO(1,I),SP1,SP2,YP,TMP,SX)                  H  233
      RHO(1,I)=CURV2(OZP(LS),MR,OZN(1,I),RHO(1,I),YP,SX,IT)                H  234
      INX=-2                                                               H  235
      IF (IT.GT.0) GO TO 210                                               H  236
      SX=SX*10.                                                            H  237
      SX=AMAX1(-50.,SX)                                                    H  238
      GO TO 205                                                            H  239
  210 IF (RHO(1,I).GT.0.9*RHO(2,I)) RHO(1,I)=0.9*RHO(2,I)                  H  240
      IF (RHO(1,I).LE.0.) RHO(1,I)=.5*RHO(2,I)                             H  241
      IF (RHO(1,I).GE.RHO(2,I)) RHO(1,I)=0.5*RHO(2,I)                      H  242
  215 XNX=RHO(1,I)/F(I)                                                    H  243
      HCC=XNX*R(I)                                                         H  244
      OZN(1,I)=OZP(LS)                                                     H  245
      IF (OZP(LS).LT.OC(2).AND.I.EQ.NCR) HCLL(1)=XNX                       H  246
      CALL SIM (HCC,XNX,OZN(1,I),INX)                                      H  247
      IF (INX.NE.-2) GO TO 235                                             H  248
      IF (OZN(1,I)-OZP(LS)) 220,230,225                                    H  249
  220 RHO(1,I)=0.8*RLBK((RHO(2,I)-RHO(1,I)),OZP(LS),OZN(1,I),OZN(2,I))+R   H  250
     1HO(1,I)                                                              H  251
      GO TO 230                                                            H  252
  225 RHO(1,I)=0.9*RLBK(RHO(1,I),OZP(LS),OC(1),OZN(1,I))                   H  253
  230 INX=1                                                                H  254
      GO TO 215                                                            H  255
  235 KSS=0                                                                H  256
  240 CONTINUE                                                             H  257
C  CHECK FOR INCREASING RATIOS                                            H  258
  245 DO 260 I=1,NR                                                        H  259
      K=I                                                                  H  260
      DO 250 J=I,NR                                                        H  261
  250 IF (R(J).LT.R(K)) K=J                                                H  262
      IF (K.EQ.I) GO TO 260                                                H  263
      SV=R(I)                                                              H  264
      R(I)=R(K)                                                            H  265
      R(K)=SV                                                              H  266
      SV=F(I)                                                              H  267
      F(I)=F(K)                                                            H  268
      F(K)=SV                                                              H  269
      DO 255 J=1,MR                                                        H  270
      SV=OZN(J,I)                                                          H  271
      OZN(J,I)=OZN(J,K)                                                    H  272
      OZN(J,K)=SV                                                          H  273
      SV=RHO(J,I)                                                          H  274
      RHO(J,I)=RHO(J,K)                                                    H  275
  255 RHO(J,K)=SV                                                          H  276
  260 CONTINUE                                                             H  277
C  DO SPECIAL CALCULATIONS                                                H  278
      KSS1=KSS+1                                                           H  279
      IF (OZP(LS).LT.OC(2)) NCR1=NCR-1                                     H  280
      IF (OZP(LS).GE.OC(2)) NCR1=NCR                                       H  281
      NN=NCR1+1                                                            H  282
      SX=-20.*SIG/FLOAT(NN)                                                H  283
      IF (NCR.NE.1) GO TO 265                                              H  284
      OT(1)=OC(2)                                                          H  285
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      HCT(1)=0.                                                          H  286
      OT(2)=OHC                                                          H  287
      HCT(2)=HCG                                                         H  288
      OT(3)=OC(3)                                                        H  289
      HCT(3)=HC                                                          H  290
      III=0                                                              H  291
      NN=3                                                               H  292
      GO TO 295                                                          H  293
  265 DO 270 I=1,NCR1                                                    H  294
      IF (OZP(LS).LT.OC(2)) L=I+1                                        H  295
      IF (OZP(LS).GE.OC(2)) L=I                                          H  296
      OT(I+2)=OZN(NR,L)                                                  H  297
  270 HCT(I+2)=RHO(NR,L)*R(L)/F(L)                                       H  298
      OT(1)=OC(2)                                                        H  299
      HCT(1)=0.                                                          H  300
      OT(2)=OHC                                                          H  301
      HCT(2)=HCG                                                         H  302
      NN=NN+1                                                            H  303
      IF (KSS1.GT.1) GO TO 300                                           H  304
      IT=1                                                               H  305
  275 CALL CURV1 (NN,OT,HCT,SP1,SP2,YP,TMP,SX)                           H  306
      DO 280 LK=1,NL                                                     H  307
  280 IF (OZP(LK).GE.OC(2)) GO TO 285                                    H  308
      LK=NL                                                              H  309
  285 HCS=CURV2(OZP(LK),NN,OT,HCT,YP,SX,IT)                              H  310
      IF (IT.GT.0) GO TO 290                                             H  311
      SX=SX*10.                                                          H  312
      SX=AMAX1(-30.,SX)                                                  H  313
      GO TO 275                                                          H  314
  290 IF (HCS.GT.TOL*HCT(3)) HCS=TOL*HCT(3)                              H  315
  295 IF (NCR.EQ.1) HCS=HC/3.                                            H  316
      IF(HCS.GE.HCT(3).OR.HCS.LE.HCT(1)) HCS=(HCT(1)+HCT(3))/2.          H  317
      CALL SIM (HCS,XN,OS(1),INX)                                        H  318
  300 OT(2)=OS(1)                                                        H  319
      HCT(2)=HCS                                                         H  320
      NT=NN                                                              H  321
      IF (KSS1.GT.2) GO TO 340                                           H  322
      SX=-SIG*20./FLOAT(NN)                                              H  323
      XNN=HC/RTO(NR)                                                     H  324
      IF (NCR.EQ.1) GO TO 335                                            H  325
      IF (OZN(NR,NR).LT.1.1*OZP(LS)) XNS=XNN*0.5                         H  326
      IF (OC(4).GT.OZP(LS)) XNS=XNN*0.5                                  H  327
      IF (XNS.EQ.XNN*0.5) GO TO 335                                      H  328
      DO 305 I=1,NCR                                                     H  329
      J=NR+1-I                                                           H  330
      OE(I+1)=OZN(NR,J)                                                  H  331
  305 XNE(I+1)=RHO(NR,J)/F(J)                                            H  332
      OE(1)=OC(4)                                                        H  333
      XNE(1)=0.                                                          H  334
      NN=NCR+1                                                           H  335
  310 IF (OE(NN).LT.OE(NN-1)) NN=NN-1                                    H  336
      IF (NN.EQ.1) XNS=XNN*0.5                                           H  337
      IF (NN.EQ.1) GO TO 335                                             H  338
      IF (OE(NN).LT.OE(NN-1)) GO TO 310                                  H  339
      IF (XNG.GE.XNE(2)) GO TO 320                                       H  340
      IF (ABS(XNE(2)-XNG).LT..0001) GO TO 325                            H  341
      NN=NN+1                                                            H  342
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      NNR=NN-2                                                          H  343
      DO 315 I=1,NNR                                                    H  344
      II=NN-I+1                                                         H  345
      XNE(II)=XNE(II-1)                                                 H  346
  315 OE(II)=OE(II-1)                                                   H  347
      XNE(2)=XNG                                                        H  348
      OE(2)=OXN                                                         H  349
      SX=-SIG*20./FLOAT(NN)                                             H  349A
  320 IT=1                                                              H  350
  325 CALL CURV1 (NN,OE,XNE,SP1,SP2,YP,TMP,SX)                          H  351
      XNS=CURV2(OZP(LS),NN,OE,XNE,YP,SX,IT)                             H  352
      IF (IT.GT.0) GO TO 330                                            H  353
      SX=SX*10.                                                         H  354
      SX=AMAX1(-50.,SX)                                                 H  355
      GO TO 325                                                         H  356
  330 IF (XNS.GT.TOL*XNE(2)) XNS=TOL*XNE(2)                             H  357
      IF(XNS.GE.XNE(3).OR.XNS.LE.XNE(1)) XNS=(XNE(1)+XNE(3))/2.         H  357A
  335 IF (NCR.EQ.1) XNS=XN/3.                                           H  358
      CALL SIM (HC,XNS,OS(2),INX)                                       H  359
  340 RETURN                                                            H  360
  345 WRITE (IOUT,350)                                                  H  361
      STOP                                                              H  362
C                                                                       H  363
C                                                                       H  364
C                                                                       H  365
  350 FORMAT (1H1,40HTHE LOWEST OZONE LINE CANNOT BE PLOTTED./1H0,39HINC H  366
     1REASE THE MAXIMUM HC AND NOX VALUES.)                             H  367
  355 FORMAT (1H1,24HNO LINES CAN BE PLOTTED./1H0,40HBACKGROUND ONLY PRO H  368
     1DUCES TOO MUCH OZONE,,F3.2,3H PPM.)                               H  369
  360 FORMAT (1H0,67HDUE TO HIGH BACKGROUND CONDITIONS THE LOWEST OZONE  H  370
     1PLOTTED WILL BE ,F3.2,3H PPM.)                                    H  371
  365 FORMAT (1H1,//,14X,36HTHE FOLLOWING SIMULATIONS WERE DONE./1H0/1H  H  372
     1,16X,2HHC,18X,3HNOX,13X,5HRATIO,16X,5HOZONE)                      H  373
  370 FORMAT (1H1,//,14X,36HTHE FOLLOWING SIMULATIONS WERE DONE./1H0/1H  H  374
     1,16X,2HHC,18X,3HNOX,13X,5HRATIO,16X,5HOZONE,16X,4HTIME)           H  375
      END                                                               H  376-
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      SUBROUTINE SIM (HC,XN,ZN,INO                                          I     1
      COMMON /CALC/ NR,ER(77,3),A(77),S(77),R(77),ITYPE(77),IA(34),JA(21    I     2
     18),DILUT,TEMP,ERR,START,STOPP,SPECIS(34),TPRNT,TSTEP                  I     3
      COMMON /TITL/ ITTL(18)                                                I     4
      COMMON /HOUR/ OZN,NGO,TM                                              I     5
      COMMON /CNTRL/ SIG,SIGMA,INFO,NPTO,XNF,RCTY,ALDX,OZIN,OZAL,HCIN,HC    I     6
     1AL,XNIN,XNAL,TSRT,DTIM,Z1,Z2,DCON,EHC,EXN,FLST,TLST                   I     7
      COMMON /INOUT/ IN,IOUT,ITAPE                                          I     8
      COMMON /PHOTON/ CF(45,8),P(15,9),IPH(9)                               I     9
      DIMENSION C(34), RT(77), XR(8)                                        I    10
      DATA IN1/1/                                                           I    11
      START=0.                                                              I    12
      T=START                                                               I    13
      FLST=1.0                                                              I    14
      TLST=START                                                            I    15
      TCI=800.                                                              I    16
      EHC=HC                                                                I    17
      EXN=XN                                                                I    18
      IF (IN1.EQ.1) SAV=STOPP                                               I    20
      STOPP=SAV                                                             I    21
      IF (NPTO.EQ.0) TPRNT=STOPP                                            I   21A
      IN1=0                                                                 I    22
      H=1.E-10                                                              I    23
      NS=33                                                                 I    24
      N=33                                                                  I    25
      M=32                                                                  I    26
      DO 5 I=1,N                                                            I    27
    5 C(I)=0.                                                               I    28
      C(1)=XN*XNF+XNIN                                                      I    29
      C(2)=XN*(1.-XNF)                                                      I    30
      C(4)=OZIN                                                             I    31
      C(12)=(HC*RCTY+HCIN*0.1)/3.                                           I    32
      C(21)=HC*.4*ALDX                                                      I    33
      C(22)=HC*.3*ALDX                                                      I    34
      C(24)=(HC*(1.-RCTY)+HCIN*0.9)*0.25                                    I    35
      IN=1                                                                  I    36
      CALL DIFSET (N,START,C,RT)                                            I    37
      IF (NPTO.EQ.0) GO TO 10                                               I    38
      CALL ISOPLT (HC,XN)                                                   I    39
      WRITE (IOUT,125)                                                      I    40
      WRITE (IOUT,135) (ITTL(I),I=1,18)                                     I    41
      IF (INFO.LT.1) WRITE (IOUT,170)                                       I    42
      IF (INFO.LT.1) GO TO 10                                               I    43
      WRITE (IOUT,150) ERR                                                  I    44
      WRITE (IOUT,155) (R(IR),IR=1,NR)                                      I    45
      WRITE (IOUT,160) (IPH(IR),IR=1,8)                                     I    46
      DO 8 I=1,8                                                            I    47
      J=IPH(I)                                                              I    48
    8 XR(I)=R(J)                                                            I    49
      WRITE (IOUT,165) (XR(IR),IR=1,8)                                      I    50
   10 DILUT=DCON                                                            I    51
      IF (TSRT.LE.START.AND.DTIM.NE.0.) DILUT=ALOG(Z2/Z1)/DTIM              I    52
      TNEXT=1.                                                              I    53
      IF (NPTO.EQ.0) GO TO 50                                               I    54
      IF (T-START) 73,73,30                                                 I    55
   15 IF (DTIM.EQ.0.) GO TO 45                                              I    56
      IF (T.GE.TSRT) GO TO 30                                               I    57
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      DILUT=DCON                                                        I   58
      IF (TSRT-TPRNT) 20,20,25                                          I   59
   20 TNEXT=TSRT                                                        I   60
      IN=2                                                              I   61
      GO TO 50                                                          I   62
   25 TNEXT=TPRNT                                                       I   63
      IN=0                                                              I   64
      GO TO 50                                                          I   65
   30 IF (T.GE.TSRT+DTIM) GO TO 45                                      I   66
      DILUT=ALOG(Z2/Z1)/DTIM                                            I   67
      FLST=EXP(-DCON*TSRT)                                              I   68
      TLST=TSRT                                                         I   69
      TNEXT=TSRT+DTIM                                                   I   70
      IF (TNEXT-TPRNT) 35,35,40                                         I   71
   35 IN=2                                                              I   72
      GO TO 50                                                          I   73
   40 TNEXT=TPRNT                                                       I   74
      IN=0                                                              I   75
      GO TO 50                                                          I   76
   45 TNEXT=AMIN1(TPRNT,STOPP)                                          I   77
      FLST=EXP(-DCON*TSRT-DILUT*DTIM)                                   I   78
      TLST=TSRT+DTIM                                                    I   79
      DILUT=DCON                                                        I   80
   50 CALL DRIVES (M,T,H,C,TNEXT,ERR,21,IN,IA,JA)                       I   81
      T=TNEXT                                                           I   82
      IF (NPTO.NE.0) GO TO 60                                           I   83
      IF (T.LT.STOPP) GO TO 15                                          I   84
      IF (INX.GT.-1) GO TO 60                                           I   85
      IF (INX.EQ.-1.AND.OZM.GT.0.75*ZN) GO TO 60                        I   86
      IF (INX.NE.-2) GO TO 55                                           I   87
      IF (OZM.LT.1.25*ZN.AND.OZM.GT.0.75*ZN) GO TO 60                   I   88
   55 ZN=OZM                                                            I   89
      RETURN                                                            I   90
   60 ZN=OZM                                                            I   91
      IF (NPTO.NE.0) GO TO 70                                           I   92
      INX=1                                                             I   93
      IF (T.LT.STOPP) GO TO 15                                          I   94
      IF (XN.EQ.0.) RR=0.                                               I   95
      IF (XN.NE.0.) RR=HC/XN                                            I   96
      IF (INFO.LT.0) GO TO 65                                           I   97
      IF (TM.GT.0.) WRITE (IOUT,100) HC,XN,RR,ZN                        I   98
      IF (TM.LE.0.) WRITE (IOUT,120) HC,XN,RR,ZN                        I   99
      RETURN                                                            I  100
   65 IF (TM.GT.0.) WRITE (IOUT,140) HC,XN,RR,ZN,TM                     I  101
      IF (TM.LT.0.) WRITE (IOUT,145) HC,XN,RR,ZN                        I  102
      RETURN                                                            I  103
   70 IF (IN.NE.0) RETURN                                               I  104
      IF (T.GE.STOPP) TPRNT=STOPP                                       I  105
      IF (T.LT.TPRNT) GO TO 15                                          I  106
   75 HCC=3.0*C(12)+4.0*C(24)                                           I  108
      IF (HCC.GT.0.0000001) GO TO 80                                    I  109
      FPROP=0.                                                          I  110
      ALDC=0.                                                           I  111
      GO TO 85                                                          I  112
   80 FPROP=3.0*C(12)/HCC                                               I  113
      ALDC=(C(21)+2.0*C(22))/HCC                                        I  114
   85 CNOX=C(1)+C(2)                                                    I  115
```

```
      IF (CNOX.LE.0.0000001) FNO2=0.                                    I  116
      IF (CNOX.GT.0.0000001) FNO2=C(1)/CNOX                             I  117
      CO3=C(4)                                                          I  118
      IF (INFO.GT.0) WRITE (IOUT,125)                                   I  119
      IF (INFO.GT.0) WRITE (IOUT,170)                                   I  120
      IF (T.EQ.START) TIMNW=START                                       I  121
      IF (T.NE.START) TIMNW=TPRNT                                       I  122
      CTIME=CLOCK(TCI,IFIX(TIMNW))                                      I  123
      WRITE (IOUT,175) CTIME,HCC,FPROP,ALDC,CNOX,FNO2,CO3               I  124
      IF (INFO.LE.0) GO TO 95                                           I  125
      WRITE (IOUT,115) (SPECIS(I),I=1,MD                                I  126
      WRITE (IOUT,130) CTIME,(C(I),I=1,10),H,(C(I),I=11,MD              I  127
      CALL DIFFUN (N,TIMNW,C,RT)                                        I  128
      WRITE (IOUT,105) (RT(I),I=1,MD                                    I  129
      DO 90 I=1,NR                                                      I  130
      J=KR(I,1)                                                         I  131
      K=KR(I,2)                                                         I  132
      IF (J.EQ.0) RT(I)=0.                                              I  133
      IF (J.EQ.0) GO TO 90                                              I  134
      IF (J.EQ.99) J=0                                                  I  135
      IF (J.EQ.0) TJ=1.                                                 I  136
      IF (J.NE.0) TJ=C(J)                                               I  137
      IF (K.EQ.0) TK=1.                                                 I  138
      IF (K.NE.0) TK=C(K)                                               I  139
      RT(I)=TJ*TK*R(I)                                                  I  140
   90 CONTINUE                                                          I  141
      WRITE (IOUT,110) (RT(I),I=1,NR)                                   I  142
      DO 91 IR=1,8                                                      I  143
      J=IPH(IR)                                                         I  143A
   91 XR(IR)=R(J)                                                       I  143B
      WRITE (IOUT,165) (XR(IR),IR=1,8)                                  I  144
   95 IF (TIMNW.EQ.START) GO TO 50                                      I  145
      IF (NPTO.NE.0) IN1=1                                              I  146
      IF (T.GE.STOPP) RETURN                                            I  147
      TPRNT=TPRNT+TSTEP                                                 I  148
      GO TO 15                                                          I  149
C                                                                       I  150
C                                                                       I  151
  100 FORMAT (1H0,4F20.5)                                               I  152
  105 FORMAT (/,10H NET RATES,1X,1P10E12.3,/,(11X,1P10E12.3))           I  153
  110 FORMAT (//,1X,22HTHE REACTION RATES ARE,/,(1H ,1P10E13.2))        I  154
  115 FORMAT (//,3X,5HTIME ,4X,10(4X,A4,4X),/,1X,8HINTERVAL,3X,10(4X,A4,  I  155
     14X),/,(12X,10(4X,A4,4X)))                                        I  156
  120 FORMAT (1H0,4F20.5,8H NOT MAX)                                    I  157
  125 FORMAT (1H1//////////)                                            I  158
  130 FORMAT (1PE11.3,10E12.3/,E11.3,10E12.3/,(11X,10E12.3))            I  159
  135 FORMAT (46X,18A4)                                                 I  160
  140 FORMAT (1H0,4F20.5,F21.9)                                         I  161
  145 FORMAT (1H0,4F20.5,14X,7HNOT MAX)                                 I  162
  150 FORMAT (24H0THE ERROR TOLERANCE IS ,1PE10.3)                      I  163
  155 FORMAT (29H0THE RATE CONSTANTS USED WERE,//,(1H0,1P10E13.3))      I  164
  160 FORMAT (29H0THE PHOTOLYSIS REACTIONS ARE,/(1H0,9I13))             I  165
  165 FORMAT (34H0THE PHOTOLYTIC RATE CONSTANTS ARE,/,(1H0,4X,1P9E13.3))  I  166
  170 FORMAT (1H0,30X,4HTIME,6X,2HHC,7X,9HPROPYLENE,5X,8HALDEHYDE,6X,3HN  I  167
     10X,10X,3HNO2,8X,5HOZONE,/,30X,6H(LDT ),4X,5HTOTAL,5X,8HFRACTION,6X  I  168
     2,8HFRACTION,5X,5HTOTAL,7X,8HFRACTION,3X,9H( INSTANT))             I  169
  175 FORMAT (1H0,26X,F6.0,1X,F10.5,2X,F10.5,3X,F10.5,1X,F10.5,3X,F10.5,  I  170
     12X,F10.5)                                                         I  171
      END                                                               I  172-
```

```
      SUBROUTINE DRIVES (N,T0,H0,Y0,TOUT,EPS,MF,INDEX,IA,JA)                J     1
      DIMENSION Y(032,06), IA(1), JA(1), Y0(N)                              J     2
      COMMON /CNTRL/ SIG,SIGMA,INFO,NPTO,XNF,RCTY,ALDX,OZIN,OZAL,HCIN,HC    J     3
     1AL,XNIN,XNAL,TSRT,DTIM,Z1,Z2,DCON,EHC,EXN,FLST,TLST                   J     4
      COMMON /GEAR1/ T,H,HMIN,HMAX,EPSC,UROUND,NC,MFC,KFLAG,JSTART          J     5
      COMMON /GEAR2/ YMAX(032)/GEAR3/ERROR(32)/GEAR4/W1(32,3)               J     6
      COMMON /GEAR5/ IW1(33,9)/GEAR6/W2(1500)/GEAR7/IW2(660)                J     7
      COMMON /GEAR8/ EPSJ,IPTI2,IPTI3,IPTI4,IPTR2,IPTR3,NGRP                J     8
      COMMON /GEAR9/ HUSED,NQUSED,NSTEP,NFE,NJE,NZA,NPL,NPU,NZL,NZU,NZRO    J     9
      COMMON /INOUT/ INP,LOUT,ITAPE                                         J    10
      DATA NMX/032/,LENW2/1500/,LENIW2/660/                                 J    11
      DATA UROUND/7.5E-9/                                                   J    12
      KOZ=4                                                                 J    13
      NGP=0                                                                 J    14
      IF (INDEX.EQ.4) GO TO 5                                               J    15
      IF (INDEX.EQ.0) GO TO 20                                              J    16
      IF (INDEX.EQ.2) GO TO 25                                              J    17
      IF (INDEX.EQ.-1) GO TO 30                                             J    18
      IF (INDEX.EQ.3) GO TO 35                                              J    19
      IF (EPS.LE.0.) GO TO 105                                              J    20
      MITER=MF-10*(MF/10)                                                   J    21
      IF ((MITER.NE.1).AND.(MITER.NE.2)) GO TO 5                            J    22
      NP1=N+1                                                               J    23
      NZA=IA(NP1)-1                                                         J    24
      IPTI2=NZA+1                                                           J    25
      MAXPL=(LENIW2-NZA)/2                                                  J    26
      IPTI3=IPTI2+MAXPL                                                     J    27
      NPL=IW1(N,4)                                                          J    28
      NPU=IW1(N,6)                                                          J    29
      NZL=IW1(N+1,3)                                                        J    30
      NZU=IW1(N+1,5)                                                        J    31
      IPTR2=NZA+1                                                           J    32
      IPTR3=IPTR2+MAX0(NZA,NZL)                                             J    33
    5 DO 10 I=1,N                                                           J    34
      YMAX(I)=ABS(Y0(I))                                                    J    35
      IF (YMAX(I).EQ.0.) YMAX(I)=1.E-10                                     J    36
   10 Y(I,1)=Y0(I)                                                          J    37
      NC=N                                                                  J    38
      T=T0                                                                  J    39
      H=H0                                                                  J    40
      NZRO=0                                                                J    41
      TST=EPS*1.E-10                                                        J    42
      DO 15 I=1,N                                                           J    43
   15 IF (Y(I,1).GT.TST) NZRO=NZRO+1                                        J    44
      NZRO=MAX0(NZRO,1)                                                     J    45
      NOLD=NZRO                                                             J    46
      HMIN=ABS(H0)                                                          J    47
      HMAX=ABS(T0-TOUT)*10.                                                 J    48
      HMAX=AMIN1(HMAX,20.)                                                  J    49
      EPSC=EPS                                                              J    50
      MFC=MF                                                                J    51
      JSTART=0                                                              J    52
      N0=N                                                                  J    53
      CALL OZMX (Y,TL,TOUT,N0)                                              J    54
      NMX1=NMX+1                                                            J    55
      EPSJ=SQRT(UROUND)                                                     J    56
      NHCUT=0                                                               J    57
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      GO TO 40                                                          J   5E
   20 HMAX=ABS(TOUT-TOUTP)*10.                                          J   59
      HMAX=AMIN1(HMAX,20.)                                              J   60
      GO TO 65                                                          J   61
   25 HMAX=ABS(TOUT-TOUTP)*10.                                          J   62
      HMAX=AMIN1(HMAX,20.)                                              J   63
      IF ((T-TOUT)*H.GE.0.) GO TO 110                                   J   64
      GO TO 70                                                          J   65
   30 JSTART=-1                                                         J   66
      NC=N                                                              J   67
      EPSC=EPS                                                          J   68
      MFC=MF                                                            J   69
   35 CONTINUE                                                          J   70
   40 CALL STIFFS (Y,N0,IA,JA,W1,NMX,IW1,NMX1)                          J   71
      IF (NPTO.NE.0) CALL SAVLIN (T,Y(KOZ,1))                           J   72
      KGO=1-KFLAG                                                       J   73
      GO TO (45,80,95,85),KGO                                           J   74
   45 CONTINUE                                                          J   75
      IF (T.GE.TL) CALL OZMX (Y,TL,TOUT,N0)                             J   76
      D=0.                                                              J   77
      NZRO=0                                                            J   78
      DO 60 I=1,N                                                       J   79
      IF (Y(I,1).GE.0.) GO TO 55                                        J   80
      NGP=NGP+1                                                         J   81
      DO 50 J=1,6                                                       J   82
   50 Y(I,J)=0.                                                         J   83
   55 CONTINUE                                                          J   84
      IF (Y(I,1).GT.TST) NZRO=NZRO+1                                    J   85
      AYI=ABS(Y(I,1))                                                   J   86
      YMAX(I)=AMAX1(1.E-10,AYI)                                         J   87
   60 D=D+(AYI/YMAX(I))**2                                              J   88
      NZRO=MAX0(NZRO,1)                                                 J   89
      IF (NZRO.NE.NOLD) JSTART=-1                                       J   90
      D=D*(UROUND/EPS)**2                                               J   91
      IF (D.GT.FLOAT(N)) GO TO 100                                      J   92
      IF (INDEX.EQ.3) GO TO 110                                         J   93
      IF (INDEX.EQ.2) GO TO 70                                          J   94
   65 IF ((T-TOUT)*H.LT.0.) GO TO 35                                    J   95
      CALL INTERP (TOUT,Y,N0,Y0)                                        J   96
      GO TO 120                                                         J   97
   70 IF (T.GE.TOUT) GO TO 75                                           J   98
      IF (((T+H)-TOUT).LE.0.) GO TO 35                                  J   99
      H=(TOUT-T)*(1.+4.*UROUND)                                         J  100
      JSTART=-1                                                         J  101
      GO TO 35                                                          J  102
   75 JSTART=-1                                                         J  103
      H=AMIN1(H,1.)                                                     J  104
      GO TO 110                                                         J  105
   80 CONTINUE                                                          J  106
   85 IF (NHCUT.EQ.10) GO TO 90                                         J  107
      NHCUT=NHCUT+1                                                     J  108
      HMIN=.1*HMIN                                                      J  109
      H=.1*H                                                            J  110
      JSTART=-1                                                         J  111
      GO TO 35                                                          J  112
   90 WRITE (LOUT,125)                                                  J  113
      IF (KGO.EQ.4) WRITE (LOUT,140) T                                  J  114
```

```
      STOP                                                              J  115
   95 WRITE (LOUT,130) T,H                                              J  116
      STOP                                                              J  117
  100 WRITE (LOUT,135) T                                                J  118
      KFLAG=-2                                                          J  119
      STOP                                                              J  120
  105 WRITE (LOUT,145)                                                  J  121
      STOP                                                              J  122
  110 TOUT=T                                                            J  123
      DO 115 I=1,N                                                      J  124
  115 Y0(I)=Y(I,1)                                                      J  125
  120 INDEX=KFLAG                                                       J  126
      TOUTP=TOUT                                                        J  127
      H0=HUSED                                                          J  128
      IF (KFLAG.NE.0) H0=H                                              J  129
      RETURN                                                            J  130
C                                                                       J  131
C                                                                       J  132
  125 FORMAT (//44H PROBLEM APPEARS UNSOLVABLE WITH GIVEN INPUT//)      J  133
  130 FORMAT (//35H KFLAG = -2 FROM INTEGRATOR AT T = ,E16.8,5H  H =,E16 J  134
     1.8/52H . THE REQUESTED ERROR IS SMALLER THAN CAN BE HANDLED//)    J  135
  135 FORMAT (//37H INTEGRATION HALTED BY DRIVER AT T = ,E16.8/56H  EPS  J  136
     1TOO SMALL TO BE ATTAINED FOR THE MACHINE PRECISION/)              J  137
  140 FORMAT (//35H KFLAG = -3 FROM INTEGRATOR AT T = ,E16.8/45H  CORREC J  138
     1TOR CONVERGENCE COULD NOT BE ACHIEVED/)                           J  139
  145 FORMAT (//28H ILLEGAL INPUT.. EPS .LE. 0.//)                      J  140
      END                                                               J  141-
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```
      SUBROUTINE STIFFS (Y,N0,IA,JA,W1,NMX,IW1,NMX1)                    K     1
      COMMON /GEAR1/ T,H,HMIN,HMAX,EPS,UROUND,N,MF,KFLAG,JSTART         K     2
      COMMON /GEAR2/ YMAX(032)/GEAR3/ERROR(32)                          K     3
      COMMON /GEAR6/ W2(1500) /GEAR7/ IW2(660)                          K     4
      COMMON /GEAR8/ EPSJ,IPTI2,IPTI3,IPTI4,IPTR2,IPTR3,NGRP            K     5
      COMMON /GEAR9/ HUSED,NQUSED,NSTEP,NFE,NJE,IDUMMY(5),NZRO          K     6
      COMMON /CALC/ NR,KR(77,5),A(77),S(77),R(77),ITYPE(77),II(34),JJ(21 K     7
     18),DILUT,TEMP,ERR,START,STOPP,SPECIS(34),TPRNT,TSTEP              K     8
      DIMENSION Y(N0,1), IA(1), JA(1), W1(NMX,1), IW1(NMX1,1)           K     9
      DIMENSION EL(13), TQ(4), RT(3)                                    K    10
      DATA EL(2)/1./,OLDL0/1./                                          K    11
      KFLAG=0                                                           K    12
      TOLD=T                                                            K    13
      IF (JSTART.GT.0) GO TO 50                                         K    14
      IF (JSTART.NE.0) GO TO 10                                         K    15
      CALL DIFFUN (N,T,Y,W1)                                            K    16
      DO 5 I=1,N                                                        K    17
    5 Y(I,2)=H*W1(I,1)                                                  K    18
      METH=MF/10                                                        K    19
      MITER=MF-10*METH                                                  K    20
      NQ=1                                                              K    21
      L=2                                                               K    22
      IDOUB=3                                                           K    23
      RMAX=1.E4                                                         K    24
      RC=0.                                                             K    25
      CRATE=1.                                                          K    26
      HOLD=H                                                            K    27
      MFOLD=MF                                                          K    28
      NSTEP=0                                                           K    29
      NSTEPJ=0                                                          K    30
      NFE=1                                                             K    31
      NJE=0                                                             K    32
      IRET=3                                                            K    33
      GO TO 15                                                          K    34
   10 IF (MF.EQ.MFOLD) GO TO 25                                         K    35
      MEO=METH                                                          K    36
      MIO=MITER                                                         K    37
      METH=MF/10                                                        K    38
      MITER=MF-10*METH                                                  K    39
      MFOLD=MF                                                          K    40
      IF (MITER.NE.MIO) IWEVAL=MITER                                    K    41
      IF (METH.EQ.MEO) GO TO 25                                         K    42
      IDOUB=L+1                                                         K    43
      IRET=1                                                            K    44
   15 CALL COSET (METH,NQ,EL,TQ,MAXDER)                                 K    45
      LMAX=MAXDER+1                                                     K    46
      RC=RC*EL(1)/OLDL0                                                 K    47
      OLDL0=EL(1)                                                       K    48
   20 FN=FLOAT(NZRO)                                                    K    49
      EDN=FN*(TQ(1)*EPS)**2                                             K    50
      E=FN*(TQ(2)*EPS)**2                                               K    51
      EUP=FN*(TQ(3)*EPS)**2                                             K    52
      BND=FN*(TQ(4)*EPS)**2                                             K    53
      EPSOLD=EPS                                                        K    54
      NOLD=NZRO                                                         K    55
      GO TO (30,35,50),IRET                                             K    56
   25 IF(EPS.EQ.EPSOLD.AND.NZRO.EQ.NOLD) GO TO 30                       K    57
```

```
      IRET=1                                                            K   58
      GO TO 20                                                          K   59
   30 IF (H.EQ.HOLD) GO TO 50                                           K   60
      RH=H/HOLD                                                         K   61
      H=HOLD                                                            K   62
      IREDO=3                                                           K   63
      GO TO 40                                                          K   64
   35 RH=AMAX1(RH,HMIN/ABS(H))                                          K   65
   40 RH=AMIN1(RH,HMAX/ABS(H),RMAX)                                     K   66
      R1=1.                                                             K   67
      DO 45 J=2,L                                                       K   68
      R1=R1*RH                                                          K   69
      DO 45 I=1,N                                                       K   70
   45 Y(I,J)=Y(I,J)*R1                                                  K   71
      H=H*RH                                                            K   72
      RC=RC*RH                                                          K   73
      IDOUB=L+1                                                         K   74
      IF (IREDO.EQ.0) GO TO 290                                         K   75
   50 IF (ABS(RC-1.).GT.0.3) IWEVAL=MITER                               K   76
      IF (NSTEP.GE.NSTEPJ+20) IWEVAL=MITER                              K   77
      T=T+H                                                             K   78
      DO 55 J1=1,NQ                                                     K   79
      DO 55 J2=J1,NQ                                                    K   80
      J=(NQ+J1)-J2                                                      K   81
      DO 55 I=1,N                                                       K   82
   55 Y(I,J)=Y(I,J)+Y(I,J+1)                                            K   83
   60 DO 65 I=1,N                                                       K   84
   65 ERROR(I)=0.                                                       K   85
      M=0                                                               K   86
      CALL DIFFUN (N,T,Y,W1(1,2))                                       K   87
      NFE=NFE+1                                                         K   88
      IF (IWEVAL.LE.0) GO TO 130                                        K   89
      IWEVAL=0                                                          K   90
      RC=1.                                                             K   91
      NJE=NJE+1                                                         K   92
      NSTEPJ=NSTEP                                                      K   93
      CON=-H*EL(1)                                                      K   94
      ISV=M                                                             K   95
      LSV=L                                                             K   96
      NZ=IA(N+1)-1                                                      K   97
      DO 75 I=1,NZ                                                      K   98
   75 W2(I)=0.                                                          K   99
      DO 115 IR=1,NR                                                    K  100
      MT=ITYPE(IR)                                                      K  101
      DO 80 I=1,MT                                                      K  102
      JX=I+1-I/2*2                                                      K  103
      J=KR(IR,JX)                                                       K  104
      IF (J.EQ.0) XX=1.                                                 K  105
      IF (J.GT.0) XX=Y(J,1)                                             K  106
   80 RT(I)=R(IR)*XX                                                    K  107
      DO 110 K=1,MT                                                     K  108
      I=KR(IR,K)                                                        K  109
      DO 90 L=1,MT                                                      K  110
      J=KR(IR,L)                                                        K  111
      M=IA(J)-1                                                         K  112
   85 M=M+1                                                             K  113
      IF (I-JA(M)) 85,90,85                                             K  114
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```
 90 W2(M)=W2(M)-RT(L)                                                    K  115
    DO 105 L=3,5                                                        K  116
    J=KR(IR,L)                                                          K  117
    M=IA(I)-1                                                           K  118
    IF (J) 105,110,95                                                   K  119
 95 M=M+1                                                               K  120
    IF (J-JA(M)) 95,100,95                                              K  121
100 W2(M)=W2(M)+RT(K)                                                   K  122
105 CONTINUE                                                            K  123
110 CONTINUE                                                            K  124
115 CONTINUE                                                            K  125
    DO 125 J=1,N                                                        K  126
    KMIN=IA(J)                                                          K  127
    KMAX=IA(J+1)-1                                                      K  128
    DO 120 K=KMIN,KMAX                                                  K  129
    W2(K)=W2(K)*CON                                                     K  130
    IF (JA(K).EQ.J) W2(K)=W2(K)+1.-CON*DILUT                            K  131
120 CONTINUE                                                            K  132
125 CONTINUE                                                            K  133
    CALL NSCORA (N,IA,JA,W2,IW1(1,2),W2(IPTR3),W2(IPTR2),IW1,IW1(1,7),  K  134
   1IW1(1,8))                                                           K  135
    CALL NSNFAC (N,IW1(1,2),IW2,W2,IW1(1,3),IW2(IPTI2),IW1(1,4),W2(IPT  K  136
   1R2),W1(1,3),IW1(1,5),IW2(IPTI3),IW1(1,6),W2(IPTR3),W1,IW1(1,7),IWI  K  137
   2(1,8),IER)                                                          K  138
    M=ISV                                                               K  139
    L=LSV                                                               K  140
    IF (IER.NE.0) GO TO 160                                             K  141
130 DO 135 I=1,N                                                        K  142
    IF (M.LE.0) GO TO 135                                               K  143
    IF (-H*W1(I,2)*10..GT.Y(I,1)) GO TO 155                             K  144
135 W1(I,1)=H*W1(I,2)-(Y(I,2)+ERROR(I))                                 K  145
    CALL NSBSLV (N,IW1,IW1,IW1(1,3),IW2(IPTI2),IW1(1,4),W2(IPTR2),W1(1  K  146
   1,3),IW1(1,5),IW2(IPTI3),IW1(1,6),W2(IPTR3),W1(1,2),W1,W2)           K  147
    D=0.                                                                K  148
    DO 145 I=1,N                                                        K  149
    ERROR(I)=ERROR(I)+W1(I,2)                                           K  150
    D=D+(W1(I,2)/YMAX(I))**2                                            K  151
145 W1(I,1)=Y(I,1)+EL(1)*ERROR(I)                                       K  152
    IF (M.NE.0) CRATE=AMAX1(.9*CRATE,D/D1)                              K  153
    IF ((D*AMIN1(1.,2.*CRATE)).LE.BND) GO TO 175                        K  154
    D1=D                                                                K  155
    M=M+1                                                               K  156
    IF (M.EQ.3) GO TO 155                                               K  157
    CALL DIFFUN (N,T,W1,W1(1,2))                                        K  158
    GO TO 130                                                           K  159
155 NFE=NFE+2                                                           K  160
    IF (IWEVAL.EQ.-1) GO TO 170                                         K  161
160 T=TOLD                                                              K  162
    RMAX=2.                                                             K  163
    DO 165 J1=1,NQ                                                      K  164
    DO 165 J2=J1,NQ                                                     K  165
    J=(NQ+J1)-J2                                                        K  166
    DO 165 I=1,N                                                        K  167
165 Y(I,J)=Y(I,J)-Y(I,J+1)                                              K  168
    IF (ABS(H).LE.HMIN*1.00001) GO TO 285                               K  169
    RH=.25                                                              K  170
    IREDO=1                                                             K  171
```

```
      GO TO 35                                                          K  172
  170 IWEVAL=MITER                                                      K  173
      GO TO 60                                                          K  174
  175 IF (MITER.NE.0) IWEVAL=-1                                         K  175
      NFE=NFE+M                                                         K  176
      D=0.                                                              K  177
      DO 180 I=1,N                                                      K  178
  180 D=D+(ERROR(I)/YMAX(I))**2                                         K  179
      IF (D.GT.E) GO TO 195                                             K  180
      KFLAG=0                                                           K  181
      IREDO=0                                                           K  182
      NSTEP=NSTEP+1                                                     K  183
      HUSED=H                                                           K  184
      NQUSED=NQ                                                         K  185
      DO 185 J=1,L                                                      K  186
      DO 185 I=1,N                                                      K  187
  185 Y(I,J)=Y(I,J)+EL(J)*ERROR(I)                                      K  188
      IF (IDOUB.EQ.1) GO TO 205                                         K  189
      IDOUB=IDOUB-1                                                     K  190
      IF (IDOUB.GT.1) GO TO 295                                         K  191
      IF (L.EQ.LMAX) GO TO 295                                          K  192
      DO 190 I=1,N                                                      K  193
  190 Y(I,LMAX)=ERROR(I)                                                K  194
      GO TO 295                                                         K  195
  195 KFLAG=KFLAG-1                                                     K  196
      T=TOLD                                                            K  197
      DO 200 J1=1,NQ                                                    K  198
      DO 200 J2=J1,NQ                                                   K  199
      J=(NQ+J1)-J2                                                      K  200
      DO 200 I=1,N                                                      K  201
  200 Y(I,J)=Y(I,J)-Y(I,J+1)                                            K  202
      RMAX=2.                                                           K  203
      IF (ABS(H).LE.HMIN*1.00001) GO TO 275                             K  204
      IF (KFLAG.LE.-3) GO TO 265                                        K  205
      IREDO=2                                                           K  206
      PR3=1.E+20                                                        K  207
      GO TO 215                                                         K  208
  205 PR3=1.E+20                                                        K  209
      IF (L.EQ.LMAX) GO TO 215                                          K  210
      D1=0.                                                             K  211
      DO 210 I=1,N                                                      K  212
  210 D1=D1+((ERROR(I)-Y(I,LMAX))/YMAX(I))**2                           K  213
      ENQ3=.5/FLOAT(L+1)                                                K  214
      PR3=((D1/EUP)**ENQ3)*1.4+1.4E-6                                   K  215
  215 ENQ2=.5/FLOAT(L)                                                  K  216
      PR2=((D/E)**ENQ2)*1.2+1.2E-6                                      K  217
      PR1=1.E+20                                                        K  218
      IF (NQ.EQ.1) GO TO 225                                            K  219
      D=0.                                                              K  220
      DO 220 I=1,N                                                      K  221
  220 D=D+(Y(I,L)/YMAX(I))**2                                           K  222
      ENQ1=.5/FLOAT(NQ)                                                 K  223
      PR1=((D/EDN)**ENQ1)*1.3+1.3E-6                                    K  224
  225 IF (PR2.LE.PR3) GO TO 230                                         K  225
      IF (PR3.LT.PR1) GO TO 240                                         K  226
      GO TO 235                                                         K  227
  230 IF (PR2.GT.PR1) GO TO 235                                         K  228
```

```
      NEWQ=NQ                                                          K  229
      RH=1./PR2                                                        K  230
      GO TO 255                                                        K  231
  235 NEWQ=NQ-1                                                        K  232
      RH=1./PR1                                                        K  233
      GO TO 255                                                        K  234
  240 NEWQ=L                                                           K  235
      RH=1./PR3                                                        K  236
      IF (RH.LT.1.1) GO TO 250                                         K  237
      DO 245 I=1,N                                                     K  238
  245 Y(I,NEWQ+1)=ERROR(I)*EL(L)/FLOAT(L)                              K  239
      GO TO 260                                                        K  240
  250 IDOUB=10                                                         K  241
      GO TO 295                                                        K  242
  255 IF ((KFLAG.EQ.0).AND.(RH.LT.1.1)) GO TO 250                      K  243
      IF (NEWQ.EQ.NQ) GO TO 35                                         K  244
  260 NQ=NEWQ                                                          K  245
      L=NQ+1                                                           K  246
      IRET=2                                                           K  247
      GO TO 15                                                         K  248
  265 IF (KFLAG.EQ.-9) GO TO 280                                       K  249
      RH=10.**KFLAG                                                    K  250
      RH=AMAX1(HMIN/ABS(H),RH)                                         K  251
      H=H*RH                                                           K  252
      CALL DIFFUN (N,T,Y,W1)                                           K  253
      NFE=NFE+1                                                        K  254
      DO 270 I=1,N                                                     K  255
  270 Y(I,2)=H*W1(I,1)                                                 K  256
      IWEVAL=MITER                                                     K  257
      IDOUB=10                                                         K  258
      IF (NQ.EQ.1) GO TO 50                                            K  259
      NQ=1                                                             K  260
      L=2                                                              K  261
      IRET=3                                                           K  262
      GO TO 15                                                         K  263
  275 KFLAG=-1                                                         K  264
      GO TO 295                                                        K  265
  280 KFLAG=-2                                                         K  266
      GO TO 295                                                        K  267
  285 KFLAG=-3                                                         K  268
      GO TO 295                                                        K  269
  290 RMAX=100.                                                        K  270
  295 HOLD=H                                                           K  271
      JSTART=NQ                                                        K  272
      RETURN                                                           K  273
      END                                                              K  274-
```

Subroutine DIFFUN

```
      SUBROUTINE DIFFUN (L,T,X,XT)                                          L     1
      COMMON /CALC/ NR,KR(77,5),A(77),S(77),R(77),ITYPE(77),IA(34),JA(21    L     2
     18),DILUT,TEMP,ERR,START,STOPP,SPECIS(34),TPRNT,TSTEP                  L     3
      COMMON /CNTRL/ SIG,SIGMA,INFO,NPTO,XNF,RCTY,ALDX,OZIN,OZAL,HCIN,HC    L     4
     1AL,XNIN,XNAL,TSRT,DTIM,Z1,Z2,DCON,EHC,EXN,FLST,TLST                   L     5
      COMMON /EMIS/ NEM,EM(11),EMHC(11),EMNOX(11),ESTRT(2),ESTOP,ESLP,EH    L     6
     1SLP,ENSLP,B(2),EC(36),BB(2),EH(36),CC(2),EX(36)                       L     7
      COMMON /PHOTON/ CF(45,8),P(15,9),IPH(9)                               L     8
      DIMENSION XT(L), X(L)                                                 L     9
      N=L                                                                   L    10
      DILU=AMAX1(DILUT,0.)                                                  L    11
      DO 5 I=1,N                                                            L    12
    5 XT(I)=-DILU*X(I)                                                      L    13
      IF (T.LT.TSRT.OR.T.GT.TSRT+DTIM) GO TO 10                             L    14
      XT(1)=DILU*(XNAL-X(1))                                                L    15
      XT(4)=DILU*(OZAL-X(4))                                                L    16
      XT(12)=DILU*(0.03333333*HCAL-X(12))                                   L    17
      XT(24)=DILU *(0.225*HCAL-X(24))                                       L   17A
   10 IF (T.GE.ESTOP) GO TO 25                                              L    18
      FNOW=FLST*EXP(-DILUT*(T-TLST))                                        L    19
      IF (T.GT.60.) GO TO 15                                                L    20
      ENOW=0.                                                               L    21
      IF (NEM.GT.0) ENOW=(ESTRT(1)+T*ESLP)*FNOW                             L    22
      ENOW1=ENOW                                                            L    23
      ENOW2=ENOW                                                            L    24
      IF (NEM.LE.-1.AND.EMHC(1).GE.-0.) ENOW1=(ESTRT(1)+T*EHSLP)*FNOW       L    25
      IF (NEM.LE.-1.AND.EMNOX(1).GE.-0.) ENOW2=(ESTRT(2)+T*ENSLP)*FNOW      L    26
      GO TO 20                                                              L    27
   15 I=IFIX(T/60.)                                                         L    28
      ENOW=0.                                                               L    29
      IF (NEM.GT.0) ENOW=(((T*EC(4*I)+EC(4*I-1))*T+EC(4*I-2))*T+EC(4*I-3    L    30
     1))*FNOW                                                               L    31
      ENOW1=ENOW                                                            L    32
      ENOW2=ENOW                                                            L    33
      IF (NEM.LE.-1.AND.EMHC(1).GE.-0.) ENOW1=(((T*EH(4*I)+EH(4*I-1))*T+    L    34
     1EH(4*I-2))*T+EH(4*I-3))*FNOW                                          L    35
      IF (NEM.LE.-1.AND.EMNOX(1).GE.-0.) ENOW2=(((T*EX(4*I)+EX(4*I-1))*T    L    36
     1+EX(4*I-2))*T+EX(4*I-3))*FNOW                                         L    37
   20 XT(1)=XT(1)+ENOW2*EXN*0.1                                             L    38
      XT(2)=XT(2)+ENOW2*EXN*0.9                                             L    39
      XT(12)=XT(12)+ENOW1*EHC*RCTY/3.                                       L    40
      XT(21)=XT(21)+ENOW1*EHC*ALDX*.4                                       L    41
      XT(22)=XT(22)+ENOW1*EHC*ALDX*.3                                       L    42
      XT(24)=XT(24)+ENOW1*EHC*(1.-RCTY)*0.25                                L    43
   25 IF (T.EQ.TOLD) GO TO 35                                               L    44
      I=IFIX(T/60.+2.001)                                                   L    45
      IF (I.GT.16) I=16                                                     L    46
      Z=T/60.-FLOAT(I-2)                                                    L    47
      DO 30 J=1,8                                                           L    48
      IR=IPH(J)                                                             L    49
      IF (P(I-1,J).EQ.0.) R(IR)=0.                                          L    50
      IF (P(I-1,J).EQ.0.) GO TO 30                                          L    51
      R(IR)=((Z*CF(3*I-3,J)+CF(3*I-4,J))*Z+CF(3*I-5,J))*Z+P(I-1,J)          L    52
   30 IF (R(IR).LT.0.) R(IR)=0.                                             L    53
   35 DO 55 IR=1,NR                                                         L    54
      I=KR(IR,1)                                                            L    55
      IF (ITYPE(IR).EQ.2) GO TO 40                                          L    56
```

```
      RT=R(IR)*X(I)                                                     L   57
      GO TO 45                                                          L   58
   40 J=KR(IR,2)                                                        L   59
      RT=R(IR)*X(I)*X(J)                                                L   60
      XT(J)=XT(J)-RT                                                    L   61
   45 XT(I)=XT(I)-RT                                                    L   62
      DO 50 K=3,5                                                       L   63
      I=KR(IR,K)                                                        L   64
      IF (I.EQ.0) GO TO 55                                              L   65
   50 XT(I)=XT(I)+RT                                                    L   66
   55 CONTINUE                                                          L   67
      TOLD=T                                                            L   68
      RETURN                                                            L   69
C     ENTRY DIFSET                                                      L   70
      ENTRY DIFSET (L,T,X,XT)                                           L   71
      TOLD=T                                                            L   72
      I=2                                                               L   73
      Z=1./60.                                                          L   74
      DO 60 J=1,8                                                       L   75
      IR=IPH(J)                                                         L   76
   60 R(IR)=P(1,J)                                                      L   77
      RETURN                                                            L   78
      END                                                               L   79-
```

```
      SUBROUTINE OZMX (C,TL,TOUT,NO)                                    M    1
C                                                                       M    2
      DIMENSION C(NO,6), RUN(61), OZ(61)                                M    3
      COMMON /GEAR1/ T,H,HMIN,HMAX,EPSC,UROUND,NC,MFC,KFLAG,JSTART      M    4
      COMMON /HOUR/ OZM,NCO,TM                                          M    5
      COMMON /CALC/ NR,KR(77,5),A(77),S(77),R(77),ITYPE(77),IA(34),JA(21 M    6
     18),DILUT,TEMP,ERR,START,STOPP,SPECIS(34),TPRNT,TSTEP              M    7
      NQ=JSTART                                                         M    8
      IF (T.NE.START) GO TO 5                                           M    9
      KOZ=4                                                             M   10
      RUN(1)=C(KOZ,1)                                                   M   11
      NT=1                                                              M   12
      TL=START+1.                                                       M   13
      OZM=0.                                                            M   14
      OZA=0.                                                            M   15
      RETURN                                                            M   16
    5 DO 10 I=1,61                                                      M   17
      RR=(TL+FLOAT(I-1)-T)/H                                            M   18
      IF (RR.GT.0.) GO TO 15                                            M   19
      IF (TL+FLOAT(I-1).GT.STOPP) GO TO 15                              M   20
      OZ(I)=C(KOZ,1)                                                    M   21
      RH=1.                                                             M   22
      DO 10 J=1,NQ                                                      M   23
      RH=RH*RR                                                          M   24
   10 OZ(I)=OZ(I)+RH*C(KOZ,J+1)                                         M   25
      I=61                                                              M   26
   15 I=I-1                                                             M   27
      TL=TL+FLOAT(I)                                                    M   28
      DO 35 J=1,I                                                       M   29
      IF (NT.GT.60) GO TO 25                                            M   30
      RUN(NT+1)=OZ(J)                                                   M   31
      NT=NT+1                                                           M   32
      IF (NT.LT.61) GO TO 35                                            M   33
      SIX=0.                                                            M   34
      S2=RUN(60)                                                        M   35
      DO 20 K=1,29                                                      M   36
      SIX=SIX+RUN(2*K+1)                                                M   37
   20 S2=S2+RUN(2*K)                                                    M   38
   25 OZA=2.*SIX+4.*S2+RUN(1)+OZ(J)                                     M   39
      SV=SIX                                                            M   40
      SIX=S2-RUN(2)                                                     M   41
      S2=SV+OZ(J)                                                       M   42
      RUN(61)=OZ(J)                                                     M   43
      DO 30 K=1,60                                                      M   44
   30 RUN(K)=RUN(K+1)                                                   M   45
      IF (OZA.GT.OZM) OZM=OZA                                           M   46
      IF (OZA.EQ.OZM) TM=TL+FLOAT(J-I-31)                               M   47
   35 CONTINUE                                                          M   48
      IF (TL-T.LT.0..AND.T.LT.STOPP) GO TO 5                            M   49
      IF (NCO.NE.0) GO TO 40                                            M   50
      IF (T.GT.360..AND.OZA.LT.OZM) GO TO 45                            M   51
   40 IF (T.LT.STOPP) RETURN                                            M   52
      GO TO 50                                                          M   53
   45 TOUT=T                                                            M   54
      STOPP=T                                                           M   55
   50 OZM=OZM/180.                                                      M   56
      OZA=OZA/180.                                                      M   57
      IF (OZA.LT.OZM) RETURN                                            M   58
      IF(T.GT.STOPP.AND.OZM.GT.0.00001) TM=-TM                          M   59
      RETURN                                                            M   60
      END                                                               M   61-
```

```
      SUBROUTINE COSET (METH,NQ,EL,TQ,MAXDER)                                   N    1
      DIMENSION PERTST(12,2,3), EL(13), TQ(4)                                   N    2
      DATA PERTST/1.,1.,2.,1.,.3158,.07407,.01391,.002182,.0002945,.0000       N    3
     13492,.000003692,.0000003524,1.,1.,.5,.1667,.04167,1.,1.,1.,1.,1.,1       N    4
     2.,1.,2.,12.,24.,37.89,53.33,70.08,87.97,106.9,126.7,147.4,168.8,19       N    5
     31.0,2.0,4.5,7.333,10.42,13.7,1.,1.,1.,1.,1.,1.,1.,12.0,24.0,37.89,      N    6
     453.33,70.08,87.97,106.9,126.7,147.4,168.8,191.0,1.,3.0,6.0,9.167,1       N    7
     52.5,1.,1.,1.,1.,1.,1.,1./                                                N    8
    5 MAXDER=5                                                                 N    9
      GO TO (10,15,20,25,30),NQ                                                N   10
   10 EL(1)=1.0                                                                N   11
      GO TO 35                                                                 N   12
   15 EL(1)=6.6666666666667E-01                                                N   13
      EL(3)=3.3333333333333E-01                                                N   14
      GO TO 35                                                                 N   15
   20 EL(1)=5.4545454545455E-01                                                N   16
      EL(3)=EL(1)                                                              N   17
      EL(4)=9.0909090909091E-02                                                N   18
      GO TO 35                                                                 N   19
   25 EL(1)=0.48                                                               N   20
      EL(3)=0.7                                                                N   21
      EL(4)=0.2                                                                N   22
      EL(5)=0.02                                                               N   23
      GO TO 35                                                                 N   24
   30 EL(1)=4.3795620437956E-01                                                N   25
      EL(3)=8.2116788321168E-01                                                N   26
      EL(4)=3.1021897810219E-01                                                N   27
      EL(5)=5.4744525547445E-02                                                N   28
      EL(6)=3.6496350364964E-03                                                N   29
   35 DO 40 K=1,3                                                              N   30
   40 TQ(K)=PERTST(NQ,METH,K)                                                  N   31
      TQ(4)=.5*TQ(2)/FLOAT(NQ+2)                                               N   32
      RETURN                                                                   N   33
      END                                                                      N   34
```

```
      SUBROUTINE NSCORA (N,IA,JA,A,IAP,JAWORK,AWORK,C,IR,ICT)          0     1
      INTEGER IA(1),JA(1),IAP(1),JAWORK(1),C(1),IR(1),ICT(1)           0     2
      REAL A(1),AWORK(1)                                               0     3
      DO 5 K=1,N                                                       0     4
      ICK=C(K)                                                         0     5
    5 IR(ICK)=K                                                        0     6
      JMIN=1                                                           0     7
      DO 15 K=1,N                                                      0     8
      ICK=C(K)                                                         0     9
      JMAX=JMIN+IA(ICK+1)-IA(ICK)-1                                    0    10
      IF (JMIN.GT.JMAX) GO TO 15                                       0    11
      IAINK=IA(ICK)-1                                                  0    12
      DO 10 J=JMIN,JMAX                                                0    13
      IAINK=IAINK+1                                                    0    14
      JAOUTJ=JA(IAINK)                                                 0    15
      JAOUTJ=IR(JAOUTJ)                                                0    16
      JAWORK(J)=JAOUTJ                                                 0    17
   10 AWORK(J)=A(IAINK)                                                0    18
   15 JMIN=JMAX+1                                                      0    19
      DO 20 I=1,N                                                      0    20
   20 ICT(I)=IAP(I)                                                    0    21
      JMIN=1                                                           0    22
      DO 30 I=1,N                                                      0    23
      ICK=C(I)                                                         0    24
      JMAX=JMIN+IA(ICK+1)-IA(ICK)-1                                    0    25
      IF (JMIN.GT.JMAX) GO TO 30                                       0    26
      DO 25 J=JMIN,JMAX                                                0    27
      JAOUTJ=JAWORK(J)                                                 0    28
      ICTJ=ICT(JAOUTJ)                                                 0    29
      A(ICTJ)=AWORK(J)                                                 0    30
      ICT(JAOUTJ)=ICTJ+1                                               0    31
   25 CONTINUE                                                         0    32
   30 JMIN=JMAX+1                                                      0    33
      RETURN                                                           0    34
      END                                                              0    35-
```

```
      SUBROUTINE NSNFAC (N,IA,JA,A,IL,JL,ISL,L,D,IU,JU,ISU,U,X,IRL,JRL,I P     1
     1ER)                                                               P     2
      INTEGER IA(1),JA(1),IL(1),JL(1),ISL(1)                            P     3
      INTEGER IU(1),JU(1),ISU(1),IRL(1),JRL(1)                          P     4
      REAL A(1),L(1),D(1),U(1),X(1)                                     P     5
      REAL LKI                                                          P     6
      IER=0                                                             P     7
      DO 5 K=1,N                                                        P     8
      IRL(K)=IL(K)                                                      P     9
    5 JRL(K)=0                                                          P    10
      DO 95 K=1,N                                                       P    11
      X(K)=0.                                                           P    12
      I1=0                                                              P    13
      IF (JRL(K).EQ.0) GO TO 15                                         P    14
      I=JRL(K)                                                          P    15
   10 I2=JRL(I)                                                         P    16
      JRL(I)=I1                                                         P    17
      I1=I                                                              P    18
      X(I)=0.                                                           P    19
      I=I2                                                              P    20
      IF (I.NE.0) GO TO 10                                              P    21
   15 JMIN=ISU(K)                                                       P    22
      JMAX=JMIN+IU(K+1)-IU(K)-1                                         P    23
      IF (JMIN.GT.JMAX) GO TO 25                                        P    24
      DO 20 J=JMIN,JMAX                                                 P    25
      JUJ=JU(J)                                                         P    26
   20 X(JUJ)=0.                                                         P    27
   25 JMIN=IA(K)                                                        P    28
      JMAX=IA(K+1)-1                                                    P    29
      DO 30 J=JMIN,JMAX                                                 P    30
      JAJ=JA(J)                                                         P    31
   30 X(JAJ)=A(J)                                                       P    32
      I=I1                                                              P    33
      IF (I.EQ.0) GO TO 50                                              P    34
   35 IRLI=IRL(I)                                                       P    35
      LKI=-X(I)                                                         P    36
      L(IRLI)=-LKI                                                      P    37
      JMIN=IU(I)                                                        P    38
      JMAX=IU(I+1)-1                                                    P    39
      IF (JMIN.GT.JMAX) GO TO 45                                        P    40
      ISUB=ISU(I)-1                                                     P    41
      DO 40 J=JMIN,JMAX                                                 P    42
      ISUB=ISUB+1                                                       P    43
      JUJ=JU(ISUB)                                                      P    44
   40 X(JUJ)=X(JUJ)+LKI*U(J)                                            P    45
   45 I=JRL(I)                                                          P    46
      IF (I.NE.0) GO TO 35                                              P    47
   50 IF (X(K).EQ.0.) GO TO 100                                         P    48
      DK=1./X(K)                                                        P    49
      D(K)=DK                                                           P    50
      IF (K.EQ.N) GO TO 95                                              P    51
      JMIN=IU(K)                                                        P    52
      JMAX=IU(K+1)-1                                                    P    53
      IF (JMIN.GT.JMAX) GO TO 60                                        P    54
      ISUB=ISU(K)-1                                                     P    55
      DO 55 J=JMIN,JMAX                                                 P    56
      ISUB=ISUB+1                                                       P    57
```

```
      JUJ=JU(ISUB)                                                    P   58
   55 U(J)=X(JUJ)*DK                                                  P   59
   60 CONTINUE                                                        P   60
      I=I1                                                            P   61
      IF (I.EQ.0) GO TO 90                                            P   62
   70 IRL(I)=IRL(I)+1                                                 P   63
      I1=JRL(I)                                                       P   64
      IF (IRL(I).GE.IL(I+1)) GO TO 85                                 P   65
      ISLB=IRL(I)-IL(I)+ISL(I)                                        P   66
      J=JL(ISLB)                                                      P   67
   75 IF (I.GT.JRL(J)) GO TO 80                                       P   68
      J=JRL(J)                                                        P   69
      GO TO 75                                                        P   70
   80 JRL(I)=JRL(J)                                                   P   71
      JRL(J)=I                                                        P   72
   85 I=I1                                                            P   73
      IF (I.NE.0) GO TO 70                                            P   74
   90 ISLK=ISL(K)                                                     P   75
      IF (IRL(K).GE.IL(K+1)) GO TO 95                                 P   76
      J=JL(ISLK)                                                      P   77
      JRL(K)=JRL(J)                                                   P   78
      JRL(J)=K                                                        P   79
   95 CONTINUE                                                        P   80
      RETURN                                                          P   81
  100 IER=K                                                           P   82
      RETURN                                                          P   83
      END                                                             P   84-
```

```
      SUBROUTINE NSBSLV (N,R,C,IL,JL,ISL,L,D,IU,JU,ISU,U,X,B,Y)          Q     1
      DIMENSION R(1), IL(1), JL(1), IU(1), JU(1), C(1), ISL(1), ISU(1)   Q     2
      DIMENSION L(1), X(1), B(1), U(1), Y(1), D(1)                       Q     3
      INTEGER R,RK,C,CK                                                  Q     4
      REAL L                                                             Q     5
      DO 5 K=1,N                                                         Q     6
      RK=R(K)                                                            Q     7
    5 Y(K)=B(RK)                                                         Q     8
      DO 15 K=1,N                                                        Q     9
      JMIN=IL(K)                                                         Q    10
      JMAX=IL(K+1)-1                                                     Q    11
      YK=-D(K)*Y(K)                                                      Q    12
      Y(K)=-YK                                                           Q    13
      IF (JMIN.GT.JMAX) GO TO 15                                         Q    14
      ISLB=ISL(K)-1                                                      Q    15
      DO 10 J=JMIN,JMAX                                                  Q    16
      ISLB=ISLB+1                                                        Q    17
      JLJ=JL(ISLB)                                                       Q    18
   10 Y(JLJ)=Y(JLJ)+YK*L(J)                                              Q    19
   15 CONTINUE                                                           Q    20
      K=N                                                                Q    21
      DO 30 I=1,N                                                        Q    22
      SUM=-Y(K)                                                          Q    23
      JMIN=IU(K)                                                         Q    24
      JMAX=IU(K+1)-1                                                     Q    25
      IF (JMIN.GT.JMAX) GO TO 25                                         Q    26
      ISUB=ISU(K)-1                                                      Q    27
      DO 20 J=JMIN,JMAX                                                  Q    28
      ISUB=ISUB+1                                                        Q    29
      JUJ=JU(ISUB)                                                       Q    30
   20 SUM=SUM+U(J)*Y(JUJ)                                                Q    31
   25 Y(K)=-SUM                                                          Q    32
      CK=C(K)                                                            Q    33
      X(CK)=-SUM                                                         Q    34
   30 K=K-1                                                              Q    35
      RETURN                                                             Q    36
      END                                                                Q    37-
```

```
      SUBROUTINE YSMER (A,K,A1)                                    R    1
      INTEGER A,A1(2)                                              R    2
      COMMON /INOUT/ INP,LOUT,ITAPE                                R    3
      WRITE (LOUT,5) A,K,A1(1),A1(2)                               R    4
      RETURN                                                       R    5
C                                                                  R    6
    5 FORMAT (1X,A10,I6,2A10)                                      R    7
      END                                                          R    8
```

```
      SUBROUTINE INTERP (TOUT,Y,N0,Y0)                                  S     1
      COMMON /GEAR1/ T,H,DUMMY(4),N,IDUMMY(2),JSTART                    S     2
      DIMENSION Y0(N0), Y(N0,1)                                         S     3
      DO 5 I=1,N                                                        S     4
    5 Y0(I)=Y(I,1)                                                      S     5
      L=JSTART+1                                                        S     6
      S=(TOUT-T)/H                                                      S     7
      S1=1.                                                             S     8
      DO 15 J=2,L                                                       S     9
      S1=S1*S                                                           S    10
      DO 10 I=1,N                                                       S    11
   10 Y0(I)=Y0(I)+S1*Y(I,J)                                             S    12
   15 CONTINUE                                                          S    13
      RETURN                                                            S    14
      END                                                               S    15-
```

Subroutine LINER

```
      SUBROUTINE LINER (SIG,KALCMP,F)                                    T     1
      COMMON /NEED/ HC,XN,NL,NR,R(20),OZP(20),OZN(8,20),RHO(8,20),MR,OC(  T     2
     14),OS(2),HCS,XNS,LS,HCLL(8)                                        T     3
      COMMON /VVLBL/ FACTOR,DISTNC,CHRSZ,NCHR,OZLBL                      T     4
      COMMON /PLTVEC/ HCT(20),OT(20),NT,OHC,HCG,PLTGRD,OXN,XNG,HCC,XNC,T T     5
     1ICZ,DIGZ,CHRZ                                                      T     6
      COMMON /CNTRL/ SGG,SIGMA,INFO,NPTO,XNF,RCTY,ALDX,OZIN,OZAL,HCIN,HC T     7
     1AL,XNIN,XNAL,TSRT,DTIM,Z1,Z2,DCON,EHC,EXN,FLST,TLST                T     8
      COMMON /INOUT/ IN,IOUT,ITAPE                                       T     9
      COMMON /TITL/ ITTL(18)                                             T     10
      COMMON /GEAR6/ RPL(20,20),RTL(20,20),NRL(20),NSL(20),NTL(20),NUL(2 T     11
     10),W(20),WW(20),OE(20),HCTP(20),XNE(20),XNEP(20),YP(20),TM(20),XNA T     12
     2P(20),HCAP(20),HCLP(20),ITTL1(18),U(44),V(44),DUM1(294)            T     13
      DIMENSION F(20), RBL(20,20), NBL(20), NTOL(20)                     T     14
C                                                                        T     15
C  FIRST SET CALCOMP OPTION                                              T     16
C                                                                        T     17
      IF (KALCMP.LE.0) GO TO 5                                           T     18
      CHRSZ=TICZ                                                         T     19
      IDIG1=1                                                            T     20
      IDIG2=2                                                            T     21
      IHY=IFIX(HC*10.+0.5)                                               T     22
      IHZ=IFIX(XN*1000.+0.5)                                             T     23
      IF (MOD(IHY,10).NE.0) IDIG1=2                                      T     24
      IF (MOD(IHZ,7).NE.0.OR.IHZ.LT.10) IDIG2=3                          T     25
      HCC=HCC/HC                                                         T     26
      HCX=0.                                                             T     27
      HCM=HC/10.                                                         T     28
      XNC=XNC/XN                                                         T     29
      XNX=0.                                                             T     30
      XNM=XN/7.                                                          T     31
      XX=((10.0-(HCC*HC))/2.0)+0.3                                       T     32
      YY=((8.0-(XNC*XN))/2.0)+0.3                                        T     33
      ORGY=-.75                                                          T     34
      CALL PLOTS (I1,I2,14)                                              T     35
      CALL PLOT (XX,YY,-3)                                               T     36
    5 M=MR+1                                                             T     38
      NLL=0                                                              T     39
      DO 10 I=1,NL                                                       T     40
      NUL(I)=0                                                           T     41
      NTL(I)=0                                                           T     42
      NTOL(I)=0                                                          T     43
      NBL(I)=0                                                           T     44
      NSL(I)=0                                                           T     45
   10 NRL(I)=0                                                           T     46
      OE(1)=OC(4)                                                        T     47
      OE(2)=OS(2)                                                        T     48
      XNE(1)=0.                                                          T     49
      XNE(2)=XNS                                                         T     50
      DO 15 I=1,NR                                                       T     51
      K=NR+1-I                                                           T     52
      OE(I+2)=OZN(MR,K)                                                  T     53
      XNE(I+2)=HC/R(K)                                                   T     54
      IF (XNE(I+2).GT.XN) GO TO 20                                       T     55
   15 CONTINUE                                                           T     56
      I=NR+1                                                             T     57
```

```
20 I=I-1                                                                    T   88
   NE=I+2                                                                   T   89
   TOL=1.0-(0.17/(SQRT(FLOAT(NR))))                                         T   90
   NCR=(NR+1)/2                                                             T   91
   CALL EDGMX (XNE,OE,NE,XMX,OZX,LX)                                        T   92
   NDIF=NE-LX+1                                                             T   93
   NEW=NE                                                                   T   94
   NE=LX+1                                                                  T   95
   OE(NE)=OZX                                                               T   96
   XNE(NE)=XMX                                                              T   97
   CALL EDGMX (HCT,OT,NT,HMX,OZHX,LHX)                                      T   98
   NDIF1=NT-LHX+1                                                           T   99
   NDIF2=NT-LHX-1                                                           T  100
   NEW1=NT                                                                  T  101
   NT=LHX+1                                                                 T  102
   OT(NT)=OZHX                                                              T  103
   HCT(NT)=HMX                                                              T  104
   SX=-SIG*0.25                                                             T  105
   IF (OZP(NL).LT.OC(2)) GO TO 30                                           T  106
   CALL NEWLIN (NT,OT,HCT,SX,LS,NL,1,0,HCTP,NPL,TOL,0,0,0)                  T  107
   NTT=NPL                                                                  T  108
   IF (OZP(LS).GE.OC(2)) NLL=0                                              T  108A
   IF (OZP(LS).GE.OC(2)) GO TO 50                                           T  109
30 SX=-SIG*10.                                                              T  110
   IF (NR.GT.1) GO TO 35                                                    T  111
   OT(1)=OC(1)                                                              T  112
   HCT(1)=0.                                                                T  113
   OT(2)=OC(2)                                                              T  114
   HCT(2)=XN                                                                T  115
   NR2=2                                                                    T  116
   GO TO 45                                                                 T  117
35 DO 40 II=1,NR                                                            T  118
   OT(II+1)=OZN(II,1)                                                       T  119
40 HCT(II+1)=HCLL(II)                                                       T  120
   OT(1)=OC(1)                                                              T  121
   HCT(1)=0.                                                                T  122
   NR2=NR+1                                                                 T  123
45 CALL NEWLIN (NR2,OT,HCT,SX,LS,NL,2,0,HCLP,NLL,TOL,0,0,0)                 T  124
   IF (OZP(NL).LT.OC(2)) NPL=NLL                                            T  125
50 NPLI=NPL+1                                                               T  126
   IF (NPLI.GE.NL) GO TO 60                                                 T  127
   DO 55 J=NPLI,NL                                                          T  128
55 IF (OZP(J).LT.OE(NE)) NPL=NPL+1                                          T  129
60 SX=-SIG*10.                                                              T  130
   CALL NEWLIN (NE,OE,XNE,SX,LS,NL,3,0,XNEP,NEL,TOL,0,0,0)                  T  131
   IF (NDIF2.EQ.0) GO TO 75                                                 T  132
   DO 65 II=LHX,NEW1                                                        T  133
   JJ=LHX-II+1                                                              T  134
   IF (IABS(JJ).GT.NCR) GO TO 70                                            T  135
   JO=II-LHX+1                                                              T  136
   OT(JO)=OZN(NR,NCR+JJ-1)                                                  T  137
65 HCT(JO)=R(NCR+JJ-1)*XN                                                   T  138
70 OT(NDIF1)=OZHX                                                           T  139
   HCT(NDIF1)=HMX                                                           T  140
   SX=-SIG*10.                                                              T  141
   CALL NEWLIN (NDIF1,OT,HCT,SX,NEL+1,NPL,4,NEL,HCAP,II,TOL,0,0,0)          T  142
75 IF ((NTT+NLL).GE.NPL) GO TO 90                                           T  143
```

```
      DO 80 II=LX,NEW                                                    T  114
      JJ=II-LX+1                                                         T  115
      IF (JJ.GT.NCR) GO TO 83                                            T  116
      OE(JJ)=OZN(NR,NCR+JJ-1)                                            T  117
   80 XNE(JJ)=HC/R(NCR+JJ-1)                                             T  118
   83 OE(NDIF)=OZX                                                       T  119
      XNE(NDIF)=XNX                                                      T  120
      SX=-SIG*10.                                                        T  121
      CALL NEWLIN (NDIF,OE,XNE,SX,NTT+1,NPL,3,NTT,XNAP,II,TOL,0,0,0)     T  122
   90 IF (OZP(LS).LT.OC(2)) NR1=NR-1                                     T  123
      IF (OZP(LS).GE.OC(2)) NR1=NR                                       T  124
      NOZLST=0                                                           T  125
      IF (OZP(LS).LT.OC(2)) IK=1                                         T  126
      IF (OZP(LS).GE.OC(2)) IK=0                                         T  127
      XOZ=AMAX1(OZHX,OZX,OC(3))                                          T  128
      IF (XOZ.EQ.OZHX) NOZLST=NT-2                                       T  129
      IF (XOZ.EQ.OC(3)) NOZLST=NCR                                       T  130
      IF (XOZ.EQ.OZX) NOZLST=NCR+NDIF-2                                  T  131
      DO 110 LL=1,NR1                                                    T  132
      IF (OZP(LS).LT.OC(2)) I=LL+1                                       T  133
      IF (OZP(LS).GE.OC(2)) I=LL                                         T  134
      IF (NR.EQ.1) I=LL                                                  T  135
      U(1)=OC(1)                                                         T  136
      V(1)=0.                                                            T  137
      DO 95 J=2,M                                                        T  138
      U(J)=OZN(J-1,I)                                                    T  139
   95 V(J)=RHO(J-1,I)                                                    T  140
      SX=-SIG*3.0                                                        T  141
      IF (M.GT.2) SX=-SIG*60./(FLOAT(M-2)**2)                            T  142
      CALL EDGMX (V,U,M,HHMX,OZMMX,MM1)                                  T  143
      MM=MM1+1                                                           T  144
      IF (MM.GE.M) GO TO 105                                             T  145
      U(MM)=OZMMX                                                        T  146
      V(MM)=HHMX                                                         T  147
      W(1)=OZN(NR,I)                                                     T  148
      WW(1)=RHO(NR,I)                                                    T  149
      MDIF=M-MM1+1                                                       T  150
      DO 100 J=2,MDIF                                                    T  151
      W(J)=OZN(M-J+1,I)                                                  T  152
  100 WW(J)=RHO(M-J+1,I)                                                 T  153
      W(MDIF)=OZMMX                                                      T  154
      WW(MDIF)=HHMX                                                      T  155
      IF ((LL-IK).LE.NOZLST) CALL NEWLIN (MDIF,W,WW,SX,LS,NL,6,0,RTL(1,I T  156
     1),IJ,TOL,NUL,NTL,I)                                                T  157
      IF ((LL-IK).GT.NOZLST) CALL NEWLIN (MDIF,W,WW,SX,LS,NL,6,0,RBL(1,I T  158
     1),IJ,TOL,NTOL,NBL,I)                                               T  159
      SX=-SIG*3.0                                                        T  160
      IF (MM.GT.2) SX=-SIG*60./(FLOAT(MM-2)**2)                          T  161
  105 CALL NEWLIN (MM,U,V,SX,LS,NL,7,0,RPL(1,I),II,TOL,NRL,NSL,I)        T  162
  110 CONTINUE                                                           T  163
      CALL ISOPLT (HCTP,XN)                                              T  164
      SX=SIGMA*30./FLOAT(NR)                                             T  165
      NTT2=NTT+NLL                                                       T  165A
      IF (NTT.NE.0.AND.NLL.NE.0) NTT2=NTT                                T  165B
      NW=0                                                               T  165C
      DO 185 I=LS,NPL                                                    T  166
      K=1                                                                T  167
```

```
      IF (I.LE.NTT2) GO TO 115                                          T  168
      U(1)=HC                                                           T  169
      V(1)=XNAP(I-NTT)                                                  T  170
      GO TO 125                                                         T  171
  115 IF (OZP(LS).GT.OC(2)) GO TO 120                                   T  172
      IF (I.GT.NLL) GO TO 120                                           T  173
      U(1)=0.                                                           T  174
      V(1)=HCLP(I)                                                      T  175
      GO TO 125                                                         T  176
  120 U(1)=HCTP(I)                                                      T  177
      V(1)=XN                                                           T  178
  125 NT=NUL(I)                                                         T  179
      NE=NTL(I)                                                         T  180
      IF (NE.EQ.0) GO TO 135                                            T  181
      DO 130 JI=NE,NT                                                   T  182
      J=NT-JI+1                                                         T  183
      K=K+1                                                             T  184
      V(K)=RTL(I,J)/F(J)                                                T  185
  130 U(K)=V(K)*R(J)                                                    T  186
  135 NT=NRL(I)                                                         T  187
      NE=NSL(I)                                                         T  188
      IF (NE.EQ.0) GO TO 145                                            T  189
      DO 140 J=NE,NT                                                    T  190
      K=K+1                                                             T  191
      V(K)=RPL(I,J)/F(J)                                                T  192
  140 U(K)=V(K)*R(J)                                                    T  193
  145 NT=NTOL(I)                                                        T  194
      NE=NBL(I)                                                         T  195
      IF (NE.EQ.0) GO TO 155                                            T  196
      DO 150 JI=NE,NT                                                   T  197
      J=NT-JI+1                                                         T  198
      K=K+1                                                             T  199
      V(K)=RBL(I,J)/F(J)                                                T  200
  150 U(K)=V(K)*R(J)                                                    T  201
  155 IF (I.GT.NEL) GO TO 160                                           T  202
      K=K+1                                                             T  203
      U(K)=HC                                                           T  204
      V(K)=XNEP(I)                                                      T  205
      GO TO 165                                                         T  206
  160 IF (NDIF2.EQ.0) GO TO 165                                         T  207
      K=K+1                                                             T  208
      U(K)=HCAP(I-NEL)                                                  T  209
      V(K)=XN                                                           T  210
  165 U(K+1)=0.                                                         T  211
      U(K+2)=1./HCC                                                     T  212
      V(K+1)=0.                                                         T  213
      V(K+2)=1./XNC                                                     T  214
      IF (K.LE.2) GO TO 185                                             T  215
      OZLBL=OZP(I)                                                      T  216
      NW=NW+1                                                           T  216A
      W(NW)=OZP(I)                                                      T  216B
      NCHR=4                                                            T  217
      NCNT=0                                                            T  218
  170 VAL=OZLBL*(10.**NCNT)                                             T  219
      IF (VAL.GT.0.01) GO TO 175                                        T  220
      NCNT=NCNT+1                                                       T  221
      GO TO 170                                                         T  222
```

```
  175 NCHR=NCHR+NCNT                                                    T  223
      REMB=OZLBL-FLOAT(IFIX(OZLBL*(10.**(NCNT+2))+0.1))/(10.**(NCNT+2))  T  224
      IF (REMB.GE.(0.001/(10.**NCNT))) NCHR=NCHR+1                      T  225
      CALL CURVE (U,V,K,1,KALCMP,0,0,SX)                                T  226
  185 CONTINUE                                                          T  227
      IF (KALCMP.LE.0) GO TO 220                                        T  228
      CALL FRAME (0.,0.,0.,HC,HCC,HCX,HCM,IDIG1,0.,XN,XNC,XNX,XNM,IDIG2, T  229
     19HNMHC,PPMC,9,7HNOX,PPM,7,1H ,1,1H ,1)                            T  230
      NCNT=0                                                            T  231
      DO 190 I=1,18                                                     T  232
      IF (ITTL(I).NE.4H     ) GO TO 195                                 T  233
      NCNT=NCNT+1                                                       T  234
  190 CONTINUE                                                          T  235
  195 NLST=18-NCNT                                                      T  236
      DO 200 I=1,NLST                                                   T  237
  200 ITTL1(I)=ITTL(I+NCNT)                                             T  238
      NCNT1=18                                                          T  239
      DO 205 I=1,18                                                     T  240
      II=19-I                                                           T  241
      IF (ITTL1(II).NE.4H     ) GO TO 210                               T  242
      NCNT1=NCNT1-1                                                     T  243
  205 CONTINUE                                                          T  244
  210 NCNT1=NCNT1-NCNT                                                  T  245
      ORGX=((HCC*HC)-(FLOAT(NCNT1)*4.*CHRZ))/2.0                        T  246
      DO 215 I=1,NCNT1                                                  T  247
      CALL SYMBOL (ORGX,ORGY,CHRZ,ITTL1(I),0.,4)                        T  248
      ORGX=ORGX+4.0*CHRZ                                                T  249
  215 CONTINUE                                                          T  250
      CALL PLOT (10.,2.,999)                                            T  251
  220 HCS=FLOAT(NW)                                                     T  252
      XNS=FLOAT(NLL)                                                    T  253
C 155 CALL LINPRT                                                       T  254
      CALL LINPRT (HC,XN)                                               T  255
      RETURN                                                            T  256
      END                                                               T  257-
```

```
      SUBROUTINE CURVE (XARRAY,YARRAY,NPTS,INC,KALCMP,LINTYP,INTEQ,SIGMA U     1
     1)                                                                 U     2
C                                                                       U     3
C     *** PURPOSE -- PLOTS A SMOOTH CURVE THROUGH THE DATA VALUES FROM T U     4
C         GW LUNDBERG/SAI   JULY 177                                    U     5
C                                                                       U     6
C          MODIFIED BY H HOGO AUG 1977                                  U     7
C                                                                       U     8
C         XARRAY  ARRAY CONTAINING X VALUES                             U     9
C         YARRAY  ARRAY CONTIANING Y VALUES                             U    10
C         NPTS     NUMBER OF DATA POINTS IN THE ARRAYS ACTUALLY USED    U    11
C                ) 0  SCALING AT TOP OF ARRAYS                          U    12
C         INC      EVERY INC POINT WILL BE USED                         U    13
C         LINTYP   PLOT SPECIAL SYMBOL EVERY LINTYP POINT               U    14
C                ) 0  CONNECTED SYMBOL PLOT                             U    15
C                = 0  LINE PLOT                                         U    16
C                ( 0  UNCONNECTED SYMBOL PLOT                           U    17
C         INTEQ    INTEGER EQUIVALENT OF SPECIAL SYMBOL                 U    18
C         THIS ROUTINE CALLS  SYMBOL, PLOT, KURV1 AND KURV2             U    19
C                                                                       U    20
      COMMON /VVLBL/ FCTR,DIST,CHRSZ,NCHR,OZLBL                         U    21
      DIMENSION XARRAY(1), YARRAY(1), XI(50), YI(50), XP(50), YP(50), TE U    22
     1MP(50)                                                            U    23
C                                                                       U    24
      DATA NSLOPE/0/,SLOPE1,SLOPEN/0.,0./                               U    25
C                                                                       U    26
C                                                                       U    27
C     *** LOCATE SCALING (FIRSTV AND DELTAV) FOR EACH ARRAY             U    28
C         ------ -------- ------- --- -------- --- ---- -----          U    29
C                                                                       U    30
C                                                                       U    31
C     *** SCALING IN TOP OF ARRAYS -- CALCOMP STANDARD                  U    32
      N=NPTS*INC+1                                                      U    33
      FIRSTX=XARRAY(N)                                                  U    34
      FIRSTY=YARRAY(N)                                                  U    35
      N=N+INC                                                           U    36
      DELTAX=XARRAY(N)                                                  U    37
      DELTAY=YARRAY(N)                                                  U    38
C                                                                       U    39
      NUM=IABS(NPTS)                                                    U    40
      IF (KALCMP.LE.0) GO TO 10                                         U    41
C                                                                       U    42
C     *** CHECK IF SYMBOL PLOT WANTED -- LINTYP () 0                    U    43
      IF (LINTYP.EQ.0) GO TO 10                                         U    44
C                                                                       U    45
C     *** CENTERED SYMBOL PLOT                                          U    46
C         -------- ------ ----                                         U    47
C                                                                       U    48
C     *** SCALE FIRST DATA POINT AND PLOT CENTERED SYMBOL               U    49
      X=(XARRAY(1)-FIRSTX)/DELTAX                                       U    50
      Y=(YARRAY(1)-FIRSTY)/DELTAY                                       U    51
      CALL SYMBOL (X,Y,0.1,INTEQ,0.,-1)                                 U    52
C                                                                       U    53
C     *** PLOT REMAINING SYMBOLS AT INCREMENTS OF MARK                  U    54
      MARK=IABS(LINTYP)                                                 U    55
      N=1                                                               U    56
C                                                                       U    57
```

```
      DO 5 J=2,NUM                                                      U   58
      N=N+INC                                                           U   59
      IF (MOD(N,MARK).NE.0) GO TO 5                                     U   60
      X=(XARRAY(N)-FIRSTX)/DELTAX                                       U   61
      Y=(YARRAY(N)-FIRSTY)/DELTAY                                       U   62
      CALL SYMBOL (X,Y,0.1,INTEQ,0.,-1)                                 U   63
    5 CONTINUE                                                          U   64
C                                                                       U   65
C     *** IF THE SYMBOLS ARE NOT TO BE CONNECTED, RETURN                U   66
      IF (LINTYP.LT.0) GO TO 30                                         U   67
C                                                                       U   68
C     *** LINE PLOT (OR CONNECT SYMBOLS)                                U   69
C         ---- ---- -- ------ --------                                  U   70
C                                                                       U   71
C     *** SCALE FIRST DATA POINT AND MOVE PEN THERE                     U   72
   10 XI(1)=(XARRAY(1)-FIRSTX)/DELTAX                                   U   73
      YI(1)=(YARRAY(1)-FIRSTY)/DELTAY                                   U   74
C                                                                       U   75
C                                                                       U   76
C     *** SCALE THE REMAINING POINTS                                    U   77
      N=1                                                               U   78
      DO 15 J=2,NUM                                                     U   79
      N=N+INC                                                           U   80
      XI(J)=(XARRAY(N)-FIRSTX)/DELTAX                                   U   81
      YI(J)=(YARRAY(N)-FIRSTY)/DELTAY                                   U   82
   15 CONTINUE                                                          U   83
C                                                                       U   84
      NSLP=NSLOPE                                                       U   85
C                                                                       U   86
C     *** CHECK IF PERIODIC                                             U   87
      IF (ABS(XI(NUM)-XI(1)).LT.0.01.AND.ABS(YI(NUM)-YI(1)).LT.0.01) NSL U   88
     1P=-1                                                              U   89
C                                                                       U   90
C     *** SET UP SPLINE INTERPOLATION                                   U   91
      NSLP=1                                                            U   92
      SLOPE1=57.29578*ATAN((YI(1)-YI(2))/(XI(1)-XI(2)))                 U   93
      IF (SLOPE1.GT.0.) SLOPE1=SLOPE1-180.                              U   94
      SLOPE1=AMIN1(SLOPE1,-90.)                                         U   95
      SLOPEN=28.64789*ATAN((YI(N)-YI(N-1))/(XI(N)-XI(N-1)))             U   96
      CALL KURV1 (NUM,XI,YI,NSLP,SLOPE1,SLOPEN,XP,YP,TEMP,S,SIGMA)      U   97
      CALL KURV2 (0.,X,Y,NUM,XI,YI,XP,YP,S,SIGMA)                       U   98
      X=AMAX1(0.,X)                                                     U   99
      Y=AMAX1(0.,Y)                                                     U  100
      USX=X*DELTAX+FIRSTX                                               U  101
      USY=Y*DELTAY+FIRSTY                                               U  102
      CALL SAVLIN (USX,USY)                                             U  103
C                                                                       U  104
C     *** LITE SEGMENTS WILL BE A TENTH INCH LONG -- S IS THE ARCLENGTH U  105
      NP=10.*S+1                                                        U  106
      CONST=1./NP                                                       U  107
      DIST=S                                                            U  108
      IF (KALCMP.LE.0) GO TO 20                                         U  109
      CALL VVLBLF (XI(1),YI(1))                                         U  110
C                                                                       U  111
C     *** MAP AND PLOT SEGMENTS                                         U  112
   20 DO 25 J=1,NP                                                      U  113
      T=-J*CONST                                                        U  114
```

```
      CALL KURV2 (T,X,Y,NUM,XI,YI,XP,YP,S,SIGMA)                    U  115
      X=AMAX1(0.,X)                                                 U  116
      Y=AMAX1(0.,Y)                                                 U  117
      USX=X*DELTAX+FIRSTX                                           U  118
      USY=Y*DELTAY+FIRSTY                                           U  119
      CALL SAVLIN (USX,USY)                                         U  120
      IF (KALCMP.LE.0) GO TO 25                                     U  121
      CALL VVLBLC (X,Y)                                             U  122
   25 CONTINUE                                                      U  123
      IF (KALCMP.LE.0) GO TO 30                                     U  124
      CALL VVLBLL (0.,0.)                                           U  125
C                                                                   U  126
   30 RETURN                                                        U  127
C                                                                   U  128
      END                                                           U  129-
```

```
      SUBROUTINE ISOPLT (SAVHC,SAVNOX)                                  V     1
      COMMON /NEED/ HC,XN,NL,NRTO,RTO(20),OZZ(20),OZN(8,20),RHO(8,20),MR V     2
     1,OC(4),OS(2),HCS,XNS,LS,HCLL(8)                                   V     3
      COMMON /TITL/ ITTL(18)                                            V     4
      COMMON /INOUT/ IN,IOUT,ITAPE                                      V     5
      COMMON /CALC/ NR,KR(77,3),A(77),S(77),R(77),ITYPE(77),IA(34),JA(21 V     6
     18),DILUT,TEMP,ERR,START,STOPP,SPECIS(34),TPRN,TSTP                V     7
      COMMON /CNTRL/ SIG,SIGMA,INFO,NPTO,XNF,RCTY,ALDX,OZIN,OZAL,HCIN,HC V     8
     1AL,XNIN,XNAL,TSRT,DTIM,Z1,Z2,DCON,EHC,EXN,FLST,TLST               V     9
      COMMON /GEAR6/ DUM1(880),OZP(20),DUM2(306),NGRID(101,2),DUM3(92)  V     9A
      COMMON /HOUR/ OZM,NGO,TM                                          V    10
      DIMENSION TVERT(52,2), JGRID(101,42), TPRINT(11), NLINE(3)        V    11
      DIMENSION CVERT(9),TV(7),SAVDAT(101),TV1(7)                       V    12
      DATA JBLANK/4H    /,MAXHC/101/,MAXNOX/42/,MAXPNT/80/,TGRID/100./,C V    13
     1GRID/42./,JPLUS/1H+/,JBAR/1H1/,JSYMB/1H+/                         V    14
      DATA CVERT /4H O  ,4H Z  ,4H O  ,4H N  ,4H E  ,4H    ,4H P  ,4H P  V    15
     1 ,4H M  /                                                         V    16
      DATA TV/4H N  ,4H O  ,4H X  ,4H    ,4H P  ,4H P  ,4H M  /         V    17
      DATA TVERT/104*4H    /,NGRID(1,1)/1HI/,NGRID(1,2)/1HI/,NGRID(101,1 V    18
     1)/1HI/,NGRID(101,2)/1HI/                                          V    18A
      DO 5 J=1,42                                                       V    19
      JGRID(1,J)=JBAR                                                   V    20
      JGRID(101,J)=JBAR                                                 V    21
    5 CONTINUE                                                          V    22
      DO 15 I=1,52                                                      V    23
      TVERT(I,1)=4H                                                     V    24
      IF (NPTO.EQ.0) GO TO 10                                           V    25
      IF (I.LT.18.OR.I.GT.26) GO TO 15                                  V    26
      K=I-17                                                            V    27
      TVERT(I,1)=CVERT(K)                                               V    28
      GO TO 15                                                          V    29
   10 IF (I.LT.17.OR.I.GT.23) GO TO 15                                  V    30
      K=I-16                                                            V    31
      TVERT(I,1)=TV(K)                                                  V    32
   15 CONTINUE                                                          V    33
      DO 20 I=1,101                                                     V    34
   20 SAVDAT(I)=0.                                                      V    35
      DO 25 J=1,42,3                                                    V    36
      JGRID(1,J)=JPLUS                                                  V    37
      JGRID(101,J)=JPLUS                                                V    38
   25 CONTINUE                                                          V    39
                                                                        V    40
C                                                                       V    41
C SET NORMALIZATION FACTORS AND VERTICAL LABELS                         V    42
C                                                                       V    43
      CLOW=0.                                                           V    44
      TLOW=0.                                                           V    45
      IF (NPTO.NE.0) GO TO 35                                           V    46
      CHIGH=XN                                                          V    47
      CSPAN=CGRID/CHIGH                                                 V    48
      THIGH=HC                                                          V    49
      DO 30 I=1,7                                                       V    50
      M=8-I                                                             V    51
      TV1(I)=(FLOAT(M)/7.)*CHIGH                                        V    52
   30 CONTINUE                                                          V    54
      GO TO 40                                                          V    55
C                                                                       V    56
```

```
C SET HORIZONTAL LABELS                                                  V   57
C                                                                        V   58
   35 THIGH=STOPP                                                        V   59
   40 TSPAN=TGRID/THIGH                                                  V   60
      DO 45 J=1,11                                                       V   61
      TPRINT(J)=(FLOAT(J-1)/10.)*THIGH                                   V   62
   45 CONTINUE                                                           V   63
C                                                                        V   64
C CLEAR GRID                                                             V   65
C                                                                        V   66
      MAXHC1=MAXHC-1                                                     V   67
      DO 50 K=1,MAXNOX                                                   V   68
      DO 50 J=2,MAXHC1                                                   V   69
      JGRID(J,K)=JBLANK                                                  V   70
      IF (K.LE.2) NGRID(J,K)=JBLANK                                      V   70A
   50 CONTINUE                                                           V   71
      RETURN                                                             V   72
C                                                                        V   73
C ENTRY FOR SAVING INTERPOLATED POINTS                                   V   74
C                                                                        V   75
C     ENTRY SAVLIN                                                       V   76
      ENTRY SAVLIN (SAVHC,SAVNOX)                                        V   77
      KHC=IFIX((SAVHC-TLOW)*TSPAN+1.5)                                   V   78
      IF (NPTO.NE.0) GO TO 55                                            V   79
      KNOX=IFIX((SAVNOX-CLOW)*CSPAN-0.5)                                 V   80
      KNOX=MAXNOX-KNOX                                                   V   81
      IF (KNOX.LT.1) GO TO 60                                            V   82
      IF (KNOX.GT.MAXNOX) GO TO 60                                       V   83
   55 IF (KHC.LT.2) GO TO 60                                             V   84
      IF (KHC.GT.MAXHC1) GO TO 60                                        V   85
      IF (NPTO.EQ.0) JGRID(KHC,KNOX)=JSYMB                               V   86
      IF (NPTO.NE.0) SAVDAT(KHC)=SAVNOX                                  V   87
   60 RETURN                                                             V   88
C                                                                        V   89
C ENTRY FOR PLOTTING GRID                                                V   90
C                                                                        V   91
C     ENTRY LINPRT                                                       V   92
      ENTRY LINPRT (SAVHC,SAVNOX)                                        V   93
      IF (NPTO.NE.0) GO TO 95                                            V   94
      NPL=IFIX(HCS+0.1)                                                  V   95
      NLL=IFIX(XNS+0.5)                                                  V   96
      KOUNT=0                                                            V   97
      IF (NLL.EQ.0) GO TO 80                                             V   98
      NJ=1                                                               V   99
   65 NJ=NJ+1                                                           V  100
      J=MAXNOX-NJ                                                        V  101
      IF (JGRID(3,J).EQ.JBLANK) GO TO 65                                 V  102
      KOUNT=KOUNT+1                                                      V  103
      IF (KOUNT.GT.NLL) GO TO 75                                         V  104
      IF (NJ.GT.MAXNOX-1) GO TO 75                                       V  105
      NVAR=IFIX(OZP(KOUNT)*100.+0.5)                                     V  106
      CALL CONVT (NVAR,NLINE)                                            V  107
      DO 70 II=1,3                                                       V  108
   70 IF (NLINE(II).NE.1H ) JGRID(2+II,J)=NLINE(II)                      V  109
      NJ=NJ+1                                                            V  110
      GO TO 65                                                           V  111
   75 KOUNT=KOUNT-1                                                      V  112
```

```
   80 I=1                                                                V  113
   83 I=I+1                                                              V  114
      IF (I.GT.MAXHC1) GO TO 110                                         V  115
      IF (JGRID(I,1).EQ.JBLANK) GO TO 83                                 V  116
      KOUNT=KOUNT+1                                                      V  117
      IF (KOUNT.GT.NPL) GO TO 110                                        V  118
      NVAR=IFIX(OZP(KOUNT)*100.+0.5)                                     V  119
      CALL CONVT (NVAR,NLINE)                                            V  120
      DO 90 II=2,3                                                       V  121
   90 IF (NLINE(II).NE.1H ) NGRID(I,II-1)=NLINE(II)                      V  122
      I=I+1                                                              V  124
      GO TO 83                                                           V  125
   95 CHIGH=OZM+(0.2*OZM                                                 V  126
      IF (OZM.EQ.0.0) RETURN                                             V  126A
      CSPAN=CGRID/CHIGH                                                  V  127
      DO 100 I=1,7                                                       V  128
      M=8-I                                                              V  129
      TV1(I)=(FLOAT(M)/7.)*CHIGH                                         V  130
  100 CONTINUE                                                           V  132
      DO 105 I=2,100                                                     V  133
      IF (SAVDAT(I).EQ.0.) GO TO 105                                     V  134
      KNOX=IFIX(SAVDAT(I)*CSPAN-0.5)                                     V  135
      KNOX=MAXNOX-KNOX                                                   V  136
      IF (KNOX.LT.1) GO TO 105                                           V  137
      IF (KNOX.GT.MAXNOX) GO TO 105                                      V  138
      JGRID(I,KNOX)=1HO                                                  V  139
  105 CONTINUE                                                           V  140
  110 IF (NPTO.EQ.0) WRITE (IOUT,125) ((NGRID(I,J),I=1,101),J=1,2)       V  141
      IF (NPTO.NE.0) WRITE (IOUT,120) TVERT(1,1),TVERT(1,2)              V  142
      IF (NPTO.EQ.0) KFRST=1                                             V  143
      IF (NPTO.NE.0) KFRST=2                                             V  144
      DO 115 K=KFRST,MAXNOX                                              V  145
      L=MOD((K-1),6)                                                     V  146
      I=(K-1)/6+1                                                        V  147
      IF (L.EQ.0) WRITE (IOUT,130) TVERT(K,1),TV1(I),(JGRID(J,K),J=1,MAX V  148
     1HC)                                                                V  149
      IF (L.NE.0) WRITE (IOUT,135) TVERT(K,1),(JGRID(J,K),J=1,MAXHC)     V  150
  115 CONTINUE                                                           V  151
      WRITE (IOUT,140) CLOW                                              V  152
      IF (NPTO.EQ.0) WRITE (IOUT,143) TPRINT                             V  153
      IF (NPTO.NE.0) WRITE (IOUT,153) TPRINT                             V  154
      WRITE (IOUT,150) (ITTL(I),I=1,18)                                  V  155
      IF (NPTO.EQ.0) WRITE (IOUT,160) (OZP(I),I=1,NPL)                   V  155A
      RETURN                                                             V  156
C                                                                        V  157
C                                                                        V  158
C                                                                        V  159
  120 FORMAT (1H1,/////////,9X,A4,F3.3,1H+,10(10H---------+))            V  160
  125 FORMAT (1H1,//////,18X,1H+,10(10H---------+),/,18X,101A1,/,18X,    V  161
     1101A1)                                                             V  162
  130 FORMAT (9X,A4,F5.3,101A1)                                          V  163
  135 FORMAT (9X,A4,5X,101A1)                                            V  164
  140 FORMAT (13X,F3.3,1H+,10(10H---------+))                            V  165
  143 FORMAT (F21.3,10F10.2,/,64X,11HNMHC (PPMC),//)                     V  166
  150 FORMAT (46X,18A4)                                                  V  167
  153 FORMAT (F21.1,10F10.1,/,63X,14HTIME (MINUTES),//)                  V  168
  160 FORMAT (1H0,/,20X,20HTHE OZONE LINES ARE  ,10F8.5,/,40X,10F8.5)    V  168A
      END                                                                V  169-
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```
      SUBROUTINE CURV1 (N,X,Y,SLP1,SLPN,YP,TEMP,SIGMA)                  W    1
C                                                                       W    2
C     THIS SUBROUTINE DETERMINES THE PARAMETERS NECESSARY TO            W    3
C     COMPUTE AN INTERPOLATORY SPLINE UNDER TENSION THROUGH             W    4
C     A SEQUENCE OF FUNCTIONAL VALUES.  THE SLOPES AT THE TWO           W    5
C     ENDS OF THE CURVE MAY BE SPECIFIED OR OMITTED.  FOR ACTUAL        W    6
C     COMPUTATION OF POINTS ON THE CURVE IT IS NECESSARY TO CALL        W    7
C     THE FUNCTION CURV2.                                               W    8
C                                                                       W    9
C     ON INPUT --                                                       W   10
C     N = THE NUMBER OF VALUES TO BE INTERPOLATED (N.GE.2),             W   11
C     X = AN ARRAY OF THE N INCREASING ABCISSAE OF THE                  W   12
C         FUNCTIONAL VALUES,                                            W   13
C     Y = AN ARRAY OF THE N ORDINATES OF THE VALUES, (I.E.Y(K)          W   14
C         IS THE FUNCTIONAL VALUE CORRESPONDING TO X(K)),               W   15
C     SLP1,SLPN CONTAIN THE DESIRED VALUES FOR THE FIRST                W   16
C         DERIVATIVE TO THE CURVE AT X(1) AND X(N), RESPECTIVELY,       W   17
C         IF THE QUANTITY SIGMA IS NEGATIVE THESE VALUES WILL BE        W   18
C         DETERMINED INTERNALLY AND THE USER NEED ONLY FURNISH          W   19
C         PLACE-HOLDING PARAMETERS FOR SLP1 AND SLPN.  SUCH PLACE-      W   20
C         HOLDING PARAMETERS WILL BE IGNORED BY NOT DESTROYED,          W   21
C     YP = AN ARRAY OF LENGTH AT LEAST N                                W   22
C     TEMP = AN ARRAY OF LENGTH AT LEAST N WHICH IS USED FOR            W   23
C         SCRATCH STORAGE,                                              W   24
C     SIGMA = THE TENSION FACTOR.  THIS IS NON-ZERO AND                 W   25
C         INDICATES THE CURVINESS DESIRED. IF ABS(SIGMA) IS NEARLY      W   26
C         ZERO (E.G. .001) THE RESULTING CURVE IS APPROXIMATELY A       W   27
C         CUBIC SPLINE.  IF ABS(SIGMA) IS LARGE (E.G. 50.) THE          W   28
C         RESULTING CURVE IS NEARLY A POLYGONAL LINE.  THE SIGN         W   29
C         OF SIGMA INDICATES WHETHER THE DERIVATIVE INFORMATION         W   30
C         HAS BEEN INPUT OR NOT.  IF SIGMA IS NEGATIVE THE ENDPOINT     W   31
C         DERIVATIVES WILL BE DETERMINED INTERNALLY.  A STANDARD        W   32
C         VALUE FOR SIGMA IS APPROXIMATELY 1. IN ABSOLUTE VALUE         W   33
C                                                                       W   34
C     ON OUTPUT --                                                      W   35
C     YP = VALUES PROPORTIONAL TO THE SECOND DERIVATIVE                 W   36
C         OF THE CURVE AT THE GIVEN NODES.                              W   37
C     N,X,Y,SLP1 AND SIGMA ARE UNALTERED,                               W   38
C                                                                       W   39
C     *** AK CLINE/NCAR, COMM. ACM 17,4(APR.1974), 221.                 W   40
C                                                                       W   41
      DIMENSION X(N), Y(N), YP(N), TEMP(N)                              W   42
      DATA EXPMAX/87.4/                                                 W   43
C                                                                       W   44
      NCYC=0                                                            W   45
      NCHG=0                                                            W   46
      NM1=N-1                                                           W   47
      NP1=N+1                                                           W   48
      DELX1=X(2)-X(1)                                                   W   49
      IF (ABS(DELX1/X(2)).LT.0.02) GO TO 55                             W   50
      DX1=(Y(2)-Y(1))/DELX1                                             W   51
C                                                                       W   52
C     *** DETERMINE SLOPES IF NECESSARY                                 W   53
      IF (SIGMA.LT.0.) GO TO 45                                         W   54
      SLPP1=SLP1                                                        W   55
      SLPPN=SLPN                                                        W   56
C                                                                       W   57
```

```
C     *** DENORMALIZE TENSION FACTOR                                    W   58
    5 IF (ABS(X(N)-X(1))/X(N).LT.0.02) GO TO 55                         W   59
      SIGMAP=ABS(SIGMA)*FLOAT(N-1)/(X(N)-X(1))                          W   60
      DX1=(Y(2)-Y(1))/DELX1                                             W   61
C                                                                       W   62
C     *** SET UP RIGHT HAND SIDE OF TRIDIAGONAL SYSTEM                  W   63
C         FOR YP AND PERFORM FORWARD ELIMINATION                        W   64
      DELS=SIGMAP*DELX1                                                 W   65
      IF (DELS.GE.EXPMAX) GO TO 55                                      W   66
      EXPS=EXP(DELS)                                                    W   67
      SINHS=0.5*(EXPS-1./EXPS)                                          W   68
      SINHIN=1./(DELX1*SINHS)                                           W   69
      DIAG1=SINHIN*(DELS*0.5*(EXPS+1./EXPS)-SINHS)                      W   70
      DIAGIN=1./DIAG1                                                   W   71
      YP(1)=DIAGIN*(DX1-SLPP1)                                          W   72
      SPDIAG=SINHIN*(SINHS-DELS)                                        W   73
      TEMP(1)=DIAGIN*SPDIAG                                             W   74
      IF (N.EQ.2) GO TO 15                                              W   75
      DO 10 I=2,NM1                                                     W   76
      DELX2=X(I+1)-X(I)                                                 W   77
      IF (ABS(DELX2)/X(I+1).LT.0.02) GO TO 55                           W   78
      DX2=(Y(I+1)-Y(I))/DELX2                                           W   79
      DELS=SIGMAP*DELX2                                                 W   80
      IF (DELS.GE.EXPMAX) GO TO 55                                      W   81
      EXPS=EXP(DELS)                                                    W   82
      SINHS=.5*(EXPS-1./EXPS)                                           W   83
      SINHIN=1./(DELX2*SINHS)                                           W   84
      DIAG2=SINHIN*(DELS*(.5*(EXPS+1./EXPS))-SINHS)                     W   85
      DIAGIN=1./(DIAG1+DIAG2-SPDIAG*TEMP(I-1))                          W   86
      YP(I)=DIAGIN*(DX2-DX1-SPDIAG*YP(I-1))                             W   87
      SPDIAG=SINHIN*(SINHS-DELS)                                        W   88
      TEMP(I)=DIAGIN*SPDIAG                                             W   89
      DX1=DX2                                                           W   90
      DIAG1=DIAG2                                                       W   91
   10 CONTINUE                                                          W   92
   15 DIAGIN=1./(DIAG1-SPDIAG*TEMP(NM1))                                W   93
      YP(N)=DIAGIN*(SLPPN-DX2-SPDIAG*YP(NM1))                           W   94
C                                                                       W   95
C     ***  PERFORM BACK SUBSTITUTION                                    W   96
      DO 20 I=2,N                                                       W   97
      IBAK=NP1-I                                                        W   98
      YP(IBAK)=YP(IBAK)-TEMP(IBAK)*YP(IBAK+1)                           W   99
   20 CONTINUE                                                          W  100
      IF (SIGMA.GT.0.) RETURN                                           W  101
      IF (N.EQ.3) RETURN                                                W  102
      IF (NCYC.GT.15) RETURN                                            W  103
      IF (NCYC.GT.0) GO TO 25                                           W  104
      XTEST=(X(3)+X(2))/2.                                              W  105
      YCORD=(Y(3)+Y(2))/2.                                              W  106
      FACT=SQRT(ABS(SIGMA))                                             W  107
      YTEST=(YCORD*FACT+CIRC(XTEST,X(1),Y(1))+CIRC(XTEST,X(2),Y(2)))/(2. W  108
     1+FACT)                                                            W  109
      DY2=CURV2(XTEST,N,X,Y,YP,SIGMA,1)-YTEST                           W  110
      DSAV=DY2                                                          W  111
      SN=-1.                                                            W  112
      IF (DY2.GT.0.) SN=1.                                              W  113
      FACT=0.3*(SN+2.)                                                  W  114
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```
      DY2=0.                                                            W  115
      IT=1                                                              W  116
   25 NCYC=NCYC+1                                                       W  117
      DY1=DY2                                                           W  118
      DY2=CURV2(XTEST,N,X,Y,YP,SIGMA,IT)-YTEST                          W  119
      IF (NCYC.GT.15) RETURN                                            W  120
      IF (NCYC.GT.13.AND.NCHG.LT.2) GO TO 40                            W  121
      IF (SIGN(1.,DY1).NE.SIGN(1.,DY2)) GO TO 30                        W  122
      IF (ABS(DY2).LT.ABS(DY1)) GO TO 35                                W  123
   30 SN=-SN                                                            W  124
      NCHG=NCHG+1                                                       W  125
      FACT=SN*((1./(1.-SN*FACT))**(1./3.)-1.)                           W  126
   35 SLPP1=SLPP1*(1.+SN*FACT)                                          W  127
      GO TO 5                                                           W  128
C                                                                       W  129
   40 IF (DY2/DSAV.LT.0.2) GO TO 35                                     W  130
      SLPP1=SLPPX                                                       W  131
      NCYC=15                                                           W  132
      GO TO 5                                                           W  133
   45 IF (N.EQ.2) GO TO 50                                              W  134
C                                                                       W  135
C     *** IF NO DERIVATIVES ARE GIVEN USE SECOND ORDER POLYNOMIAL       W  136
C         INTERPOLATION ON INPUT DATA FOR VALUES AT ENDPOINTS.          W  137
      SLPP1=(Y(2)-Y(1))/(X(2)-X(1))                                     W  138
      DELN=X(N)-X(NM1)                                                  W  139
      DELNM1=X(NM1)-X(N-2)                                              W  140
      DELNN=X(N)-X(N-2)                                                 W  141
      IF (ABS(DELN)/X(N).LT.0.02) GO TO 55                              W  142
      IF (ABS(DELN)/X(N).LT.0.02) GO TO 55                              W  143
      IF (ABS(DELNM1)/X(NM1).LT.0.02) GO TO 55                          W  144
      IF (ABS(DELNN)/X(N).LT.0.02) GO TO 55                             W  145
      C1=(DELNN+DELN)/DELNN/DELN                                        W  146
      C2=-DELNN/DELN/DELNM1                                             W  147
      C3=DELN/DELNN/DELNM1                                              W  148
      SLPPN=C3*Y(N-2)+C2*Y(NM1)+C1*Y(N)                                 W  149
      DX2=X(3)-X(2)                                                     W  150
      DX31=X(3)-X(1)                                                    W  151
      IF (ABS(DX2)/X(3).LT.0.02) GO TO 55                               W  152
      IF (ABS(DX31)/X(3).LT.0.02) GO TO 55                              W  153
      C1=-(DX31+DELX1)/DX31/DELX1                                       W  154
      C2=DX31/DELX1/DX2                                                 W  155
      C3=-DELX1/DX31/DX2                                                W  156
      SLPPX=C1*Y(1)+C2*Y(2)+C3*Y(3)                                     W  157
      IF (Y(2).GT.Y(1)) SLPPX=AMAX1(0.,SLPPX)                           W  158
      FACT2=SQRT(ABS(SIGMA))                                            W  159
      SLPPX=(SLPPX+FACT2*SLPP1)/(1.+FACT2)                              W  160
      SLPP1=SLPPX                                                       W  161
      IF (Y(N).GT.Y(NM1)) SLPPN=AMAX1(0.,SLPPN)                         W  162
      SLPNL=(Y(N)-Y(NM1))/DELN                                          W  163
      SLPPN=(SLPPN+SLPNL*FACT2)/(1.+FACT2)                              W  164
      SLPPN=(SLPPN-SLPNL*SIGMA)/(1.-SIGMA)                              W  165
      GO TO 5                                                           W  166
C                                                                       W  167
C     *** IF ONLY TWO POINTS AND NO DERIVATIVES ARE GIVEN, USE          W  168
C         STRAIGHT LINE FOR CURVE                                       W  169
C                                                                       W  170
   50 YP(1)=0.                                                          W  171
      YP(2)=0.                                                          W  172
      RETURN                                                            W  173
   55 SIGMA=-50.                                                        W  174
      RETURN                                                            W  175
      END                                                               W  176-
```

```
      FUNCTION CURV2 (T,N,X,Y,YP,SIGMA,IT)                              X    1
C                                                                       X    2
C     THIS FUNCTION INTERPOLATES A CURVE AT A GIVEN POINT               X    3
C     USING A SPLINE UNDER TENSION.  THE SUBROUTINE CURV1 SHOULD        X    4
C     BE CALLED EARLIER TO DETERMINE CERTAIN NECESSARY                  X    5
C     PARAMETERS.                                                       X    6
C                                                                       X    7
C     ON INPUT--                                                        X    8
C     T = A REAL VALUE TO BE MAPPED ONTO THE                            X    9
C         INTERPOLATING CURVE.                                          X   10
C     N = THE NUMBER OF POINTS WHICH WERE INTERPOLATED                  X   11
C         TO DETERMINE THE CURVE.                                       X   12
C     X,Y = ARRAYS CONTAINING THE ORDINATES AND ABCISSAS                X   13
C         OF THE INTERPOLATED POINTS.                                   X   14
C     YP = AN ARRAY WITH VALUES PROPORTIONAL TO THE SECOND              X   15
C         DERIVATIVE OF THE CURVE AT THE NODES                          X   16
C     SIGMA = THE TENSION FACTOR (ITS SIGN IS IGNORED)                  X   17
C         IT IS AN INTEGER SWITCH.  IF IT IS NOT 1 THIS INDICATES       X   18
C         THAT THE FUNCTION HAS BEEN CALLED PREVIOUSLY (WITH N,X,       X   19
C         Y,YP, AND SIGMA UNALTERED) AND THAT THIS VALUE OF T           X   20
C         EXCEEDS THE PREVIOUS VALUE.  WITH SUCH INFORMATION THE        X   21
C         FUNCTION IS ABLE TO PERFORM THE INTERPOLATION MUCH MORE       X   22
C         RAPIDLY.  IF A USER SEEKS TO INTERPOLATE AT A SEQUENCE        X   23
C         OF POINTS, EFFICIENCY IS GAINED BY ORDERING THE VALUES        X   24
C         INCREASING AND SETTING IT TO THE INDEX OF THE CALL.           X   25
C         IF IT IS 1 THE SEARCH FOR THE INTERVAL (X(K),X(K+1))          X   26
C         CONTAINING T STARTS WITH K=1.                                 X   27
C         THE PARAMETERS N,X,Y,YP AND SIGMA SHOULD BE INPUT             X   28
C         UNALTERED FROM THE OUTPUT OF CURV1.                           X   29
C                                                                       X   30
C     ON OUTPUT--                                                       X   31
C     CURV2 = THE INTERPOLATED VALUE.  FOR T LESS THAN                  X   32
C         X(1) CURV2 = Y(1).  FOR T GREATER THAN X(N) CURV2 = Y(N).     X   33
C                                                                       X   34
C     NONE OF THE INPUT PARAMETERS ARE ALTERED.                         X   35
C                                                                       X   36
C      *** AK CLINE/NCAR, COMM. ACM 17,4(APR.1974), 221                 X   37
C                                                                       X   38
      DIMENSION X(N), Y(N), YP(N)                                       X   39
C                                                                       X   40
      S=X(N)-X(1)                                                       X   41
      IT=IABS(IT)                                                       X   42
C                                                                       X   43
C     *** DENORMALIZE SIGMA                                             X   44
      SIGMAP=ABS(SIGMA)*FLOAT(N-1)/S                                    X   45
C                                                                       X   46
C     *** IF IT.NE. 1 START SEARCH WHERE PREVIOUSLY TERMINATED,         X   47
C         OTHERWISE START SEARCH FROM BEGINNING                         X   48
      IF (IT.EQ.1) I1=2                                                 X   49
C                                                                       X   50
C     *** SEARCH FOR INTERVAL                                           X   51
    5 DO 10 I=I1,N                                                      X   52
      IF (X(I)-T) 10,10,15                                              X   53
   10 CONTINUE                                                          X   54
      I=N                                                               X   55
C                                                                       X   56
C     *** CHECK TO INSURE CORRECT INTERVAL                              X   57
```

```
   15 IF (X(I-1).LE.T.OR.T.LE.X(1)) GO TO 20                                X   58
C                                                                           X   59
C     *** RESTART SEARCH AND RESET I1                                       X   60
C         (INPUT (IT( WAS INCORRECT)                                        X   61
      I1=2                                                                  X   62
      GO TO 5                                                               X   63
C                                                                           X   64
C     *** SET UP AND PERFORM INTERPOLATION                                  X   65
   20 IF (SIGMA.EQ.-50.) GO TO 25                                           X   66
      DEL1=T-X(I-1)                                                         X   67
      DEL2=X(I)-T                                                           X   68
      DELS=X(I)-X(I-1)                                                      X   69
      EXPS1=EXP(SIGMAP*DEL1)                                                X   70
      SINHD1=.5*(EXPS1-1./EXPS1)                                            X   71
      EXPS=EXP(SIGMAP*DEL2)                                                 X   72
      SINHD2=.5*(EXPS-1./EXPS)                                              X   73
      EXPS=EXPS1*EXPS                                                       X   74
      SINHS=.5*(EXPS-1./EXPS)                                               X   75
      CURV2=(YP(I)*SINHD1+YP(I-1)*SINHD2)/SINHS+((Y(I)-YP(I))*DEL1+(Y(I-    X   76
     11)-YP(I-1))*DEL2)/DELS                                                X   77
      IF ((ABS(Y(I)-CURV2)+ABS(Y(I-1)-CURV2)).GT.1.001*(ABS(Y(I)-Y(I-1))    X   78
     1)) IT=-IT                                                             X   79
      I1=1                                                                  X   80
      RETURN                                                                X   81
   25 IF (ABS(X(I)-X(I-1))/X(I).LT.0.02) I=I+1                              X   82
      IF (I.GT.N) I=I-2                                                     X   83
      CURV2=((T-X(I-1))*(Y(I)-Y(I-1))/(X(I)-X(I-1)))+Y(I-1)                 X   84
      IT=1                                                                  X   85
      RETURN                                                                X   86
      END                                                                   X   87-
```

Subroutine KURV1

```
      SUBROUTINE KURV1 (NPTS,X,Y,NSLOPE,SLOPE1,SLOPEN,XP,YP,TEMP,S,SIGMA Y    1
     1)                                                                  Y    2
C                                                                        Y    3
C     THIS SUBROUTINE DETERMINES THE PARAMETERS NECESSARY TO             Y    4
C     COMPUTE AN SPLINE UNDER TENSION PASSING THROUGH A SEQUENCE         Y    5
C     OF PAIRS (X(1),Y(1),.....,X(N),Y(N)) IN THE PLANE, THE             Y    6
C     SLOPES AT THE TWO ENDS OF THE CURVE MAY BE SPECIFIED OR            Y    7
C     OMITTED, FOR ACTUAL COMPUTATION OF POINTS ON THE CURVE IT          Y    8
C     IS NECESSARY TO CALL THE SUBROUTINE KURV2.                         Y    9
C                                                                        Y   10
C     ON INPUT --                                                        Y   11
C     NPTS = THE NUMBER OF POINTS TO BE INTERPOLATED (N.GE.2),           Y   12
C     X = AN ARRAY CONTAINING THE N X-COORDINATES OF THE                 Y   13
C         POINTS,                                                        Y   14
C     Y = AN ARRAY CONTAIING THE N Y-COODINATES OF THE                   Y   15
C         POINTS,                                                        Y   16
C     NSLOPE = A FLAG FOR ENDPOINT SLOPES.  IF = 0, THIS IS A CLOSED     Y   17
C         LOOP AND NO SLOPES ARE GIVEN.  IF = 0, THIS IS AN OPEN CURVE   Y   18
C         AND NO SLOPES ARE GIVEN.  IF ) 0, BOTH ENDPOINT SLOPES ARE     Y   19
C         GIVEN                                                          Y   20
C     SLOPE1,SLOPEN = THE DESIRED VALUES FOR THE SLOPE                   Y   21
C         OF THE CURVE AT (X(1),Y(1)) AND (X(N),Y(N)), RESPEC-           Y   22
C         TIVELY.  THESE QUANTITIES ARE IN DEGREES AND MEASURED          Y   23
C         COUNTER CLOCKWISE FROM THE POSITIVE X-AXIS.  THE POSITIVE      Y   24
C         SENSE OF THE CURVE IS ASSUMED TO BE THAT MOVING FROM THE       Y   25
C         POINT 1 TO POINT N.                                            Y   26
C     XP,YP = ARRAYS OF LENGTH AT LEAST N,                               Y   27
C     TEMP = AN ARRAY OF LENGTH AT LEAST N WHICH IS USED FOR             Y   28
C         SCRATCH STORAGE,                                               Y   29
C     SIGMA = THE TENSION FACTOR.  THIS IS NON-ZERO AND                  Y   30
C         INDICATES THE CURVINESS DESIRED.  IF SIGMA IS VERY             Y   31
C         LARGE (E.G. 50.) THE RESULTING CURVE IS VERY NEARLY A          Y   32
C         POLYGONAL LINE.  A STANDARD VALUE FOR SIGMA IS 1.              Y   33
C                                                                        Y   34
C     ON OUTPUT -                                                        Y   35
C     N,X,Y,SLOPE1,SLOPEN, AND SIGMA ARE UNALTERED,                      Y   36
C     XP,YP CONTAIN INFORMATION ABOUT THE CURVATURE OF THE               Y   37
C         CURVE AT THE GIVEN NODE,                                       Y   38
C     S = THE POLYGONAL ARCLENGTH OF THE CURVE.                          Y   39
C                                                                        Y   40
C      *** AK CLINE, COMM. ACM 17,4(APR.1974), 221                       Y   41
C          MODIFIED BY CW LUNDBERG/SAI  MAY :77                          Y   42
C                                                                        Y   43
      DIMENSION X(NPTS), Y(NPTS), XP(NPTS), YP(NPTS), TEMP(NPTS)         Y   44
C                                                                        Y   45
      DATA EXPMAX/87.4/                                                  Y   45A
      TEMAX=-9999.                                                       Y   45B
      DEGRAD=3.1415926/180.                                              Y   46
      N=NPTS                                                             Y   47
      SLP1=SLOPE1                                                        Y   48
      SLPN=SLOPEN                                                        Y   49
      NM1=N-1                                                            Y   50
      NP1=N+1                                                            Y   51
      DELX1=X(2)-X(1)                                                    Y   52
      DELY1=Y(2)-Y(1)                                                    Y   53
      DELS1=SQRT(DELX1*DELX1+DELY1*DELY1)                                Y   54
      DX1=DELX1/DELS1                                                    Y   55
```

```
      DY1=DELY1/DELS1                                                    Y   56
C                                                                        Y   57
C      *** DETERMINE SLOPES IF NECESSARY                                 Y   58
       IF (NSLOPE) 50,40,5                                               Y   59
     5 SLPP1=SLP1*DEGRAD                                                 Y   60
       SLPPN=SLPN*DEGRAD                                                 Y   61
C                                                                        Y   62
C      *** SET UP RIGHT HAND SIDES OF TRIDIAGONAL LINEAR SYSTEM FOR      Y   63
C          XP AND YP                                                     Y   64
    10 XP(1)=DX1-COS(SLPP1)                                              Y   65
       YP(1)=DY1-SIN(SLPP1)                                              Y   66
       TEMP(1)=DELS1                                                     Y   67
       S=DELS1                                                           Y   68
       IF (N.EQ.2) GO TO 20                                              Y   69
       DO 15 I=2,NM1                                                     Y   70
       DELX2=X(I+1)-X(I)                                                 Y   71
       DELY2=Y(I+1)-Y(I)                                                 Y   72
       DELS2=SQRT(DELX2*DELX2+DELY2*DELY2)                               Y   73
       DX2=DELX2/DELS2                                                   Y   74
       DY2=DELY2/DELS2                                                   Y   75
       XP(I)=DX2-DX1                                                     Y   76
       YP(I)=DY2-DY1                                                     Y   77
       TEMP(I)=DELS2                                                     Y   78
       TEMAX=AMAX1(TEMAX,TEMP(I))                                        Y   78A
       DELX1=DELX2                                                       Y   79
       DELY1=DELY2                                                       Y   80
       DELS1=DELS2                                                       Y   81
       DX1=DX2                                                           Y   82
       DY1=DY2                                                           Y   83
C                                                                        Y   84
C      *** ACCUMULATE POLYGONAL ARCLENGTH                                Y   85
       S=S+DELS1                                                         Y   86
    15 CONTINUE                                                          Y   87
    20 XP(N)=COS(SLPPN)-DX1                                              Y   88
       YP(N)=SIN(SLPPN)-DY1                                              Y   89
C                                                                        Y   90
C      *** DENORMALIZE TENSION FACTOR                                    Y   91
       SIGMAP=ABS(SIGMA)*FLOAT(N-1)/S                                    Y   92
       DELT1=SIGMAP*TEMAX                                                Y   92A
       IF (DELT1.LT.EXPMAX) GO TO 21                                     Y   92B
       SIGMAP=0.9*EXPMAX/TEMAX                                           Y   92C
       SGN=1.0                                                           Y   92D
       IF (SIGMA.LT.0.) SGN=-1.0                                         Y   92E
       SIGMA=SIGMAP*SGN*S/FLOAT(N-1)                                     Y   92F
    21 CONTINUE                                                          Y   92G
C                                                                        Y   93
C      *** PERFORM FORWARD ELIMINATION ON TRIDIAGONAL SYSTEM             Y   94
       DELS=SIGMAP*TEMP(1)                                               Y   95
       EXPS=EXP(DELS)                                                    Y   96
       SINHS=.5*(EXPS-1./EXPS)                                           Y   97
       SINHIN=1./(TEMP(1)*SINHS)                                         Y   98
       DIAG1=SINHIN*(DELS*.5*(EXPS+1./EXPS)-SINHS)                       Y   99
       DIAGIN=1./DIAG1                                                   Y  100
       XP(1)=DIAGIN*XP(1)                                                Y  101
       YP(1)=DIAGIN*YP(1)                                                Y  102
       SPDIAG=SINHIN*(SINHS-DELS)                                        Y  103
       TEMP(1)=DIAGIN*SPDIAG                                             Y  104
```

```
      IF (N.EQ.2) GO TO 30                                              Y  105
      DO 25 I=2,NM1                                                     Y  106
      DELS=SIGMAP*TEMP(I)                                               Y  107
      EXPS=EXP(DELS)                                                    Y  108
      SINHS=.5*(EXPS-1./EXPS)                                           Y  109
      SINHIN=1./(TEMP(I)*SINHS)                                         Y  110
      DIAG2=SINHIN*(DELS*(.5*(EXPS+1./EXPS))-SINHS)                     Y  111
      DIAGIN=1./(DIAG1+DIAG2-SPDIAG*TEMP(I-1))                          Y  112
      XP(I)=DIAGIN*(XP(I)-SPDIAG*XP(I-1))                               Y  113
      YP(I)=DIAGIN*(YP(I)-SPDIAG*YP(I-1))                               Y  114
      SPDIAG=SINHIN*(SINHS-DELS)                                        Y  115
      TEMP(I)=DIAGIN*SPDIAG                                             Y  116
      DIAG1=DIAG2                                                       Y  117
   25 CONTINUE                                                          Y  118
   30 DIAGIN=1./(DIAG1-SPDIAG*TEMP(NM1))                                Y  119
      XP(N)=DIAGIN*(XP(N)-SPDIAG*XP(NM1))                               Y  120
      YP(N)=DIAGIN*(YP(N)-SPDIAG*YP(NM1))                               Y  121
C                                                                       Y  122
C     *** PERFORM BACK SUBSTITUTION                                     Y  123
      DO 35 I=2,N                                                       Y  124
      IBAK=NP1-I                                                        Y  125
      XP(IBAK)=XP(IBAK)-TEMP(IBAK)*XP(IBAK+1)                           Y  126
      YP(IBAK)=YP(IBAK)-TEMP(IBAK)*XP(IBAK+1)                           Y  127
   35 CONTINUE                                                          Y  128
      RETURN                                                            Y  129
   40 IF (N.EQ.2) GO TO 45                                              Y  130
C                                                                       Y  131
C     *** IF NO SLOPES ARE GIVEN, USE SECOND ORDER INTERPOLATION ON     Y  132
C         INPUT DATA FOR SLOPES AT ENDPOINTS                            Y  133
      DELS2=SQRT((X(3)-X(2))**2+(Y(3)-Y(2))**2)                         Y  134
      DELS12=DELS1+DELS2                                                Y  135
      C1=-(DELS12+DELS1)/DELS12/DELS1                                   Y  136
      C2=DELS12/DELS1/DELS2                                             Y  137
      C3=-DELS1/DELS12/DELS2                                            Y  138
      SX=C1*X(1)+C2*X(2)+C3*X(3)                                        Y  139
      SY=C1*Y(1)+C3*Y(2)+C3*Y(3)                                        Y  140
      SLPP1=ATAN2(SY,SX)                                                Y  141
      DELNM1=SQRT((X(N-2)-X(NM1))**2+(Y(N-2)-Y(NM1))**2)                Y  142
      DELN=SQRT((X(NM1)-X(N))**2+(Y(NM1)-Y(N))**2)                      Y  143
      DELNN=DELNM1+DELN                                                 Y  144
      C1=(DELNN+DELN)/DELNN/DELN                                        Y  145
      C2=-DELNN/DELN/DELNM1                                             Y  146
      C3=DELN/DELNN/DELNM1                                              Y  147
      SX=C3*X(N-2)+C2*X(NM1)+C1*X(N)                                    Y  148
      SY=C3*Y(N-2)+C2*Y(NM1)+C1*Y(N)                                    Y  149
      SLPPN=ATAN2(SY,SX)                                                Y  150
      GO TO 10                                                          Y  151
C                                                                       Y  152
C     *** IF ONLY TWO POINTS AND NO SLOPES ARE GIVEN, USE STRAIGHT      Y  153
C         LINE SEGMENT FOR CURVE                                        Y  154
   45 XP(1)=0.                                                          Y  155
      XP(2)=0.                                                          Y  156
      YP(1)=0.                                                          Y  157
      YP(2)=0.                                                          Y  158
      RETURN                                                            Y  159
C                                                                       Y  160
C     *** CLOSED LOOP -- PERIODIC SPLINE -- CALCULATE SLOPES            Y  161
```

```
C          FOR JOIN                                                    Y  162
   50 DELN=SQRT((X(NM1)-X(N))**2+(Y(NM1)-Y(N))**2)                     Y  163
      DELNN=DELS1+DELN                                                 Y  164
      C1=-DELS1/DELN/DELNN                                             Y  165
      C2=(DELS1-DELN)/DELS1/DELN                                       Y  166
      C3=DELN/DELNN/DELS1                                              Y  167
      SX=C1*X(NM1)+C2*X(1)+C3*X(2)                                     Y  168
      SY=C1*Y(NM1)+C2*Y(1)+C3*Y(2)                                     Y  169
      IF (SX.EQ.0..AND.SY.EQ.0.) SX=1                                  Y  170
      SLPP1=ATAN2(SY,SX)                                               Y  171
      SLPPN=SLPP1                                                      Y  172
      GO TO 10                                                         Y  173
      END                                                              Y  174-
```

```
      SUBROUTINE KURV2 (T,XS,YS,N,X,Y,XP,YP,S,SIGMA)                    Z    1
C                                                                       Z    2
C     THIS SUBROUTINE PERFORMS THE MAPPING OF POINTS IN THE             Z    3
C     INTERVAL (0.,1.) ONTO A CURVE IN THE PLANE.  THE SUBROUTINE       Z    4
C     KURV1 SHOULD BE CALLED EARLIER TO DETERMINE CERTAIN               Z    5
C     NECESSARY PARAMETERS.  THE RESULTING CURVE HAS A PARAMETRIC       Z    6
C     REPRESENTATION BOTH OF WHOSE COMPONENTS ARE SPLINES UNDER         Z    7
C     TENSION AND FUNCTIONS OF THE POLYGONAL ARCLENGTH PARAMETER.       Z    8
C                                                                       Z    9
C     ON INPUT--                                                        Z   10
C     T = A REAL VALUE OF ABSOLUTE VALUE LESS THAN OR                   Z   11
C         EQUAL TO 1.  TO BE MAPPED TO A POINT ON THE CURVE.  THE       Z   12
C         SIGN OF T IS IGNORED AND THE INTERVAL (0.,1.) IS MAPPED       Z   13
C         ONTO THE ENTIRE CURVE.  IF T IS NEGATIVE THIS INDICATES       Z   14
C         THAT THE SUBROUTINE HAS BEEN CALLED PREVIOUSLY (WITH ALL      Z   15
C         OTHER INPUT VARIABLES UNALTERED) AND THAT THIS VALUE OF       Z   16
C         T EXCEEDS THE PREVIOUS VALUE IN ABSOLUTE VALUE.  WITH         Z   17
C         SUCH INFORMATION THE SUBROUTINE IS ABLE TO MAP THE POINT      Z   18
C         MUCH MORE RAPIDLY.  THUS IF THE USER SEEKS TO MAP A           Z   19
C         SEQUENCE OF POINTS ONTO THE SAME CURVE, EFFICIENCY IS         Z   20
C         GAINED BY ORDERING THE VALUES INCREASING IN MAGNITUDE         Z   21
C         AND SETTING THE SIGNS OF ALL BUT THE FIRST, NEGATIVE.         Z   22
C     N = THE NUMBER OF POINTS WHICH WERE INTERPOLATED                  Z   23
C         TO DETERMINE THE CURVE,                                       Z   24
C     X,Y = ARRAYS CONTAINING THE X- AND Y-COORDINATES                  Z   25
C         OF THE INTERPOLATED POINTS,                                   Z   26
C     XP,YP = THE ARRAYS OUTPUT FROM KURV2 CONTAINING                   Z   27
C         CURVATURE INFORMATION,                                        Z   28
C     S = THE POLYGONAL ARCLENGTH OF THE CURVE,                         Z   29
C     SIGMA = THE TENSION FACTOR (ITS SIGN IS IGNORED).                 Z   30
C                                                                       Z   31
C     THE PARAMETERS N,X,Y,XP,UP,S, AND SIGMA SHOULD BE INPUT           Z   32
C     UNALTERED FROM THE OUTPUT OF KURV1.                               Z   33
C                                                                       Z   34
C     ON  OUTPUT--                                                      Z   35
C     XS,YS = THE X- AND Y-COORDINATES OF THE IMAGE                     Z   36
C         POINT ON THE CURVE.                                           Z   37
C     T,N,X,Y,XP,YP,S, AND SIGMA ARE UNALTERED.                         Z   38
C                                                                       Z   39
      DIMENSION X(N), Y(N), XP(N), YP(N)                                Z   40
C                                                                       Z   41
C     *** DENORMALIZE SIGMA                                             Z   42
      SIGMAP=ABS(SIGMA)*FLOAT(N-1)/S                                    Z   43
C                                                                       Z   44
C     *** STRETCH UNIT INTERVAL INTO ARCLENGTH DISTANCE                 Z   45
      TN=ABS(T*S)                                                       Z   46
C                                                                       Z   47
C     *** FOR NEGATIVE T START SEARCH WHERE PREVIOUSLY TERMINATED.      Z   48
C         OTHERWISE START FROM BEGINNING                                Z   49
      IF (T.LT.0.) GO TO 5                                              Z   50
      I1=2                                                              Z   51
      XS=X(1)                                                           Z   52
      YS=Y(1)                                                           Z   53
      SUM=0.                                                            Z   54
      IF (T.LE.0.) RETURN                                               Z   55
    5 CONTINUE                                                          Z   56
C                                                                       Z   57
```

```
C       *** DETERMINE INTO WHICH SEGMENT TN IS MAPPED                          Z   58
        DO 15 I=I1,N                                                          Z   59
        DELX=X(I)-X(I-1)                                                      Z   60
        DELY=Y(I)-Y(I-1)                                                      Z   61
        DELS=SQRT(DELX*DELX+DELY*DELY)                                        Z   62
        IF (SUM+DELS-TN) 10,20,20                                             Z   63
   10   SUM=SUM+DELS                                                          Z   64
   15   CONTINUE                                                              Z   65
C                                                                            Z   66
C       *** IF ABS(T) IS GREATER THAN 1., RETURN TERMINAL POINT ON             Z   67
C           CURVE                                                             Z   68
C                                                                            Z   69
        XS=X(N)                                                               Z   70
        YS=Y(N)                                                               Z   71
        RETURN                                                                Z   72
C                                                                            Z   73
C       *** SET UP AND PERFORM INTERPOLATION                                  Z   74
   20   DEL1=TN-SUM                                                           Z   75
        DEL2=DELS-DEL1                                                        Z   76
        EXPS1=EXP(SIGMAP*DEL1)                                                Z   77
        SINHD1=.5*(EXPS1-1./EXPS1)                                            Z   78
        EXPS=EXP(SIGMAP*DEL2)                                                 Z   79
        SINHD2=.5*(EXPS-1./EXPS)                                              Z   80
        EXPS=EXPS1*EXPS                                                       Z   81
        SINHS=.5*(EXPS-1./EXPS)                                               Z   82
        XS=(XP(I)*SINHD1+XP(I-1)*SINHD2)/SINHS+((X(I)-XP(I))*DEL1+(X(I-1)-    Z   83
       1XP(I-1))*DEL2)/DELS                                                   Z   84
        YS=(YP(I)*SINHD1+YP(I-1)*SINHD2)/SINHS+((Y(I)-YP(I))*DEL1+(Y(I-1)-    Z   85
       1YP(I-1))*DEL2)/DELS                                                   Z   86
        I1=I                                                                  Z   87
        RETURN                                                                Z   88
        END                                                                   Z   89-
```

```
      SUBROUTINE FRAME (X,Y,FRSTX,FINX,SIZX,TICX,STEPX,NDECX,FRSTY,FINY,  AA   1
     1SIZY,TICY,STEPY,NDECY,LBLBOT,NB,LBLLFT,NL,LBLTOP,NT,LBLRGT,NR)      AA   2
C                                                                         AA   3
C     *** PURPOSE -- PREPARES AN ANNOTATED FOUR SIDED FRAME               AA   4
C         WITH LOWER LEFT CORNER AT (X,Y)                                 AA   5
C             GWL/SAI   MARCH 1977                                        AA   6
C                                                                         AA   7
C         SEE SUBROUTINE AXES FOR DESCRIPTION OF ARGUMENTS                AA   8
C                                                                         AA   9
      COMMON /PLTVEC/ HCT(20),OT(20),NH,OHC,HCG,PLTGRD,OXN,XNG,HCC,XNC,T  AA  10
     1ICZ,DIGZ,CHRZ                                                       AA  11
C                                                                         AA  12
C     *** CALCULATE THE AXES LENGTHS                                      AA  13
      XLEN=(FINX-FRSTX)*SIZX                                              AA  14
      YLEN=(FINY-FRSTY)*SIZY                                              AA  15
C                                                                         AA  16
C     *** PLACE GRIDDED LINES ON PLOT                                     AA  17
C                                                                         AA  18
      IF (ABS(PLTGRD).EQ.0.) GO TO 40                                     AA  19
      IF (PLTGRD.LT.0.) GO TO 25                                          AA  20
      CALL NEWPEN (2)                                                     AA  21
      STINC=(STEPY/10.)*SIZY                                              AA  22
      ILP=FINY/STEPY+.005                                                 AA  23
      ILP=ILP*10-1                                                        AA  24
      STVAL=STINC                                                         AA  25
      J=1                                                                 AA  26
      DO 10 I=1,ILP                                                       AA  27
      IF (J.EQ.2) GO TO 5                                                 AA  28
      CALL PLOT (X,STVAL,3)                                               AA  29
      CALL PLOT (XLEN,STVAL,2)                                            AA  30
      STVAL=STVAL+STINC                                                   AA  31
      J=2                                                                 AA  32
      GO TO 10                                                            AA  33
    5 CALL PLOT (XLEN,STVAL,3)                                            AA  34
      CALL PLOT (X,STVAL,2)                                               AA  35
      STVAL=STVAL+STINC                                                   AA  36
      J=1                                                                 AA  37
   10 CONTINUE                                                            AA  38
      STINC=(STEPX/10.)*SIZX                                              AA  39
      ILP=FINX/STEPX+.005                                                 AA  40
      ILP=ILP*10-1                                                        AA  41
      STVAL=STINC                                                         AA  42
      J=1                                                                 AA  43
      DO 20 I=1,ILP                                                       AA  44
      IF (J.EQ.2) GO TO 15                                                AA  45
      CALL PLOT (STVAL,Y,3)                                               AA  46
      CALL PLOT (STVAL,YLEN,2)                                            AA  47
      STVAL=STVAL+STINC                                                   AA  48
      J=2                                                                 AA  49
      GO TO 20                                                            AA  50
   15 CALL PLOT (STVAL,YLEN,3)                                            AA  51
      CALL PLOT (STVAL,Y,2)                                               AA  52
      STVAL=STVAL+STINC                                                   AA  53
      J=1                                                                 AA  54
   20 CONTINUE                                                            AA  55
      CALL NEWPEN (1)                                                     AA  56
      GO TO 40                                                            AA  57
```

```
C                                                                       AA  58
C  PLOT GRIDDED LINES WITH MATRIX PLOTTER                              AA  59
C                                                                       AA  60
   25 IPLT=IFIX(PLTGRD)                                                 AA  61
      CALL NEWPEN (IPLT)                                                AA  62
      STINC=(STEPY/10.)*SIZY                                            AA  63
      ILP=IFIX(FINY/STEPY+0.005)*10-1                                   AA  64
      STVAL=STINC                                                       AA  65
      DO 30 I=1,ILP                                                     AA  66
      IF (MOD(I,10).EQ.0) CALL NEWPEN (IPLT+1)                          AA  67
      CALL PLOT (X+0.01,STVAL,3)                                        AA  68
      CALL PLOT (XLEN,STVAL,2)                                          AA  69
      IF (MOD(I,10).EQ.0) CALL NEWPEN (IPLT)                            AA  70
      STVAL=STVAL+STINC                                                 AA  71
   30 CONTINUE                                                          AA  72
      STINC=(STEPX/10.)*SIZX                                            AA  73
      ILP=IFIX(FINX/STEPX+0.005)*10-1                                   AA  74
      STVAL=STINC                                                       AA  75
      DO 35 I=1,ILP                                                     AA  76
      IF (MOD(I,10).EQ.0) CALL NEWPEN (IPLT+1)                          AA  77
      CALL PLOT (STVAL,Y-0.02,3)                                        AA  78
      CALL PLOT (STVAL,Y,3)                                             AA  79
      CALL PLOT (STVAL,YLEN,2)                                          AA  80
      IF (MOD(I,10).EQ.0) CALL NEWPEN (IPLT)                            AA  81
      STVAL=STVAL+STINC                                                 AA  82
   35 CONTINUE                                                          AA  83
      CALL NEWPEN (0)                                                   AA  84
   40 CONTINUE                                                          AA  85
C                                                                       AA  86
C     *** PLOT THE FOUR SIDES WITH ANNOTATIONS                          AA  87
      CALL AXES (X,Y,FRSTX,FINX,SIZX,TICX,STEPX,NDECX,0.,LBLBOT,-NB,1)  AA  88
      CALL AXES (X,Y,FRSTY,FINY,SIZY,TICY,STEPY,NDECY,90.,LBLLFT,NL,1)  AA  89
      CALL AXES (X,Y+YLEN,FRSTX,FINX,SIZX,TICX,STEPX,NDECX,0.,LBLTOP,NT, AA  90
     1-1)                                                               AA  91
      CALL AXES (X+XLEN,Y,FRSTY,FINY,SIZY,TICY,STEPY,NDECY,90.,LBLRGT,-N AA  92
     1R,-1)                                                             AA  93
C                                                                       AA  94
      RETURN                                                            AA  95
      END                                                               AA  96-
```

```
      SUBROUTINE AXES (X,Y,FIRSTV,FINALV,SCALE,TSTEP,ASTEP,NDEC,ANGLE,IB AB   1
     1CD,NCHAR,LABEL)                                                    AB   2
C                                                                        AB   3
C     *** SAI SUBROUTINE AXES                                            AB   4
C         GW LUNDBERG/SAI  DEC 76                                        AB   5
C                                                                        AB   6
C         X,Y = COORDINATES IN INCHES OF AXIS LINE STARTING              AB   7
C               POINT                                                    AB   8
C         FIRSTV = STARTING VALUE FOR THE AXIS                           AB   9
C         FINALV = ENDING VALUE FOR THE AXIS                             AB  10
C         SCALE = INCHES/UNIT FOR FIRSTV,FINALV,TSTEP,ASTEP              AB  11
C         TSTEP = STEP SIZE FOR TICS                                     AB  12
C         ASTEP = STEP SIZE FOR LABELED TICS                             AB  13
C         NDEC = FORMAT FOR LABELS -- SEE SUBROUTINE NUMBER              AB  14
C         ANGLE = ANGLE OF AXIS IN DEGRES FROM HORIZONTAL                AB  15
C         IBCD = THE AXIS TITLE AS ARRAY OR HOLLERITH STRING             AB  16
C         NCHAR = NUMBER OF CHARACTERS IN TITLE                          AB  17
C               ) 0, TIC MARKS, ANNOTATION AND TITLE PLOTTED ON          AB  18
C                  CLOCKWISE SIDE OF AXIS LINE                           AB  19
C               ( 0, ON COUNTER CLOCKWISE SIDE                           AB  20
C                                                                        AB  21
C         THIS ROUTINE WAS WRITTEN FOR A MATRIX PLOTTER -- IT DOES       AB  22
C         NOT OPTIMIZE PEN MOVEMENTS.  THE ROUTINE SHOULD BE MACHINE     AB  23
C         INDEPENDENT                                                    AB  24
C                                                                        AB  25
C                                                                        AB  26
C     *** FOLLOWING ARE ADJUSTABLE -- IF LABEL ) 0, ALL TICS ARE         AB  27
C         LABELED, IF LABEL = 0, THE LAST TIC IS NOT LABELED,            AB  28
C         IF LABEL ( 0, THE FIRST AND LAST ARE NOT LABELED               AB  29
C                                                                        AB  30
C     *** DEFINE VARIOUS CHARACTER SIZES                                 AB  31
      COMMON /PLTVEC/ HCT(20),OT(20),NH,OHC,HCG,PLTGRD,OXN,XNG,HC1,XN1,T AB  32
     1ICSIZ,DIGSIZ,CHRSIZ                                                AB  33
C                                                                        AB  34
C     *** STEP 1 -- DRAW AXIS AND TIC MARKS                              AB  35
C         ---- -    ---- ---- --- --- -----                              AB  36
C                                                                        AB  37
C     *** MOVE PEN TO START OF AXIS                                      AB  38
      X0=X                                                               AB  39
      Y0=Y                                                               AB  40
      CALL PLOT (X0,Y0,3)                                                AB  41
C                                                                        AB  42
C     *** LOCATE THE OTHER END AND DRAW AXIS                             AB  43
      COSA=COS(ANGLE*0.017453294)                                        AB  44
      SINA=SIN(ANGLE*0.017453294)                                        AB  45
      AXLEN=(FINALV-FIRSTV)*SCALE                                        AB  46
      X1=X0+AXLEN*COSA                                                   AB  47
      Y1=Y0+AXLEN*SINA                                                   AB  48
      CALL PLOT (X1,Y1,2)                                                AB  49
C                                                                        AB  50
C     *** ADD THE TIC MARKS ON WRONG SIDE OF AXIS                        AB  51
      POS=FLOAT(ISIGN(1,NCHAR))                                          AB  52
      IF (TSTEP.EQ.0.) GO TO 10                                          AB  53
      NTIC=(FINALV-FIRSTV)/TSTEP+1.5                                     AB  54
      DO 5 J=1,NTIC                                                      AB  55
C                                                                        AB  56
C         *** MOVE PEN TO START OF TIC                                   AB  57
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      X1=X0+FLOAT(J-1)*TSTEP*SCALE*COSA                                  AB  58
      Y1=Y0+FLOAT(J-1)*TSTEP*SCALE*SINA                                  AB  59
      CALL PLOT (X1,Y1,3)                                                AB  60
C                                                                        AB  61
C         *** DRAW A TIC NORMAL TO AXIS                                  AB  62
      X1=X1+TICSIZ*POS*SINA                                              AB  63
      Y1=Y1-TICSIZ*POS*COSA                                              AB  64
      CALL PLOT (X1,Y1,2)                                                AB  65
    5 CONTINUE                                                           AB  66
C                                                                        AB  67
C     *** STEP 2 -- SET IN LABELED TICS ON CORRECT SIDE OF AXIS          AB  68
C         ---- -    --- -- ------- ---- -- ------- ---- -- ----         AB  69
C                                                                        AB  70
   10 IF (ASTEP.EQ.0.) GO TO 25                                          AB  71
      NTIC=(FINALV-FIRSTV)/ASTEP+1.5                                     AB  72
      NFRST=1                                                            AB  73
      NLST=NTIC                                                          AB  74
      IF (LABEL.LE.0) NLST=NLST-1                                        AB  75
      IF (LABEL.LT.0) NFRST=NFRST+1                                      AB  76
      DO 15 J=NFRST,NLST                                                 AB  77
      X1=X0+FLOAT(J-1)*ASTEP*SCALE*COSA                                  AB  78
      Y1=Y0+FLOAT(J-1)*ASTEP*SCALE*SINA                                  AB  79
      CALL PLOT (X1,Y1,3)                                                AB  80
C                                                                        AB  81
      X1=X1-TICSIZ*POS*SINA                                              AB  82
      Y1=Y1+TICSIZ*POS*COSA                                              AB  83
      CALL PLOT (X1,Y1,2)                                                AB  84
   15 CONTINUE                                                           AB  85
C                                                                        AB  86
C     *** STEP 3 -- ANNOTATE THE TIC MARKS                               AB  87
C         ---- -    -------- --- --- -----                              AB  88
C                                                                        AB  89
C     *** DETERMINE PERPENDICULAR OFFSET TO BOTTOM OF CHARACTER          AB  90
      OFFSET=TICSIZ+0.03                                                 AB  91
      IF (POS.NE.1) OFFSET=OFFSET+DIGSIZ                                 AB  92
C                                                                        AB  93
C     *** CALCULATE LOCATION OF FIRST CHARACTER                          AB  94
      X0=X0-DIGSIZ*COSA                                                  AB  95
      Y0=Y0-DIGSIZ*SINA                                                  AB  96
      X0=X0-OFFSET*POS*SINA                                              AB  97
      Y0=Y0+OFFSET*POS*COSA                                              AB  98
C                                                                        AB  99
C     *** ANNOTATE THE TIC MARKS                                         AB 100
      NFRST=1                                                            AB 101
      NLAST=NTIC                                                         AB 102
      IF (LABEL.LE.0) NLAST=NLAST-1                                      AB 103
      IF (LABEL.LT.0) NFRST=NFRST+1                                      AB 104
      DO 20 J=NFRST,NLAST                                                AB 105
C                                                                        AB 106
C         *** GET FLOATING POINT VALUE OF ANNOTATION                     AB 107
      FPN=FIRSTV+FLOAT(J-1)*ASTEP                                        AB 108
C                                                                        AB 109
C         *** GET LOCATION AND PLOT FPN                                  AB 110
      X1=X0+FLOAT(J-1)*ASTEP*SCALE*COSA                                  AB 111
      Y1=Y0+FLOAT(J-1)*ASTEP*SCALE*SINA                                  AB 112
      CALL NUMBER (X1,Y1,DIGSIZ,FPN,ANGLE,NDEC)                          AB 113
   20 CONTINUE                                                           AB 114
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C                                                                       AB 115
C     *** STEP 4 -- ADD AXIS TITLE                                      AB 116
C         ---- -    --- ---- -----                                     AB 117
C                                                                       AB 118
   25 IF (NCHAR.EQ.0) GO TO 30                                          AB 119
C     *** SET TITLE OFFSET -- DISTANCE FROM AXIS TO CHARACTERS          AB 120
      OFFSET=TICSIZ+DIGSIZ+0.10                                         AB 121
      IF (NCHAR.LT.0) OFFSET=OFFSET+CHRSIZ                              AB 122
C                                                                       AB 123
C     *** CALCULATE TITLE SIZE                                          AB 124
      TSIZ=CHRSIZ*IABS(NCHAR)                                           AB 125
C                                                                       AB 126
C     *** CALCULATE OFFSET FROM BEGINNING OF AXIS TO FIRST CHARACTER    AB 127
      OFF=0.5*(AXLEN-TSIZ)                                              AB 128
C                                                                       AB 129
C     *** CALCULATE LOCATION OF FIRST CHARACTER AND PLOT TITLE          AB 130
      X0=X+OFF*COSA                                                     AB 131
      Y0=Y+OFF*SINA                                                     AB 132
      X0=X0-OFFSET*POS*SINA                                             AB 133
      Y0=Y0+OFFSET*POS*COSA                                             AB 134
      CALL SYMBOL (X0,Y0,CHRSIZ,IBCD,ANGLE,IABS(NCHAR))                 AB 135
C                                                                       AB 136
C         FINISHED                                                      AB 137
   30 RETURN                                                            AB 138
      END                                                               AB 139-
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```
      BLOCK DATA SUN                                                    AC    1
      COMMON /SUNLIT/ XJ(47,10),SIGMA(31,10),PHI(31,10),Z(10),RTCON(10),  AC    2
     1LAM1,INC,SLA,SLO,TZ,IY,IM,ID,ISTRT,ISTOP,IINC,IEND,SPECIE,MAXZ,ITI  AC    3
     2ME(015),XZ(015),K(015),JSTRT,JSTOP,SPEC(11),MNLM(11),MXLM(11),MAXL  AC    4
     3,MAXJ                                                             AC    5
      COMMON /PHOTON/ CF(45,8),P(15,9),IPH(9)                           AC    6
      DATA IPH/1,12,19,18,50,49,17,53,0/                                AC    7
      DATA MAXL,MAXZ,MAXJ,LAM1,INC/09,10,47,2900,100/                   AC    8
      DATA (Z(I),I=1,10)/0.,10.,20.,30.,40.,50.,60.,70.,78.,86./        AC    9
      DATA (XJ(1,J),J=1,10)/0.00015,0.00015,8*0.0/                      AC   10
      DATA (XJ(2,J),J=1,10)/.039835,.038015,0.032546,.024647,.0155188,.0 AC   11
     1074586,.002285,.0003046,2*0.0/                                    AC   12
      DATA (XJ(3,J),J=1,10)/.4394,.4313000,.4012000,.3505500,.2814000,.1 AC   13
     1978000,.1104300,.039249,.009269,.0009416/                         AC   14
      DATA (XJ(4,J),J=1,10)/.9551,.9438000,.9006000,.8261000,.7174000,.5 AC   15
     1706000,.3890000,.19372,.06372,.008893/                            AC   16
      DATA (XJ(5,J),J=1,10)/1.6132,1.5944000,1.5384000,1.4402000,1.29220 AC   17
     100,1.0832000,.8031000,.4628,.20291,.03894/                        AC   18
      DATA (XJ(6,J),J=1,10)/1.7134,1.6964000,1.6450000,1.5547000,1.41600 AC   19
     100,1.2153000,.9357000,.5726,.2689,.06149/                         AC   20
      DATA (XJ(7,J),J=1,10)/1.8924,1.8748000,1.8237000,1.7327000,1.59150 AC   21
     100,1.3834000,1.2429000,.6841,.3276,.07653/                        AC   22
      DATA (XJ(8,J),J=1,10)/1.9508,1.9335000,1.8849000,1.7982000,1.66210 AC   23
     100,1.4590000,1.1638000,.7493,.3626,.08341/                        AC   24
      DATA (XJ(9,J),J=1,10)/2.3974,2.3782000,2.3233000,2.2238000,2.06680 AC   25
     100,1.8310000,1.4799000,.9722,.4767,.10653/                        AC   26
      DATA (XJ(10,J),J=1,10)/2.3177,2.3008000,2.2508000,2.1609000,2.0189 AC   27
     1000,1.8026000,1.4751000,.9879,.4913,.1065/                        AC   28
      DATA (XJ(11,J),J=1,10)/2.3415,2.3254000,2.2769000,2.1947000,2.0594 AC   29
     1000,1.8520000,1.5336000,1.0468,.5291,.11136/                      AC   30
      DATA (XJ(12,J),J=1,10)/3.1737,3.1530000,3.0929000,2.9841000,2.8100 AC   31
     1000,2.5412000,2.1246000,1.4744,.758,.15557/                       AC   32
      DATA (XJ(13,J),J=1,10)/3.9935,3.9685000,3.8957000,3.7652000,3.5559 AC   33
     1000,3.2319000,2.7246000,1.9188,1.0035,.20173/                     AC   34
      DATA (XJ(14,J),J=1,10)/4.1188,4.0949000,4.0250000,3.8985000,3.6956 AC   35
     1000,3.3780000,2.8754000,2.0589,1.0973,.21538/                     AC   36
      DATA (XJ(15,J),J=1,10)/4.22245,4.1180000,4.0599500,3.9301500,3.734 AC   37
     18000,3.4279500,2.9379000,2.12855,1.15135,.222625/                 AC   38
      DATA (XJ(16,J),J=1,10)/4.6172,4.5120000,4.4421000,4.3168499,4.1135 AC   39
     1000,3.7932000,3.2742000,2.40225,1.3207,.250665/                   AC   40
      DATA (XJ(17,J),J=1,10)/5.2089,5.1817000,5.1007500,4.9576500,4.7279 AC   41
     1500,4.3661000,3.7832500,2.79965,1.55895,.292135/                  AC   42
      DATA (XJ(18,J),J=1,10)/5.6146,5.5851500,5.4983500,5.3444500,5.0991 AC   43
     1000,4.7150000,4.0991000,3.05525,1.72055,.318635/                  AC   44
      DATA (XJ(19,J),J=1,10)/5.7505,5.7211000,5.6363000,5.4851000,5.2420 AC   45
     1000,4.8484500,4.2483000,3.19345,1.82055,.333/                     AC   46
      DATA (XJ(20,J),J=1,10)/5.7988,5.7708000,5.6876500,5.5407500,5.3036 AC   47
     1000,4.9180000,4.3271000,3.2775,1.88745,.3398/                     AC   48
      DATA (XJ(21,J),J=1,10)/5.78355,5.7564500,5.6759000,5.5333000,5.304 AC   49
     16500,4.9435500,4.3521500,3.3168,1.9265,.3416/                     AC   50
      DATA (XJ(22,J),J=1,10)/5.8866,5.8571500,5.7735000,5.6254000,5.3897 AC   51
     1000,5.0215500,4.4222500,3.3773,1.97045,.34205/                    AC   52
      DATA (XJ(23,J),J=1,10)/5.93495,5.9050500,5.8182500,5.6660000,5.424 AC   53
     17000,5.0527000,4.4501500,3.405,1.99415,.3394/                     AC   54
      DATA (XJ(24,J),J=1,10)/5.9353,5.9032000,5.8178500,5.6686000,5.4327 AC   55
     1000,5.0667000,4.4724000,3.43375,2.0198,.3376/                     AC   56
      DATA (XJ(25,J),J=1,10)/5.9797,5.9503500,5.8656000,5.7171000,5.4816 AC   57
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1500,5.1156000,4.5209500,3.4756,2.0455,0.33125/                          AC  58
 DATA (XJ(26,J),J=1,10)/5.92715,5.8988000,5.8161500,5.6701500,5.439      AC  59
12500,5.0801500,4.4947500,3.46155,2.03995,0.3217/                        AC  60
 DATA (XJ(27,J),J=1,10)/5.90955,5.8814500,5.7972500,5.6504500,5.419      AC  61
17000,5.0612000,4.4787000,3.4521,2.03715,0.3147/                         AC  62
 DATA (XJ(28,J),J=1,10)/5.96875,5.9396500,5.8528500,5.7025500,5.467      AC  63
11000,5.1035000,4.5142000,3.47855,2.05155,0.30885/                       AC  64
 DATA (XJ(29,J),J=1,10)/6.0576,6.0280000,5.9412000,5.7889500,5.5507      AC  65
1000,5.1827500,4.5650500,3.53355,2.0813,0.30345/                         AC  66
 DATA (XJ(30,J),J=1,10)/6.1739,6.1445000,6.0576000,5.9047000,5.6665      AC  67
1000,5.2964000,4.7142000,3.6287,2.1482,0.3108/                           AC  68
 DATA (XJ(31,J),J=1,10)/6.2265,6.1975000,6.1110000,5.9585000,5.7225      AC  69
1000,5.3540000,4.7538500,3.6857,2.1941,0.3201/                           AC  70
 DATA (XJ(32,J),J=1,10)/6.26925,6.2397500,6.1517500,5.9972500,5.757      AC  71
17500,5.3875000,4.7846750,3.714,2.2183,0.323675/                         AC  72
 DATA (XJ(33,J),J=1,10)/6.312,6.2820000,6.1925000,6.0360000,5.79300      AC  73
100,5.4210000,4.8155000,3.7423,2.2425,0.32725/                           AC  74
 DATA (XJ(34,J),J=1,10)/6.321,6.2917500,6.2047500,5.9370000,5.63775      AC  75
100,5.4517500,4.8578000,3.79835,2.30265,0.34945/                         AC  76
 DATA (XJ(35,J),J=1,10)/6.33,6.3015000,6.2170000,5.8380000,5.482500      AC  77
10,5.4825000,4.9001000,3.8544,2.3628,0.37165/                            AC  78
 DATA (XJ(36,J),J=1,10)/6.4215,6.3922500,6.3060000,6.0392500,5.7432      AC  79
1500,5.5620000,4.9790500,3.93455,2.437625,0.400375/                      AC  80
 DATA (XJ(37,J),J=1,10)/6.513,6.4830000,6.3950000,6.2405000,6.00400      AC  81
100,5.6415000,5.0580000,4.0147,2.51245,0.4291/                           AC  82
 DATA (XJ(38,J),J=1,10)/6.59375,6.5630000,6.4720000,6.3142500,6.074      AC  83
10000,5.7002500,5.1225000,4.078575,2.5737,0.454825/                      AC  84
 DATA (XJ(39,J),J=1,10)/6.6745,6.6436000,6.5490000,6.3880000,6.1440      AC  85
1000,5.7750000,5.1870000,4.14245,2.63495,0.48055/                        AC  86
 DATA (XJ(40,J),J=1,10)/6.659,6.6265000,6.5367500,6.3787500,6.13925      AC  87
100,5.7772500,5.1992500,4.167625,2.670625,0.49945/                       AC  88
 DATA (XJ(41,J),J=1,10)/6.6435,6.6100000,6.5245000,6.3695000,6.1345      AC  89
1000,5.7795000,5.2115000,4.1928,2.7063,0.5184/                           AC  90
 DATA (XJ(42,J),J=1,10)/6.46,6.45,6.35,6.20,5.98,5.71,5.15,4.09,2.7      AC  91
14,0.53/                                                                 AC  92
 DATA (XJ(43,J),J=1,10)/6.40,6.38,6.29,6.14,5.91,5.65,5.11,4.07,2.7      AC  93
15,0.54/                                                                 AC  94
 DATA (XJ(44,J),J=1,10)/6.34,6.32,6.22,6.08,5.87,5.60,5.05,4.05,2.7      AC  95
16,0.56/                                                                 AC  96
 DATA (XJ(45,J),J=1,10)/6.27,6.25,6.16,6.02,5.80,5.55,5.02,4.04,2.7      AC  97
17,0.56/                                                                 AC  98
 DATA (XJ(46,J),J=1,10)/6.21,6.19,6.10,5.96,5.75,5.49,4.97,4.02,2.7      AC  99
18,0.58/                                                                 AC 100
 DATA (XJ(47,J),J=1,10)/6.14,6.12,6.03,5.90,5.68,5.43,4.92,4.00,2.7      AC 101
19,0.59/                                                                 AC 102
 DATA SPEC/4H NO2,4HHONO,4HO33P,4HO31D,4HFOR1,4HFOR2,4HH2O2,4HALD2,      AC 103
14HO3CH,4H    ,4H    /                                                   AC 104
 DATA MNLM/8*2900,4500,0,0/                                              AC 105
 DATA MXLM/4500,3900,3500,3100,3600,3600,3700,3400,7500,0,0/             AC 106
 DATA (SIGMA(I,1),I=1,17)/8.52E-20,1.28E-19,1.83E-19,2.47E-19,3.10E      AC 107
1-19,3.74E-19,4.49E-19,5.01E-19,5.41E-19,5.70E-19,5.82E-19,5.95E-19      AC 108
2,5.80E-19,5.45E-19,5.15E-19,4.85E-19,4.55E-19/                          AC 109
 DATA (PHI(J,1),J=1,17)/0.988,0.980,0.972,0.964,0.956,0.948,0.940,0      AC 110
1.932,0.924,0.916,0.908,0.699,0.175,0.025,0.006,0.001,0.000/            AC 111
 DATA (SIGMA(I,2),I=1,12)/0.79E-20,0.79E-20,1.14E-20,1.75E-20,2.86E      AC 112
1-20,4.23E-20,5.29E-20,3.98E-20,6.08E-20,3.33E-20,1.78E-20,0.0/          AC 113
 DATA (PHI(J,2),J=1,12)/0.0,9*1.0,2*0.0/                                 AC 114
```

```
 DATA (SIGMA(I,3),I=1,07)/1.62E-18,4.44E-19,1.19E-19,3.36E-20,8.79E AC 115
1-21,1.94E-21,3.86E-22/                                             AC 116
 DATA (PHI(J,3),J=1,07)/2*0.0,5*1.0/                                AC 117
 DATA (SIGMA(I,4),I=1,07)/1.62E-18,4.44E-19,1.19E-19,3.36E-20,8.79E AC 118
1-21,1.94E-21,3.86E-22/                                             AC 119
 DATA (PHI(J,4),J=1,7)/3*1.0,4*0.0/                                 AC 120
 DATA (SIGMA(I,5),I=1,8)/3.18E-20,3.25E-20,3.15E-20,2.34E-20,2.37E- AC 121
120,1.98E-20,8.37E-21,1.76E-21/                                     AC 122
 DATA (PHI(J,5),J=1,8)/0.81,0.66,0.52,0.40,0.29,0.18,0.09,0.01/     AC 123
 DATA (SIGMA(I,6),I=1,8)/3.18E-20,3.25E-20,3.15E-20,2.34E-20,2.37E- AC 124
120,1.98E-20,8.37E-21,1.76E-21/                                     AC 125
 DATA (PHI(J,6),J=1,8)/0.19,0.34,0.48,0.60,0.71,0.82,0.91,0.99/     AC 126
 DATA (SIGMA(I,7),I=1,09)/1.49E-20,9.94E-21,6.88E-21,4.97E-21,3.82E AC 127
1-21,3.01E-21,1.91E-21,1.15E-21,0.76E-21/                           AC 128
 DATA (PHI(J,7),J=1,9)/9*1.0/                                       AC 129
 DATA (SIGMA(I,8),I=1,6)/4.66E-20,4.09E-20,2.96E-20,1.69E-20,6.92E- AC 130
121,1.34E-21/                                                       AC 131
 DATA (PHI(J,8),J=1,6)/0.987,0.722,0.663,0.474,0.300,0.123/         AC 132
 DATA (SIGMA(I,09),I=1,31)/1.99E-22,3.60E-22,5.38E-22,7.48E-22,9.58 AC 133
1E-22,1.31E-21,1.74E-21,2.20E-21,2.76E-21,3.31E-21,3.78E-21,4.54E-2 AC 134
21,5.09E-21,4.93E-21,5.15E-21,5.52E-21,4.98E-21,4.17E-21,3.61E-21,3 AC 135
3.18E-21,2.69E-21,2.17E-21,1.79E-21,1.52E-21,1.26E-21,9.77E-22,8.06 AC 136
4E-22,6.76E-22,5.56E-22,4.84E-22,4.07E-22/                          AC 137
 DATA (PHI(J,09),J=1,31)/31*1.0/                                    AC 138
 END                                                                AC 139-
```

```
      BLOCK DATA MECH                                                   AD    1
      COMMON /CALC/ NR,KR(77,5),A(77),S(77),R(77),ITYPE(77),IA(34),JA(21 AD    2
     18),DILUT,TEMP,ERR,START,STOPP,SPECIS(34),TPRNT,TSTEP              AD    3
      DATA NR/76/                                                       AD    4
      DATA (KR(I,1),I=1,77)/1,3,4,1,1,5,1,6,6,2,7,7,8,8,9,9,10,4,4,11,11 AD    5
     1,8,4,12,13,13,13,13,13,14,12,12,24,24,2,2,2,2,2,27,28,20,18,27,28, AD    6
     220,18,16,21,21,21,22,22,22,30,30,30,29,29,29,13,13,32,31,23,32,31, AD    7
     323,26,19,25,17,15,32,31,23,0/                                     AD    8
      DATA (KR(I,2),I=1,77)/0,0,2,4,3,2,5,0,0,1,7,0,1,2,2,9,0,0,0,0,0,4, AD    9
     19,8,2,13,15,17,19,0,4,4,8,8,26,25,19,17,15,0,0,0,0,0,0,0,0,0,0,8 AD   10
     2,0,0,8,0,0,8,0,0,8,26,25,2,2,2,1,1,1,9,9,9,9,9,9,9,9,0/          AD   11
      DATA (KR(I,3),I=1,77)/2,4,1,5,2,1,6,1,0,7,2,8,0,7,1,10,8,11,3,3,8, AD   12
     19,8,13,14,14,14,14,14,21,8,8,25,26,1,1,1,1,1,21,22,21,21,29,9,30,2 AD   13
     22,21,0,9,9,0,15,23,0,17,31,0,19,32,14,14,19,17,15,12*0/           AD   14
      DATA (KR(I,4),I=1,77)/3,4*0,1,0,5,0,7,1,2,0,0,6,0,8,0,0,0,8,0,0,0, AD   15
     11,14,16,18,20,9,9,23,0,0,27,28,20,18,16,19,17,17,15,9,0,9,9,9,0,9, AD   16
     20,0,9,0,0,9,0,0,9,0,27,28,1,1,1,12*0/                             AD   17
      DATA (KR(I,5),I=1,77)/29*0,22,22,21,45*0/                         AD   18
      DATA R/.35,4.4E+6,25...045,1.3E+4,1.3E+4,5600..,22...05,2.E-5,.001, AD   19
     1.018,8000.,3000.,1200.,8400.,8.4E-4,9.5E-4,.019,8.7E+10,1.E+10,84. AD   20
     2,2.4,2.5E+4,1000.,1.2E+4,1000.,1000.,1000.,1.E+5,.008,.008,1800.,1 AD   21
     3800.,1800.,1800.,1800.,1800.,1800.,7.5E+4,1.E+5,8000.,4000.,1.5E+5 AD   22
     4,3.E+5,1.E+5,8.E+4,8.E+4,.003,.001,1.5E+4,4.2E-6,9.8E-4,1.5E+4,6.E AD   23
     5-5,.0025,4.5E+4,6.E-5,.0019,4.5E+4,1000.,1000.,800.,800.,800.,100. AD   24
     6,100.,100.,4000.,4000.,4000.,4000.,4000.,4000.,4000.,4000.,0.0/   AD   25
      DATA ITYPE/1,1,2,2,2,2,2,1,1,2,2,1,2,2,2,2,1,1,1,1,1,2,2,2,2,2,2,2 AD   26
     1,2,1,2,2,2,2,2,2,2,2,2,2,1,1,1,1,1,1,1,1,1,1,1,1,2,1,1,2,1,1,2,1,1,2,2 AD   27
     2,2,2,2,2,2,2,2,2,2,2,2,2,2,2,2,2,2,0/                             AD   28
      DATA IA/1,12,34,38,50,54,57,61,79,93,95,98,106,120,124,131,134,141 AD   29
     1,146,153,158,161,166,171,175,182,189,194,198,203,208,213,218,0/   AD   30
      DATA JA/1,2,3,4,5,6,7,8,23,31,32,1,2,4,5,7,8,9,13,14,15,16,17,18,1 AD   31
     19,20,23,25,26,27,28,31,32,1,2,3,4,1,2,3,4,5,8,9,11,12,21,22,23,1,2 AD   32
     2,5,6,1,5,6,1,2,7,8,1,2,4,7,8,9,12,13,21,22,23,24,25,26,29,30,31,32 AD   33
     3,1,2,4,8,9,10,15,17,19,23,25,26,31,32,8,10,3,8,11,4,8,9,12,13,21,2 AD   34
     42,23,1,2,13,14,15,16,17,18,19,20,25,26,27,28,9,14,21,22,1,2,9,13,1 AD   35
     54,15,16,9,16,21,1,2,9,13,14,17,18,9,15,18,21,22,1,2,9,13,14,19,20, AD   36
     69,17,20,21,30,8,9,21,8,9,15,22,23,1,2,9,15,23,8,24,25,26,1,2,9,13, AD   37
     714,25,28,1,2,9,13,14,26,27,9,19,21,27,29,9,17,22,28,8,9,19,29,32,8 AD   38
     8,9,17,30,31,1,2,9,17,31,1,2,9,19,32,0/                           AD   39
      DATA SPECIS/4HNO2 ,4HNO  ,4HO   ,4HO3  ,4HN2O3,4HN2O5,4HHONO,4HOH  AD   40
     1 ,4HHO2 ,4HNO3,4HO1D ,4HPROP,4HADD ,4HX   ,4HMEO2,4HMEO ,4HC2O2,4 AD   41
     2HC2O ,4HC3O2,4HC3O ,4HHCHO,4HALD2,4HC2O3,4HBUT ,4HSCO2,4HC4O2,4HC4 AD   42
     3O ,4HSCO ,4HALD4,4HALD3,4HC3O3,4HC4O3,4HM   ,4H    /              AD   43
      END                                                               AD   44-
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```
      BLOCK DATA GEAR                                                   AE    1
      COMMON /GEAR5/ IW1(33,9)/GEAR7/IW2(660)                           AE    2
      DIMENSION IX1(200), IX2(200), IX3(200), IX4(60)                   AE    3
      EQUIVALENCE (IW2,IX1), (IW2(201),IX2), (IW2(401),IX3), (IW2(601),I AE    4
     1X4)                                                               AE    5
      DATA (IW1(I,1),I=1,33)/6,10,5,7,11,24,3,16,29,30,28,31,32,18,12,19 AE    6
     1,26,4,23,20,25,27,8,1,2,9,13,14,15,17,21,22,0/                    AE    7
      DATA (IW1(I,2),I=1,33)/1,4,6,11,15,17,19,23,27,30,33,37,43,49,53,5 AE    8
     16,63,69,76,84,88,94,98,112,130,147,170,179,187,194,202,211,218/   AE    9
      DATA (IW1(I,3),I=1,33)/1,3,4,6,9,11,14,17,19,23,27,30,34,38,42,49, AE   10
     155,61,69,73,79,86,94,103,111,118,124,129,133,136,138,139,139/     AE   11
      DATA (IW1(I,4),I=1,33)/1,3,4,6,9,11,14,17,19,23,27,30,34,38,42,49, AE   12
     155,61,69,73,79,86,94,95,96,97,98,99,100,101,102,102,0/            AE   13
      DATA (IW1(I,5),I=1,33)/1,3,4,7,10,11,12,14,17,19,21,24,29,34,37,39 AE   14
     1,45,49,53,58,64,68,72,78,85,91,97,102,106,109,111,112,112/        AE   15
      DATA (IW1(I,6),I=1,33)/1,3,4,7,10,11,12,14,17,19,21,24,29,34,37,39 AE   16
     1,45,49,53,58,64,68,72,78,85,91,97,102,106,109,111,111,0/          AE   17
      DATA (IW1(I,7),I=1,33)/3,4,6,9,11,14,17,19,23,27,29,34,38,41,48,55 AE   18
     1,61,68,73,79,85,94,102,110,117,123,128,132,135,137,138,139,0/     AE   19
      DATA (IW1(I,9),I=1,33)/33,4*32,31,32,31,32,26,27,0,0,32,8*0,28,31, AE   20
     132,0,31,6*0/                                                      AE   21
      DATA IX1/1,3,24,2,26,1,3,18,24,25,4,23,24,25,5,18,6,23,5,7,18,24,8 AE   22
     1,25,27,29,09,22,23,10,20,23,11,21,25,27,10,12,23,24,25,26,9,13,23, AE   23
     224,25,26,14,25,27,30,15,18,23,9,13,16,22,25,26,27,6,17,23,25,26,27 AE   24
     3,7,15,18,23,24,25,26,15,18,19,23,24,25,26,32,16,20,25,27,6,21,23,2 AE   25
     45,26,27,17,22,25,27,2,4,5,6,9,10,15,18,23,24,25,26,31,32,1,3,4,7,1 AE   26
     52,13,16,17,18,19,21,23,24,25,26,27,29,30,3,4,7,12,13,16,17,18,19,2 AE   27
     61,23,24,25,26,27,29,30,8,9,10,11,12,13,14,15,16,17,18,19,20,21,22, AE   28
     723,25,26,28,29,30,31,32,15,16,17,21,23,25,27,29,30,16,17,21,25,27, AE   29
     828,29,30,14,19,25,26,27,29,32,10,11,12,20,25,26,27/               AE   30
      DATA IX2/30,8,14,15,18,20,22,23,28,31,11,14,15,18,23,28,32,3,24,23 AE   31
     1,24,25,23,24,25,7,23,17,21,23,18,24,25,26,31,13,16,23,26,12,23,26, AE   32
     230,26,30,32,24,25,26,30,16,24,25,26,26,29,31,32,18,19,23,26,27,31, AE   33
     332,20,24,25,26,27,28,22,24,25,26,27,28,19,23,24,25,26,27,31,32,24, AE   34
     425,26,29,23,24,25,26,30,31,24,25,26,27,28,30,32,23,24,25,26,27,28, AE   35
     530,31,24,25,26,27,28,29,30,31,32,26,27,28,21,11,26,16,31,22,9,24,2 AE   36
     65,18,4,23,26,15,27,31,32,19,6,21,17,9,10,12,13,24,25,7,18,3,1,4,23 AE   37
     7,19,12,13,24,25,18,3,4,23,26,27,28,29,8,30,14,16,20,19,21,17,22,11 AE   38
     8,12,13,24,25,18,23,26,2,29,30,16,19,21,17,12,13,24,25,27,28,29,8/ AE   39
      DATA IX3/30,14,16,20,21,17,22,11,26,28,31,32,24,25,26,27,28,29,8,2 AE   40
     14,25,26,27,28,30,14,23,26,31,23,26,29,32,19,231,210,109,225,3,24,2 AE   41
     26,18,24,25,23,24,25,18,23,18,24,25,27,29,22,23,20,23,21,25,27,20,2 AE   42
     33,24,25,26,22,23,24,25,26,25,27,30,18,23,22,23,24,25,26,27,23,25,2 AE   43
     46,27,23,24,25,26,23,24,25,26,32,22,23,24,25,26,27,23,25,26,27,23,2 AE   44
     55,26,27,24,25,26,27,31,32,25,26,27,29,30,31,32,26,27,29,30,31,32,2 AE   45
     67,28,29,30,31,32,28,29,30,31,32,29,30,31,32,30,31,32,31,32,32,267, AE   46
     7188,205,228,255,102,73,256,189,254,223,232,230,76,172,237,191,276, AE   47
     8236,194,287,243,173,178,242,251,264,124,250,126,118,208,211,227,25 AE   48
     93,229,190,259,129,260,258,82,280,294,195,286,265,84,186,104,197/  AE   49
      DATA IX4/272,165,200,215,238,275,78,48,290,239,278,87,285,201,266, AE   50
     1284,77,135,72,288,300,291,95,137,92,246,158,249,292,159,162,161,30 AE   51
     24,305,26*0/                                                       AE   52
      END                                                               AE   53-
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```
      FUNCTION CIRC (TI,XI,YI)                                    AF    1
      DIMENSION XI(3), YI(3)                                      AF    2
      DX=XI(3)-XI(1)                                              AF    3
      DY=YI(3)-YI(1)                                              AF    4
      X=(XI(2)-XI(1))/DX                                          AF    5
      Y=(YI(2)-YI(1))/DY                                          AF    6
      T=(TI-XI(1))/DX                                             AF    7
      IF (X.EQ.Y) GO TO 10                                        AF    8
      B=((Y*X+Y*Y)*0.5-X)/(Y-X)                                   AF    9
      TT=SQRT(B*B+2.*T*(1.-B)-T*T)                                AF   10
      CX=B+TT                                                     AF   11
      IF (X.GT.Y) CX=B-TT                                         AF   12
      IF (CX.LT.0..OR.CX.GT.1.) GO TO 10                          AF   13
    5 CIRC=CX*DY+YI(1)                                            AF   14
      RETURN                                                      AF   15
   10 CX=T*Y/X                                                    AF   16
      IF (T.GT.X) CX=(T-X)*(1.-Y)/(1.-X)+Y                        AF   17
      GO TO 5                                                     AF   18
      END                                                         AF   19-
```

Subroutine EMISS

```
      SUBROUTINE EMISS (NEM,EM,ESTRT,ESTOP,ESLP,EC)                    AG   1
      COMMON /GEAR6/ A(38,38),IX(38),SR(18)                            AG   2
      DIMENSION EM(11), EC(38), IFLAG(11)                              AG   3
      EM(NEM+1)=0.                                                     AG   4
      DO 5 I=1,11                                                      AG   5
      IFLAG(I)=3                                                       AG   6
      IF (I.LE.NEM.AND.ABS(EM(I)).EQ.0.) IFLAG(I)=0                    AG   7
      IF (I.LT.2.OR.I.GT.NEM-1) GO TO 5                                AG   8
      IF (EM(I-1).EQ.EM(I).AND.EM(I).EQ.EM(I+1)) IFLAG(I)=0            AG   9
    5 CONTINUE                                                         AG  10
      IFLAG(1)=2                                                       AG  11
      IFLG1=1                                                          AG  12
      IF (EM(1).EQ.0..AND.EM(2).NE.0.) IFLG1=-1                        AG  13
      NEM1=NEM                                                         AG  14
      DO 10 I=1,NEM1                                                   AG  15
      IK=NEM1-I+1                                                      AG  16
      IF (EM(IK).GT.0.) GO TO 15                                       AG  17
      NEM=NEM-1                                                        AG  18
   10 CONTINUE                                                         AG  19
   15 IF (NEM.EQ.0) RETURN                                             AG  20
      IF (NEM.GT.1) GO TO 20                                           AG  21
      ESLP=-EM(1)/1800.                                                AG  22
      ESTOP=60.                                                        AG  23
      ESTRT=-60.*ESLP                                                  AG  24
      RETURN                                                           AG  25
   20 N=NEM                                                            AG  26
      NM1=NEM-1                                                        AG  27
      JK=4*N-2                                                         AG  28
      DO 25 I=1,JK                                                     AG  29
      EC(I)=0.                                                         AG  30
      DO 25 J=1,JK                                                     AG  31
   25 A(I,J)=0.0                                                       AG  32
C                                                                      AG  33
C  LOOP THROUGH EACH HOUR TO SET UP A MATRIX                           AG  34
C                                                                      AG  35
C  ... BUT FIRST SET UP FIRST HOUR (SPECIAL)                           AG  36
C                                                                      AG  37
      A(1,1)=1.                                                        AG  38
      A(1,2)=60.                                                       AG  39
      DO 55 LM=1,3                                                     AG  40
      NM=NM1*(LM-1)+1                                                  AG  41
      DO 50 K=1,4                                                      AG  42
      IF (LM.EQ.1) A(NM,K+2)=-(60.**(K-1))                             AG  43
      IF (LM.EQ.2.AND.K.GT.1) A(NM,K+2)=-(FLOAT(K-1)*(60.**(K-2)))     AG  44
      IF (LM.NE.3) GO TO 50                                            AG  45
      IF (IFLG1.EQ.1) GO TO 45                                         AG  46
      IF (EM(2)-EM(3)) 40,30,30                                        AG  47
   30 DO 35 I=1,6                                                      AG  48
   35 A(NM-NM1,I)=0.                                                   AG  49
      A(NM-NM1,1)=1.                                                   AG  50
      GO TO 45                                                         AG  51
   40 A(NM,1)=1.                                                       AG  52
      GO TO 50                                                         AG  53
   45 IF (K.LE.2) GO TO 50                                             AG  54
      A(NM,K+2)=-FLOAT(K-1)*(2.0**(K-3))*(60.**(K-3))                  AG  55
   50 CONTINUE                                                         AG  56
   55 CONTINUE                                                         AG  57
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```
      IF (IFLG1.EQ.1.OR.EM(2).LT.EM(3)) A(N,2)=1.                       AG  58
      A(3*N-2,1)=60.                                                    AG  59
      A(3*N-2,2)=1800.                                                  AG  60
      EC(3*N-2)=EM(1)                                                   AG  61
C                                                                       AG  62
C  NOW SET UP REST                                                      AG  63
C                                                                       AG  64
      DO 125 I=2,NM1                                                    AG  65
      J=4*I-6                                                           AG  66
C                                                                       AG  67
C  SET UP THIRD ORDER                                                   AG  68
C                                                                       AG  69
      DO 65 LM=1,4                                                      AG  70
      M=LM-1                                                            AG  71
      NM=NM1*M+I                                                        AG  72
      T=FLOAT(I)*60.                                                    AG  73
      DO 60 K=1,4                                                       AG  74
      IF (LM.EQ.1) A(NM,J+K)=T**(K-1)                                   AG  75
      IF (LM.EQ.2.AND.K.GT.1) A(NM,J+K)=FLOAT(K-1)*(T**(K-2))           AG  76
      IF (LM.EQ.3.AND.K.GT.2) A(NM,J+K)=FLOAT(K-1)*(2.**(K-3))*(T**(K-3) AG  77
     1)                                                                 AG  78
      IF (LM.EQ.4) A(NM,J+K)=(T**K-(T-60.)**K)/FLOAT(K)                 AG  79
      IF (LM.EQ.4) EC(NM)=EM(I)                                         AG  80
      IF (LM.NE.4) A(NM,J+K+4)=-A(NM,J+K)                               AG  81
   60 CONTINUE                                                          AG  82
   65 CONTINUE                                                          AG  83
C                                                                       AG  84
C  NOW RESET A MATRIX ACCORDING TO THE                                  AG  85
C        RESPECTIVE ORDER                                               AG  86
C                                                                       AG  87
      IF (IFLAG(I).EQ.3) GO TO 125                                      AG  88
      KL=4-IFLAG(I)                                                     AG  89
      DO 120 L=2,KL                                                     AG  90
      K=4*I-L                                                           AG  91
      IK=I+NM1*(4-L)                                                    AG  92
      IF (L.EQ.4) GO TO 75                                              AG  93
      DO 70 II=1,JK                                                     AG  94
      IF (L.EQ.2) A(IK-1,II)=0.                                         AG  95
      IF (L.NE.2) A(IK,II)=0.                                           AG  96
   70 A(II,K)=0.                                                        AG  97
      IF (L.EQ.2) A(IK-1,K)=1.                                          AG  98
      IF (L.NE.2) A(IK,K)=1.                                            AG  99
      GO TO 120                                                         AG 100
   75 CONTINUE                                                          AG 101
      IF (IFLAG(I-1)-1) 80,90,100                                       AG 102
   80 DO 85 II=1,JK                                                     AG 103
      IF (I.NE.2) A(IK-1,II)=0.                                         AG 104
      IF (I.EQ.2) A(IK+NM1-1,II)=0.                                     AG 105
   85 A(II,K)=0.                                                        AG 106
      IF (I.EQ.2) A(IK+NM1-1,K)=1.                                      AG 107
      IF (I.NE.2) A(IK-1,K)=1.                                          AG 108
      GO TO 120                                                         AG 109
   90 DO 95 II=1,JK                                                     AG 110
      A(II,K)=0.                                                        AG 111
   95 A(IK+NM1-2,II)=0.                                                 AG 112
      A(IK+NM1-2,K)=1.                                                  AG 113
      GO TO 120                                                         AG 114
```

```
  100 DO 110 II=1,JK                                                    AG 115
      IF (I.NE.2) GO TO 105                                             AG 116
      IF (IFLG1.EQ.1) GO TO 105                                         AG 117
      IF (EM(2).LT.EM(3)) A(IK+NM1-1,II)=0.                             AG 118
      IF (EM(2).GE.EM(3)) A(NM1*2+1,II)=0.                              AG 119
      A(II,K)=0.                                                        AG 120
      GO TO 110                                                         AG 121
  105 A(II,K)=0.                                                        AG 122
      A(IK+NM1-1,II)=0.                                                 AG 123
  110 CONTINUE                                                          AG 124
      IF (I.NE.2) GO TO 115                                             AG 125
      IF (IFLG1.EQ.1) GO TO 115                                         AG 126
      IF (EM(2).LT.EM(3)) A(IK+NM1-1,K)=1.                              AG 127
      IF (EM(2).GE.EM(3)) A(NM1*2+1,K)=1.                               AG 128
      GO TO 120                                                         AG 129
  115 A(IK+NM1-1,K)=1.                                                  AG 130
  120 CONTINUE                                                          AG 131
  125 CONTINUE                                                          AG 132
C                                                                       AG 133
C  SET LAST EMISSION VALUE EQUAL TO ZERO                                AG 134
C                                                                       AG 135
      T=FLOAT(N)*60.                                                    AG 136
      DO 130 I=1,4                                                      AG 137
      L=JK-4+I                                                          AG 138
      A(JK-1,L)=(T**I-(T-60.)**I)/FLOAT(I)                              AG 139
  130 A(JK,L)=T**(I-1)                                                  AG 140
      EC(JK-1)=EM(N)                                                    AG 141
C                                                                       AG 142
      CALL DEC (JK,38,A,IX,IER)                                         AG 143
      CALL SOL (JK,38,A,EC,IX)                                          AG 144
C                                                                       AG 145
      IF (IFLG1.EQ.-1.OR.EM(2).EQ.0.) GO TO 135                         AG 146
      IF (EC(1).LT.0.) IFLG1=-1                                         AG 147
      IF (IFLG1.EQ.-1) GO TO 20                                         AG 148
  135 DO 170 I=2,NM1                                                    AG 149
      ISAV=IFLAG(I)                                                     AG 150
      IR=ISAV+1                                                         AG 151
      T1=FLOAT(I-1)*60.+1.                                              AG 152
      T2=FLOAT(I)*60.-1.                                                AG 153
      IF (I.LE.3.AND.EM(1).GE.0.) IFLG1=1                               AG 154
      J=4*I-2                                                           AG 155
      GO TO (165,140,145,150),IR                                        AG 156
  140 VAL1=EC(J-3)+EC(J-2)*T1                                           AG 157
      VAL2=EC(J-3)+EC(J-2)*T2                                           AG 158
      EMI=AMIN1(VAL1,VAL2)                                              AG 159
      GO TO 160                                                         AG 160
  145 TI=-EC(J-2)/(2.0*EC(J-1))                                         AG 161
      EMI=999.                                                          AG 162
      IF (TI.LT.T1.OR.TI.GT.T2) GO TO 155                               AG 163
      EMI=(EC(J-1)*TI+EC(J-2))*TI+EC(J-3)                               AG 164
      GO TO 155                                                         AG 165
  150 IF (EC(J).EQ.0.) GO TO 170                                        AG 166
      EMI=999.                                                          AG 167
      DETR=(EC(J-1)**2)-3.*EC(J)*EC(J-2)                                AG 168
      IF (DETR.LT.0.) GO TO 155                                         AG 169
      DETR=SQRT(DETR)                                                   AG 170
      Z1=(-EC(J-1)+DETR)/(3.0*EC(J))                                    AG 171
```

```
      Z2=-(EC(J-1)+DETR)/(3.0*EC(J))                                    AG 172
      Z=-1.                                                             AG 173
      IF (Z2.GT.FLOAT(I-1)*60..AND.Z2.LT.FLOAT(I)*60.) Z=Z2             AG 174
      IF (Z1.GT.FLOAT(I-1)*60..AND.Z1.LT.FLOAT(I)*60.) Z=Z1             AG 175
      IF (Z.LT.0.) GO TO 155                                            AG 176
      EMI=((Z*EC(J)+EC(J-1))*Z+EC(J-2))*Z+EC(J-3)                       AG 177
  155 VAL1=((T1*EC(J)+EC(J-1))*T1+EC(J-2))*T1+EC(J-3)                   AG 178
      VAL2=((T2*EC(J)+EC(J-1))*T2+EC(J-2))*T2+EC(J-3)                   AG 179
      EMI=AMIN1(VAL1,VAL2,EMI)                                          AG 180
  160 IF (EMI.LT.0.) IFLAG(I)=IFLAG(I)-1                                AG 181
  165 IF (IFLAG(I).NE.ISAV) GO TO 20                                    AG 182
  170 CONTINUE                                                          AG 183
C                                                                       AG 184
      ESTBT=EC(1)                                                       AG 185
      ESLP=EC(2)                                                        AG 186
      ESTOP=FLOAT(N)*60.                                                AG 187
      RETURN                                                            AG 188
      END                                                               AG 189-
```

```
      SUBROUTINE CONVT (NUM,L)                                          AH   1
C                                                                       AH   2
C     SUBROUTINE CONVT CONVERTS INTEGERS TO ALPHANUMERIC FOR            AH   3
C   PRINTING                                                            AH   4
C                                                                       AH   5
C   ASSUMES VALUE OF INTEGER IS POSITIVE                                AH   6
C                                                                       AH   7
      DIMENSION L(3), JDIGIT(10)                                        AH   8
C                                                                       AH   9
      DATA JDIGIT/1H0,1H1,1H2,1H3,1H4,1H5,1H6,1H7,1H8,1H9               AH  10
      DATA JBLANK/1H /                                                  AH  11
C                                                                       AH  12
      N=NUM                                                             AH  13
      DO 5 I=1,3                                                        AH  14
      L(I)=JBLANK                                                       AH  15
    5 CONTINUE                                                          AH  16
C                                                                       AH  17
      DO 10 K=1,3                                                       AH  18
      I=4-K                                                             AH  19
      NEXT=N/10                                                         AH  20
      NDX=(N-NEXT*10)+1                                                 AH  21
      L(I)=JDIGIT(NDX)                                                  AH  22
      NK=K                                                              AH  23
      IF (NEXT.LE.0) GO TO 15                                           AH  24
      N=NEXT                                                            AH  25
   10 CONTINUE                                                          AH  26
C                                                                       AH  27
C                                                                       AH  28
   15 RETURN                                                            AH  29
      END                                                               AH  30-
```

Subroutine EDGMX

```
      SUBROUTINE EDGMX (X,Y,N,XMX,YMX,L)                                AI   1
      DIMENSION X(N), Y(N)                                              AI   2
      LL=N-1                                                            AI   3
      IF (N.LE.2) GO TO 10                                              AI   4
      NGO=0                                                             AI   5
      DO 5  I=2,LL                                                      AI   6
      IF(Y(I).GT.Y(I-1)) GO TO 5                                        AI   7
      IF(Y(I).GT.Y(I+1)) L=I+1                                          AI   8
      IF(Y(I).GT.Y(I+1)) NGO=1                                          AI   9
    5 CONTINUE                                                          AI   9A
      IF(NGO.EQ.1) GO TO 15                                             AI   9B
   10 XMX=X(N)                                                          AI   10
      YMX=Y(N)                                                          AI   11
      L=N-1                                                             AI   12
      RETURN                                                            AI   13
   15 L=MAX0(L-1,3)                                                     AI   14
      X21=X(L-1)-X(L-2)                                                 AI   15
      X221=X(L-1)*X(L-1)-X(L-2)*X(L-2)                                  AI   16
      X32=X(L)-X(L-1)                                                   AI   17
      XL2=X(L)*X(L)                                                     AI   18
      Y21=Y(L-1)-Y(L-2)                                                 AI   19
      C=(Y21/X21-(Y(L)-Y(L-1))/X32)/(X221/X21-(XL2-X(L-1)*X(L-1))/X32)  AI   20
      B=(Y21-C*X221)/X21                                                AI   21
      A=Y(L)-B*X(L)-C*XL2                                               AI   22
      XMX=-B*0.5/C                                                      AI   23
      YMX=A+B*XMX+C*XMX*XMX                                             AI   24
      IF (XMX.GE.0.999*X(L)) YMX=Y(L)                                   AI   25
      IF (YMX.EQ.Y(L)) XMX=X(L)                                         AI   26
      IF (XMX.LT.1.001*X(L-2).AND.L.GT.3) GO TO 15                      AI   27
      L=L-1                                                             AI   28
      IF (XMX.LE.X(L)) L=L-1                                            AI   29
      RETURN                                                            AI   30
      END                                                               AI   31-
```

```
      SUBROUTINE DEC (N,ND,A,IP,IER)                                    AJ     1
      DIMENSION A(ND,N), IP(N)                                          AJ     2
      L=N                                                               AJ     3
      IER=0                                                             AJ     4
      IP(L)=1                                                           AJ     5
      IF (L.EQ.1) GO TO 30                                              AJ     6
      NM1=L-1                                                           AJ     7
      DO 25 K=1,NM1                                                     AJ     8
      K1=K+1                                                            AJ     9
      M=K                                                               AJ    10
      DO 5 I=K1,L                                                       AJ    11
    5 IF (ABS(A(I,K)).GT.ABS(A(M,K))) M=I                               AJ    12
      IP(K)=M                                                           AJ    13
      T=A(M,K)                                                          AJ    14
      IF (M.EQ.K) GO TO 10                                              AJ    15
      IP(L)=-IP(L)                                                      AJ    16
      A(M,K)=A(K,K)                                                     AJ    17
      A(K,K)=T                                                          AJ    18
   10 IF (T.EQ.0.) GO TO 35                                             AJ    19
      T=1./T                                                            AJ    20
      DO 15 I=K1,L                                                      AJ    21
   15 A(I,K)=-A(I,K)*T                                                  AJ    22
      DO 25 J=K1,L                                                      AJ    23
      T=A(M,J)                                                          AJ    24
      A(M,J)=A(K,J)                                                     AJ    25
      A(K,J)=T                                                          AJ    26
      IF (T.EQ.0.) GO TO 25                                             AJ    27
      DO 20 I=K1,L                                                      AJ    28
      A(I,J)=A(I,J)+A(I,K)*T                                            AJ    29
   20 CONTINUE                                                          AJ    30
   25 CONTINUE                                                          AJ    31
   30 K=L                                                               AJ    32
      IF (A(L,L).EQ.0.) GO TO 35                                        AJ    33
      RETURN                                                            AJ    34
   35 IER=K                                                             AJ    35
      IP(L)=0                                                           AJ    36
      RETURN                                                            AJ    37
      END                                                               AJ    38-
```

```
      SUBROUTINE SOL (L,ND,A,B,J)                                    AK    1
      DIMENSION A(ND,L), B(L), J(L)                                  AK    2
      N=L                                                            AK    3
      IF (N.EQ.1) GO TO 15                                           AK    4
      DO 5 K=2,N                                                     AK    5
      M=J(K-1)                                                       AK    6
      C=B(M)                                                         AK    7
      B(M)=B(K-1)                                                    AK    8
      B(K-1)=C                                                       AK    9
      DO 5 I=K,N                                                     AK   10
      B(I)=B(I)+A(I,K-1)*C                                           AK   11
    5 CONTINUE                                                       AK   12
      K=N                                                            AK   13
      DO 10 KB=2,N                                                   AK   14
      B(K)=B(K)/A(K,K)                                               AK   15
      C=B(K)                                                         AK   16
      K=K-1                                                          AK   17
      DO 10 I=1,K                                                    AK   18
      B(I)=B(I)-A(I,K+1)*C                                           AK   19
   10 CONTINUE                                                       AK   20
   15 B(1)=B(1)/A(1,1)                                               AK   21
      RETURN                                                         AK   22
      END                                                            AK   23-
```

```
      SUBROUTINE VVLBLF (X2,Y2)                                          AL     1
C                                                                        AL     2
C     *** SETS A LINE LABEL INTO A VECTOR PLOT PROVIDING THAT            AL     3
C         A CALL TO SUBROUTINE PLTLBL HAS PRESET THE NECESSARY           AL     4
C         PARAMETERS IN /VVLBL/                                          AL     5
C             GW LUNDBERG/SAI  DEC ;77                                   AL     6
C                                                                        AL     7
C     X2,Y2     THE TERMINAL POINT OF THE CURRENT VECTOR                 AL     8
C               IN INCHES FROM PRESENT PLOT ORIGIN                       AL     9
C                                                                        AL    10
C     *** NOTES --                                                       AL    11
C         (1) THERE ARE THREE ENTRY POINTS -- VVLBLF SETS UP THE         AL    12
C             PARAMETERS FOR VVLBLC WHICH ACTUALLY DOES THE LABELING.    AL    13
C             VVLBLL CLEANS UP IN CASE THERE WAS NOT ENOUGH              AL    14
C             ROOM FOR THE LAST LABEL                                    AL    15
C         (2) THE LABELS ARE SEPERATED BY DIST INCHES EXCEPT FOR         AL    16
C             THE FIRST LABEL WHICH STARTS FACT*DIST INCHES FROM         AL    17
C             THE BEGINNING OF THE VECTOR PLOT -- THIS PROVIDES FOR      AL    18
C             STAGGERED LABELS.                                          AL    19
C                                                                        AL    20
      DIMENSION XSV(20), YSV(20)                                         AL    21
C                                                                        AL    22
C     *** DIST IS THE DISTANCE IN INCHES BETWEEN LABELS.  FACT           AL    23
C         IS THE FACTOR (0-1) OF DIST TO USE FOR THE FIRST LABEL.        AL    24
C         CHRSZ IS THE SIZE OF THE LABEL CHARACTERS IN INCHES.           AL    25
C         NCHR IS THE NUMBER OF CHARACTERS (0-10), AND LABEL             AL    26
C         IS THE A-FORMATED TEXT OF THE LABEL                            AL    27
      COMMON /VVLBL/ FACT,DIST,CHRSZ,NCHR,OZL                            AL    28
      DATA MXSV/20/                                                      AL    29
C                                                                        AL    30
C     *** MOVE THE PEN TO THE FIRST POINT                                AL    31
      CALL PLOT (X2,Y2,3)                                                AL    32
C                                                                        AL    33
C     *** IF THERE ARE TO BE NO LABELS -- JUST RETURN                    AL    34
      IF (NCHR.EQ.0) RETURN                                              AL    35
C                                                                        AL    36
C     *** SET UP THE OFFSET NECESSARY TO CENTER THE LABEL AND            AL    37
C         THE DISTANCE REQUIRED BY THE LABEL                             AL    38
      OFF=CHRSZ/2.                                                       AL    39
      SZLBL=NCHR*CHRSZ+2.*OFF-0.3*CHRSZ                                  AL    40
C                                                                        AL    41
C     *** INITALIZE THE ACCUMULATED LENGTH OF THE VECTORS, THE           AL    42
C         LENGTH REQUIRED BEFORE FIRST LABEL, AND THE NUMBER             AL    43
C         OF SAVED POINTS (VECTORS) THAT MAY HAVE BEEN PREEMPTED         AL    44
C         BY THE LABEL                                                   AL    45
      TOTSZ=0.                                                           AL    46
      SKPSZ=FACT*DIST                                                    AL    47
      NSV=0                                                              AL    48
C                                                                        AL    49
C     *** REMEMBER THE STARTING LOCATION OF FIRST VECTOR                 AL    50
      X1=X2                                                              AL    51
      Y1=Y2                                                              AL    52
C                                                                        AL    53
      RETURN                                                             AL    54
C                                                                        AL    55
C*************************************************************           AL    56
C                   ENTRY VVLBLC                                         AL    57
```

```
C*************************************************************** AL  58
C                                                                AL  59
      ENTRY VVLBLC(X2,Y2)                                        AL  60
C                                                                AL  61
C     *** IF THERE ARE TO BE NO LABELS -- PLOT THE VECTOR AND RETURN AL  62
      IF (NCHR.GT.0) GO TO 5                                     AL  63
      CALL PLOT (X2,Y2,2)                                        AL  64
      RETURN                                                     AL  65
C                                                                AL  66
C     *** IF SEEKING ROOM FOR THE LABEL -- SKIP FOLLOWING        AL  67
    5 IF (NSV.GT.0) GO TO 15                                     AL  68
C                                                                AL  69
C     *** CALCULATE THIS VECTOR LENGTH AND ADD TO THE ACCUMULATED AL  70
C         LENGTH.  IF A LABEL IS TO START IN THIS VECTOR, SKIP TO AL  71
C         120, ELSE PLOT THE VECTOR AND RETURN                   AL  72
      VECSZ=SQRT((X2-X1)**2+(Y2-Y1)**2)                          AL  73
      TOTSZ=TOTSZ+VECSZ                                          AL  74
      IF (TOTSZ.GT.SKPSZ) GO TO 10                               AL  75
      CALL PLOT (X2,Y2,2)                                        AL  76
      X1=X2                                                      AL  77
      Y1=Y2                                                      AL  78
      RETURN                                                     AL  79
C                                                                AL  80
C     *** ITS TIME FOR A LABEL -- LOCATE START                   AL  81
   10 RATIO=(VECSZ-TOTSZ+SKPSZ)/VECSZ                            AL  82
      X1L=X1+RATIO*(X2-X1)                                       AL  83
      Y1L=Y1+RATIO*(Y2-Y1)                                       AL  84
C                                                                AL  85
C     *** PLOT SUBVECTOR AND REMEMBER THE END POINT              AL  86
      CALL PLOT (X1L,Y1L,2)                                      AL  87
      X1=X1L                                                     AL  88
      Y1=Y1L                                                     AL  89
C                                                                AL  90
C     *** FIND OUT IF THERE IS ENOUGH ROOM LEFT IN THIS VECTOR   AL  91
C         FOR THE LABEL -- IF THERE ISNT, SAVE (X2,Y2) AND RETURN AL  92
   15 HAVSZ=SQRT((X2-X1L)**2+(Y2-Y1L)**2)                        AL  93
      IF (HAVSZ.GE.SZLBL) GO TO 20                               AL  94
      NSV=NSV+1                                                  AL  95
C                                                                AL  96
C     *** CHECK FOR OVERFLOW                                     AL  97
      IF (NSV.GT.MXSV) STOP                                      AL  98
      XSV(NSV)=X2                                                AL  99
      YSV(NSV)=Y2                                                AL 100
      X1=X2                                                      AL 101
      Y1=Y2                                                      AL 102
      RETURN                                                     AL 103
C                                                                AL 104
C     *** CALCULATE THE END OF THE LABEL                         AL 105
C         IM SURE THERE IS AN EASIER WAY TO DO THIS, BUT IT      AL 106
C         ESCAPES ME                                             AL 107
   20 A=(X2-X1)**2+(Y2-Y1)**2                                    AL 108
      B=-2*((X1L-X1)*(X2-X1)+(Y1L-Y1)*(Y2-Y1))                   AL 109
      C=(X1L-X1)**2+(Y1L-Y1)**2-SZLBL*SZLBL                      AL 110
C                                                                AL 111
      SQRTD=SQRT(B*B-4*A*C)                                      AL 112
      T1=(-B+SQRTD)/(2*A)                                        AL 113
      T2=(-B-SQRTD)/(2*A)                                        AL 114
```

```
C                                                                       AL  115
C     *** PICK THE MINIMUM T BETWEEN 0-1 (MUST BE ONE)                  AL  116
      IF (T1.LT.0.) T1=1.                                               AL  117
      IF (T2.LT.0.) T2=1.                                               AL  118
      RATIO=AMIN1(T1,T2)                                                AL  119
C                                                                       AL  120
C     *** SET LABEL END POINT                                           AL  121
      X2L=X1+RATIO*(X2-X1)                                              AL  122
      Y2L=Y1+RATIO*(Y2-Y1)                                              AL  123
C                                                                       AL  124
C     *** CALCULATE LABEL ANGLE                                         AL  125
      DX=X2L-X1L                                                        AL  126
      DY=Y2L-Y1L                                                        AL  127
      ANG=0.                                                            AL  128
      IF (DY.NE.0.) ANG=ATAN2(DY,DX)                                    AL  129
C                                                                       AL  130
      XL=X1L                                                            AL  131
      YL=Y1L                                                            AL  132
      COSA=COS(ANG)                                                     AL  133
      SINA=SIN(ANG)                                                     AL  134
C                                                                       AL  135
C     *** REVERSE EVERYTHING IF ANGLE IN QUADRANTS 2 OR 3               AL  136
      IF (DX.GE.0.) GO TO 25                                            AL  137
      XL=X2L                                                            AL  138
      YL=Y2L                                                            AL  139
      COSA=-COSA                                                        AL  140
      SINA=-SINA                                                        AL  141
      IF (DY.GE.0.) ANG=ANG-3.1415926536                                AL  142
      IF (DY.LT.0.) ANG=ANG+3.1415926536                                AL  143
   25 ANGD=ANG*180./3.1415926536                                        AL  144
C                                                                       AL  145
C     *** LOCATE AND PLOT LABEL                                         AL  146
      XL=XL+OFF*COSA+OFF*SINA                                           AL  147
      YL=YL+OFF*SINA-OFF*COSA                                           AL  148
      IDG=NCHR-2                                                        AL  149
      CALL NUMBER (XL,YL,CHRSZ,OZL,ANGD,IDG)                            AL  150
C                                                                       AL  151
C     *** FINISH OFF THIS SEQMENT BY MEANS OF A PSUEDO REENTRY          AL  152
      TOTSZ=0.                                                          AL  153
      SKPSZ=DIST                                                        AL  154
      NSV=0                                                             AL  155
      X1=X2L                                                            AL  156
      Y1=Y2L                                                            AL  157
      CALL PLOT (X1,Y1,3)                                               AL  158
      GO TO 5                                                           AL  159
C                                                                       AL  160
C*********************************************************************  AL  161
C                    ENTRY VVLBLL                                       AL  162
C*********************************************************************  AL  163
C                                                                       AL  164
      ENTRY VVLBLL(X2,Y2)                                               AL  165
C                                                                       AL  166
C     *** PLOT THE SAVED VECTORS IF ANY                                 AL  167
      IF (NSV.EQ.0) RETURN                                              AL  168
      DO 30 I=1,NSV                                                     AL  169
      CALL PLOT (XSV(I),YSV(I),2)                                       AL  170
      CONTINUE                                                          AL  171
      NSV=0                                                             AL  172
      RETURN                                                            AL  173
C                                                                       AL  174
      END                                                               AL  175-
```

Subroutine NEWLIN

```
      SUBROUTINE NEWLIN (N,OT,HCT,SX,NS,NE,NL,NR,XNL,NPL,TOL,NUL,NTL,II)  AM    1
      COMMON /NEED/ HC,XN,NN,NB,R(20),OZP(20),OZN(8,20),RHO(8,20),M,OC(4  AM    2
     1),OS(2),HCS,XNS,LL,HCLL(8)                                          AM    3
      DIMENSION XNL(20), OT(20), HCT(20), YP(20), TM(20), NUL(20), NTL(2  AM    4
     10)                                                                  AM    5
      IT=1                                                                AM    6
      ISAV=0                                                              AM   6A
      IF (OT(N-1).LT.TOL*OT(N)) GO TO 3                                   AM    7
      IF (N.LE.2) GO TO 3                                                 AM    8
      DO 1 I=NS,NE                                                        AM    9
      J=NE-I+NS                                                           AM   10
      IF(OZP(J).LE.OT(N).AND.OZP(J).GE.OT(N-1)) GO TO 5                   AM   11
    1 CONTINUE                                                            AM  11A
      N=N-1                                                               AM  11B
    5 CALL CURV1 (N,OT,HCT,SP1,SP2,YP,TM,SX)                              AM   12
      DO 15 I=NS,NE                                                       AM   13
      IF (OZP(I).GT.OT(N)) GO TO 20                                       AM   14
      IF (OZP(I).LT.OT(1).AND.NL.GE.6) GO TO 20                           AM   15
      IF (NL.LT.6) GO TO 10                                               AM   16
      IF (IT.GT.0) NUL(I)=NUL(I)+1                                        AM   17
      IF(IT.LT.0.AND.ISAV.NE.1) NUL(ISAV)=NUL(ISAV)-1                     AM  17A
      IF (NUL(I).EQ.1) NTL(I)=II                                          AM   18
      IF (NUL(I).EQ.1) NUL(I)=II                                          AM   19
   10 XNL(I-NR)=CURV2(OZP(I),N,OT,HCT,YP,SX,IT)                           AM   20
      IF (IT.GT.0) GO TO 15                                               AM   21
      ISAV=I                                                              AM  21A
      SX=SX*10.                                                           AM   22
      SX=AMAX1(-50.,SX)                                                   AM   23
      GO TO 3                                                             AM   24
   15 IT=2                                                                AM   25
      I=NE+1                                                              AM   26
   20 NPL=I-1                                                             AM   27
      RETURN                                                              AM   28
      END                                                                 AM   29-
```

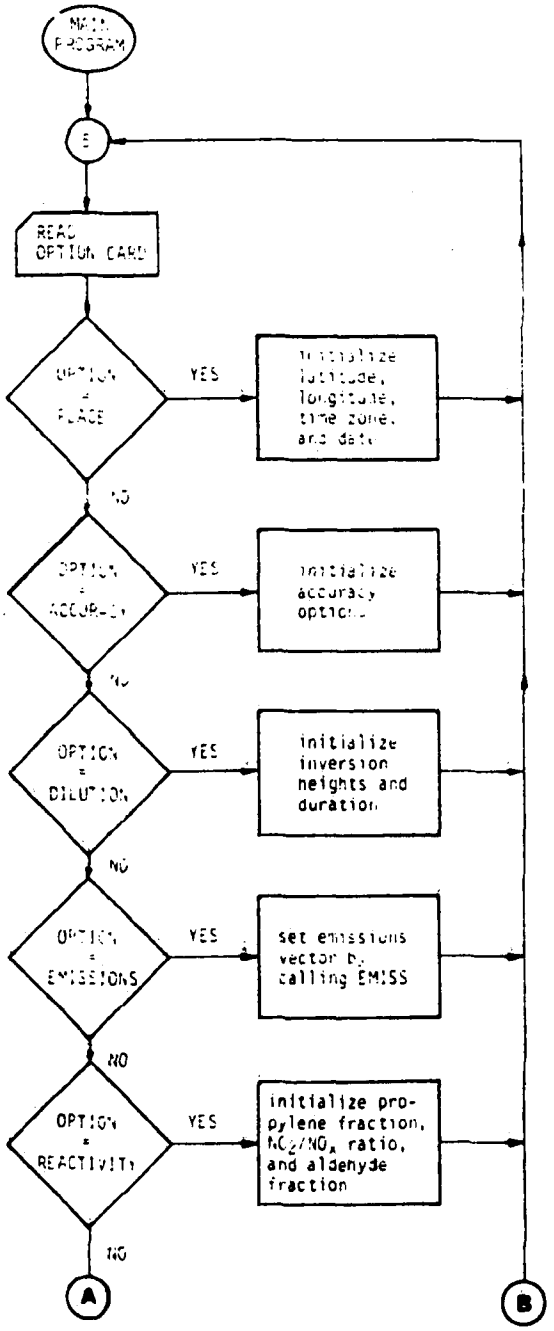
APPENDIX C

SELECTED FLOW DIAGRAMS

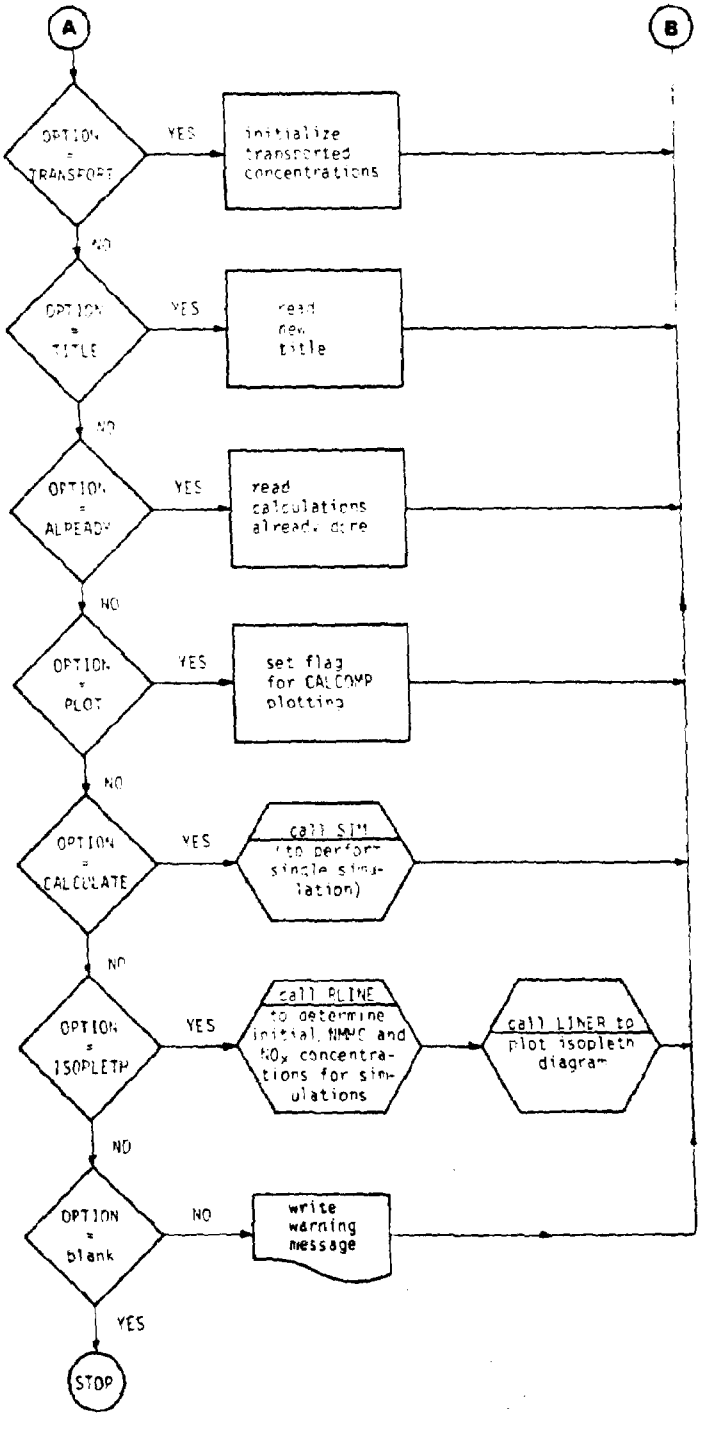
APPENDIX C

SELECTED FLOW DIAGRAMS

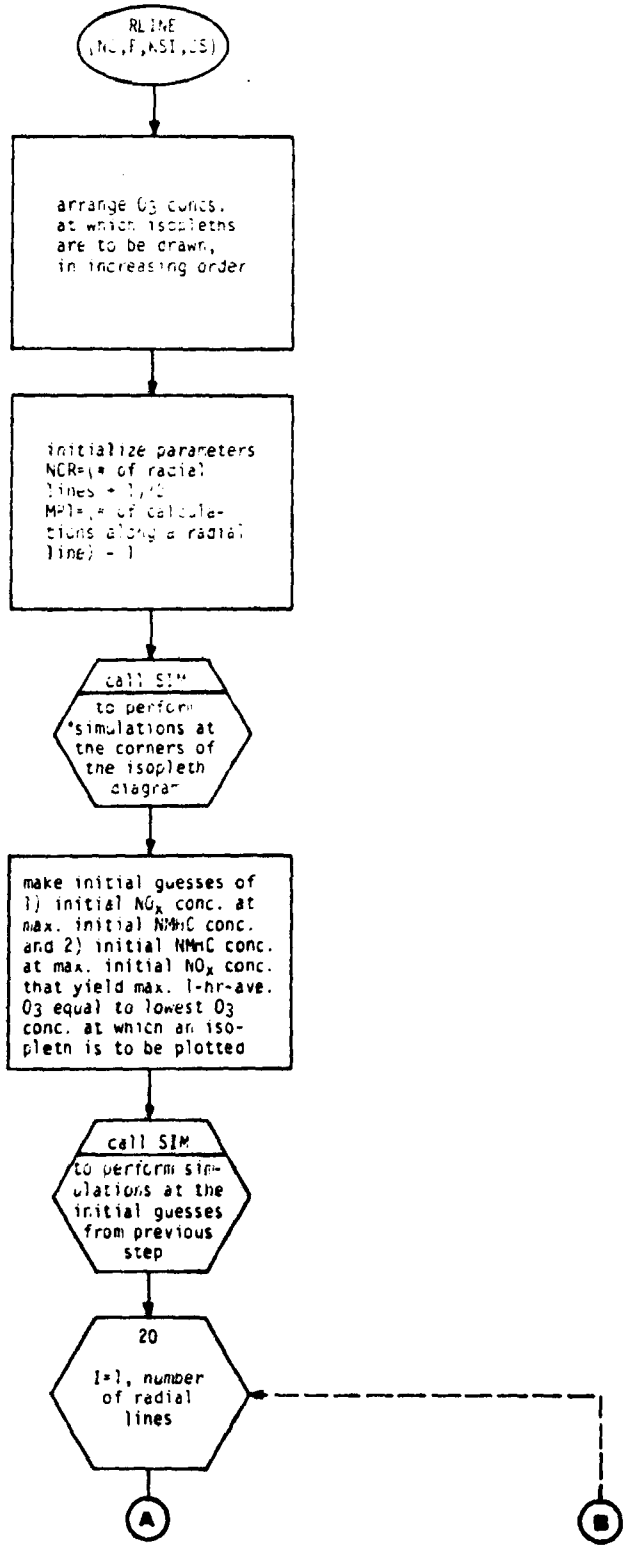
This appendix contains flow diagrams for some of the important routines of the OZIPP program. The diagrams are listed as follows:



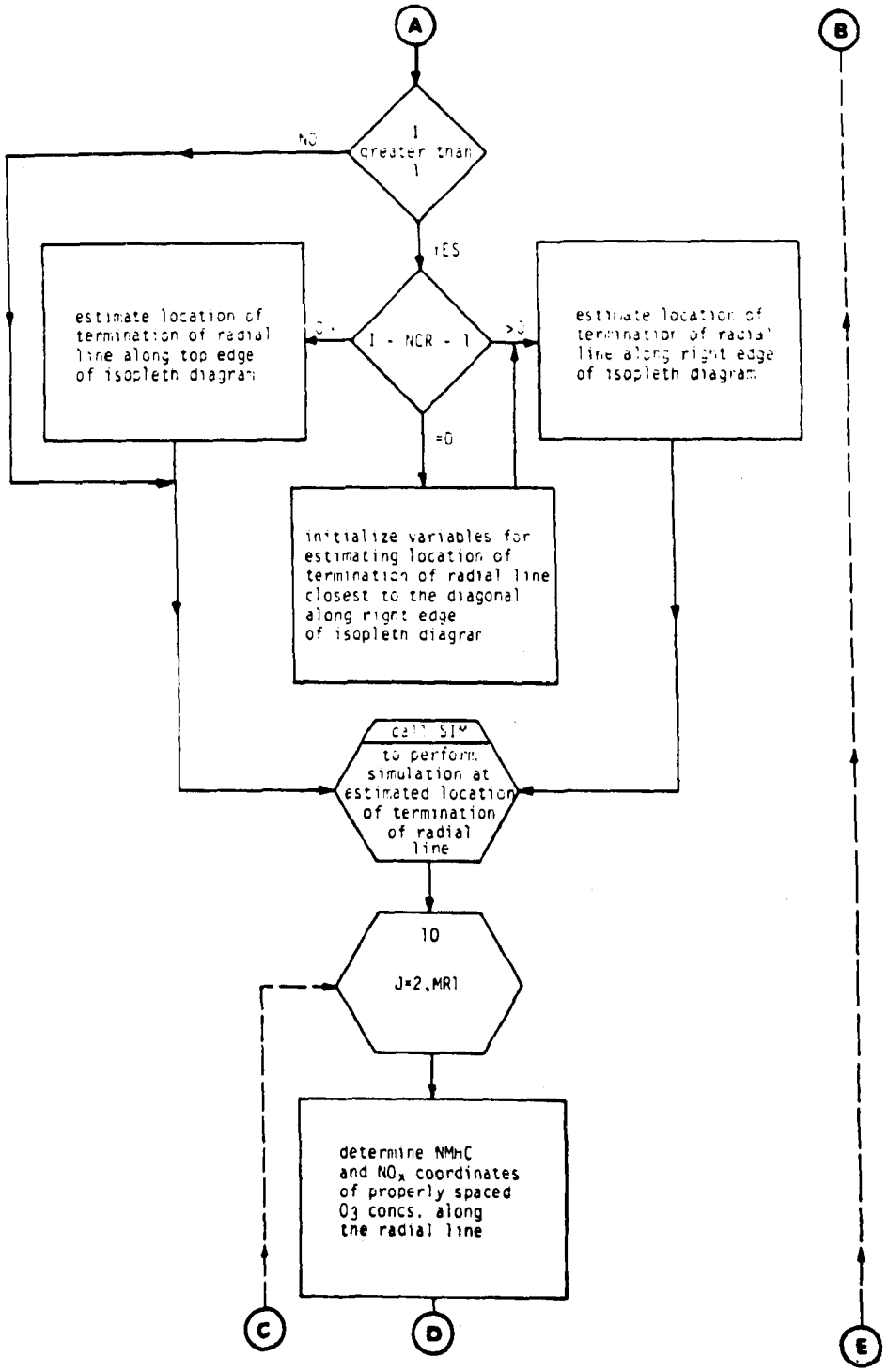
Flow diagram of the MAIN program, which processes the options, reads input data, and calls subroutines as required.



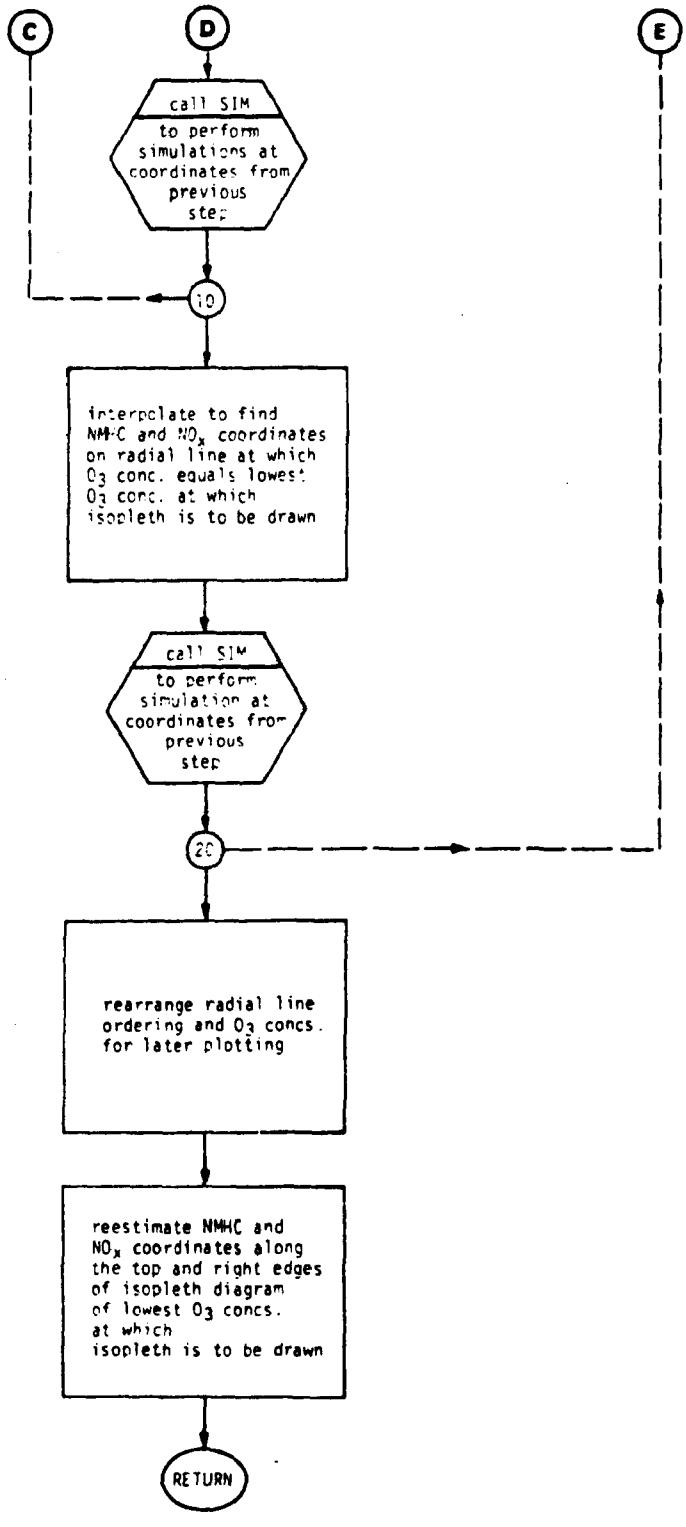
MAIN (Concluded)



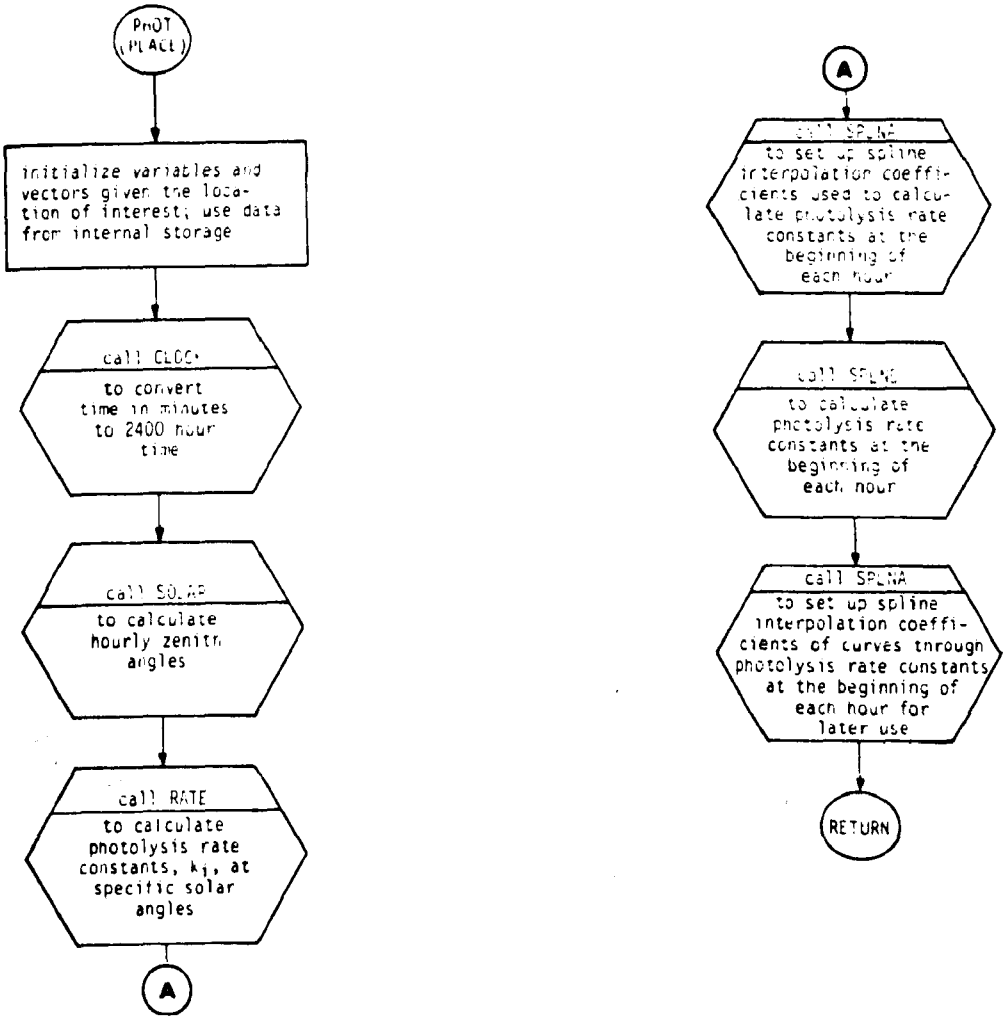
Flow diagram of subroutine RLINE, which performs the calculations for the location of the ozone value on the isopleth diagram



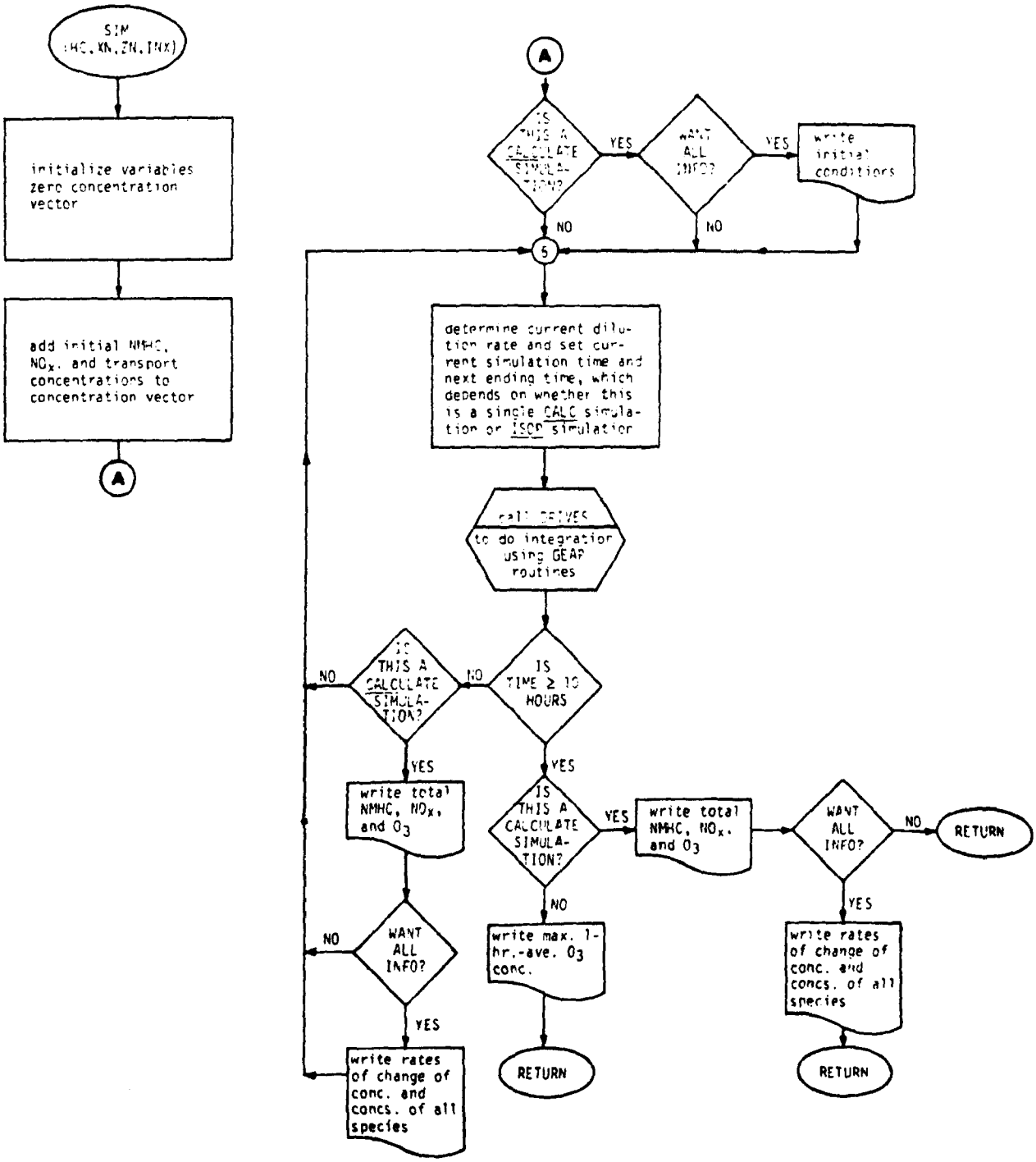
RLINE (Continued)



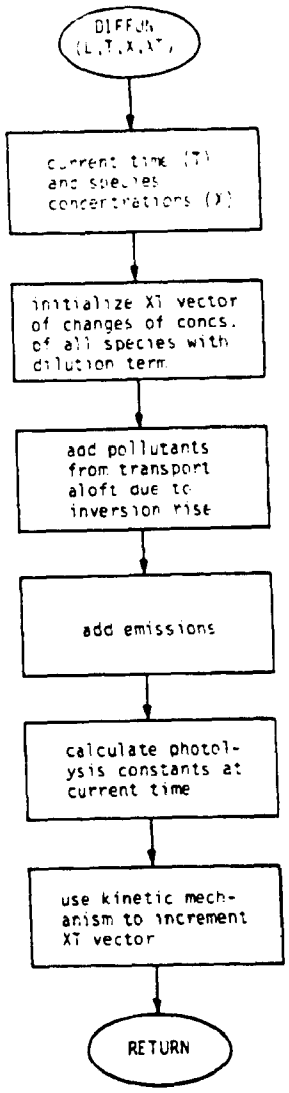
RLINE (Concluded)



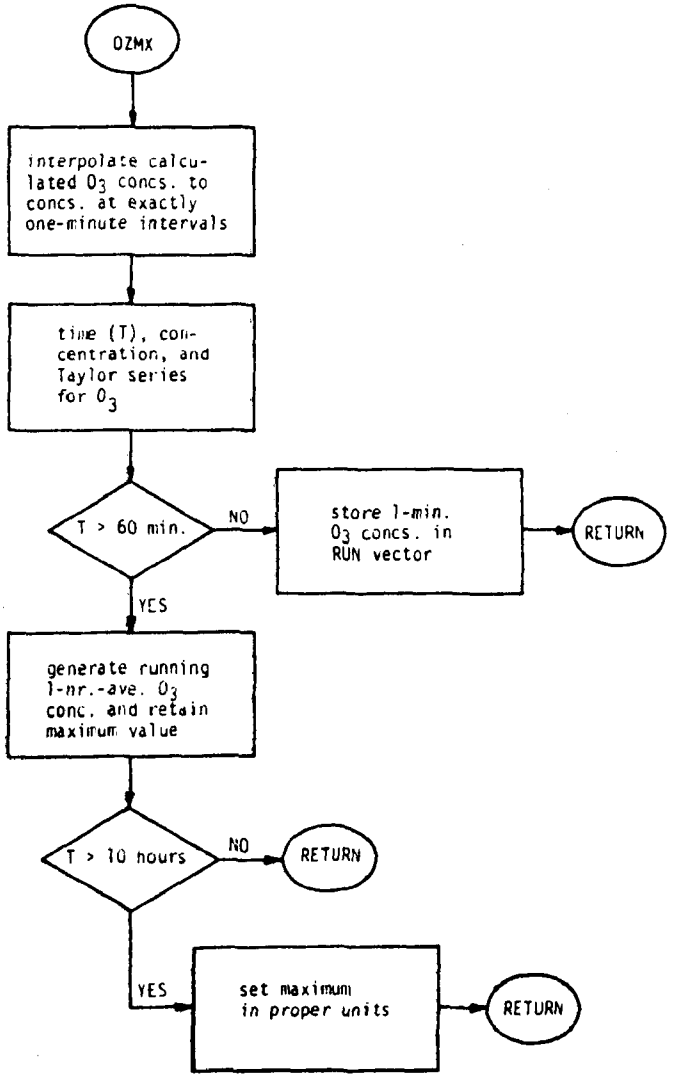
Flow diagram of subroutine PHOT, which directs calculations of photolysis rate constants



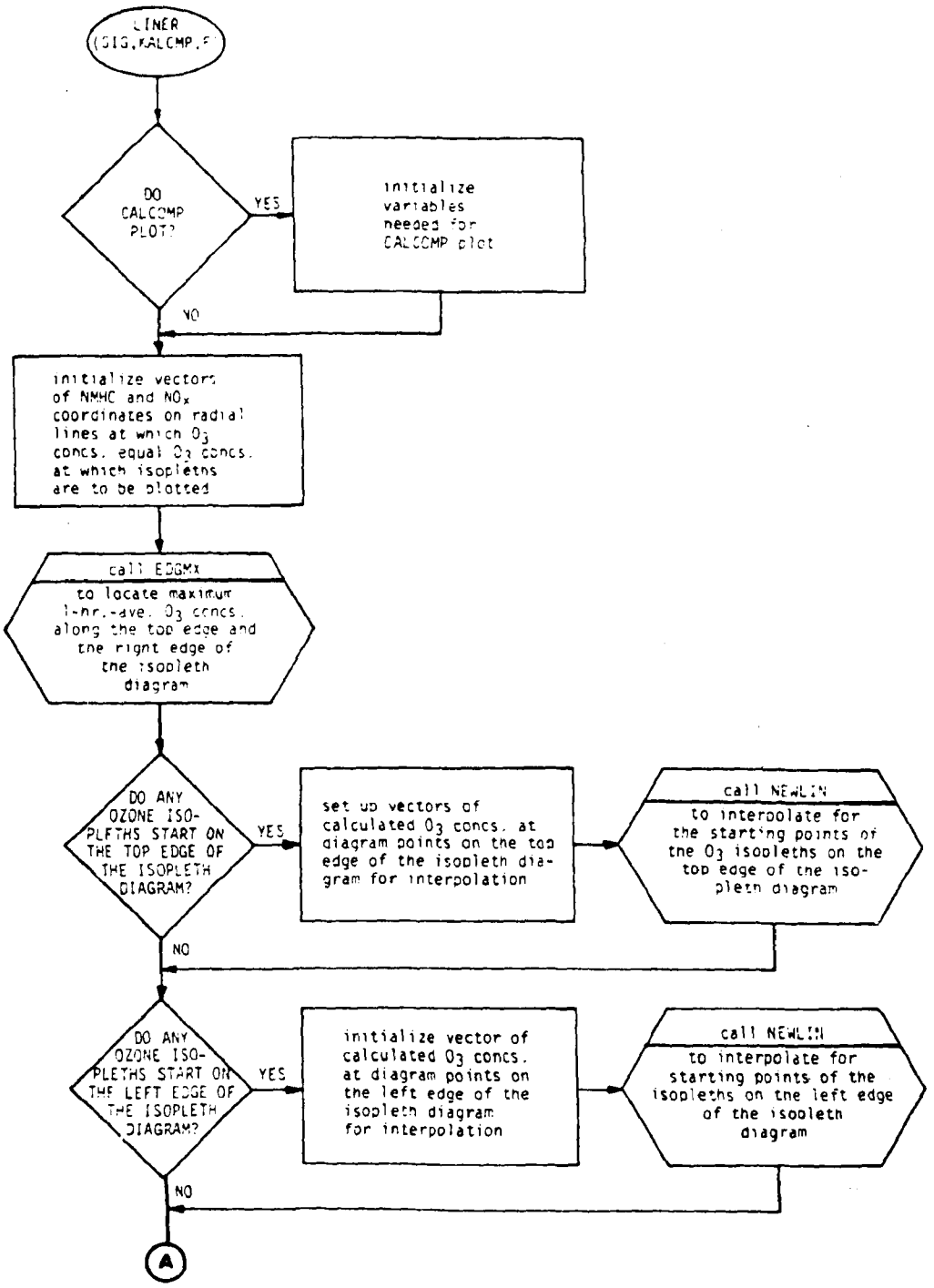
Flow diagram of subroutine SIM, which controls each calculation of the maximum one-hour average ozone concentration



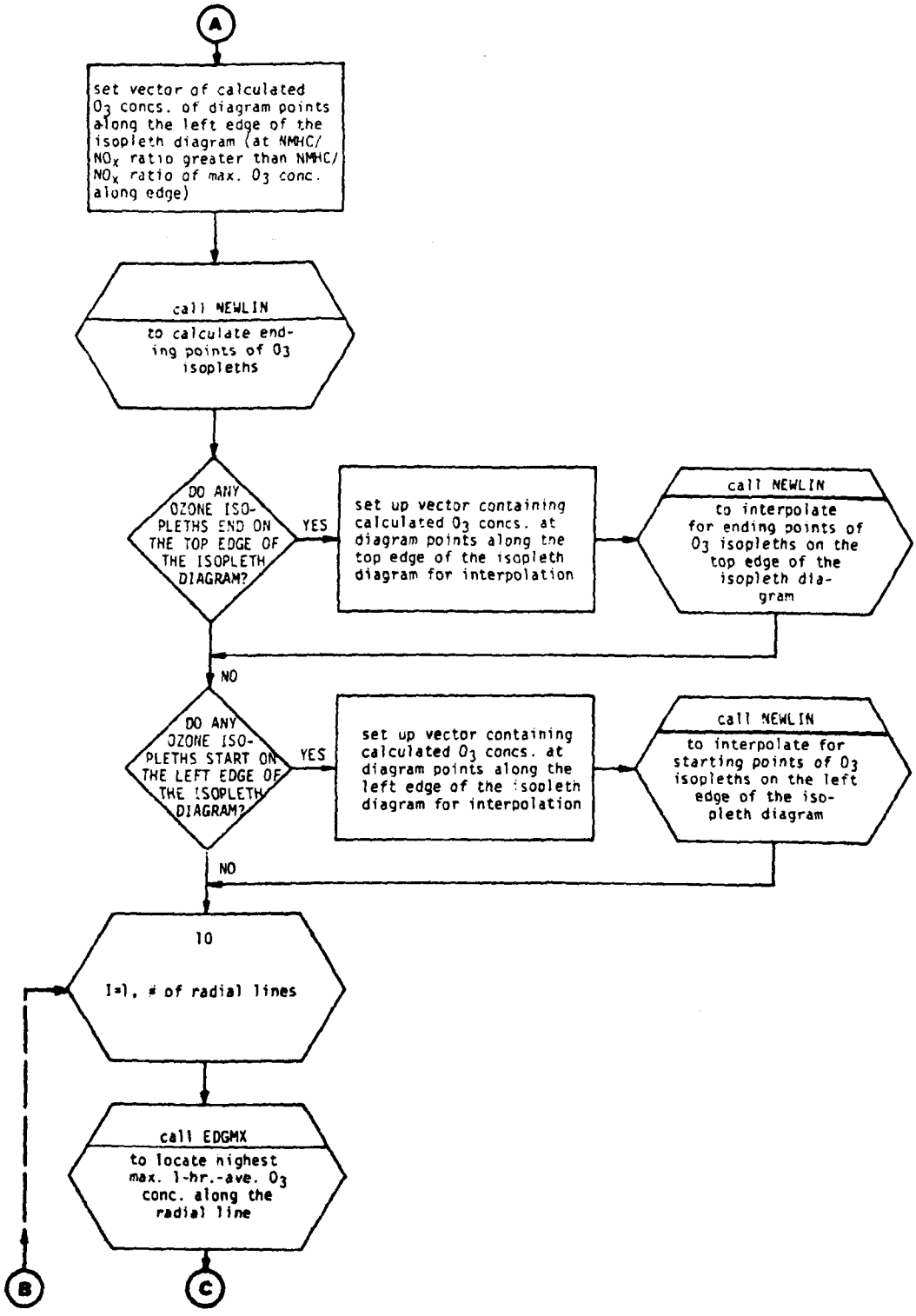
Flow diagram of subroutine DIFFUN, which updates the concentration vector based on current dilution rate (if any), emissions (if any), and chemical reactions in the kinetic mechanism. The XT vector is the vector of rates of change for each species.



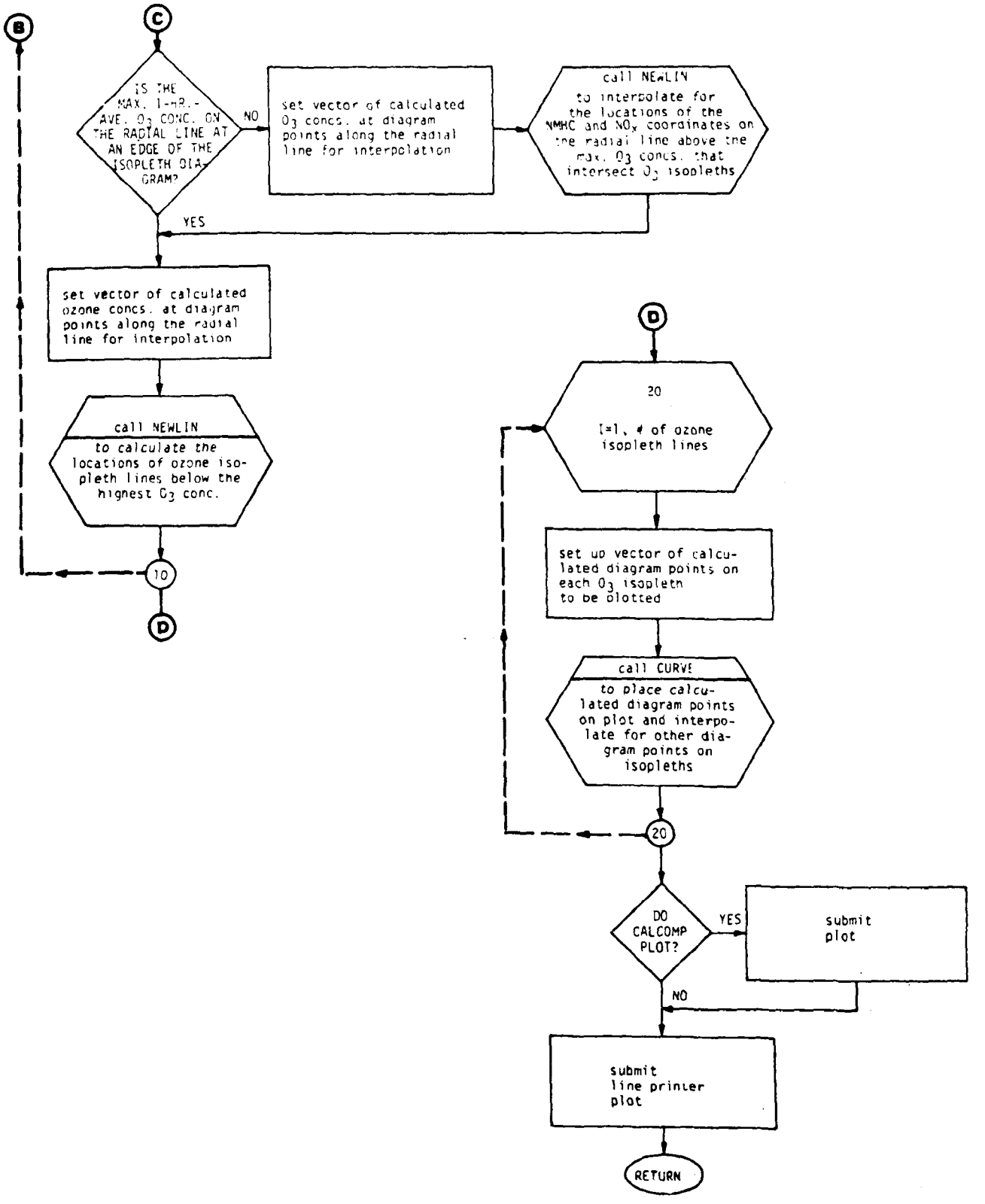
Flow diagram of subroutine OZMX, which monitors interpolation for maximum one-hour average ozone concentration



Flow diagram of subroutine LINER, which calculates the desired ozone isopleths and submits the isopleth diagram to the line printer



LINER (Continued)



LINER (Concluded)

APPENDIX D

INPUT AND OUTPUT FOR STANDARD OZONE ISOPLETH DIAGRAM EXAMPLE

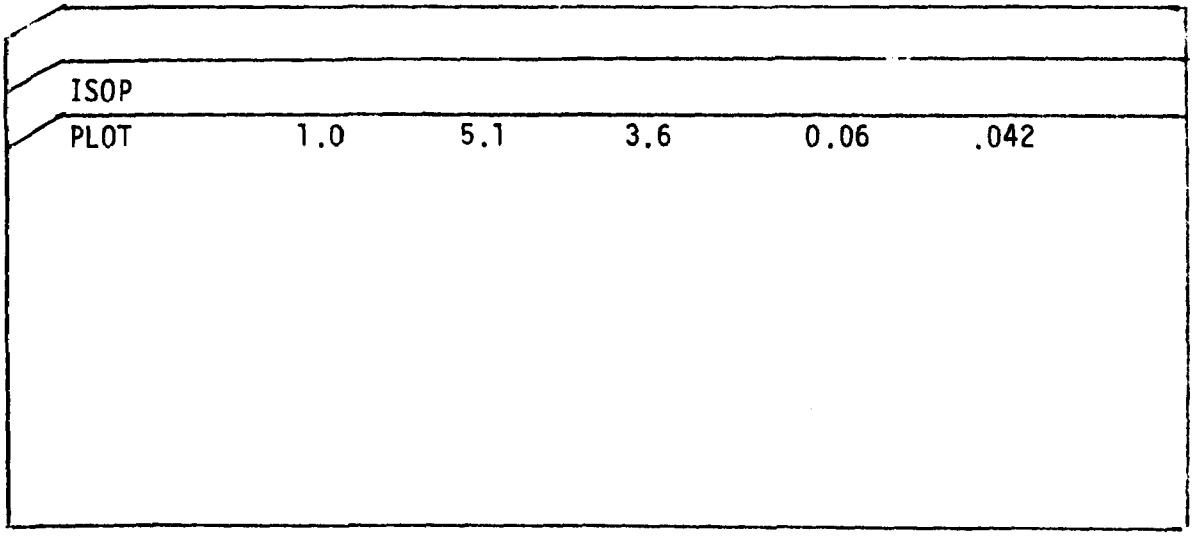


FIGURE D-1. Input Deck For Standard Diagram Example.

STANDARD OZONE ISOPLETH CONDITIONS

PHOTOLYTIC RATE CONSTANTS CALCULATED FOR

LOS ANGELES, CALIF.

LATITUDE	34.058				
LONGITUDE	-118.250				
TIME ZONE	8.0				
DATE	6,	21	1975		
TIME	800	TO	1800	LOCAL DAYLIGHT TIME	

DILUTION DETERMINED FROM THE FOLLOWING

INVERSION HEIGHTS	INITIAL	510.	FINAL	630.
TIMING	START	800.	STOP	1500.

INITIAL PROPYLENE FRACTION	.250	NO2/NOX	.250
INITIAL ALDEHYDE FRACTION	.050		

FIGURE D-2. Output For Standard Diagram Example

THE FOLLOWING SIMULATIONS WERE DONE.

HC	NOX	RATIO	OZONE	
.00000	.00000	.00000	.00000	
.00000	.28000	.00000	.00555	
2.00000	.28000	7.14286	.44847	
2.00000	.00000	.00000	.00000	
.66667	.28000	2.38095	.11901	NOT MAX
2.00000	.04995	40.04220	.20551	
1.29978	.18197	7.14286	.34608	NOT MAX
.64989	.09098	7.14286	.22120	NOT MAX
.32494	.04549	7.14286	.13778	NOT MAX
.16312	.02284	7.14286	.08438	NOT MAX
1.70176	.28000	6.07771	.42742	NOT MAX
1.11933	.18417	6.07771	.32946	NOT MAX
.55966	.09208	6.07771	.20832	NOT MAX
.27983	.04604	6.07771	.12884	NOT MAX
.15290	.02516	6.07771	.08348	NOT MAX
1.40352	.28000	5.01256	.38897	NOT MAX
.94517	.18856	5.01256	.30236	NOT MAX
.48953	.09766	5.01256	.19473	NOT MAX
.25368	.05061	5.01256	.12349	NOT MAX
.14632	.02919	5.01256	.08329	NOT MAX
1.10528	.28000	3.94742	.31779	NOT MAX
.78290	.19833	3.94742	.25539	NOT MAX
.44563	.11289	3.94742	.17657	NOT MAX
.24930	.06315	3.94742	.11971	NOT MAX
.14941	.03785	3.94742	.08416	NOT MAX

FIGURE D-2 (Continued)

.80704	.28000	2.88227	.19098 NOT MAX
.64926	.22526	2.88227	.14956 NOT MAX
.43902	.15232	2.88227	.13525 NOT MAX
.29267	.10154	2.88227	.10644 NOT MAX
.20113	.06978	2.88227	.08514 NOT MAX
.65791	.28000	2.34970	.11512 NOT MAX
.60070	.25565	2.34970	.11080 NOT MAX
.49420	.21033	2.34970	.10168 NOT MAX
.39923	.16991	2.34970	.09204 NOT MAX
.32049	.13639	2.34970	.08274 NOT MAX
2.00000	.22789	8.77622	.41815
1.32272	.15072	8.77622	.32424
.66136	.07536	8.77622	.20904 NOT MAX
.33068	.03768	8.77622	.13121 NOT MAX
.17574	.02002	8.77622	.08409 NOT MAX
2.00000	.17578	11.37803	.38096
1.35389	.11899	11.37803	.30000
.68604	.06029	11.37803	.19389
.34511	.03033	11.37803	.12355 NOT MAX
.19605	.01723	11.37803	.08367 NOT MAX
2.00000	.12367	16.17260	.32704
1.40654	.08697	16.17260	.26557
.75213	.04651	16.17260	.17910
.40261	.02489	16.17260	.11912
.24082	.01489	16.17260	.08508 NOT MAX
2.00000	.07155	27.95069	.24923
1.50541	.05386	27.95069	.21295
.89159	.03190	27.95069	.15645
.52248	.01869	27.95069	.11138

FIGURE D-2 (Continued)

.34191	.01223	27.95069	.08526 NOT MAX
2.00000	.03681	54.32763	.17397
1.64696	.03032	54.32763	.15810
1.12259	.02066	54.32763	.12835
.76637	.01411	54.32763	.10284
.54949	.01011	54.32763	.08362
.54090	.28000	1.93177	.06282
2.00000	.01354	147.71556	.09819

FIGURE D-2 (Continued)

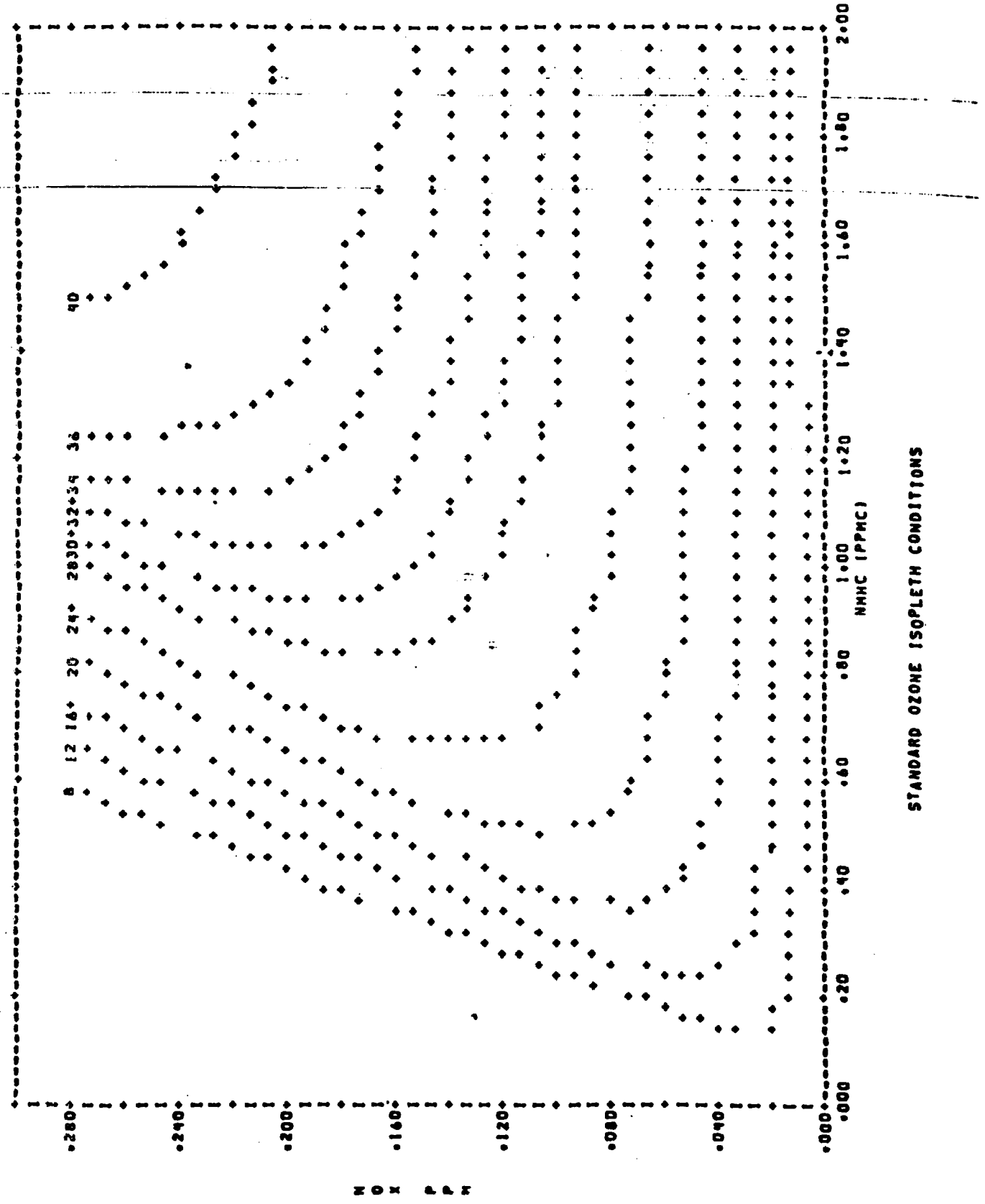


FIGURE D-2 (Continued)

THE OZONE LINES ARE .08000 .12000 .16000 .20000 .24000 .28000 .30000 .32000 .34000 .36000
.40000

FIGURE D-2 (Continued)

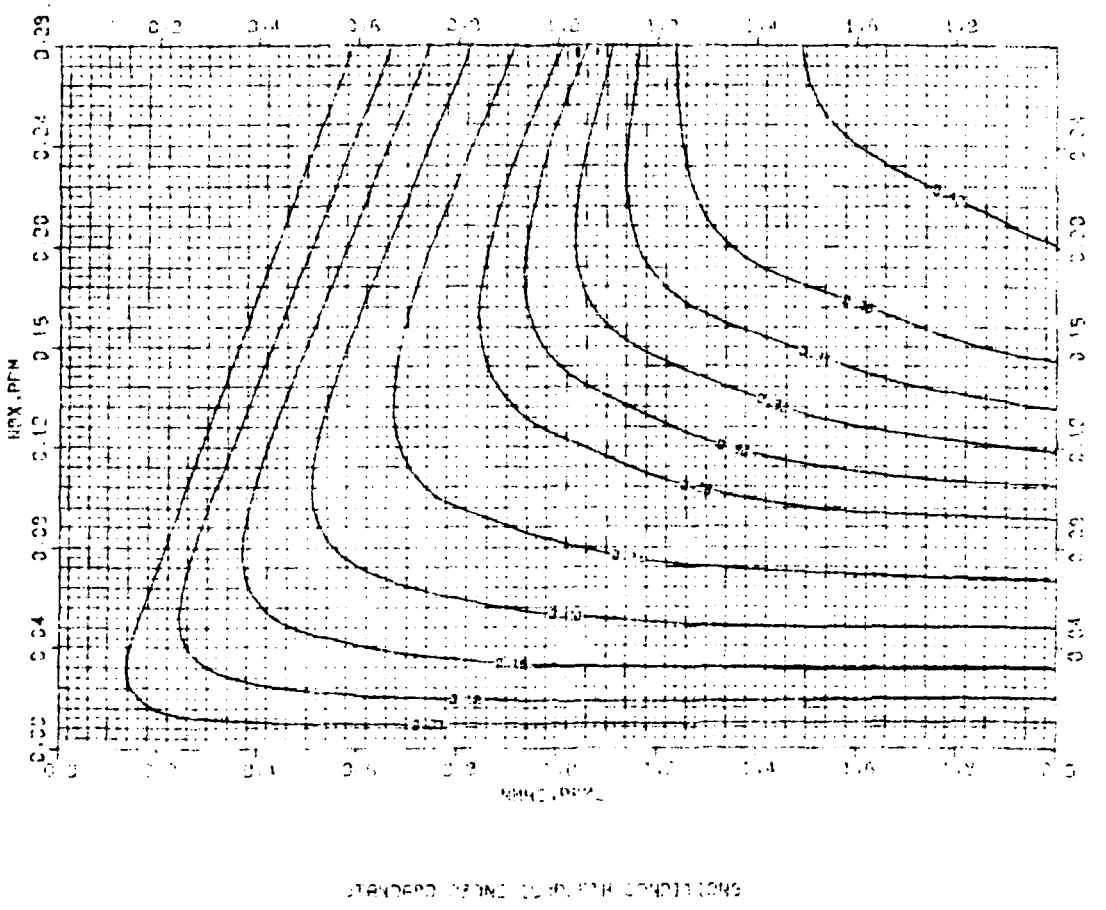


FIGURE D-3. CALCOMP Plot For Standard Diagram Example.

APPENDIX E

INPUT AND OUTPUT FOR CITY-SPECIFIC DIAGRAM EXAMPLE

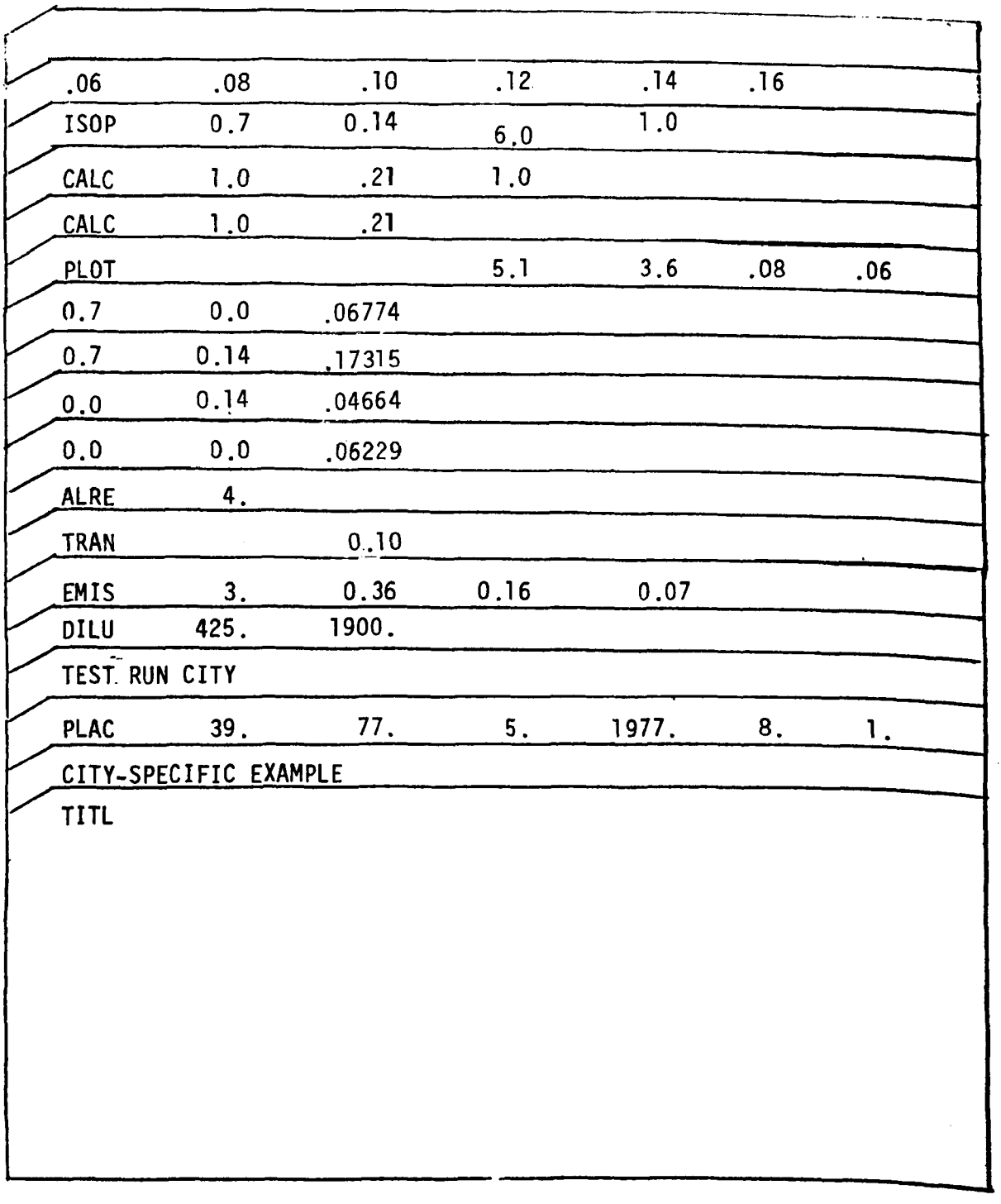


FIGURE E-1. Input Deck For City-specific Diagram Example.

THE FOLLOWING RESULTS WERE READ IN.

HC	NOX	RATIO	OZONE
.00000	.00000	.00000	.06729
.00000	.14000	.00000	.04664
.70000	.14000	5.00000	.17315
.70000	.00000	.00000	.06774

Figure E-2 Output For City-Specific Diagram Example

CITY-SPECIFIC EXAMPLE

PHOTOLYTIC RATE CONSTANTS CALCULATED FOR

TEST RUN CITY

LATITUDE	39.000			
LONGITUDE	77.000			
TIME ZONE	5.0			
DATE	8	1	1977	
TIME	800	TO	1800	LOCAL DAYLIGHT TIME
SOLAR NOON	1314			

DILUTION DETERMINED FROM THE FOLLOWING

INVERSION HEIGHTS	INITIAL	425.	FINAL	1900.
TIMING	START	800.	STOP	1500.

INITIAL PROPYLENE FRACTION	.250	NO2/NOX	.250
INITIAL ALDEHYDE FRACTION	.050		

TRANSPORTED CONCENTRATIONS

ALOFT	OZONE	.100	HYDROCARBON	.000	NOX	.000 PPM

CONTINUOUS EMISSIONS (EXPRESSED AS THE FRACTION OF

INITIAL NON-BACKGROUND CONCENTRATION EMITTED PER HOUR)

HOUR	1	2	3
FRACTION	.360	.160	.070

Figure E-2 (continued)

Figure E-2 (continued)

CITY-SPECIFIC EXAMPLE

TIME (LDT)	HC TOTAL	PROPYLENE FRACTION	ALDEHYDE FRACTION	NOX TOTAL	NO_2 FRACTION	OZONE (INSTANT)
800.	1.00000	.25000	.05000	.21000	.25000	.00000
900.	1.06317	.23397	.07178	.22767	.39099	.00831
1000.	.88886	.20057	.11404	.19618	.65288	.03020
1100.	.67768	.15350	.16177	.15052	.83232	.08668
1200.	.48401	.10062	.19604	.10230	.88829	.14797
1300.	.34851	.05925	.20207	.06590	.90567	.18170
1400.	.25300	.03202	.18766	.04052	.91155	.19317
1500.	.18658	.01693	.16519	.02425	.91387	.19061
1600.	.14996	.00877	.14308	.01772	.92390	.20001
1700.	.15888	.00490	.12599	.01338	.93572	.20517
1800.	.15209	.00314	.11533	.01080	.95242	.20742

MAXIMUM OZONE NOT REACHED, THE LAST ONE HOUR AVERAGE WAS .20645 PPM.

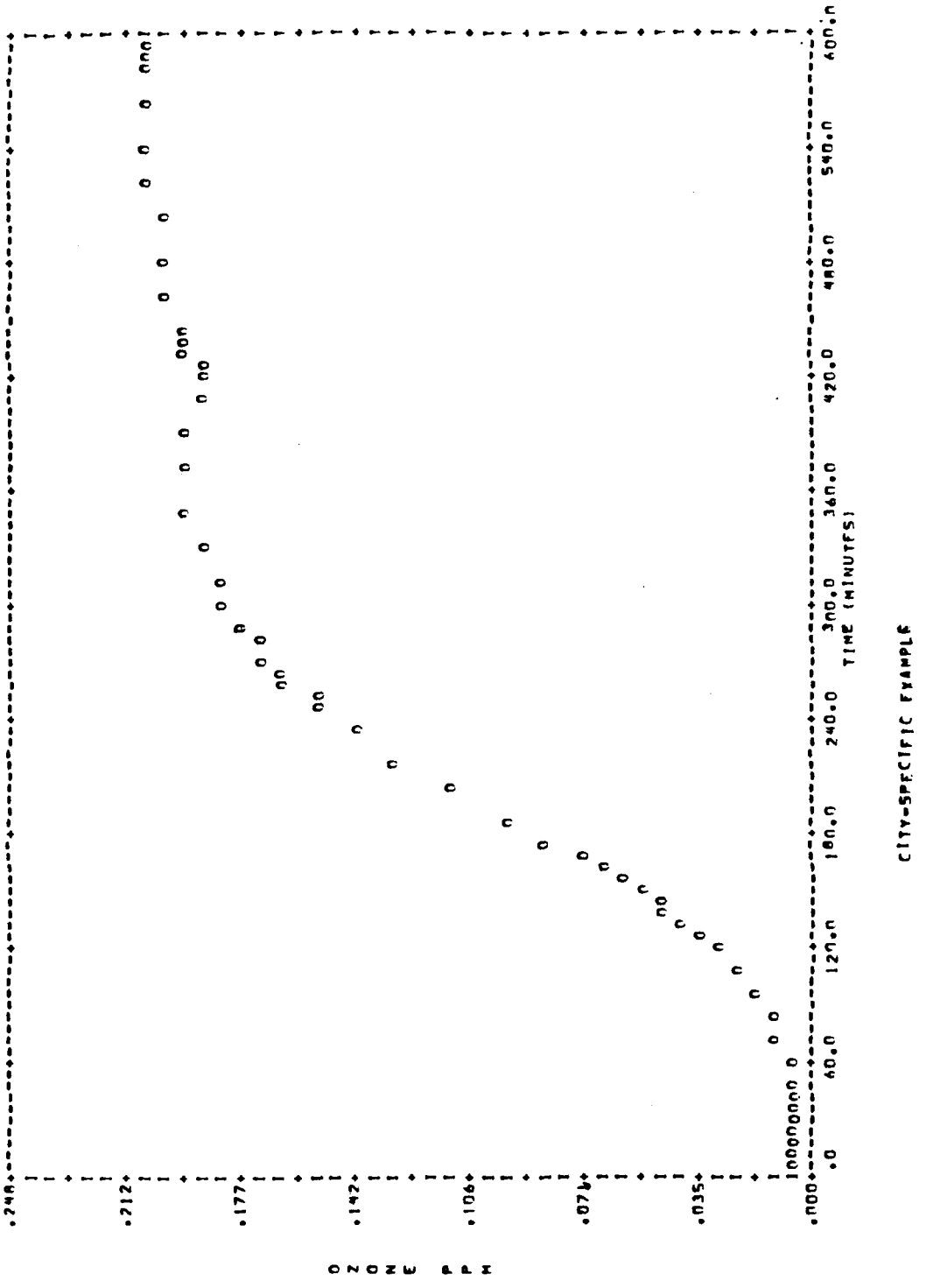


Figure E-2 (continued)

CITY-SPECIFIC EXAMPLE

PHOTOLYTIC RATE CONSTANTS CALCULATED FOR

TEST RUN CITY

LATITUDE 39.000

LONGITUDE 77.000

TIME ZONE 5.0

DATE 8 1 1977

TIME 800 TO 1800 LOCAL DAYLIGHT TIME

SOLAR NOON 1314

DILUTION DETERMINED FROM THE FOLLOWING

INVERSION HEIGHTS INITIAL 425. FINAL 1900.

TIMING START 800. STOP 1500.

INITIAL PROPYLENE FRACTION .250 NO2/NOX .250

INITIAL ALDEHYDE FRACTION .050

TRANSPORTED CONCENTRATIONS

ALOFT OZONE .100 HYDROCARBON .000 NOx .000 PPM

CONTINUOUS EMISSIONS (EXPRESSED AS THE FRACTION OF

INITIAL NON-BACKGROUND CONCENTRATION EMITTED PER HOUR)

HOUR 1 2 3

FRACTION .360 .160 .070

Figure E-2 (continued)

CITY-SPECIFIC EXAMPLE

THE ERROR TOLERANCE IS 1.000-02

THE RATE CONSTANTS USED WERE

2.058-01	4.400+06	2.500+01	4.500-02	1.300+04	1.300+04	5.600+03	2.200+01	5.000-02	2.000-05
1.000-03	1.196-02	8.000+03	3.000+03	1.200+03	8.400+03	4.579-04	2.882-04	1.705-02	8.700+10
1.000+10	8.400+01	2.900+00	2.500+04	1.000+03	1.200+04	1.000+03	1.000+03	1.000+03	1.000+05
8.000-03	8.000-03	1.800+03	1.800+03	1.800+03	1.800+03	1.800+03	1.800+03	1.800+03	7.500+04
1.000+05	8.000+03	4.000+03	1.500+05	3.000+05	1.000+05	8.000+04	8.000+04	1.615-03	4.926-04
1.500+04	4.200-06	2.031-04	1.500+04	6.000-05	2.500-03	4.500+04	6.000-05	1.900-03	4.500+04
1.000+03	1.000+03	8.000+02	8.000+02	8.000+02	1.000+02	1.000+02	1.000+02	4.000+03	4.000+03
4.000+03	4.000+03	4.000+03	4.000+03	4.000+03	4.000+03				

THE PHOTOLYSIS REACTIONS ARE

1	12	19	18	50	49	17	53

THE PHOTOLYTIC RATE CONSTANTS ARE

2.058-01	1.196-02	1.705-02	2.882-04	4.926-04	1.615-03	4.579-04	2.031-04

Figure E-2 (continued)

	TIME (LDT)	HC TOTAL	PROPYLENE FRACTION	ALDEHYDE FRACTION	NOX TOTAL	NO_2 FRACTION	OZONE (INSTANT)
	800.	1.00000	.25000	.05000	.21000	.25000	.00000

TIME INTERVAL	NO2	NO	O	O3	NO3	N2O5	HONO	OH	HO2	HO2H
	O1D	PROP	ADD	X	MEO2	MEO	C2O2	C2O	C3O2	C3O
	HCHO	ALD2	C2O3	RUT	SCO2	C4O2	C4O	SCO	ALD4	ALD3
	C3O3	C4O3								
8.000+02	5.250-02	1.575-01	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
1.000-10	0.000	8.333-02	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
	2.000-02	1.500-02	0.000	1.875-01	0.000	0.000	0.000	0.000	0.000	0.000
	0.000	0.000								
NET RATES	-1.083-02	1.171-02	1.080-02	3.566-04	0.000	0.000	3.307-07	0.000	2.275-05	0.000
	0.000	3.510-04	0.000	0.000	3.046-06	0.000	0.000	0.000	0.000	0.000
	4.210-05	6.007-05	0.000	7.898-04	0.000	0.000	0.000	0.000	0.000	0.000
	0.000	0.000								

THE REACTION RATES ARE

1.08-02	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.45-07
0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	3.23-05	9.85-06
0.00	6.30-08	3.05-06	0.00	0.00	0.00	0.00	0.00	0.00	0.00
0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
0.00	0.00	0.00	0.00	0.00	0.00				

THE PHOTOLYTIC RATE CONSTANTS ARE

2.05A-01	1.196-02	1.705-02	2.882-04	4.926-04	1.615-03	4.579-04	2.031-04

Figure E-2 (Continued)

TIME (LDT)	HC TOTAL	PROPYLENE FRACTION	ALDEHYDE FRACTION	NOX TOTAL	NO_2 FRACTION	OZONE (INSTANT)
900.	1.06117	.23397	.07178	.22767	.39099	.00831

TIME INTERVAL	NO2	NO	O	O3	NO3	N2O5	HONO	OH	HO2	HOOH
	O1D	PROP	ADD	X	MEO2	MEO	C2O2	C2O	C3O2	C3O
	HCHO	ALD2	C2O3	RUT	SCO2	C4O2	C4O	SCO	ALD4	ALD3
	C3O3	C4O3								
9.000+02	8.902-02	1.387-01	6.729-09	8.313-03	1.706-08	3.626-07	1.262-03	1.135-07	2.959-06	1.377-06
1.244+01	7.826-17	8.292-02	1.674-06	2.364-09	2.157-07	6.940-10	5.918-08	1.811-10	7.539-08	1.793-10
	2.746-02	2.443-02	3.796-07	2.036-01	1.635-07	1.635-07	1.853-10	1.042-10	8.421-04	4.756-04
	1.834-08	3.308-08								
NET RATES	7.485-06	-2.133-04	2.629-05	8.706-04	2.017-06	5.082-07	1.771-05	-1.116-05	1.167-05	6.747-08
	4.149-07	-2.579-04	2.764-06	-4.116-06	4.604-07	-1.684-06	3.078-07	-4.411-07	3.456-07	-5.519-07
	1.276-04	1.780-04	1.605-06	-1.700-04	7.815-07	7.815-07	-8.684-07	-8.684-07	1.883-05	1.259-05
	2.311-07	3.372-07								

THE REACTION RATES ARE

2.99-02	2.94-02	2.88-02	3.33-05	7.79-06	3.08-05	8.51-06	7.98-06	1.81-08	2.47-07
1.59-09	2.56-05	8.08-05	9.72-05	4.92-04	7.36-08	1.18-09	8.01-06	1.95-04	6.81-06
7.83-07	7.93-08	5.90-08	2.35-04	2.32-04	3.37-08	3.62-10	9.92-11	1.26-10	2.37-04
5.51-06	5.51-06	4.16-05	4.16-05	4.08-05	4.08-05	1.88-05	1.48-05	5.38-05	1.39-05
1.09-05	1.43-06	7.24-07	2.78-05	3.13-05	1.79-05	1.45-05	5.55-05	8.26-05	2.70-05
4.68-05	1.03-07	1.15-05	4.16-05	2.85-08	1.19-06	2.43-06	5.05-08	1.60-06	4.30-06
2.79-10	2.79-10	3.67-06	2.03-06	4.21-05	2.94-07	1.63-07	3.38-06	1.94-09	8.92-10
1.99-09	7.01-10	2.55-09	3.92-10	2.17-10	4.49-09				

THE PHOTOLYTIC RATE CONSTANTS ARE

3.307-01	2.021-02	2.395-02	9.631-04	9.841-04	3.008-03	8.545-04	4.692-04

Figure E-2 (continued)

TIME (LDT)	HC TOTAL	PROPYLENE FRACTION	ALDEHYDE FRACTION	NOX TOTAL	NO2 FRACTION	OZONE (INSTANT)
1000.	.88886	.20057	.11404	.19618	.65288	.03020

TIME INTERVAL	NO2 O1D HCHO C3O3	NO PROP ALD2 C4O3	O ADD C2O3	O3 X PAN	NO3 MEO2 SCO2	N2O5 MEO C4O2	HONO C2O2 C4O	OH C2O C5O	HO2 C3O2 ALD4	HOOH C3H ALD3
1.000+03	1.281-01	6.810-02	1.201-08	3.020-02	1.942-07	6.288-06	1.610-03	1.941-07	9.728-06	1.807-05
1.244+01	5.825-16	5.943-07	4.229-06	2.882-09	9.601-07	1.472-09	2.557-07	3.735-10	3.079-07	3.497-10
	3.366-02	3.385-02	1.676-06	1.776-01	5.057-07	5.057-07	2.757-10	1.551-10	1.908-03	1.368-03
	1.773-07	2.474-07								
NET RATES	3.960-04	-1.111-03	6.026-06	6.127-04	1.096-06	6.640-07	-6.037-06	-3.393-07	4.954-07	7.099-07
	-4.307-08	-4.945-04	-5.000-08	1.839-07	7.714-08	-7.688-08	2.739-08	-2.668-08	2.384-08	-7.742-08
	6.664-05	1.188-04	4.777-08	-5.474-04	5.137-08	5.137-08	-3.620-08	-3.620-08	1.414-05	1.465-05
	1.071-04	1.102-08								

THE REACTION RATES ARE

5.20-02	5.29-02	5.14-02	1.74-04	2.00-05	1.72-04	1.39-04	1.38-04	3.14-07	1.74-07
2.59-09	4.03-05	1.99-04	3.97-05	7.95-04	7.95-07	2.06-08	5.65-05	8.26-04	5.07-05
5.82-06	4.92-07	7.05-07	2.88-04	2.88-04	2.15-07	4.06-09	1.08-09	1.30-09	2.88-04
1.44-05	1.44-05	6.21-05	6.21-05	6.20-05	6.20-05	3.77-05	3.13-05	1.18-04	2.07-05
1.55-05	2.80-06	1.49-06	4.14-05	4.45-05	3.50-05	2.99-05	1.18-04	1.34-04	4.72-05
9.80-05	1.42-07	2.50-05	9.86-05	8.21-08	3.42-06	1.19-05	1.14-07	3.63-06	1.67-05
2.19-09	2.14-09	1.35-05	9.64-06	9.13-05	3.17-06	2.27-06	2.15-05	1.97-08	1.20-08
1.97-08	9.95-09	3.74-08	9.63-09	6.90-09	6.52-08				

THE PHOTOLYTIC RATE CONSTANTS ARE

9.061-01	2.503-02	2.736-07	1.870-03	1.402-03	3.973-03	1.140-03	7.382-04

Figure E-2 (continued)

TIME (LDT)	HC TOTAL	PROPYLENE FRACTION	ALDEHYDE FRACTION	NOX TOTAL	NO_2 FRACTION	OZONE (INSTANT)
1100.	.67768	.15350	.16177	.15052	.83732	.08668

TIME INTERVAL	NO2	NO	O	O3	NO3	N2O5	HONO	OH	HO2	HOOH
	OLD	PROP	ADD	X	MEO2	MEO	C2O2	C2O	C3O2	C3O
	HCHO	ALD2	C2O3	RUT	SCO2	C4O2	C4O	SCO	ALD4	ALD1
	C3O3	C4O3								
1.100+03	1.253-01	2.529-02	1.362-08	8.668-02	1.485-06	4.634-05	9.694-04	2.617-07	2.769-05	1.642-04
1.423+01	2.444-15	3.467-02	8.876-06	2.274-09	3.104-06	1.793-09	8.577-07	4.725-10	9.657-07	4.133-10
	3.449-07	3.757-02	5.172-06	1.434-01	1.460-06	1.460-06	2.998-10	1.686-10	2.429-03	2.009-03
	7.093-07	8.595-07								
NET RATES	-1.209-03	3.239-04	-6.445-05	1.933-03	2.003-05	-8.027-06	-1.115-05	-1.142-05	1.174-05	5.634-06
	9.654-07	-3.986-04	8.446-07	-1.460-06	7.854-07	-7.403-06	4.402-07	-7.140-07	4.601-07	-7.576-07
	-5.702-05	-1.135-05	1.696-06	-6.464-04	1.049-06	1.049-06	-1.113-06	-1.113-06	2.983-06	5.374-06
	3.649-07	3.882-07								

THE REACTION RATES ARE

5.71-02	5.99-02	5.47-02	4.89-04	2.22-05	4.74-04	1.01-03	1.02-03	2.32-06	6.32-08
9.40-10	2.76-05	2.62-04	1.98-05	8.39-04	6.44-06	2.23-07	2.38-04	2.58-03	2.13-04
2.44-05	1.91-06	5.76-06	2.27-04	2.29-04	9.45-07	2.76-08	7.61-09	8.57-09	2.27-04
2.40-05	2.40-05	6.75-05	6.75-05	6.63-05	6.63-05	4.39-05	3.90-05	1.41-04	2.25-05
1.69-05	3.31-06	1.49-06	4.50-05	5.06-05	4.13-05	3.78-05	1.43-04	1.62-04	5.92-05
1.35-04	1.58-07	3.59-05	1.47-04	1.21-07	5.02-06	2.37-05	1.46-07	4.62-06	2.86-05
1.30-08	1.30-08	1.74-05	1.43-05	1.04-04	1.08-05	8.89-06	6.48-05	1.62-07	1.07-07
1.62-07	9.50-08	3.44-07	9.52-08	7.86-08	5.73-07				

THE PHOTOLYTIC RATE CONSTANTS ARE

9.558-01	2.850-02	2.976-02	2.747-03	1.718-03	4.700-03	1.356-03	9.551-04

Figure E-2 (continued)

Figure E-2 (continued)

TIME (LDT)	HC TOTAL	PROPYLENE FRACTION	ALDEHYDE FRACTION	NOX TOTAL	NO2 FRACTION	OZONE (INSTANT)
1200.	.48401	.10062	.19609	.10230	.88829	.14797

TIME INTERVAL	NO2 O1D HCHO C303	NO PROP ALD2 C403	O AOO C203	O3 X BUT	NO3 MEO2 SCO2	N2O5 MEO C4O2	HONO C2O2 C4O	OH C2O SCO	HO2 C3O2 ALD4	HOOH C3O ALD3
1.200+03	9.087-07	1.143-07	1.114-08	1.480-01	4.036-06	9.335-05	4.711-04	3.063-07	4.739-05	7.892-04
1.423+01	5.164-15	1.623-07	1.068-05	1.242-09	5.981-06	1.533-09	1.766-06	4.379-10	1.929-06	3.676-10
	2.818-02	3.335-07	9.358-06	1.088-01	2.887-06	2.887-06	2.641-10	1.485-10	2.323-03	2.028-03
	1.515-06	1.735-06								
NET RATES	-5.172-04	-1.862-04	-1.050-05	7.521-04	6.283-06	-5.518-06	-5.460-06	1.178-06	-1.022-06	1.488-05
	-9.711-08	-2.206-04	-7.073-07	7.321-07	4.454-08	3.969-08	1.911-08	-1.079-08	1.757-08	-5.852-09
	-1.377-04	-1.160-04	4.100-08	-5.080-04	2.597-08	2.597-08	-2.644-09	-2.642-09	-5.234-06	-3.606-06
	4.190-08	4.201-08								

THE REACTION RATES ARE

4.39-02	4.90-02	4.23-07	6.05-04	1.32-05	5.99-04	2.05-03	2.05-03	4.67-06	2.08-08
2.22-10	1.43-05	2.23-04	1.05-05	6.50-04	1.89-05	1.17-06	5.01-04	4.64-03	4.49-04
5.16-05	3.81-04	1.68-05	1.24-04	1.22-04	1.37-06	6.37-08	1.89-08	2.06-08	1.74-04
1.92-05	1.92-05	6.00-05	6.00-05	5.94-05	5.94-05	3.97-05	3.63-05	1.23-04	1.98-05
1.49-05	2.94-06	1.73-06	3.96-05	4.46-05	3.68-05	3.46-05	1.23-04	1.49-04	5.39-05
1.29-04	1.40-07	3.66-05	1.53-04	1.27-07	5.07-06	2.79-05	1.39-07	4.41-06	3.70-05
3.08-08	3.08-08	1.59-05	1.38-05	8.56-05	1.58-05	1.38-05	8.50-05	5.47-07	3.66-07
5.47-07	3.15-07	1.13-06	3.29-07	2.87-07	1.77-06				

THE PHOTOLYTIC RATE CONSTANTS ARE

4.833-01	3.040-02	3.136-03	3.385-03	1.914-03	5.122-03	1.984-03	1.098-03

TIME (LDT)	HC TOTAL	PROPYLENE FRACTION	ALDEHYDE FRACTION	NOX TOTAL	NO_2 FRACTION	OZONE (INSTANT)
1300.	.34851	.05925	.20207	.06590	.90567	.18170

TIME INTERVAL	NO2	NO	O	O3	NO3	N2O5	HONO	OH	HO2	H2O2
	O1D	PROP	ADD	X	MEO2	MEO	C2O2	C2O	C3O2	C3O
	HCHO	ALD2	C2O3	RNT	SCO2	C4O2	C4O	SCO	ALD4	ALD3
	C3O3	C4O3								
1.300+03	5.968-02	6.216-03	8.161-09	1.817-01	5.981-06	9.067-05	2.504-04	3.394-07	5.647-05	1.802-03
1.000+01	6.883-15	6.883-03	9.048-06	5.841-10	8.108-06	1.135-09	2.666-06	3.556-10	2.893-06	3.001-10
	1.972-02	2.535-02	1.244-05	8.197-02	4.378-06	4.378-04	2.180-10	1.226-10	1.925-03	1.703-03
	2.327-06	2.630-06								
NET RATES	-4.561-04	-5.227-05	-2.134-07	3.562-04	3.614-07	-5.392-07	-2.353-06	-8.777-08	1.559-07	1.759-05
	2.112-09	-1.029-04	-4.569-08	1.160-09	3.687-08	-2.378-08	2.200-08	-1.107-08	2.374-08	-1.207-08
	-1.351-04	-1.398-04	6.336-08	-3.924-04	4.584-08	4.584-08	-1.997-08	-1.997-08	-7.345-06	-6.442-06
	1.911-08	2.146-08								

THE REACTION RATES ARE

2.95-02	3.59-02	2.82-02	4.88-04	6.33-06	4.83-04	2.00-03	1.99-03	4.53-06	7.42-09
6.27-11	7.80-06	1.62-04	6.33-06	4.21-04	2.68-05	2.77-06	6.68-04	5.82-03	5.99-04
6.88-05	5.18-06	2.46-05	5.84-05	5.62-05	9.82-07	7.34-08	2.41-08	2.62-08	5.84-05
1.00-05	1.00-05	5.01-05	5.01-05	4.90-05	4.90-05	3.24-05	2.98-05	9.07-05	1.63-05
1.23-05	2.40-06	1.42-06	3.27-05	3.68-05	3.00-05	2.84-05	9.08-05	1.09-04	3.94-05
1.00-04	1.06-07	2.94-05	1.29-04	1.02-07	4.26-06	2.60-05	1.16-07	3.66-06	2.94-05
3.96-08	3.96-08	1.31-05	1.16-05	6.19-05	1.57-05	1.39-05	7.43-05	9.89-07	6.53-07
9.89-07	6.02-07	1.83-06	5.94-07	5.26-07	2.81-06				

THE PHOTOLYTIC RATE CONSTANTS ARE

4.942-01	3.117-02	3.209-02	3.674-03	1.997-03	5.297-03	1.538-03	1.159-03

Figure E-2 (continued)

TIME (LOT)	HC TOTAL	PROPYLENE FRACTION	ALDEHYDE FRACTION	NOx TOTAL	NO_2 FRACTION	OZONE (INSTANT)
1400.	.25300	.03202	.18766	.04052	.91155	.19317

TIME INTERVAL	NO2	NO	O	O3	NO3	N2O5	HONO	OH	HO2	H2O2
	O1D	PROP	ADD	X	MEO2	MEO	C2O2	C2O	C3O2	C3O
	HCHO	ALD2	C2O3	RNO	SCO2	C4O2	C4O	SCO	ALD4	ALD3
	C3O3	C4O3								
1.400+03	3.693-02	3.583-03	5.652-09	1.932-01	6.823-06	6.406-05	1.500-04	3.695-07	5.779-05	7.777-03
2.000+01	7.120-15	2.701-03	6.658-06	2.497-10	9.483-06	7.657-10	3.601-06	2.775-10	3.928-06	2.355-10
	1.258-02	1.745-02	1.483-05	6.122-02	6.085-06	6.065-06	1.746-10	9.820-11	1.491-03	1.311-03
	3.197-06	3.634-06								
NET RATES	-2.932-04	-4.471-05	-2.739-06	4.069-05	1.396-06	-1.680-06	-1.191-04	6.431-07	-4.109-07	1.394-05
	-1.205-06	-4.292-05	-1.945-07	1.492-07	1.083-08	-2.642-08	5.032-08	-5.599-08	5.567-08	-6.431-08
	-9.875-05	-1.177-04	8.930-08	-2.997-04	1.276-07	1.276-07	-1.162-07	-1.162-07	-6.832-06	-6.287-06
	7.393-08	9.129-08								

THE REACTION RATES ARE

1.81-07	2.49-02	1.73-02	3.21-04	2.71-06	3.18-04	1.41-03	1.41-03	3.20-06	2.65-09
2.25-11	4.63-06	1.09-04	3.97-06	2.49-04	2.81-05	4.22-06	6.89-04	6.14-03	6.19-04
7.12-05	5.99-06	2.68-05	2.49-05	2.39-05	5.37-07	6.31-08	2.40-08	2.62-08	2.50-05
4.17-06	4.17-06	4.07-05	4.07-05	3.91-05	3.91-05	2.53-05	2.42-05	6.12-06	1.31-05
9.82-06	1.88-06	1.11-06	2.62-05	2.95-05	2.35-05	2.22-05	6.13-05	6.59-05	2.48-05
8.97-05	7.33-08	1.98-05	9.67-05	7.87-08	3.28-06	2.18-05	8.94-08	2.83-06	2.48-05
4.04-08	4.04-08	1.04-05	9.17-06	4.25-05	1.34-05	1.18-05	5.48-05	1.40-06	9.08-07
1.40-06	8.33-07	2.19-06	8.40-07	7.39-07	3.43-06				

THE PHOTOLYTIC RATE CONSTANTS ARE

4.904-01	3.090-02	3.179-02	3.569-01	1.967-03	5.235-03	1.519-03	1.137-01

Figure E-2 (continued)

TIME (LDT)	HC TOTAL	PROPYLENE FRACTION	ALDEHYDE FRACTION	NOX TOTAL	NO2 FRACTION	OZONE (INSTANT)
1500.	.18658	.01693	.16519	.02425	.91387	.19051

TIME INTERVAL	NO2 O1D HCHO C303	NO PROP ALD2 C403	O ADD C203	O3 X RUT	NO3 HE02 SC02	N2O5 ME0 C402	HONO C202 C40	OH C20 SCO	HO2 C302 ALD4	HOOH C30 ALD3
1.500+03	2.217-02	2.089-03	3.870-09	1.905-01	6.932-06	3.903-05	9.482-05	3.841-07	5.377-05	3.414-03
9.281+00	6.069-15	1.047-03	4.509-06	1.007-10	1.086-05	4.735-10	4.523-06	2.027-10	4.990-06	1.739-10
	7.781-03	1.144-02	1.643-05	4.561-02	7.909-06	7.909-08	1.323-10	7.444-11	1.116-03	9.649-04
	4.059-06	4.695-06								
NET RATES	-1.942-04	-1.929-05	-2.183-10	-1.141-04	-2.539-09	-3.491-07	-7.317-07	-1.705-11	-1.027-07	7.241-06
	2.728-12	-1.698-05	-2.634-08	4.145-11	1.584-09	-1.000-11	1.364-08	-2.501-12	1.608-08	-7.728-12
	-6.350-05	-8.321-05	1.586-08	-2.257-04	2.933-08	2.933-08	-1.329-12	-8.740-13	-5.612-06	-5.196-06
	1.204-08	1.561-08								

THE REACTION RATES ARE

1.04-02	1.68-02	9.95-03	1.90-04	1.10-06	1.88-04	8.60-04	8.59-04	1.95-06	9.26-10
8.99-12	2.80-06	6.81-05	2.41-06	1.35-04	2.43-05	4.87-06	5.89-04	5.84-03	5.28-04
6.07-05	6.15-06	2.46-05	1.01-05	9.42-06	2.44-07	4.54-08	2.04-08	2.25-08	1.01-05
1.60-06	1.60-06	3.15-05	3.15-05	2.97-05	2.97-05	1.88-05	1.70-05	3.78-05	9.92-06
7.44-06	1.39-06	8.11-07	1.98-05	2.23-05	1.74-05	1.62-05	3.79-05	3.84-05	1.42-05
4.48-05	4.80-08	1.18-05	6.59-05	5.79-08	2.41-06	1.67-05	6.70-08	2.12-06	1.93-05
3.57-08	3.57-08	7.85-06	6.78-06	2.75-05	1.04-05	9.00-06	3.64-05	1.70-06	1.07-06
1.70-06	9.73-07	2.16-06	1.01-06	8.73-07	3.53-06				

THE PHOTOLYTIC RATE CONSTANTS ARE

4.712-01	2.956-02	3.064-02	3.090-03	1.824-03	4.933-03	1.427-03	1.033-03

Figure E-2 (continued)

TIME (LDT)	HC TOTAL	PROPYLENE FRACTION	ALDEHYDE FRACTION	NOX TOTAL	NO2 FRACTION	OZONE (INSTANT)
1600.	.16996	.00877	.14308	.01772	.92390	.20001

TIME INTERVAL	NO2	NO	O	O3	NO3	N2O5	HONO	OH	HO2	HO2H
	O1D	PROP	ADD	X	HO2	HO	C2O2	C2O	C3O2	C3O
	HCHO	ALD2	C2O3		SCO2	C4O2	C4O	SCO	ALD4	ALD3
	C3O3	C4O3								
1.600+03	1.637-02	1.349-03	3.005-09	2.000-01	8.306-06	3.455-05	6.784-05	3.372-07	4.851-05	4.431-03
2.000+01	4.752-15	4.970-04	2.888-06	4.209-11	9.909-06	1.011-10	5.300-06	1.534-10	5.913-06	1.331-10
	5.910-03	9.204-03	1.628-05	4.212-02	9.732-06	9.732-06	1.051-10	5.914-11	1.016-03	8.542-04
	4.454-06	5.297-06								
NET RATES	-8.087-05	-8.709-06	-2.194-07	1.191-04	2.543-07	-2.339-07	-4.593-07	1.182-11	-1.250-07	1.422-05
	-9.746-08	-5.780-06	-2.278-08	3.907-09	-1.151-08	-4.776-10	1.069-08	-2.086-09	1.271-08	-1.725-09
	-2.626-05	-3.123-05	-2.240-08	-5.113-05	2.489-08	2.432-08	-1.679-09	-1.678-09	-1.640-06	-1.843-06
	-7.923-10	1.750-09								

THE REACTION RATES ARE

7.09-03	1.32-07	6.74-03	1.47-04	6.40-07	1.46-04	7.62-04	7.60-04	1.73-06	4.42-10
4.60-12	1.82-06	4.42-05	1.36-06	7.86-05	1.98-05	5.56-06	4.61-04	5.72-03	4.13-04
4.75-05	5.67-06	2.33-05	4.19-06	3.90-06	1.00-07	2.86-08	1.53-08	1.71-08	4.21-06
7.95-07	7.95-07	2.56-05	2.54-05	2.36-05	2.36-05	1.44-05	1.29-05	2.41-05	7.88-06
5.91-06	1.06-06	6.13-07	1.58-05	1.77-05	1.33-05	1.23-05	2.41-05	2.58-05	9.24-06
2.99-05	3.87-08	7.82-06	4.66-05	5.13-08	2.14-06	1.30-05	6.10-08	1.93-06	1.54-05
2.81-08	2.81-08	5.72-06	4.81-06	1.76-05	8.47-06	7.29-06	2.67-05	1.89-06	1.15-06
1.89-06	1.03-06	1.92-06	1.03-06	8.64-07	3.16-06				

THE PHOTOLYTIC RATE CONSTANTS ARE

4.329-01	2.690-02	2.860-02	2.304-03	1.567-03	4.358-03	1.254-03	8.496-04

Figure E-2 (continued)

TIME (LDT)	HC TOTAL	PROPYLENE FRACTION	ALDEHYDE FRACTION	NOX TOTAL	NO_2 FRACTION	OZONE (INSTANT)
1700.	.15888	.00490	.12599	.01338	.93572	.20517

TIME INTERVAL										
	NO2	NO	O	O3	NO3	N2O5	HONO	OH	HO2	H2O2
	O1D	PROP	ADD	X	MEO2	MEO	C2O2	C2O	C3O2	C3O
	HCHO	ALD2	C2O3	RNO	SCO2	C4O2	C4O	SCO	ALD4	ALD3
	C3O3	C4O3								
1.700+03	1.252-02	8.600-04	2.304-09	2.052-01	1.016-05	3.234-05	4.336-05	2.457-07	3.912-05	5.090-03
2.000+01	2.919-15	2.598-04	1.703-06	1.609-11	8.531-06	1.650-10	5.456-06	1.005-10	6.115-06	8.750-11
	4.616-03	7.701-03	1.380-05	3.953-02	1.029-05	1.029-05	7.059-11	3.971-11	9.235-04	7.529-04
	3.989-06	4.894-06								
NET RATES	-4.895-05	-6.268-04	-1.912-06	5.914-05	1.503-06	-1.083-06	-3.510-07	6.725-08	-2.038-07	7.770-06
	2.648-07	-2.498-06	-8.254-09	-5.200-09	-3.495-08	2.119-08	-1.256-08	1.696-08	-1.683-08	2.563-08
	-1.704-05	-1.899-05	-1.213-07	-3.496-05	-8.690-08	-8.690-08	7.162-08	7.162-08	-1.431-06	-1.500-06
	-3.935-08	-5.090-08								

THE REACTION RATES ARE

4.64-03	1.01-02	4.41-03	1.16-04	3.75-07	1.14-04	7.12-04	7.11-04	1.62-06	2.15-10
1.88-12	9.85-07	2.46-05	6.34-07	4.04-05	1.29-05	5.08-06	2.83-04	5.24-03	2.54-04
2.92-05	4.73-06	1.93-05	1.60-06	1.46-06	3.48-08	1.45-08	9.29-09	1.04-08	1.41-06
4.26-07	4.76-07	1.75-05	1.75-05	1.59-05	1.59-05	9.47-06	8.45-06	1.32-05	5.29-06
3.97-06	7.00-07	4.02-07	1.06-05	1.19-05	8.75-06	8.04-06	1.32-05	1.62-05	5.51-06
1.70-05	3.23-08	4.63-06	2.84-05	4.52-08	1.88-06	8.32-06	5.54-08	1.75-06	1.02-05
1.75-08	1.75-08	3.37-06	2.74-06	9.49-06	6.13-06	4.99-06	1.73-05	1.61-06	9.57-07
1.61-06	8.54-07	1.33-06	7.66-07	6.24-07	2.16-06				

THE PHOTOLYTIC RATE CONSTANTS ARE

3.705-01	2.272-02	2.556-02	1.381-03	1.194-03	3.498-03	9.989-04	6.008-04

Figure E-2 (continued)

TIME (LDT)	HC TOTAL	PROPYLENE FRACTION	ALDEHYDE FRACTION	NOX TOTAL	NO2 FRACTION	OZONE (INSTANT)
1800.	.15209	.00314	.11533	.01080	.95242	.20742

TIME INTERVAL	NO2	NO	O	O3	NO3	N2O5	HONO	OH	HO2	H2OH
	O1D	PROP	ADD	X	MEO2	MEO	C2O2	C2O	C3O2	C1O
	HCHO	ALD2	C2O3	RUT	SCO2	C4O2	C4O	SCO	ALD4	ALD3
	C3O3	C4O3								
1.800+03	1.029-02	5.138-04	1.634-09	2.074-01	1.375-05	3.609-05	2.588-05	1.316-07	2.726-05	5.401-03
1.811+01	1.171-15	1.592-04	9.384-07	5.199-12	6.011-06	6.802-11	4.972-06	5.459-11	5.449-06	4.642-11
	3.812-03	6.865-03	9.057-06	3.790-02	8.800-06	8.800-06	3.580-11	2.014-11	8.434-04	6.756-04
	2.624-06	3.276-06								
NET RATES	-1.313-05	-1.485-05	-3.331-05	3.742-05	6.359-06	-3.989-06	-2.184-07	-3.497-08	-6.748-07	2.700-06
	3.021-06	-1.052-06	-1.159-08	1.533-08	-5.781-08	1.240-07	7.348-09	1.773-08	-4.432-09	3.117-08
	-9.616-06	-8.633-06	-2.143-07	-1.795-05	-1.307-07	-1.307-07	9.313-08	9.313-08	-1.277-06	-1.088-06
	-6.293-08	-7.994-08								

THE REACTION RATES ARE

2.80-03	7.19-03	2.66-03	9.60-05	2.18-07	9.18-05	7.92-04	7.94-04	1.80-06	1.04-10
4.70-13	4.21-07	1.08-05	2.03-07	1.68-05	6.24-06	3.54-06	1.17-04	4.26-03	1.02-09
1.17-05	2.79-06	1.36-05	5.24-07	4.82-07	1.08-08	5.64-09	4.67-09	5.11-09	5.20-07
2.64-07	2.64-07	8.98-06	8.98-06	8.14-06	8.14-06	5.04-06	4.60-06	5.56-06	2.44-06
2.01-06	3.71-07	2.18-07	5.37-06	6.04-06	4.64-06	4.37-06	5.44-06	8.82-06	2.77-06
7.52-06	2.88-08	2.72-06	1.35-05	4.05-08	1.69-06	4.00-06	5.06-08	1.60-06	4.99-06
8.26-09	8.26-09	1.35-06	1.08-06	3.72-06	3.37-06	2.70-06	9.32-06	9.60-07	5.94-07
9.60-07	5.42-07	6.55-07	3.57-07	2.86-07	9.87-07				

THE PHOTOLYTIC RATE CONSTANTS ARE

2.71A-01	1.628-02	2.059-07	5.622-04	7.277-04	2.313-03	6.556-04	3.236-04

MAXIMUM OZONE NOT REACHED, THE LAST ONE HOUR AVERAGE WAS .20645 PPM.

Figure E-2 (continued)

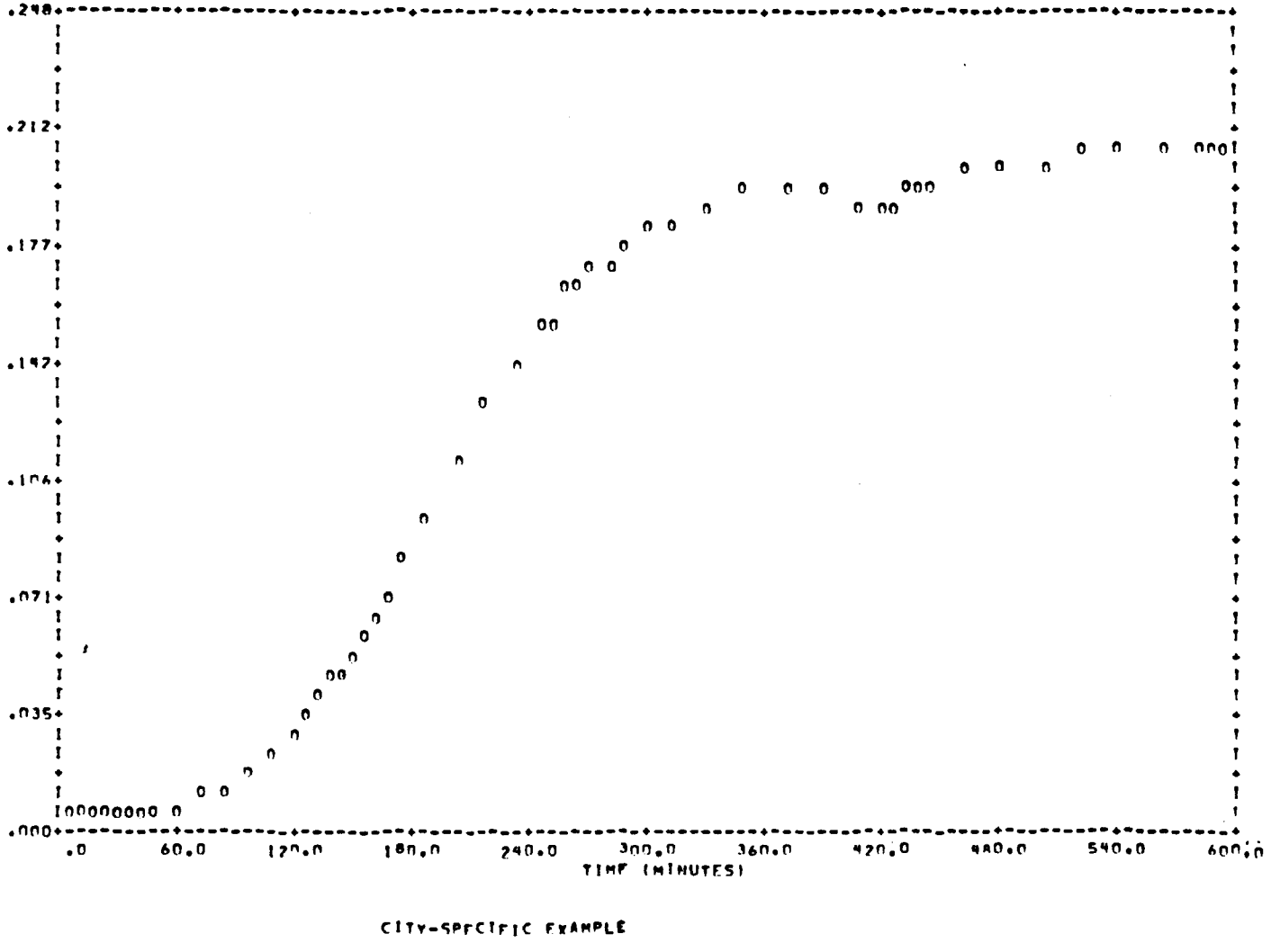


Figure E-2 (continued)

CITY-SPECIFIC EXAMPLE

PHOTOLYTIC RATE CONSTANTS CALCULATED FOR

TEST RUN CITY

LATITUDE 39.000

LONGITUDE 77.000

TIME ZONE 5.0

DATE 8 1 1977.

TIME 800 TO 1800 LOCAL DAYLIGHT TIME

SOLAR NOON 1314

DILUTION DETERMINED FROM THE FOLLOWING

INVERSION HEIGHTS	INITIAL	425.	FINAL	1000.
TIMING	START	800.	STOP	1500.

INITIAL PROPYLENE FRACTION	.250	NO2/NOX	.250
INITIAL ALDEHYDE FRACTION	.050		

TRANSPORTED CONCENTRATIONS

ALOFT	OZONE	.100	HYDROCARBON	.000	NOX	.000 PPM

CONTINUOUS EMISSIONS (EXPRESSED AS THE FRACTION OF INITIAL NON-BACKGROUND CONCENTRATION EMITTED PER HOUR)

HOUR	1	2	3
FRACTION	.340	.160	.070

Figure E-2 (continued)

THE FOLLOWING SIMULATIONS WERE DONE.

HC	NOX	RATIO	OZONE	TIME
DUE TO HIGH BACKGROUND CONDITIONS THE LOWEST OZONE PLOTTED WILL BE .08 PPM.				
.18459	.14000	1.31847	.06861	567.
.70000	.01628	42.98940	.11206	303.
.50807	.10161	5.00000	.14965	NOT MAX
.31094	.06219	5.00000	.12223	NOT MAX
.16648	.03330	5.00000	.10000	434.
.06667	.01333	5.00000	.08239	406.
.60815	.14000	4.34391	.16210	NOT MAX
.44830	.10320	4.34391	.14216	NOT MAX
.27932	.06430	4.34391	.11820	NOT MAX
.15305	.03523	4.34391	.09804	445.
.06568	.01512	4.34391	.08258	409.
.51629	.14000	3.68782	.14778	NOT MAX
.38935	.10558	3.68782	.13250	NOT MAX
.24728	.06705	3.68782	.11308	NOT MAX
.13782	.03737	3.68782	.09554	457.
.06451	.01749	3.68782	.08267	413.
.42444	.14000	3.03172	.12917	NOT MAX
.33191	.10948	3.03172	.12005	NOT MAX
.21120	.06966	3.03172	.10588	NOT MAX
.11869	.03915	3.03172	.09180	472.
.06367	.02100	3.03172	.08271	421.
.34586	.14000	2.47040	.10985	NOT MAX
.28497	.11535	2.47040	.10627	NOT MAX
.17239	.06978	2.47040	.09726	NOT MAX

Figure E-2 (continued)

.09351	.03785	2.47040	.08687	464.
.06113	.02474	2.47040	.08203	429.
.29330	.14000	2.09497	.09584	NOT MAX
.25629	.12234	2.09497	.09506	NOT MAX
.12815	.06117	2.09497	.08939	NOT MAX
.06407	.03058	2.09497	.08187	441.
.05767	.02753	2.09497	.08094	435.
.70000	.11290	6.20013	.16991	341.
.51031	.08231	6.20013	.14654	NOT MAX
.32059	.05170	6.20013	.12142	372.
.17221	.02777	6.20013	.09996	413.
.06877	.01109	6.20013	.08204	404.
.70000	.08580	8.15833	.16928	310.
.51075	.06260	8.15833	.14529	324.
.32675	.04005	8.15833	.12020	350.
.18314	.02245	8.15833	.09956	399.
.07503	.00920	8.15833	.08214	406.
.70000	.05946	11.77210	.16052	286.
.51722	.04394	11.77210	.13859	305.
.34196	.02905	11.77210	.11644	336.
.20019	.01701	11.77210	.09804	396.
.08696	.00738	11.77210	.08235	410.
.70000	.03477	19.03923	.14288	279.
.53249	.02797	19.03923	.12606	300.
.37020	.01944	19.03923	.10932	337.
.23143	.01216	19.03923	.09538	404.
.10976	.00576	19.03923	.08257	418.
.57266	.01332	42.98939	.10470	330.
.43433	.01010	42.98940	.09677	385.

Figure E-2 (continued)

.30249	.00704	42.96940	.08953	418.
.17770	.00413	42.96940	.08216	427.
.13566	.14000	.96901	.05911	521.
.70000	.00450	155.39421	.08386	418.

Figure E-2 (continued)

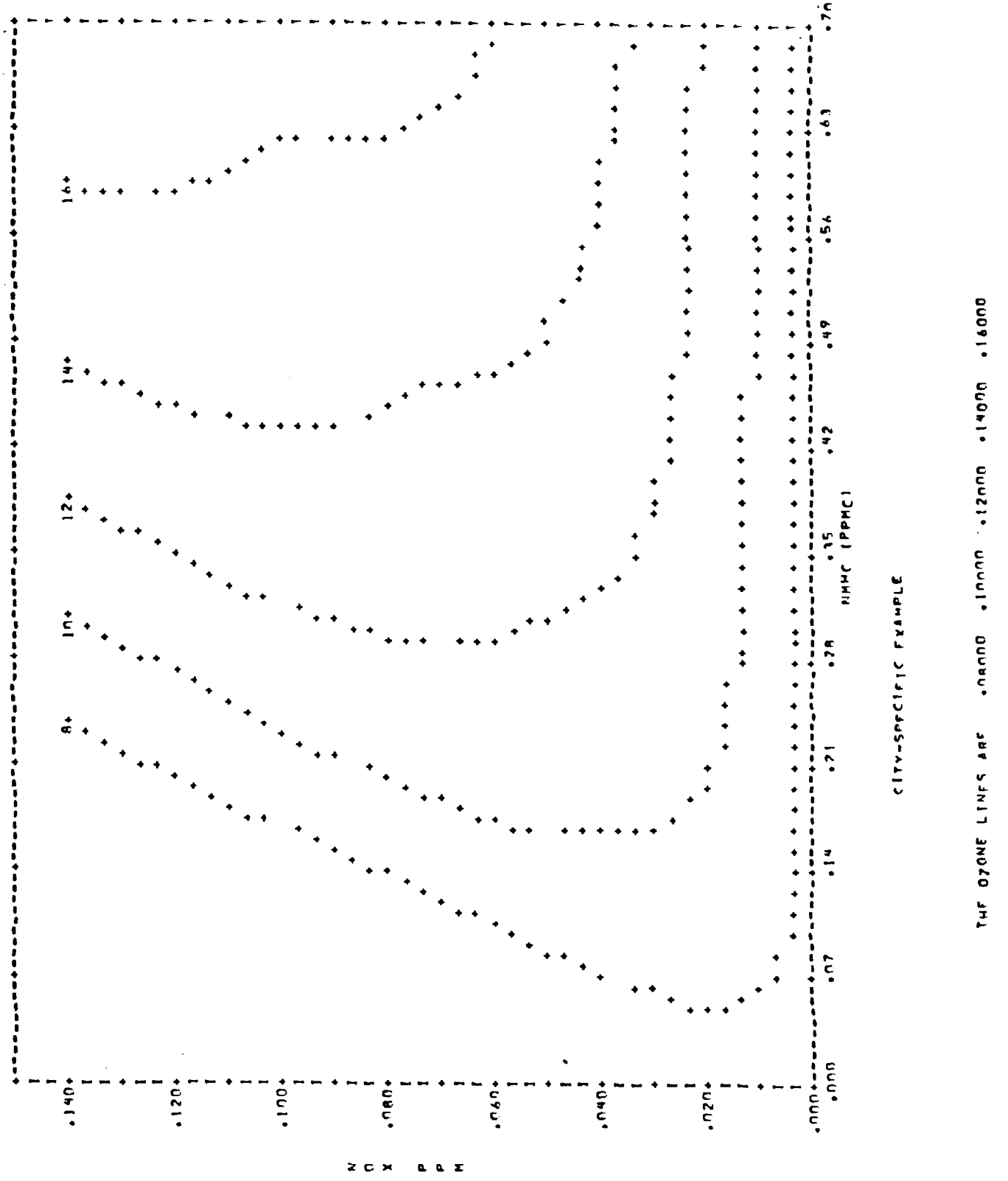


Figure E-2 (concluded)

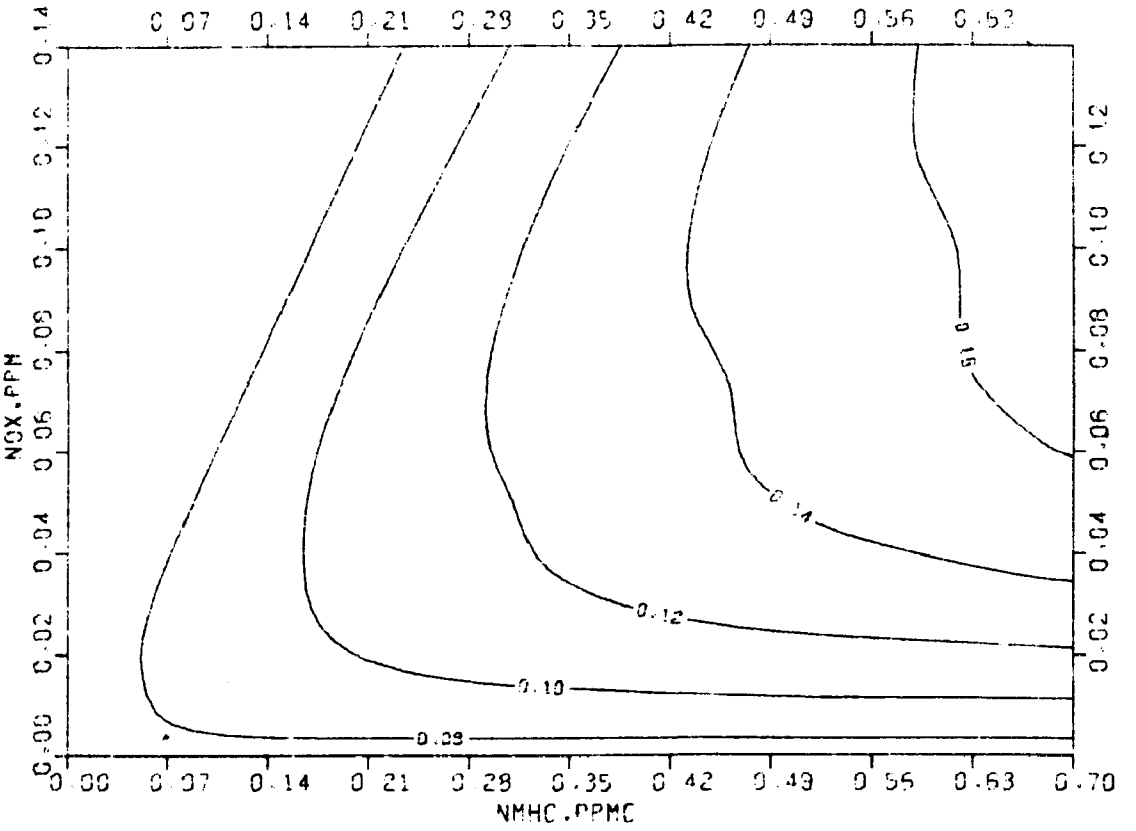


FIGURE E-3. CALCOMP Plot For City-Specific Diagram Example

TECHNICAL REPORT DATA
(Please read Instructions on the reverse before completing)

1. REPORT NO.	2.	3. RECIPIENT'S ACCESSION NO.
EPA-600/8-78-014a		

4. TITLE AND SUBTITLE
USER'S MANUAL FOR KINETICS MODEL AND OZONE ISOPLETH PLOTTING PACKAGE

5. REPORT DATE
July 1978

6. PERFORMING ORGANIZATION CODE

7. AUTHOR(S)
Gary Z. Whitten and H. Hogo

8. PERFORMING ORGANIZATION REPORT NO.

9. PERFORMING ORGANIZATION NAME AND ADDRESS
Systems Applications, Incorporated
950 Northgate Drive
San Rafael, California 94903

10. PROGRAM ELEMENT NO.
1AA603 (AC-18) FY 77

11. CONTRACT/GRANT NO.
68-02-2428

12. SPONSORING AGENCY NAME AND ADDRESS
Environmental Sciences Research Laboratory-RTP, NC
Office of Research and Development
U.S. Environmental Protection Agency
Research Triangle Park, North Carolina 27711

13. TYPE OF REPORT AND PERIOD COVERED
Interim

14. SPONSORING AGENCY CODE
EPA/600/09

15. SUPPLEMENTARY NOTES
Prepared in cooperation with the Monitoring and Data Analysis Division, Office of Air Quality Planning and Standards, U.S. Environmental Protection Agency

16. ABSTRACT

The Kinetics Model and Ozone Isopleth Plotting Package (OZIPP) is a computerized model that simulates ozone formation in urban atmospheres. OZIPP calculates maximum one-hour average ozone concentrations given a set of input assumptions about initial precursor concentrations, light intensity, dilution, diurnal and spatial emission patterns, transported pollutant concentrations, and reactivity of the precursor mix. The results of multiple simulations are used to produce an ozone isopleth diagram tailored to particular cities. Such a diagram relates maximum ozone concentrations to concentrations of non-methane hydrocarbons and oxides of nitrogen, and can be used in the Empirical Kinetic Modeling Approach (EKMA) to calculate emission reductions necessary to achieve air quality standards for photochemical oxidants. This user's manual describes the technical basis, necessary and optional input data, computer code and the use of OZIPP.

17. KEY WORDS AND DOCUMENT ANALYSIS

a. DESCRIPTORS	b. IDENTIFIERS/OPEN ENDED TERMS	c. COSATI Field/Group
* Air pollution * Ozone * Hydrocarbons * Nitrogen oxides Meteorology Atmospheric circulation * Mathematical models *Chemical kinetics * Nomographs *Programming Manuals		13B 20A 07B 05B 07C 04B 12A 07D 20K

18. DISTRIBUTION STATEMENT	19. SECURITY CLASS *(This Report)*	21. NO. OF PAGES
RELEASE TO PUBLIC	UNCLASSIFIED	251
	20. SECURITY CLASS *(This page)* UNCLASSIFIED	22. PRICE

EPA Form 2220-1 (9-73)