EPA-R4-73-013b

# CONTROLLED EVALUATION OF THE REACTIVE ENVIRONMENTAL SIMULATION MODEL (REM)

## Volume II
## User's Guide

**Pacific Environmental Services, INC.**
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# CONTROLLED EVALUATION OF THE REACTIVE ENVIRONMENTAL SIMULATION MODEL (REM)

## VOLUME II: USER'S GUIDE

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by

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WASHINGTON, D.C. 20460

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# Section I
# Introduction

This document describes the design, operation and use of the Reactive Pollution Environmental Simulation Model (REM). Its main purpose is to explain to the user how REM functions and from experience gained in operation, how it can best be utilized.

The latter includes imparting to the user the following:

- Detailed instructions for setting up input decks;
- How REM may be utilized in performing control strategies;
- An understanding of the methodology, techniques and calculational procedures employed in REM; and
- Sufficient information to enable program modifications to be accomplished.

The above tasks are facilitated by the incorporation of algorithm descriptions, flow charts, complete data input instructions, sample input decks, a glossary of program terms and program listings in this volume.

# Section II

## Description of the Reactive Environmental Simulation Model (REM)

### A. INTRODUCTION

The REM effort has been directed towards the construction of a sophisticated photochemical mechanism which is capable of closely replicating smog chamber data and then extending this capability to the urban atmosphere. REM is based on a Lagrangian (moving coordinate) system. This system enables the numerical computation of the chemical reactions to take place in a moving parcel or column of air. The parcel is bounded by the inversion base above and the ground below. The locations of the base of the column at successive points in time describe the path or trajectory that the air parcel traverses across the region. The trajectory is computed by special routines contained in the REM program from wind velocity information contained in the data base as a function of time of day and location. An overview of the model's operation is presented in Figure II-1.

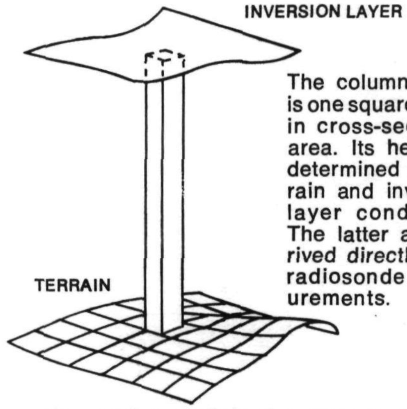
The computer program has been designed as a detailed episode model for chemical kinetics, with additional modules linked up to form a complete atmospheric system. The modules presently in the system determine the necessary meteorological parameters, the rate of absorption of actinic light by $NO_2$, and emissions due to traffic and area sources. A schematic diagram of REM appears in Figure II-2. The facility exists to incorporate modules to calculate the emissions due to large point sources and the effect of vertical diffusion should practical and effectual methods be found to perform these tasks.

# PHOTOCHEMICAL MODELING

For pollution modeling, the air space within each *geographic grid is assumed to emit an approximate* mean value of pollutants for a given time. The model includes nitrogen oxides, high and low reactive hydrocarbons and carbon monoxide. Values are provided by local environmental control agencies.

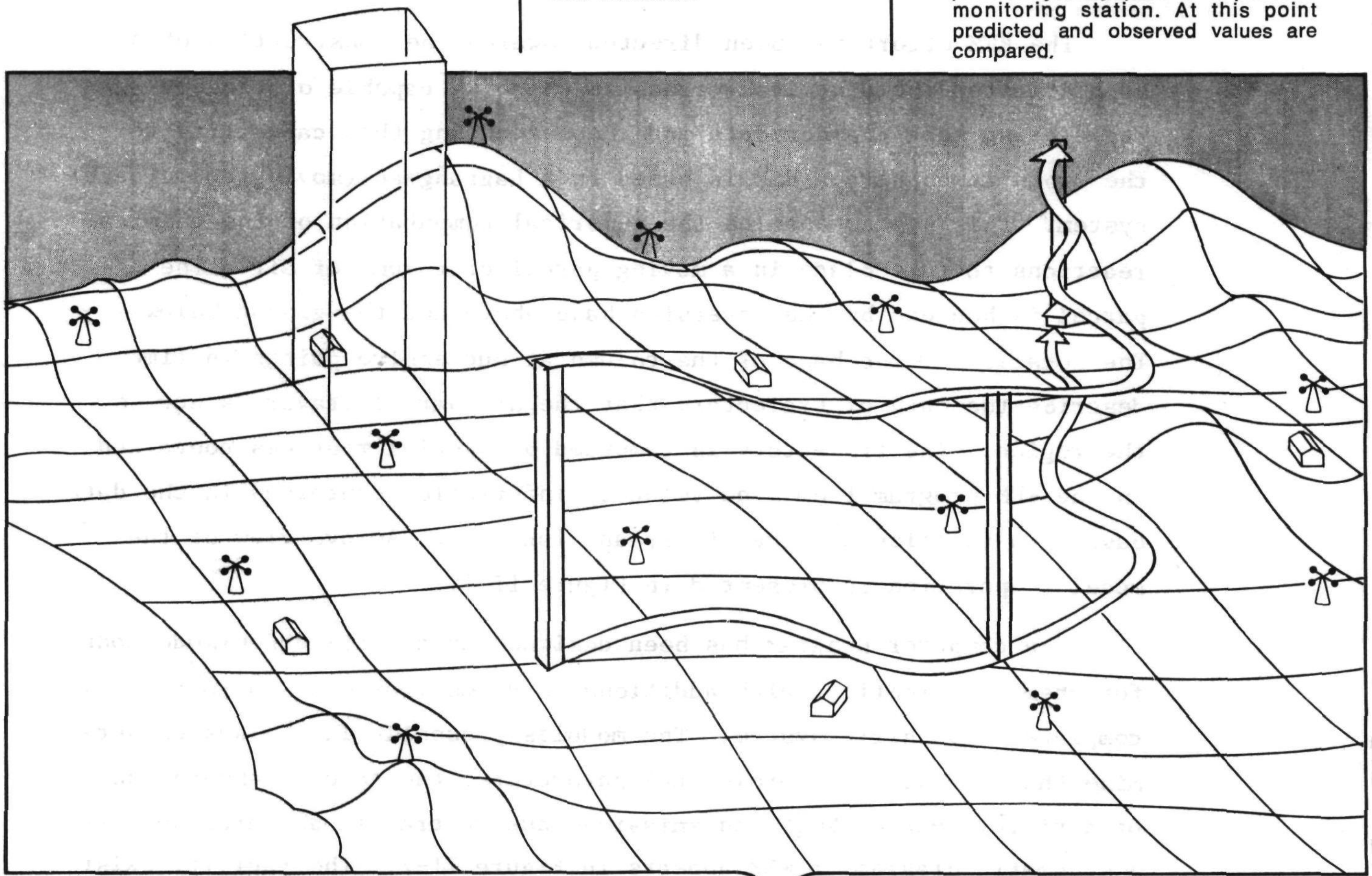
Meteorological stations provide current data on winds, temperature, pressure, dew point, etc., to the model for predictive movement of air parcels through the various grids.

Pollutant monitoring stations measure types and amounts of pollutants, i.e., oxidants, hydrocarbons, nitrogen oxides, carbon monoxide.

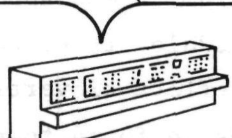



The column of air is one square meter in cross-sectional area. Its height is determined by terrain and inversion layer conditions. The latter are de*rived directly from* radiosonde measurements.

The model predicts the amount and type of photochemicals present in a column of air as it traverses a computed trajectory path to a pollutant monitoring station. At this point predicted and observed values are compared.



This model *simulates* a *region's photochemical pollutant content* by representing in a computer the chemical reactions occurring in a column of air as it traverses a dynamic wind trajectory. The model is tested by acquiring appropriate meteorological and *pollutant data from a dense network of monitoring* stations.




The path of a moving parcel of air is computed on the basis of wind station data. As the parcel passes over the urban area it picks up pollutants from vehicular traffic, power plants, factories and other sources. Pollutants, or emission rates, for each grid are contained in the data base. With the sun's energy acting as the catalyst, the pollutants are transformed into a variety of photochemical pollutants, producing the well known effects of smog. Predicted concentrations for these pollutants are printed out for points along the air parcel path and compared with values measured at actual air monitoring stations.

In a given area this photochemical model could predict the effects of new smog control devices for any given time period after introduction, determine a proposed freeway's effect on pollutant concentrations, or the contributory effects of new industries and proposed rapid transit systems. Decreases in pollutants that would result if modified or advanced propulsion systems are used in vehicles or if nuclear power plants are installed also could be predicted by the model.

Figure II-1. PES Reactive Environmental Model (REM)

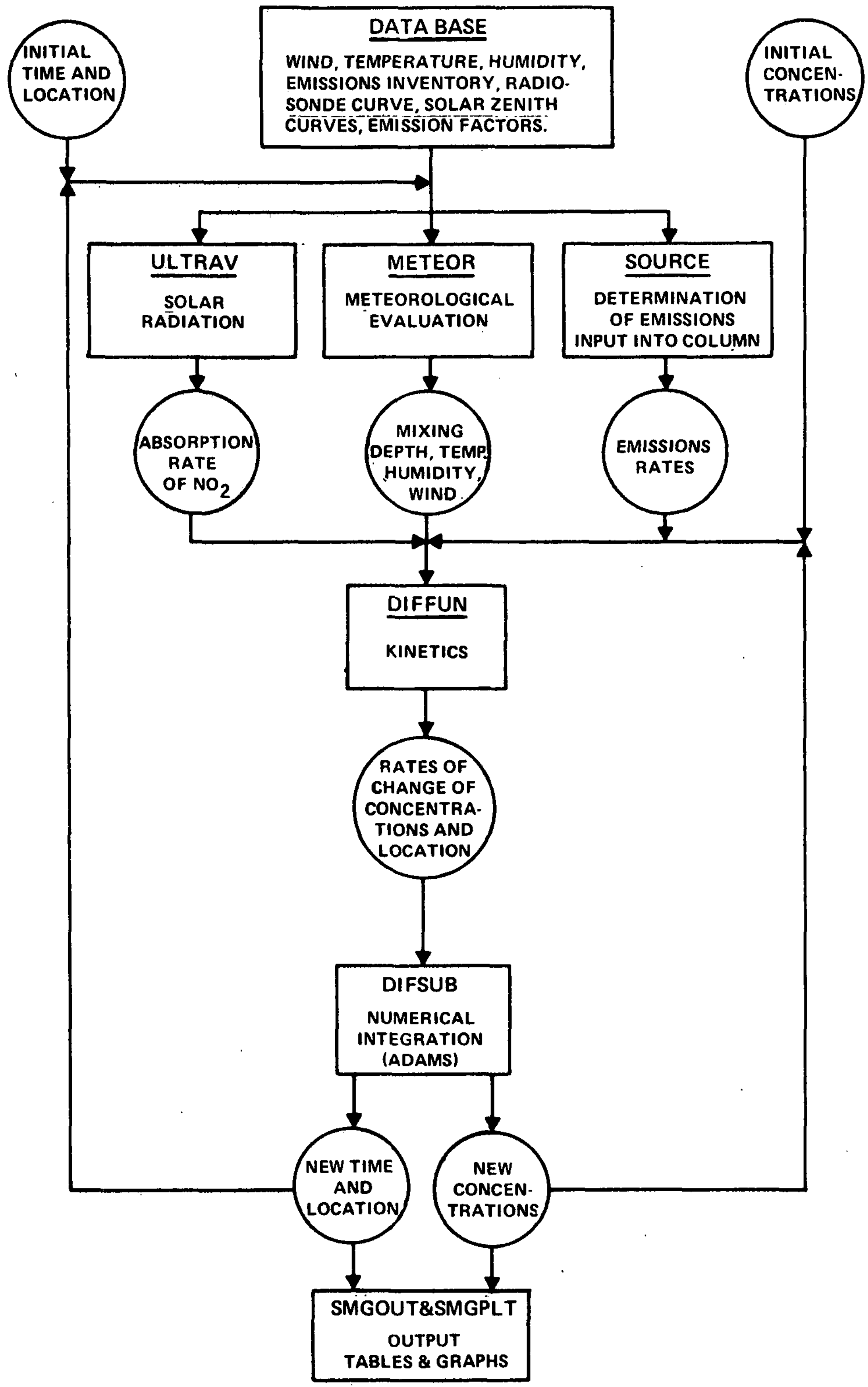



Figure II.2. Schematic of the PES Reactive Environmental Model (REM)

## B. GRID SYSTEM

The geometric setting for REM is a standard two-dimensionsl coordinate system. REM utilizes the mile as the standard unit of measure with all urban grid squares chosen as 4-square miles. The kilometer can also be used as the standard.

To set up the grid system, the origin is placed at a point such that the region of interest resides entirely in the positive quadrant. The coordinate positions of all air monitoring and meteorological stations are established in either miles or kilometers. These values are then fed into the model at execution time. In this manner, REM can be applied in any region.

Figure II-3 illustrates the grid system used by REM for the Los Angeles Basin. The locations of the air monitoring stations are designated as circles and the coordinate points are given in miles.

## C. PROGRAM CODE AND MACHINE USE

REM is coded in the FORTRAN IV computer language and has operated with both the Level G and H compilers. It is thus operational on any computer system with 150K in core and a standard FORTRAN compiler.

The Los Angeles validation version of the model has been successfully run on the IBM System 360, Models 50 and 65, and the IBM System 370, Models 155 and 165. The ratio of simulation time to computer time used was approximately 150:1 on the 370/155 and 550:1 on the 370/165. In regions where much less data is available than in Los Angeles, REM will operate at even greater speeds.

## D. OPERATION OF REM

REM has been designed to operate as a multi-receptor point model. The user is required to provide a minimum number of inputs after the data base has been prepared. In its execution mode, the model transports a parcel of air, bounded by the ground and the inversion layer,

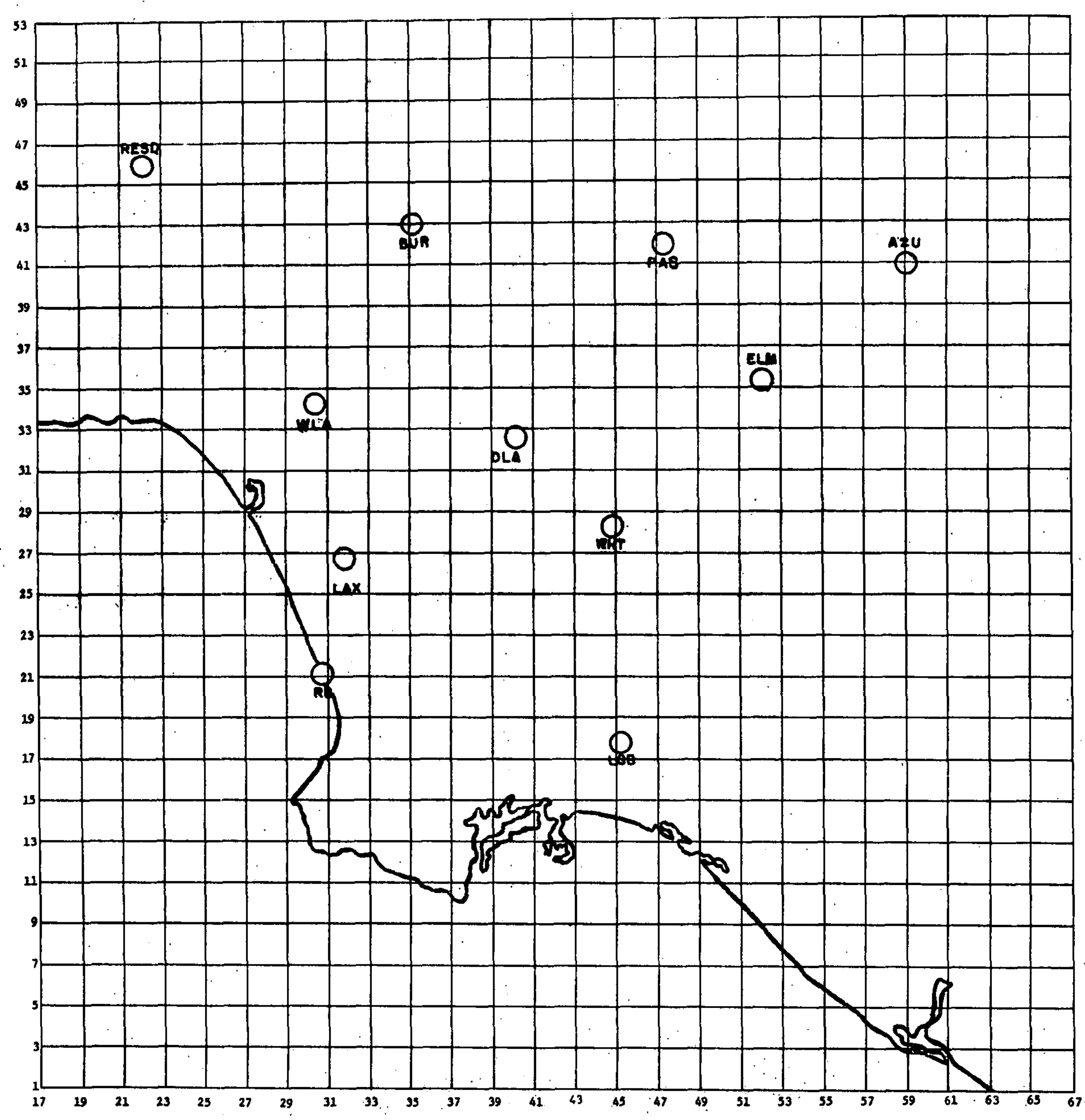



Figure II.3. REM Grid System for the Los Angeles Basin along a dynamic trajectory that is generated utilizing wind data from numerous meteorological stations. At each point along the path, the speed and direction of the trajectory are recalculated.

The user may select the starting point or the terminus for each simulation run. In either case, he must indicate the length and starting time (of day) of the simulation, and initial values for the major pollutants.

If the user selects the terminus, he must first operate the reverse trajectory program (see Section F.10) to determine the correct starting position and major pollutant values. The starting location is necessary because this point must be input into REM in order for the trajectory to reach the selected terminus at the end of the full simulation run. The initial pollutant concentrations are determined by interpolation of observed values at air monitoring stations to the trajectory starting point. Once the location and starting values have been calculated for a simulation run, the same trajectory may be run many times over without utilizing the reverse trajectory program again.

If the user executes the model by selecting a starting point, he may wish to choose a monitoring station where the initial pollutant values will be known. As an alternative, he may select another point of interest, or pick a completely random location. For these latter cases, some assumptions may be made regarding the starting values, or minimum or standard background values may be input.

## E. CONTROL STRATEGIES

After a given full simulation run has been made, it may be considered as a standard run for the purposes of evaluating particular control strategies. Control strategies are implemented to reduce pollutant concentrations and to attain required air quality standards.

By varying any of the numerous emissions inputs to the REM, either individually or in combination, the possible effects of control strategies can be determined before they are actually implemented. These strategies may include for example: reducing total traffic, reducing traffic in specified areas, reducing emission rates, varying traffic patterns, or altering operating times of area sources.

## F. REM MODULES

The modular construction of REM has facilitated the model's development and alteration, when necessary. Any given module may be unplugged and replaced as desired; or special modules may be created and added to handle special situations.

### 1. Initialization Program

The initialization program reads in the data base and the information needed for a complete simulation run. This program converts all of the data, except station locations, to the metric system for easy utilization by the other modules, and calls the numerical integration, output and plotting routines as required by monitoring the simulation time. At the end of the run, it checks to see if another simulation is to take place. To make additional runs, only control information must be input thereby facilitating the operation of REM for the user.

The initialization routine outputs the data base that has been read in to provide the user with a permanent record of the information employed in the simulation. A complete list of the data categories required for input follows:

- Trajectory start position and time of day;
- Length of simulation;
- Starting pollutant concentration values;

- Control parameters for numerical integration routine;
- Meteorological stations - location and elevation;
- Meteorological variables - hourly data (wind speed and direction, temperature, dew point);
- Emission factors for freeway and street traffic in grams per vehicle mile;
- Grid distribution of hourly area emissions;
- Radiosonde data - temperature vs. elevation profile; and
- Solar zenith angle as a function of time.

2. Numerical Integration

The numerical integration module is the heart of REM. This routine accepts as input derivatives calculated by the kinetics and meteorological modules and computes pollutant concentrations and the parcel position forward in simulated time. The kinetics module supplies the derivative of each of the photochemical pollutants computed as a function of time. The meteorological module provides wind velocity outputs as the time derivatives of the position vectors.

The economic use of REM is dependent upon the numerical integration routine. By attaining larger step sizes, the program will execute faster, use less computer time, and be less expensive to operate.

REM utilizes the Adams method of integrating ordinary differential equations of the Gear numerical integration package.[1] A sensitivity analysis has been conducted on the Adams routine in REM. As a result of this examination, it was found that the Adams method executes most economically with the maximum step size at 0.1 minutes and the error limit at .05 in pollutant concentration units.

3. Chemical Kinetics

The chemical kinetics module has operated on reaction mechanisms

[1] C. W. Gear, DIFSUB for Solution of Ordinary Differential Equations, Communications of the ACM, Volume 14, Number 3, March 1971.

containing 13-41 reactions and is based on a set of stoichiometrically valid elementary reactions. The current version contains a 32-reaction mechanism that preserves the flexibility of chemical detail necessary for adequate simulation of both primary and secondary contaminants. The set of elementary reactions, rate constants and chemical species is easily modified and expanded as required.

This routine calculates the elementary reaction rates and the derivatives of each of the accumulating chemical species as they change with time. It calls the meteorological, ultraviolet and emissions modules into operation, as necessary. The kinetics program adds the perturbations from the traffic and area sources to the derivatives computed for the chemistry for input into the numerical integration routine.

4. Meteorology

This module consists of a series of related routines that employ wind speed and velocity, temperature, relative humidity, elevation, and radiosonde data to calculate the meteorological values, mixing depth and rates of change in the wind at the pollutant column position.

a. Spatial Interpolation

Wind speed and direction, temperature, and relative humidity undergo both spatial and temporal interpolations from numerous meteorological stations to the trajectory location of the air parcel. The spatial interpolation is inversely proportional to the square of the distance from station to parcel. This procedure has two advantages over simply using a ratio inversely proportional to the distance involved. Firstly, it ensures that the meteorological values assigned to the trajectory position are more closely in keeping with the data at the nearest stations; and secondly, it permits the computer program to execute faster by eliminating the necessity of computing square roots.

b. Temporal Interpolation

The temporal interpolation is linear. The meteorological items for the current hour and the next hour are utilized in this process. The portion of each item contributing to the result is directly proportional to the number of minutes in the hour that have passed. For example, at 10:15 A.M. one-quarter of the value for hour 10 would be added to three-quarters of the value for hour 11.

c. Mixing Depth

The model calculates mixing depth on the basis of a temperature versus height profile derived from temperature soundings at various altitudes aloft recorded by radiosonde measurement or aircraft. The mixing height is taken as a function of temperature at the ground and the most recent vertical temperature soundings. The mixing depth is then obtained by subtracting ground elevation at the location of interest. The ground temperature is interpolated at the trajectory point from meteorological data at each station. In this technique the temperature versus height profile is assumed fixed during the day unless more frequent soundings are provided. The mixing depth changes with variations in ground temperature and elevation.

d. Trajectory Derivatives

The rates of change of the wind components at the air parcel position are utilized by the numerical integration routine to calculate the next trajectory position. Two differential equations are reserved for the trajectory calculation. They employ these derivatives in the same manner in which the integration of the differential equations for the chemistry occurs.

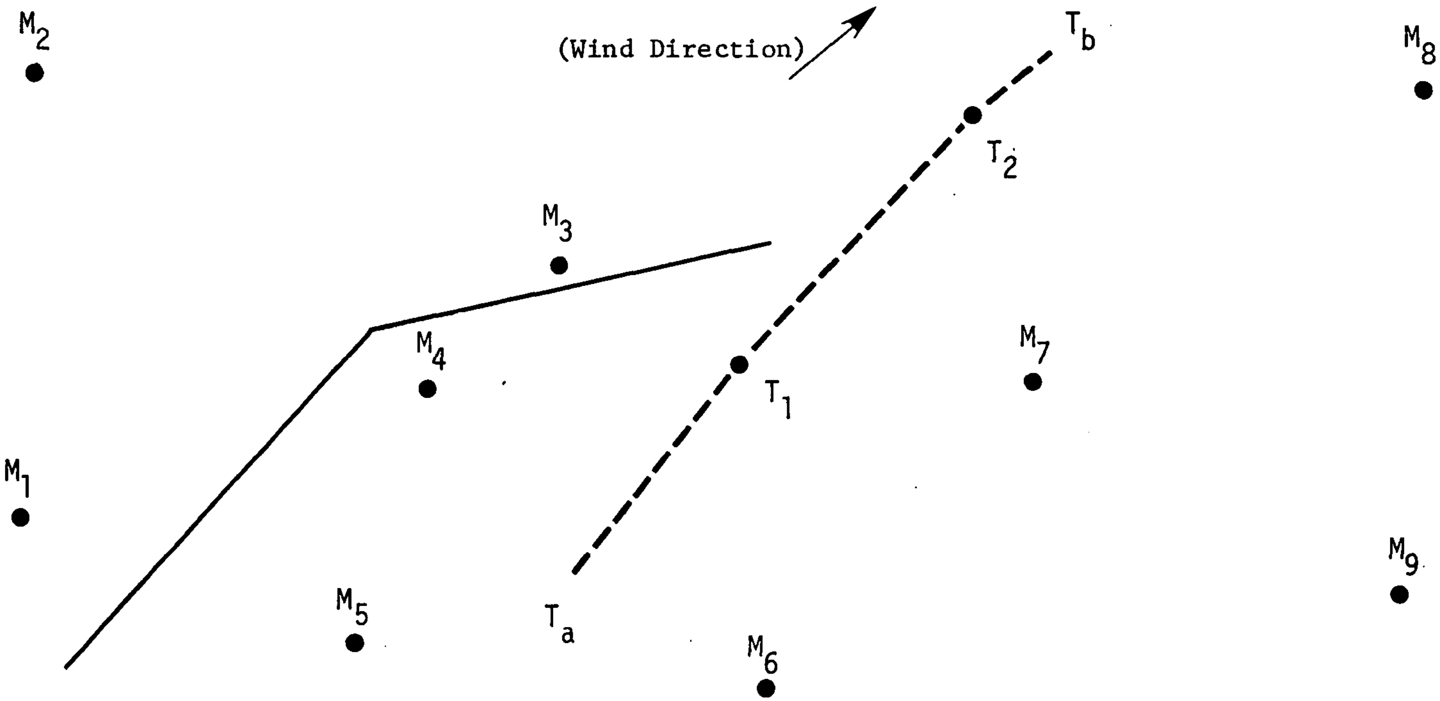
## 5. Barrier Check

A "barrier" is an imaginary line or set of connected line segments superimposed on the region of interest with the coordinate system for that area. Its purpose is to represent a topographical feature such as a mountain range which may serve to separate sections of an air quality region. The mountain range may tend to influence differing climatological characteristics and wind regimes. For example, on a given day in the Los Angeles Basin, the meteorological characteristics of the Westwood area are likely to differ from those in Van Nuys due, in part, to the intervention of the Santa Monica Mountains. Experience in the Los Angeles area has shown that significant temperature and wind regime differences between the San Fernando Valley and the central Basin tend to occur on any given day.

REM contains two such barriers. One bisects the Santa Monica Mountains and separates the San Fernando Valley from the main section of Los Angeles. The other barrier passes through the Puente and San Jose Hills at the east side of the Basin.

The main function of the barrier routine is to determine the "permissible" meteorological stations. Permissible stations are simply stations which are located in the same general section of the Basin as the trajectory point of interest, as defined by the barriers. That is, both the trajectory point and all stations to be used in the calculation of the trajectory path and the interpolated meteorological values at any trajectory point are located on the same side of each barrier. This is graphically shown in Figure II.4.

The barrier check is intended to ensure that a station which is very close in distance to a trajectory point of interest, but separated from the trajectory point by a mountain range does not exert any influence on the calculation of the trajectory path, temperature, and relative humidity at the trajectory point.




Wind direction

Line $T_a$ - $T_b$ is the trajectory path

$T_1$ - $T_a$ trajectory point of interest

$T_2$ - $T_a$ downwind trajectory point along the same trajectory

$M_i$ meteorological stations

$P_1$ Permissible meteorological stations for $T_1$ ($M_4$, $M_5$, $M_6$, $M_7$, $M_8$, $M_9$)

$P_2$ Permissible meteorological stations for $T_2$ ($M_2$, $M_3$, $M_5$, $M_6$, $M_7$, $M_8$, $M_9$)

Figure II.4 Demonstration of Barrier Check Technique

6. Ultraviolet Module

This module calculates a diurnal ultraviolet irradiance function based on measurement of sky cover, latitude and local calendar time. The irradiance determines the specific ultraviolet absorption rate of $NO_2$, which is used in the kinetics module.

7. Source Emissions

This routine computes emissions of NO, CO, reactive hydrocarbons and less reactive hydrocarbons for freeway and street traffic, and calculates emissions from area sources of NO, reactive hydrocarbons, and less reactive hydrocarbons.

The inputs to this program for vehicular sources include two diurnal traffic curves (see Figures II.5 and II.6),[2] emission factors for reactive hydrocarbons, less reactive hydrocarbons, CO and NO in grams per vehicle mile, and distributions of daily vehicle traffic on streets and freeways given in a system of 650 4-square mile grids that cover the Los Angeles Basin (see Figures II.7 and II.8).[2] The emissions of the above pollutants are computed as a function of time by applying their respective emission factors to the traffic levels at the air parcel location qualified by the daily traffic usage curve.

Emissions from area sources are also calculated as a function of time. A constant diurnal usage curve is applied to grid system distributions of hourly pollutant emissions of NO,[3] reactive hydrocarbons, and less reactive hydrocarbons (see Figures II.9, II.10 and II.11).[2]

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[2] Appendix A, Development of a Simulation Model for Estimating Ground Level Concentrations of Photochemical Pollutants by P. J. W. Roberts, P. M. Roth and C. L. Nelson; Report 71SAI-6, March 1971, prepared by Systems Applications, Inc.

[3] Oxides of nitrogen taken as NO

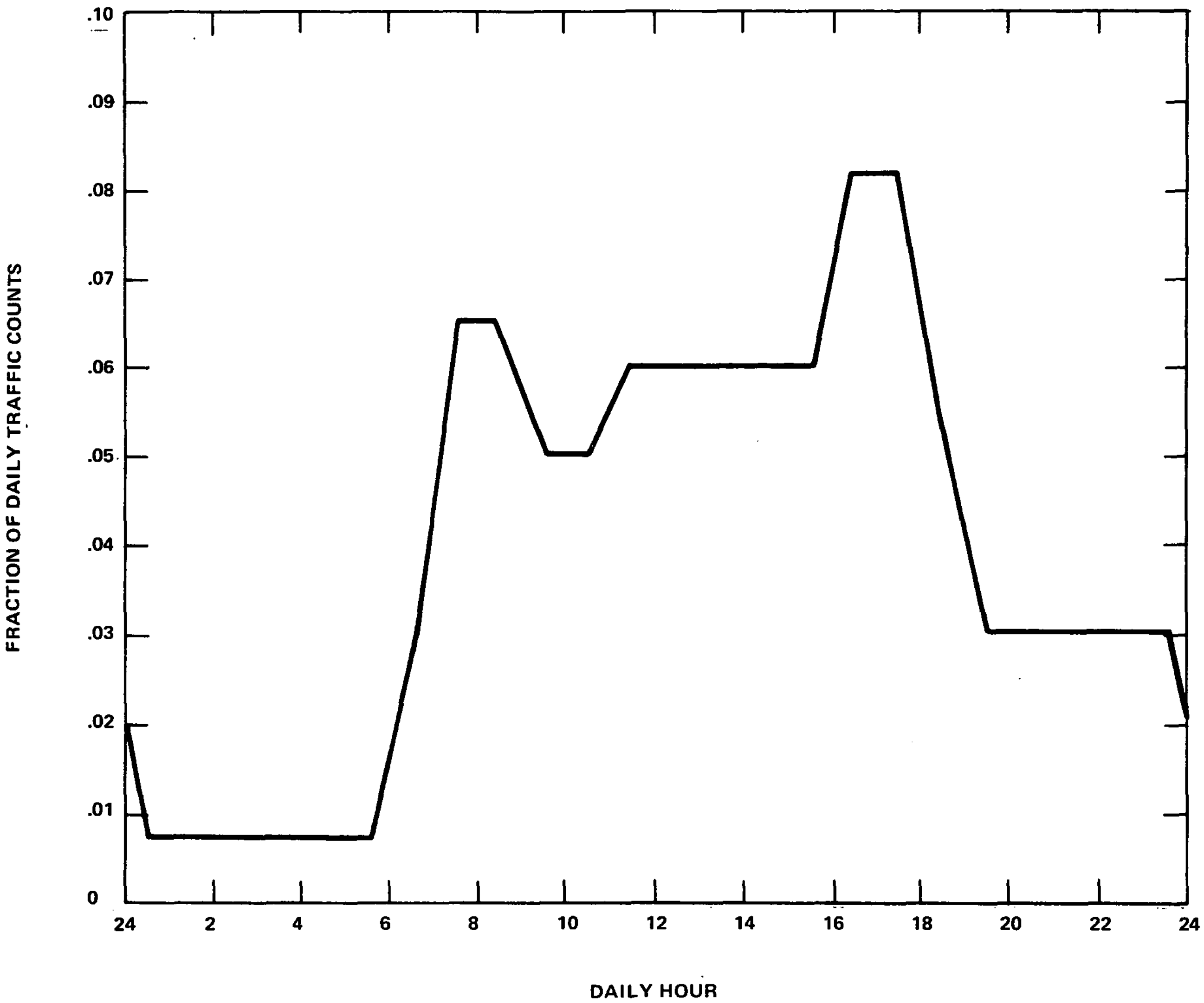



Figure II.5. Temporal Distribution of Daily Street Traffic (Interpreted from Data in Reference 2, pg. II.13)

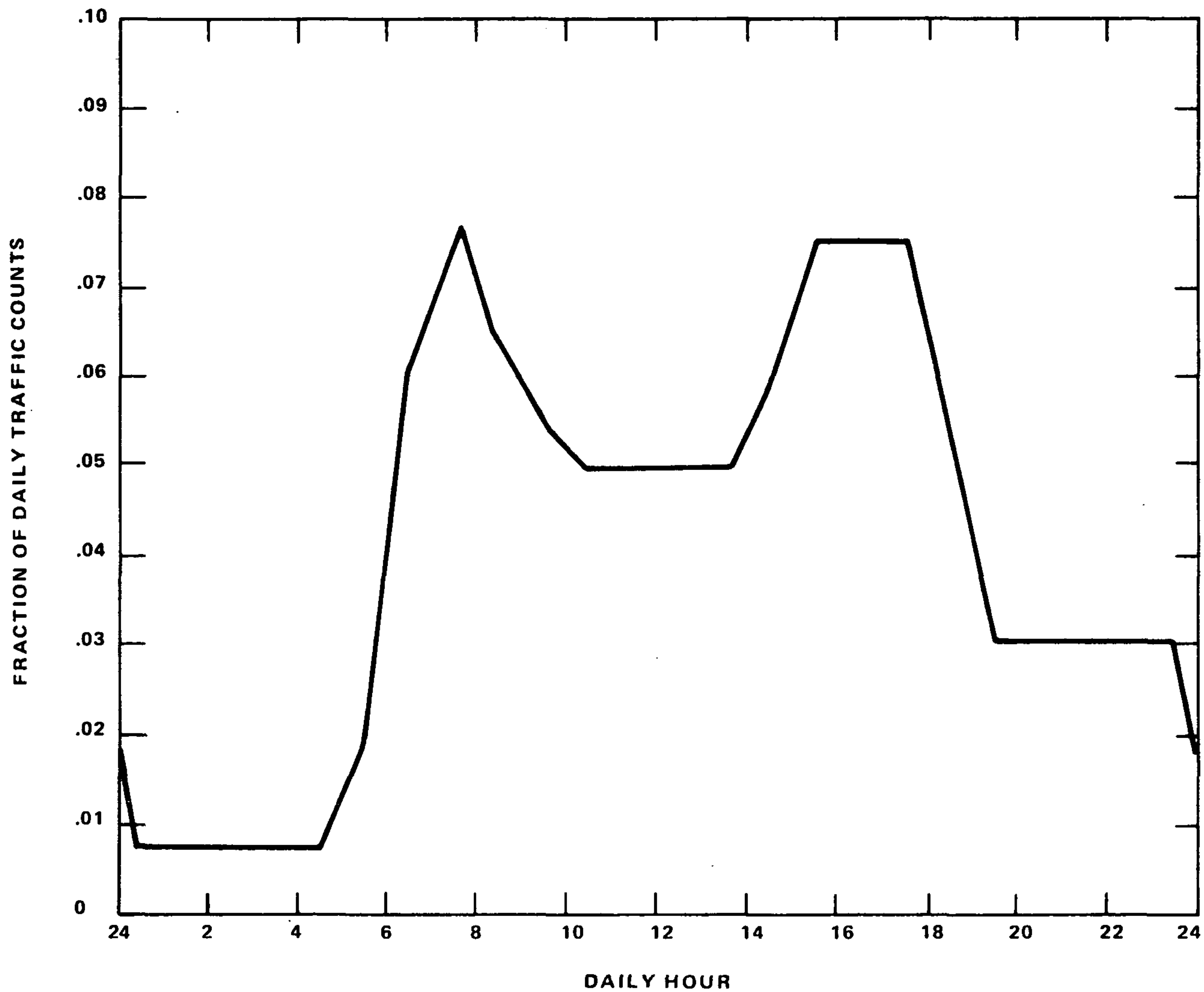



Figure II.6. Temporal Distribution of Daily Freeway Traffic (Interpreted from Data in Reference 2, pg. II.13)

| | | | | | | | | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | 60 | 125 | 50 | | | | | | | | | | | | | | | | | | |
| 35 | 12 | 34 | 149 | 146 | 172 | 135 | 43 | 28 | 17 | 1 | 0 | 0 | 4 | 2 | 1 | 2 | 2 | 1 | 0 | 0 | 0 | 2 | 0 | 0 |
| 60 | 155 | 202 | 223 | 252 | 221 | 152 | 85 | 66 | 84 | 73 | 7 | 2 | 0 | 0 | 2 | 0 | 0 | 0 | 0 | 0 | 0 | 2 | 0 | 0 |
| 137 | 255 | 238 | 238 | 266 | 295 | 251 | 233 | 54 | 20 | 27 | 157 | 50 | 4 | 0 | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 2 | 0 | 0 |
| 239 | 250 | 249 | 250 | 264 | 414 | 328 | 276 | 212 | 215 | 4 | 131 | 58 | 91 | 113 | 21 | 1 | 2 | 0 | 0 | 0 | 1 | 2 | 0 | 0 |
| 139 | 118 | 107 | 194 | 182 | 350 | 268 | 280 | 247 | 180 | 204 | 204 | 21 | 173 | 241 | 212 | 156 | 91 | 57 | 1 | 6 | 6 | 2 | 0 | 0 |
| 25 | 30 | 17 | 12 | 59 | 63 | 121 | 155 | 116 | 25 | 245 | 242 | 191 | 162 | 318 | 308 | 241 | 218 | 183 | 77 | 126 | 149 | 151 | 76 | 32 |
| 9 | 25 | 0 | 2 | 30 | 70 | 32 | 260 | 478 | 375 | 259 | 164 | 116 | 190 | 236 | 227 | 236 | 185 | 160 | 130 | 155 | 232 | 143 | 66 | 77 |
| 0 | 18 | 0 | 7 | 98 | 283 | 403 | 549 | 512 | 572 | 473 | 226 | 217 | 229 | 285 | 243 | 250 | 242 | 114 | 190 | 280 | 244 | 71 | 10 | 99 |
| 47 | 64 | 99 | 117 | 231 | 512 | 346 | 459 | 478 | 468 | 642 | 579 | 290 | 199 | 186 | 75 | 108 | 173 | 131 | 180 | 142 | 18 | 48 | 50 | 73 |
| | | | 125 | 476 | 254 | 338 | 261 | 412 | 413 | 512 | 328 | 324 | 293 | 264 | 195 | 127 | 43 | 39 | 227 | 121 | 45 | 53 | 27 | 5 |
| | | | | 88 | 305 | 255 | 255 | 311 | 478 | 477 | 364 | 292 | 273 | 299 | 198 | 185 | 69 | 21 | 82 | 42 | 90 | 33 | 12 | 0 |
| | | | | | 106 | 266 | 413 | 392 | 331 | 393 | 273 | 322 | 305 | 265 | 253 | 190 | 295 | 119 | 42 | 22 | 1 | 37 | 1 | 5 |
| | | | | | 22 | 261 | 296 | 397 | 285 | 314 | 254 | 292 | 255 | 386 | 263 | 229 | 234 | 181 | 240 | 156 | 103 | 21 | 9 | 7 |
| | | | | | | 189 | 255 | 328 | 358 | 176 | 265 | 293 | 257 | 298 | 241 | 230 | 135 | 114 | 62 | 129 | 114 | 95 | 57 | 4 |
| | | | | | | 124 | 215 | 412 | 322 | 210 | 121 | 270 | 312 | 301 | 93 | 96 | 104 | 270 | 179 | 290 | 197 | 82 | 48 | 30 |
| | | | | | | 9 | 360 | 324 | 231 | 124 | 79 | 204 | 288 | 430 | 204 | 138 | 186 | 305 | 242 | 323 | 241 | 113 | 31 | 6 |
| | | | | | | 1 | 239 | 304 | 249 | 175 | 94 | 283 | 192 | 282 | 165 | 155 | 173 | 259 | 228 | 304 | 169 | 123 | 109 | 11 |
| | | | | | | 46 | 121 | 188 | 266 | 254 | 157 | 413 | 386 | 317 | 162 | 75 | 116 | 209 | 220 | 255 | 149 | 168 | 163 | 28 |
| | | | | | | 30 | 49 | 28 | 142 | 145 | 75 | 157 | 126 | 153 | 175 | 60 | 125 | 212 | 200 | 219 | 249 | 266 | 182 | 32 |
| | | | | | | 4 | 5 | 25 | 176 | 88 | | | | | 32 | 48 | 114 | 195 | 116 | 166 | 203 | 190 | 98 | 19 |
| | | | | | | | | | 5 | 5 | | | | | | 36 | 24 | 133 | 135 | 116 | 74 | 80 | 11 | 26 |
| | | | | | | | | | | | | | | | | | 36 | 126 | 107 | 248 | 215 | 100 | 29 | 15 |
| | | | | | | | | | | | | | | | | | | 34 | 104 | 277 | 94 | 114 | 10 | 0 |
| | | | | | | | | | | | | | | | | | | | 7 | 218 | 196 | 52 | 0 | 0 |
| | | | | | | | | | | | | | | | | | | | | | 5 | 119 | 18 | 0 |

Figure II.7. Distribution of Street Traffic by Grid Area
(thousands of vehicle miles per day)
[From Reference 2, pg. II.13]

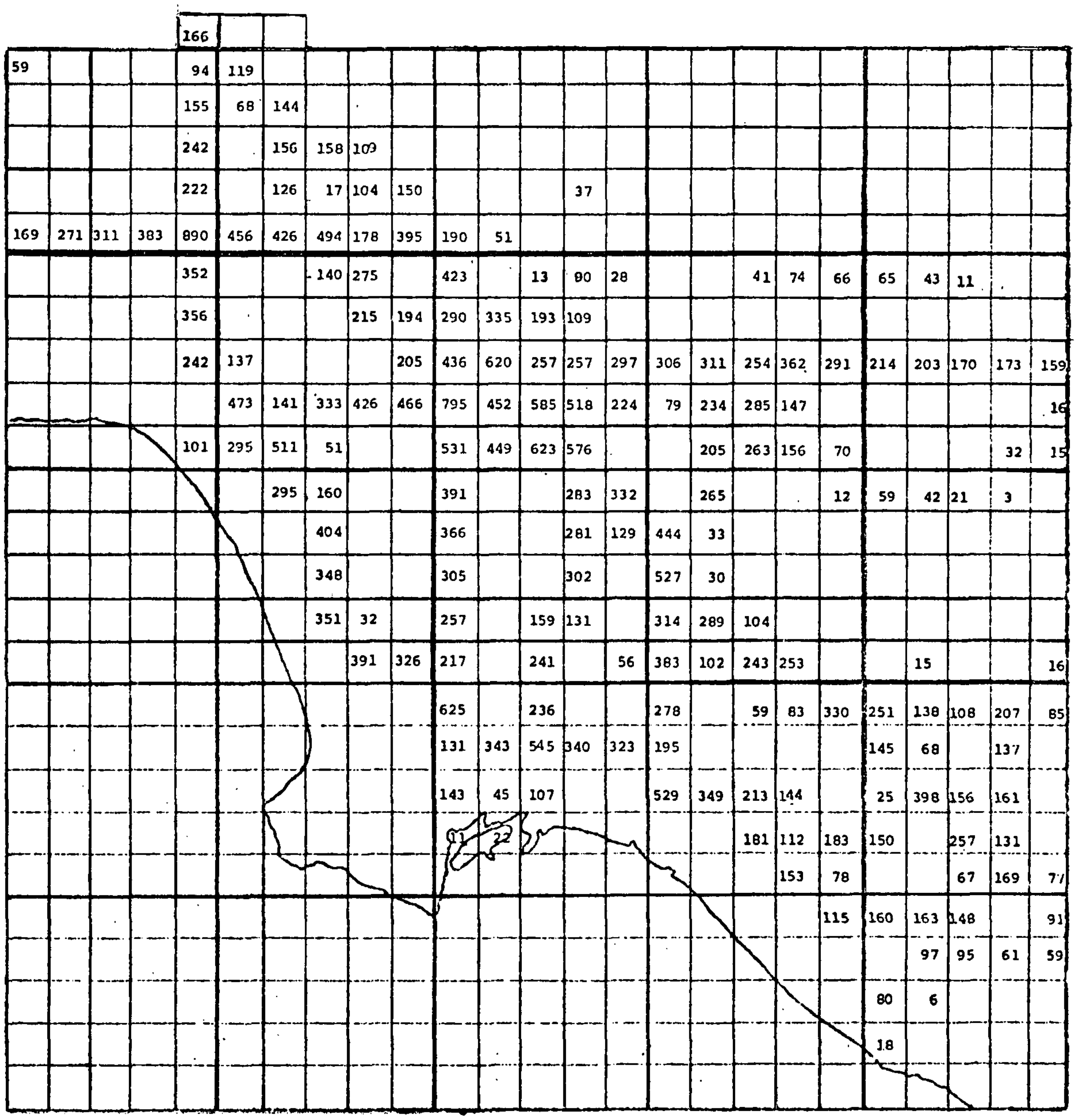



Figure II.8. Distribution of Freeway Traffic by Grid Area
(thousands of vehicle miles per day)
[From Reference 2, pg. II.13]

| | | | | | | | | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 0 | 0 | 0 | 0 | 9 | 9 | 9 | 9 | 1 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 1 | 1 | 1 | 10 | 10 | 12 | 12 | 11 | 9 | 7 | 2 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 8 | 9 | 9 | 18 | 17 | 15 | 15 | 15 | 12 | 1 | 1 | 8 | 4 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 8 | 9 | 13 | 18 | 15 | 15 | 17 | 15 | 12 | 7 | 4 | 8 | 8 | 8 | 8 | 3 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 8 | 8 | 12 | 14 | 12 | 8 | 8 | 8 | 9 | 10 | 10 | 9 | 1 | 9 | 10 | 10 | 16 | 19 | 16 | 14 | 13 | 9 | 9 | 9 | 8 |
| 0 | 0 | 0 | 0 | 4 | 4 | 4 | 8 | 9 | 10 | 10 | 9 | 9 | 18 | 16 | 8 | 16 | 18 | 18 | 14 | 13 | 9 | 9 | 7 | 0 |
| 0 | 0 | 0 | 1 | 3 | 7 | 9 | 18 | 19 | 19 | 19 | 19 | 19 | 18 | 18 | 18 | 19 | 19 | 20 | 20 | 20 | 17 | 17 | 9 | 9 |
| 0 | 0 | 0 | 1 | 6 | 10 | 10 | 10 | 11 | 12 | 12 | 12 | 12 | 11 | 10 | 10 | 13 | 13 | 12 | 11 | 11 | 9 | 9 | 1 | 10 |
| 8 | 8 | 8 | 9 | 19 | 19 | 19 | 20 | 20 | 21 | 21 | 21 | 21 | 20 | 19 | 19 | 22 | 22 | 21 | 20 | 20 | 1 | 1 | 1 | 10 |
| | | | 4 | 9 | 18 | 20 | 20 | 20 | 19 | 19 | 37 | 37 | 29 | 21 | 21 | 9 | 1 | 6 | 15 | 19 | 18 | 18 | 9 | 8 |
| | | | | 10 | 19 | 21 | 21 | 20 | 19 | 20 | 38 | 38 | 29 | 21 | 21 | 19 | 5 | 3 | 9 | 2 | 1 | 1 | 0 | 0 |
| | | | | | 13 | 25 | 25 | 22 | 20 | 20 | 31 | 31 | 26 | 22 | 22 | 22 | 18 | 7 | 0 | 0 | 0 | 0 | 0 | 0 |
| | | | | | 6 | 29 | 29 | 25 | 22 | 22 | 24 | 24 | 24 | 23 | 23 | 27 | 27 | 23 | 11 | 11 | 5 | 0 | 0 | 0 |
| | | | | | | 28 | 29 | 25 | 22 | 22 | 24 | 24 | 24 | 23 | 23 | 27 | 27 | 23 | 11 | 11 | 11 | 8 | 0 | 0 |
| | | | | | | 6 | 21 | 27 | 34 | 34 | 25 | 25 | 24 | 23 | 23 | 19 | 19 | 11 | 11 | 11 | 11 | 11 | 2 | 0 |
| | | | | | | 5 | 21 | 27 | 34 | 34 | 25 | 25 | 24 | 23 | 23 | 19 | 11 | 11 | 11 | 11 | 11 | 11 | 5 | 0 |
| | | | | | | 0 | 19 | 24 | 29 | 29 | 30 | 30 | 26 | 22 | 22 | 18 | 11 | 11 | 11 | 11 | 11 | 11 | 8 | 0 |
| | | | | | | 10 | 18 | 21 | 23 | 23 | 35 | 35 | 28 | 21 | 21 | 11 | 11 | 11 | 11 | 11 | 11 | 11 | 11 | 0 |
| | | | | | | 14 | 18 | 21 | 23 | 25 | 37 | 37 | 30 | 22 | 13 | 11 | 11 | 11 | 11 | 11 | 11 | 11 | 11 | 0 |
| | | | | | | 4 | 6 | 15 | 20 | 2 | | | | | 5 | 11 | 11 | 11 | 11 | 11 | 11 | 11 | 0 | 0 |
| | | | | | | | | | | | | | | | | 5 | 11 | 11 | 11 | 11 | 0 | 0 | 0 | 0 |
| | | | | | | | | | | | | | | | | | 5 | 11 | 11 | 11 | 11 | 0 | 0 | 0 |
| | | | | | | | | | | | | | | | | | | 5 | 11 | 11 | 11 | 0 | 0 | 0 |
| | | | | | | | | | | | | | | | | | | | 3 | 11 | 11 | 0 | 0 | 0 |
| | | | | | | | | | | | | | | | | | | | | 1 | 3 | 0 | 0 | 0 |

Figure II.9. Distribution of Reactive Hydrocarbon Emissions (average kilograms/hour) by Grid Area [From Reference 2, pg. II.13]

| | | | | | | | | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 0 | 0 | 0 | 1 | 32 | 32 | 31 | 31 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 3 | 36 | 36 | 42 | 42 | 40 | 37 | 27 | 10 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 30 | 31 | 31 | 35 | 39 | 39 | 53 | 53 | 48 | 13 | 13 | 31 | 16 | 5 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 30 | 31 | 31 | 35 | 39 | 39 | 53 | 53 | 48 | 33 | 23 | 31 | 31 | 30 | 25 | 15 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 30 | 31 | 31 | 30 | 30 | 30 | 34 | 34 | 38 | 42 | 42 | 36 | 6 | 35 | 35 | 35 | 37 | 37 | 39 | 41 | 41 | 30 | 15 | 0 | 0 |
| 0 | 1 | 1 | 0 | 15 | 15 | 19 | 34 | 38 | 42 | 42 | 36 | 36 | 35 | 35 | 35 | 37 | 37 | 39 | 41 | 41 | 30 | 30 | 20 | 10 |
| 0 | 0 | 0 | 0 | 5 | 15 | 23 | 33 | 36 | 39 | 39 | 48 | 48 | 44 | 40 | 40 | 49 | 49 | 43 | 38 | 38 | 31 | 31 | 32 | 30 |
| 0 | 0 | 0 | 5 | 24 | 39 | 33 | 33 | 35 | 37 | 37 | 60 | 60 | 53 | 45 | 45 | 62 | 62 | 49 | 36 | 36 | 31 | 31 | 4 | 30 |
| 30 | 30 | 30 | 35 | 39 | 39 | 33 | 33 | 35 | 37 | 37 | 60 | 60 | 53 | 45 | 45 | 62 | 62 | 49 | 36 | 36 | 1 | 1 | 4 | 30 |
| | | | 20 | 40 | 40 | 45 | 45 | 47 | 49 | 49 | 110 | 110 | 82 | 56 | 56 | 34 | 4 | 22 | 39 | 39 | 32 | 32 | 1 | 0 |
| | | | | 25 | 40 | 45 | 45 | 47 | 49 | 49 | 110 | 110 | 82 | 56 | 56 | 34 | 19 | 12 | 34 | 9 | 2 | 2 | 1 | 0 |
| | | | | | 30 | 51 | 51 | 51 | 51 | 51 | 90 | 90 | 69 | 50 | 50 | 35 | 35 | 20 | 4 | 4 | 0 | 0 | 0 | 0 |
| | | | | | 10 | 56 | 56 | 56 | 56 | 56 | 70 | 70 | 57 | 45 | 45 | 36 | 36 | 33 | 11 | 11 | 5 | 0 | 0 | 0 |
| | | | | | | 51 | 56 | 56 | 56 | 56 | 70 | 70 | 57 | 45 | 45 | 36 | 36 | 33 | 11 | 11 | 11 | 6 | 0 | 0 |
| | | | | | | 6 | 31 | 46 | 61 | 61 | 36 | 36 | 36 | 36 | 36 | 34 | 34 | 13 | 11 | 11 | 11 | 11 | 2 | 0 |
| | | | | | | 6 | 31 | 46 | 61 | 61 | 36 | 36 | 36 | 36 | 36 | 34 | 15 | 13 | 11 | 11 | 11 | 11 | 5 | 0 |
| | | | | | | 1 | 31 | 39 | 47 | 47 | 34 | 34 | 34 | 34 | 34 | 32 | 13 | 11 | 11 | 11 | 11 | 11 | 10 | 0 |
| | | | | | | 15 | 30 | 32 | 33 | 33 | 33 | 33 | 33 | 33 | 33 | 11 | 11 | 11 | 11 | 11 | 11 | 11 | 11 | 0 |
| | | | | | | 25 | 30 | 32 | 33 | 18 | 18 | 18 | 18 | 3 | 14 | 11 | 11 | 11 | 11 | 11 | 11 | 11 | 11 | 0 |
| | | | | | | 10 | 15 | 21 | 31 | 11 | | | | | 5 | 11 | 11 | 11 | 11 | 11 | 11 | 11 | 0 | 0 |
| | | | | | | | | | 5 | | | | | | | 5 | 11 | 11 | 11 | 11 | 0 | 0 | 0 | 0 |
| | | | | | | | | | | | | | | | | | 5 | 11 | 11 | 11 | 11 | 0 | 0 | 0 |
| | | | | | | | | | | | | | | | | | | 5 | 11 | 11 | 11 | 0 | 0 | 0 |
| | | | | | | | | | | | | | | | | | | | | 10 | 11 | 0 | 0 | 0 |
| | | | | | | | | | | | | | | | | | | | | | 5 | 0 | 0 | 0 |

Figure II.10. Distribution of Oxides of Nitrogen Emissions Taken as Nitric Oxide (average kilograms/hour) by Grid Area [From Reference 2, pg. II.13]

| | | | | | | | | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 0 | 0 | 0 | 6 | 91 | 91 | 85 | 85 | 3 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 3 | 3 | 8 | 108 | 108 | 133 | 133 | 101 | 107 | 83 | 22 | 2 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 80 | 84 | 84 | 105 | 125 | 125 | 180 | 180 | 158 | 56 | 56 | 81 | 52 | 11 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 80 | 84 | 84 | 105 | 125 | 125 | 180 | 180 | 158 | 116 | 76 | 81 | 81 | 80 | 70 | 30 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 79 | 81 | 81 | 81 | 80 | 80 | 96 | 96 | 113 | 129 | 129 | 103 | 24 | 102 | 101 | 101 | 108 | 108 | 118 | 129 | 129 | 80 | 41 | 2 | 1 |
| 0 | 2 | 2 | 2 | 41 | 41 | 57 | 96 | 113 | 129 | 129 | 103 | 103 | 102 | 101 | 101 | 108 | 108 | 118 | 128 | 128 | 80 | 80 | 62 | 21 |
| 0 | 1 | 1 | 11 | 21 | 41 | 74 | 93 | 105 | 118 | 118 | 153 | 153 | 136 | 122 | 122 | 159 | 159 | 137 | 117 | 117 | 82 | 82 | 90 | 97 |
| 0 | 0 | 0 | 20 | 79 | 118 | 90 | 90 | 98 | 106 | 106 | 204 | 204 | 174 | 143 | 143 | 212 | 212 | 158 | 104 | 104 | 85 | 85 | 21 | 115 |
| 79 | 79 | 79 | 99 | 118 | 118 | 90 | 90 | 98 | 106 | 106 | 204 | 204 | 174 | 143 | 143 | 212 | 212 | 158 | 104 | 104 | 6 | 6 | 21 | 115 |
| | | | 41 | 120 | 121 | 145 | 145 | 150 | 156 | 156 | 426 | 426 | 307 | 189 | 189 | 98 | 19 | 69 | 117 | 117 | 86 | 86 | 4 | 0 |
| | | | | 11 | 120 | 145 | 145 | 150 | 156 | 156 | 426 | 426 | 307 | 189 | 189 | 98 | 59 | 99 | 108 | 38 | 7 | 7 | 4 | 0 |
| | | | | 10 | 90 | 189 | 189 | 179 | 175 | 175 | 333 | 333 | 267 | 170 | 170 | 118 | 118 | 68 | 19 | 19 | 1 | 1 | 1 | 0 |
| | | | | | 30 | 233 | 233 | 214 | 193 | 193 | 245 | 245 | 197 | 150 | 150 | 137 | 137 | 109 | -44 | 44 | 23 | 1 | 0 | 0 |
| | | | | | | 214 | 233 | 214 | 193 | 193 | 245 | 245 | 197 | 150 | 150 | 137 | 137 | 109 | 44 | 44 | 45 | 31 | 0 | 0 |
| | | | | | | 54 | 96 | 173 | 251 | 251 | 131 | 131 | 120 | 108 | 108 | 94 | 94 | 51 | 44 | 44 | 44 | 44 | 5 | 0 |
| | | | | | | 24 | 96 | 173 | 251 | 251 | 131 | 131 | 120 | 108 | 108 | 94 | 59 | 51 | 44 | 44 | 44 | 44 | 20 | 0 |
| | | | | | | 3 | 78 | 130 | 182 | 182 | 144 | 144 | 122 | 101 | 101 | 86 | 51 | 44 | 44 | 44 | 44 | 44 | 40 | 0 |
| | | | | | | 40 | 79 | 96 | 111 | 111 | 156 | 156 | 125 | 94 | 94 | 44 | 44 | 44 | 44 | 44 | 44 | 44 | 44 | 0 |
| | | | | | | 60 | 79 | 96 | 111 | 63 | 91 | 91 | 91 | 131 | 55 | 44 | 44 | 44 | 44 | 44 | 44 | 44 | 44 | 0 |
| | | | | | | 11 | 26 | 72 | 95 | 26 | | | | | 20 | 44 | 44 | 44 | 44 | 44 | 44 | 44 | 0 | 0 |
| | | | | | | | | | 10 | | | | | | | 20 | 44 | 44 | 44 | 44 | 0 | 0 | 0 | 0 |
| | | | | | | | | | | | | | | | | | 20 | 44 | 44 | 44 | 44 | 0 | 0 | 0 |
| | | | | | | | | | | | | | | | | | | 20 | 44 | 44 | 44 | 0 | 0 | 0 |
| | | | | | | | | | | | | | | | | | | | | 40 | 44 | 0 | 0 | 0 |
| | | | | | | | | | | | | | | | | | | | | | 15 | 0 | 0 | 0 |

Figure II.11. Distribution of Less Reactive Hydrocarbon Emissions (average kilograms/hour) by Grid Area [From Reference 2, pg. II.13]

TIME= 0.38019937D 03 MINUTES    STEP= 66    POSITION= 58.4039, 40.3573    STEP SIZE= 0.10000000D 00    PAGE 13

EXPECTED RATE OF CHANGE OF CONCENTRATIONS DUE TO EMISSIONS FROM REGIONAL SOURCES

| | PPHM/MIN | | | | GRAM-MOLES/MIN | | | |
|---|---|---|---|---|---|---|---|---|
| | PROPYLENE | NO | CO | DUMHC | PROPYLENE | NO | CO | DUMHC |
| STREET TRAFFIC | 0.3660D-02 | 0.1025D-01 | 0.2196D 00 | 0.4918D-01 | 0.5274E-06 | 0.1477E-05 | 0.3165E-04 | 0.7089E-05 |
| FREEWAY TRAFFIC | 0.1446D-02 | 0.4049D-02 | 0.8677D-01 | 0.1944D-01 | 0.2084E-06 | 0.5836E-06 | 0.1251E-04 | 0.2801E-05 |
| AREA SOURCES | 0.1752D-02 | 0.1547D-02 | | 0.7252D-01 | 0.2525E-06 | 0.2230E-06 | | 0.1045E-04 |

| TEMPERATURE (CENT.) | RELATIVE HUMIDITY | ELEVATION (METERS) | MIXING HEIGHT (METERS) | MIXING DEPTH (METERS) |
|---|---|---|---|---|
| 27.2137 | 0.2871 | 181.3918 | 757.9106 | 576.5190 |

| COMPOUND | CONC PPHM | CHANGE, PPHM/MIN |
|---|---|---|
| 1 NO2 | 0.10570770 02 | -0.1501666D-01 |
| 2 NO | 0.7426092D 00 | -0.2883168D-02 |
| 3 O3 | 0.1308366D 02 | 0.2785062D-01 |
| 4 C3H6 | 0.5829044D 00 | -0.4806162D-02 |
| 5 HNO3 | 0.2953317D 01 | 0.1119049D-01 |
| 6 CH3CHO | 0.7138339D 01 | -0.5582240D-04 |
| 7 HCHO | 0.3470503D 01 | -0.7033884D-02 |
| 8 CO (PPM) | 0.4641978D 01 | -0.3806332D-02 |
| 9 CH3ONO2 | 0.3984505D 00 | -0.1581540D-03 |
| 10 C2H3NO5 | 0.5547380D 00 | 0.4134232D-03 |
| 11 FIXED O2 | 0.0 | 0.0 |
| 12 DUMHC | 0.1175608D 03 | -0.3339904D-01 |
| 13 | 0.0 | |
| 14 H | 0.3816246D-07 | |
| 15 OH | 0.1244696D-04 | |
| 16 HO2 | 0.5258254D-02 | |
| 17 CH3 | 0.6893148D-08 | |
| 18 CH3O | 0.4025991D-04 | |
| 19 CH3O2 | 0.3855134D-02 | |
| 20 C2H3O | 0.1420276D-06 | |
| 21 C2H3O2 | 0.7953880D-03 | |
| 22 C2H4O2 | 0.1095992D-05 | |
| 23 O | 0.2803847D-05 | |
| 24 NO3 | 0.1116167D-05 | |
| 25 C2H3O3 | 0.5799575D-03 | |

Figure II.12. Sample REM Output

## 8. Output Routine

This program prints output data at various times along the trajectory route. The user may specify the times at which the printouts are to occur and the routine checks to see if a requested output time has been reached. A sample output is shown in Figure II.12. The primary data categories printed include:

- Time of output and trajectory position;
- Step size;
- Rate of change of concentrations from source routine in pphm/minute and in gram-moles/minute;
- Meteorological values at the trajectory point including mixing depth;
- Pollutant concentrations;
- Rates of change of accumulating (primary) pollutants; and
- Rates of the elementary reactions.

## 9. Plotting Routine

At the end of the simulation run, this program outputs three digital plots containing the history of each accumulating pollutant represented in time vs. concentration curves. An example of this output is shown in Figure II.13.

## 10. Reverse Trajectory Program

The reverse trajectory program calculates wind trajectories and interpolates initial concentration values for use by the simulation model. Its primary inputs consist of hourly average wind data monitored at a network of meteorological stations, and hourly average pollutant data recorded at a group of pollutant monitoring stations. The coordinate positions of these stations are also required.

In addition, the user must specify a coordinate position and the length of time for which the simulated trajectory is to be calculated. The program then considers the given coordinate position to be the

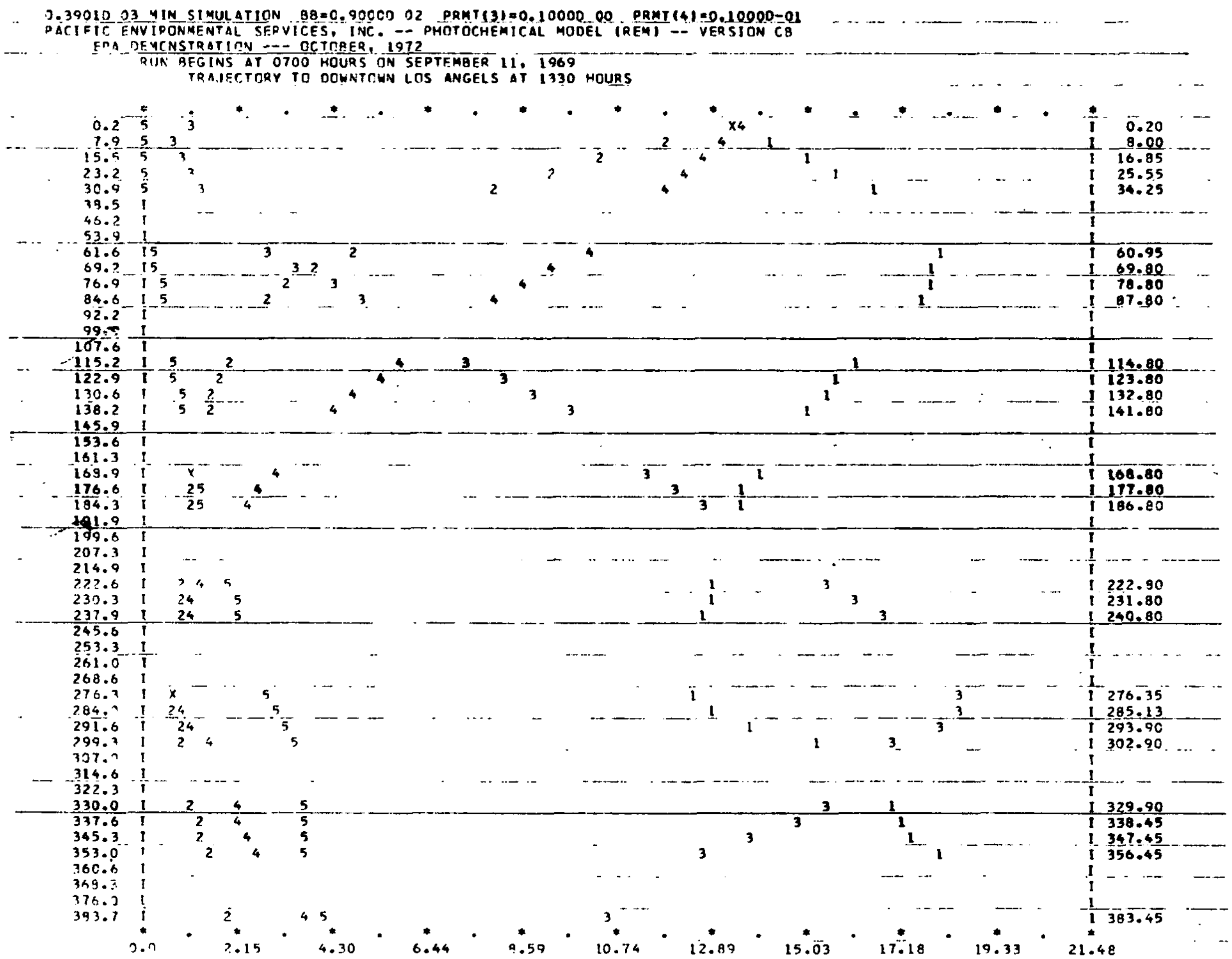



Figure II.13. Digital Plot of Primary Pollutant Time vs. Concentration Histories

Vertical axis represents time in minutes; horizontal axis depicts pollutant concentrations in pphm. The species plotted are as follows: 1 - $NO_2$, 2 - NO, 3 - $O_3$, 4 - $C_3H_6$, and 5 - $HNO_3$.

terminus of the trajectory, and computes consecutive points along the trajectory in a direction opposite to that of the wind. At the conclusion of the trajectory (the determination of the starting point), an interpolation routine calculates initial concentrations for nitrogen dioxide, nitric oxide, ozone and carbon monoxide from the pollutant data.

Although its primary use has been for calculating reverse trajectories, the program may also be used for computing forward trajectories. In this case, the pollutant interpolation routine would yield concentration values which could be considered as validation points.

Theoretically, the program could operate with one meteorological and one pollutant station. However, the greater the number of stations utilized, the more realistic and accurate will be the results.

# Section III

## Mathematical Description of the Reactive Pollution Simulation Model (REM)

### A. METEOROLOGICAL MODULE

#### 1. Introduction

The meteorological module calculates weather parameters at the air parcel location after considering the effect of natural barriers such as mountain ranges. This routine also determines the mixing depth and the rates of change of the wind components at this point.

#### 2. Derivations

##### a. The Barrier Routine and Definition of Permissible Stations

A barrier is a set of adjoining line segments utilized by the REM to represent a natural obstacle such as a mountain range. The barrier program's function is to determine the set of "permissible" meteorological stations employable by the meteorological routine for interpolating wind speed and direction, temperature, relative humidity and ground elevation. A station is permissible if and only if it is located on the same side of a barrier as is the air parcel. This is expressed mathematically below.

Each barrier is defined by an integer $N_B$, which is one greater than the number of barrier sides, and a sequence of points $(x_i, y_i)$, $i=1, 2, \ldots, N_B$, with each consecutive pair of points defining a side of the barrier. Let $(x_o, y_o)$ and $(x_s, y_s)$ be, respectively, the coordinate of the trajectory point and a given station. Let $m = (y_s-y_o)/(x_s-x_o)$, $b = y_o-mx_o$ be the slope and y the intercept of the line joining the trajectory point to the station. For each $i = 1, 2, \ldots, N_B-1$ let

$$m_i = (y_{i+1}-y_i)/(x_{i+1}-x_i)$$

$$b_i = y_i-m_ix_i$$

$$\lambda_i = \frac{y_s-m_ix_i-b_i}{m_i(x_o-x_s)-(y_o-y_s)}$$

$$\mu_i = \frac{y_{i+1}-mx_{i+1}-b}{m(x_i-x_{i+1})-(y_i-y_{i+1})}$$

A station located at $(x_s, y_s)$ is said to be <u>permissible</u> if, and only if, for each $i=1, 2, \ldots, N_B-1$ either

$$\lambda_i \geq 0,\ \lambda_i \geq 1,\ \mu_i \leq 0 \text{ or } \mu_i \geq 1.$$

## b. Interpolation of Meteorological Variables

A spatial interpolation is performed automatically for the data values from two successive hours. This is followed by a linear temporal interpolation for the two spatially interpolated values for each of four meteorological variables. The spatial interpolation is given as follows: Let $(x_j, y_j)$ be the coordinates of each permissible station $(j=1,2,\ldots N_p)$. Let $d_1,d_2,d_3,\ldots,d_{N_p}$ be the distance from these stations to the trajectory point and let $\dot{x}_1,\dot{x}_2,\ldots,\dot{x}_{N_p}$ be, for example, the corresponding set of observed x components of wind velocity. The x component of wind velocity, $\dot{x}_o$, at the trajectory point is estimated according to:

$$\dot{x}_o=\left(\sum_{j=1}^{N_p}\dot{x}_j/d_j^{\,2}\right)/A \qquad \text{(III.1)}$$

Each of the three remaining trajectory point variables is estimated by the corresponding analogue to equation (III.1).

For example, if the calculation is being conducted for a trajectory point at 0715 hours, then two interpolations are conducted for each of four variables (x and y wind components, temperature, and relative humidity). One interpolation is calculated for 0700 and the other for 0800.

This is followed by a temporal interpolation for each set of spatially interpolated variables given by:

$$x = x_1 + (x_2-x_1)-(t-t_1) \qquad \text{(III.2)}$$

where: $x$ is the interpolated value;

$x_1$ is the spatially interpolated value at hour 1;

$x_2$ is the spatially interpolated value at hour 2;

$t_1$ is the time of hour 1;

$t$ is the time of day where $t \geq t_1$.

In the example above, equation (III.2) would cause 25% of the 0700 value to be added to 75% of the 0800 value.

## c. Rates of Change of the Wind Components

The wind component rates of change are easily computed by dividing the hourly interpolations of these variables by 60. These values are then passed to the numerical integration routine where they are utilized in the integration process by the ordinary differential equations reserved for the trajectory calculation.

## d. Computation of Mixing Height

The mixing height is computed by passing a straight line of slope -.00986 (the dry adiabatic lapse rate) through the trajectory height-temperature point and determining the abscissa of its intersection with the radiosonde curve. The mixing depth is calculated by subtracting interpolated height-above-sea-level from the mixing height.

Given the interpolated values $(z_o,T_o)$ of height above sea level and temperature at our trajectory point, the module selects the appropriate A.M. or P.M. radiosonde curve depending of the value $t_o$. Each of these curves is defined by an integer $N_{a.m.}$ or $N_{p.m.}$ and a sequence of points $(z_k, T_k)$ $k=1,2,\ldots N_{a.m.(p.m.)}$. The mixing height, $h_m$, is computed according to:

$$h_m = \frac{T_o - T_k + m_k z_k - \alpha z_o}{m_k - \alpha}$$

where k is the first integer such that $1 \le k < N_{a.m.(p.m.)}$, $z_k < h_m < z_{k+1}$, $z_o \le h_m$, $m_k = (T_{k+1} - T_k)/(z_{k+1} - z_k)$, and $\alpha = -.00986$ °C/meter.

### 3. Symbol Glossary and Units

$t_o$ [hours] = time of day
$\dot{x}_o$ [meters/minute] = x component of wind velocity
$\dot{y}_o$ [meters/minute] = y component of wind velocity
$T_o$ [degree centigrade (°C)] = temperature
$P_o$ [millibar] = pressure
$H_o$ [dimensionless] = relative humidity
$w_o$ [dimensionless] = cloud cover
$z_o$ [meters] = height-above-sea-level
$h_m$ [meters] = mixing height

## B. ULTRAVIOLET IRRADIANCE MODULE

### 1. Introduction

The basic physical hypotheses underlying this module's computations have been taken almost directly from [1]. Our departure is in the formulation of a total irradiance equation which takes into account albedo and weather effects and which reduces to a standard form (see equation II-29 of [1] when the cloud cover and albedo are both zero. Thus, our final formulation (see equation III.3) will differ from any developed on the basis of equation (II-38) of [1]. The input to the module is the time $t_o$, the height above sea level of the trajectory point, $z_o$, the relative humidity at the trajectory point $H_o$, the corresponding atmospheric pressure $p_o$, the mixing height, $h_m$, the weather cover, $w_o$, and the average concentration of $NO_2$, $\bar{C}_{NO_2}$, in the column. The module's output is the specific absorption rate of $NO_2$, $k_{NO_2}$.

## 2. Derivations

As a function of the time of day, $t_o$ (Pacific Standard Time), a value of the solar zenith angle $\theta$, is interpolated from a table derived from the equinox curve of Figure 2 in Chapter II of [1]. The air mass, m, is interpolated as a function of $\theta$ in Table 2 of [1].

Depending of an input cloud-type parameter, a value of average fraction of radiation transmitted, $\beta$, is interpolated in Table 10 of [1]. For each wavelength band of 100Å in a wavelength region of 3000Å≤λ≤4000Å, the molecular scattering coefficient $(s_{m\lambda})_o$ is selected from Table 3 of [1]. From equation (II-9) of [1], the transmissivity relative to molecular scattering, $T_{m\lambda}$, may be computed from the formula

$$\log_{10} T_{m\lambda} = -(s_{m\lambda})_o \frac{p_o m}{1013.250}$$

where $p_o$ is the interpolated pressure in millibars.

The transmissivity relative to particle scattering, $T_{p\lambda}$, may be computed from the formula (II-11) of [1] (with λ in microns)

$$\log_{10} T_{p\lambda} = -(3.75\text{x}10^{-3}\lambda^{-2}W+3.5\text{x}10^{-2}\lambda^{-.75}d)m$$

where W is the amount of precipitable water vapor in the atmosphere, measured vertically above the trajectory point, computed as in equation (II-2) of [1], in units of centimeters, according to:

$$W = 1.722\text{x}10^{-1}P_W 10^{-(z_o/22,000)}$$

$P_W$ is the partial pressure in millibars of water vapor at the trajectory point. $P_W$ is interpolated from a vapor pressure table in [2], and d is a dimensionless parameter of preset nominal value 1.

The ozone absorption coefficient $\alpha_\lambda$ [meters$^{-1}$] is interpolated from Table 5 of [1] and the transmissivity of ozone, $T_{a\lambda}$, as in equation (II-13) of [1], may be computed from

$$\log_{10} T_{a\lambda} = -\alpha_\lambda (O_3) m$$

where $(O_3)$ is a preset parameter of nominal value $2.2 \times 10^{-3}$ [meters] (of ozone).

The mean solar spectral irradiance $I_{0\lambda}$, is selected from Table 1 of [1] and the direct and sky radiation $I_{d\lambda}$ and $I_{s\lambda}$ are computed from equations (II-15) and (II-16) of [1]:

$$I_{d\lambda} = T_{s\lambda} T_{a\lambda} I_{0\lambda} \cos\theta$$

$$I_{s\lambda} = g(1-T_{s\lambda}) T_{a\lambda} I_{0\lambda} \cos\theta$$

where $T_{s\lambda} = T_{m\lambda} T_{p\lambda}$ and g is a preset dimensionless parameter of nominal value .5.

Following the development from equations (II-17) through (II-28) of [1] and taking average weather cover and an average albedo effect into account we obtain the formula for the average rate of absorption per unit pollutant column volume for direct and sky radiation over a wavelength band of 100Å centered at wavelength $\lambda$, $I_{a\lambda}$:

$$I_{a\lambda} = \frac{\left\{1+a\right\}\left\{I_{d\lambda}(1-w_o)(1-10^{-\alpha_\lambda \bar{C}_{NO_2} h_m \sec\theta}) + \left[\beta w_o I_{d\lambda} + (1-w_o+\beta w_o) I_{s\lambda}\right](1-10^{-2\alpha_\lambda \bar{C}_{NO_2} h_m})\right\}}{h_m} \quad \text{(III.3)}$$

where a is the albedo (preset nominal value of .235), $w_o$ is the weather cover, and $\bar{C}_{NO_2}$ is the average column concentration of $NO_2$. $\alpha\lambda$ now refers to $NO_2$.

Finally, the specific absorption rate of $NO_2$, $k_{NO_2}$ derived from equations (II-31) and (II-32) of [1] is computed as:

$$k_{NO_2} = \frac{1}{7.2} \times 10^{-16}\left(\frac{273+T_o}{p_o \bar{C}_{NO_2}}\right)\sum_{\lambda=3000Å}^{4000Å} I_{a\lambda}$$

In passing we note that in our formulation equation (III.3) reduces to (II-29) of [1] when a=0 and $w_o=0$ ($\gamma=w_o$), but equation (II-38) does not.

### 3. Units

All lengths are in meters.

Time is in minutes.

Temperature is in °C.

All pressures are in millibars.

$I_{0\lambda}$ are in photons meters$^{-2}$ minutes$^{-1}$(100Å)$^{-1}$.

$\bar{C}_{NO_2}$ is in pphm.

$k_{NO_2}$ is in minutes$^{-1}$.

$w_o$ is dimensionless.

$\beta$ is dimensionless.

### 4. References

[1] P. A. Leighton, Photochemistry of Air Pollution, Academic Press, New York, 1961.

[2] Handbook of Physics and Chemistry

## C. KINETICS MODULE EQUATIONS

### 1. Introduction

We first characterize an abstract k step -$N_\sigma$ species constant mass, constant volume chamber photochemical mechsnism. As a consequence of this characterization, using standard principles of chemical kinetics, we can write, in compact notation, the differential equations of species concentration for the constant volume, constant mass situation. Next we expand our conceptual framework to the chemical kinetics of the contents of a pollutant column whose motion over a time-varying field of urban emission sources induces variations in average column temperature, colume mass, etc. This is accomplished by adding a series of appropriate first order perturbation terms to the species concentration time derivatives. It is to be emphasized that the number of reactions and number of species characterizing our imbedded kinetic mechanism are limited only by computer storage and computation time considerations. For this reason we are utilizing the IBM 370/155, a high-speed, large storage computer, in conjunction with an auxiliary FORTRAN system whose function is to derive a set of differential equations from a corresponding set of photochemical equations. Thus, we have complete flexibility in reaction number, species number and, more importantly, the photochemical equations themselves.

The inputs to the module are the outputs of the weather, diffusion, and ultraviolet irradiance modules.

## 2. Derivations

An abstract k-reaction, $N_\sigma$-species, constant-volume, constant-mass photochemical mechanism is characterized by (i) a binary valued $k x N_\sigma$ matrix B whose (i,j) element, $b_{ij}$, is 1 if, and 0 unless, the jth species appears as a reactant in the $i^{th}$ (elementary) step; (ii) an integer valued $k x N_\sigma$ species conservation matrix, P, whose (i,j) element, $P_{ij}$, is the number of molecules of species j produced ($p_{ij} \geq 0$) or consumed ($p_{ij} < 0$) in the $i^{th}$ step; (iii) a K-element vector F of reaction rate factors $k_j$, j=1, 2,...K; and (iv) a $N_\sigma$-element vector, $C_o$, of initial concentrations, $C_\ell(0)$, $\ell$=1, 2,...,$N_\sigma$. From the above definitions and elementary considerations of chemical kinetics, we may formulate the following set of differential equations:

$$\dot{C}_i(t) = \sum_{j=i}^{k} p_{ji} k_j \left( \prod_{\{\ell : b_{j\ell} = 1\}}^{N_\sigma} C_\ell(t) \right), \tag{III.4}$$

$$C_i(0) = C_{io}$$

$$(i = 1,2,\ldots,N_\sigma)$$

or, in matrix-vector form:

$$\dot{C}(t) = P^T R(t)$$

$$C(0) = C_o,$$

where

$$\dot{C}(t) = \begin{bmatrix} \dot{C}_1(t) \\ \dot{C}_2(t) \\ \dot{C}_3(t) \\ \cdot \\ \cdot \\ \cdot \\ \cdot \\ \dot{C}_{N_\sigma}(t) \end{bmatrix}$$

$$R(t) = \begin{bmatrix} k_1 \prod_{\{\ell : b_{1\ell}=1\}} C_\ell(t) \\ \vdots \\ \vdots \\ k_K \prod_{\{\ell : b_{K\ell}=1\}} C_\ell(t) \end{bmatrix},$$

and $P^T$ is the transpose of P.

Taking equation (III.4) as our starting point, we permit F to be time-varying (i.e., $k_j$ are replaced by $k_j(t)$) and add first order perturbations due to stationary sources, $\dot{C}_S(t)$, traffic sources, $\dot{C}_T(t)$, and the rate of change of column volume, $\dot{C}_V(t)$, to derive the pollutant column concentration differential equations:

$$\dot{C}(t) = P^T R(t) + \dot{C}_S(t) + \dot{C}_T(t) + \dot{C}_V(t),$$

$$C(0) = C_o$$

where

$$\dot{C}_V(t) = \begin{cases} 0 \text{ if } h_m \leq 0 \\ \dfrac{-\dot{h}_m}{h_m} C(t) \text{ if } h_m > 0 \end{cases}$$

## 3. Units

All concentrations are in parts per hundred million except CO, which is in ppm. Rates of change of concentration are in pphm $\cdot$ min$^{-1}$ and $h_m$

(mixing depth) is in meters.

## D. EMISSION MODULE

### 1. Introduction

The emission module computes the contributions to the pollutant column of street vehicular traffic, freeway traffic and stationary area sources. In characterizing the module, the Los Angeles Basin is subdivided into a grid system of 650 equal 4-square-mile squares corresponding to a 50-by-52-mile square total area. To each of these grid areas is assigned the total number of vehicular freeway and non-freeway miles travelled daily; and the rate of emission in kilograms per hour of reactive hydrocarbons, nitric oxide*, and less reactive hydrocarbons from area sources. The traffic section of the routine requires emission factors in grams/vehicle mile for reactive hydrocarbons, nitric oxide, carbon monoxide, and less reactive hydrocarbons.

The inputs to the module are the time(t), the position of the pollutant column (x,y), the mixing depth ( $h_m$ ), the emission distributions described above, emission factors described above, and diurnal usage curves. The diurnal curves are illustrated in Figures II.5 and II.6. The grid distributions are shown in Figures II.7 - II.11.

The module's outputs include the emissions from the five sources

$$\left.\begin{array}{l}\text{street traffic}\\ \text{freeway traffic}\end{array}\right\}\quad\text{vehicular sources}$$

$$\left.\begin{array}{l}\text{reactive hydrocarbons (propylene)}\\ \text{nitric oxide}\\ \text{less reactive hydrocarbons}\end{array}\right\}\quad\text{area source emissions}$$

in propylene, nitric oxide, carbon monoxide, and less reactive hydrocarbons. These results are given in both pphm/min and gram-moles/min.

*Oxides of nitrogen taken as nitric oxide

## 2. Derivations

Given the air parcel or column location (x,y) (in miles) such that $17 \leq x \leq 67$ and $1 \leq y \leq 53$, the projection of the column centroid falls in grid sub-area i, where is is computed according to:

$$i = \left[\frac{x+1}{2}\right] + 25\left[\frac{y+1}{2} - 1\right] - 8$$

where [z] = integer part of z.

Once the primary grid square is selected, the program determines the three next closest grids to the pollutant column; that is, the three grids whose midpoints are nearest the column. At this point, the emissions attributable to the column are computed utilizing values from four grids. The contribution to each of the sources for each of the pollutants is calculated on the basis of the distance of the grid midpoint to the pollutant column and is inversely proportional to the square of this distance. These contributions are then modified by the appropriate diurnal usage curves.

## 3. Units

All computations are calculated in metric units with the exception of distances which remain in miles.

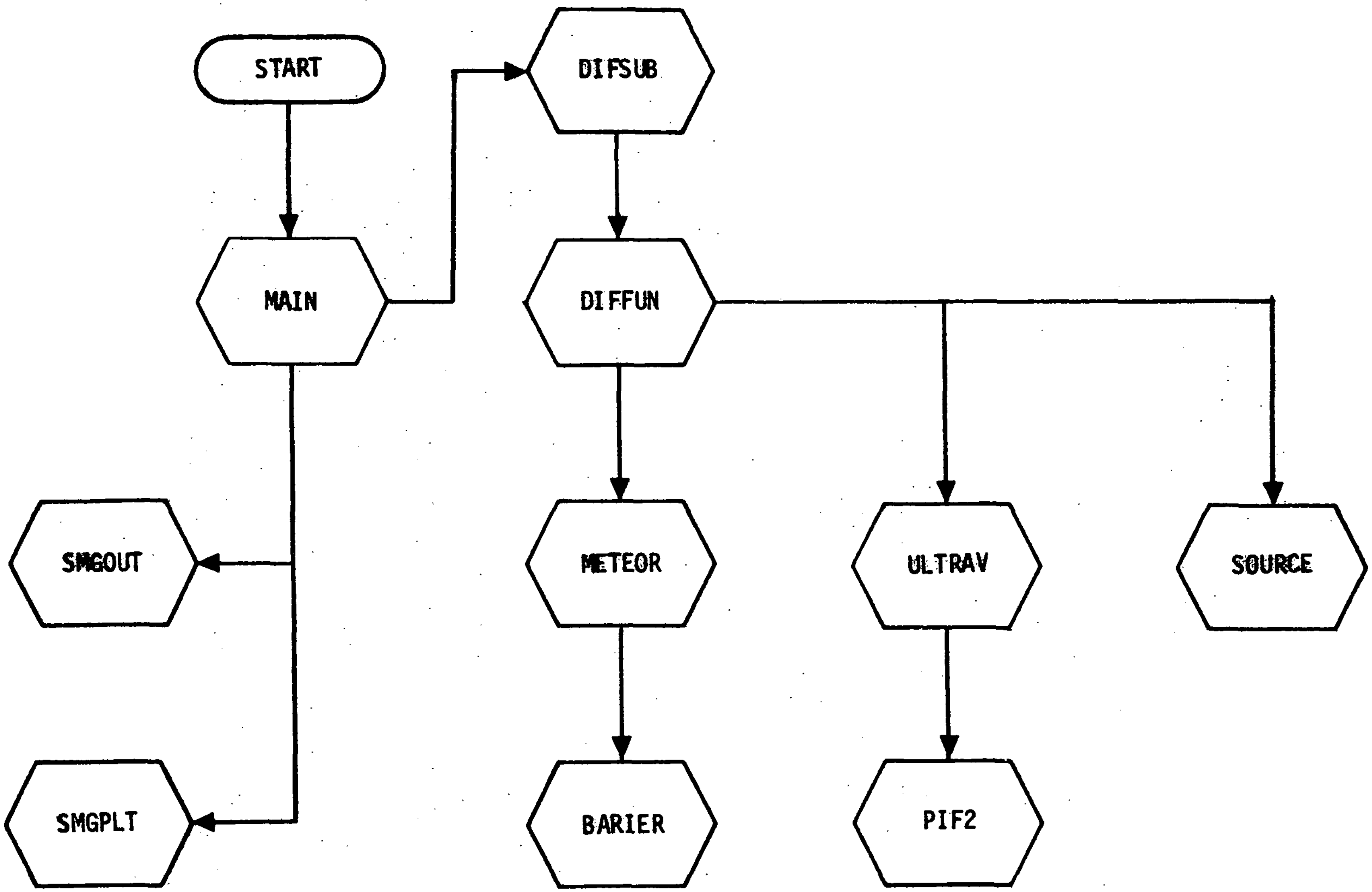
# E. NUMERICAL INTEGRATION

DIFSUB is the numerical integration program. It is more commonly known as the Gear routine named after its developer, Professor C. W. Gear of the University of Illinois.

This routine has three numerical integration routines imbedded in it. REM utilizes the option known as the Adams method.

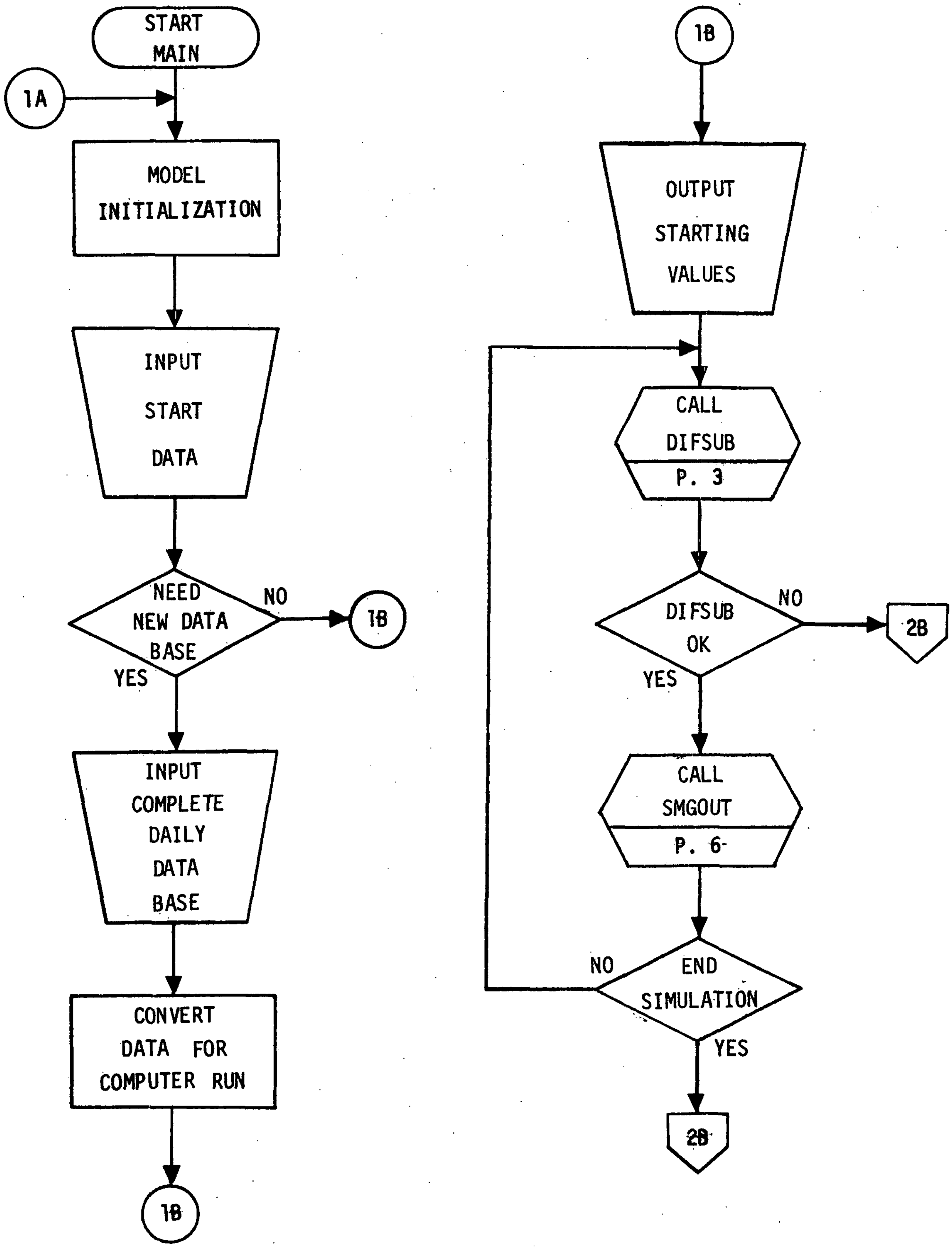
No flowchart or other descriptive material is provided for DIFSUB since this routine was not programmed by PES staff. For additional information contact Professor Gear at the Department of Computer Science, University of Illinois; or see the Communications of the Association for Computing Machinery, March, 1971.

# Section IV
# Flowcharts



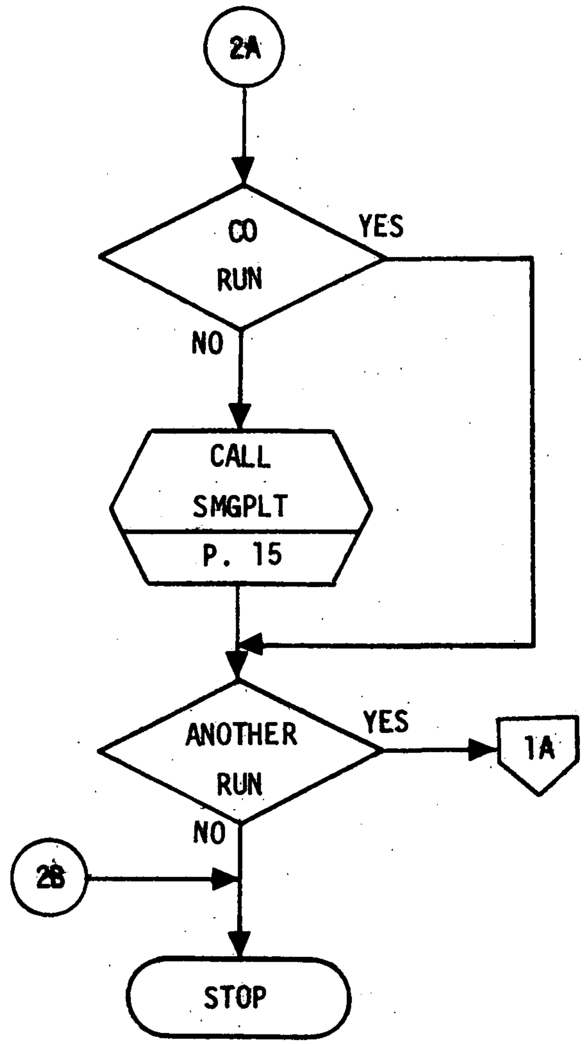

OVERVIEW OF REM

IV.3




FLOW OF MAIN PROGRAM

IV.4



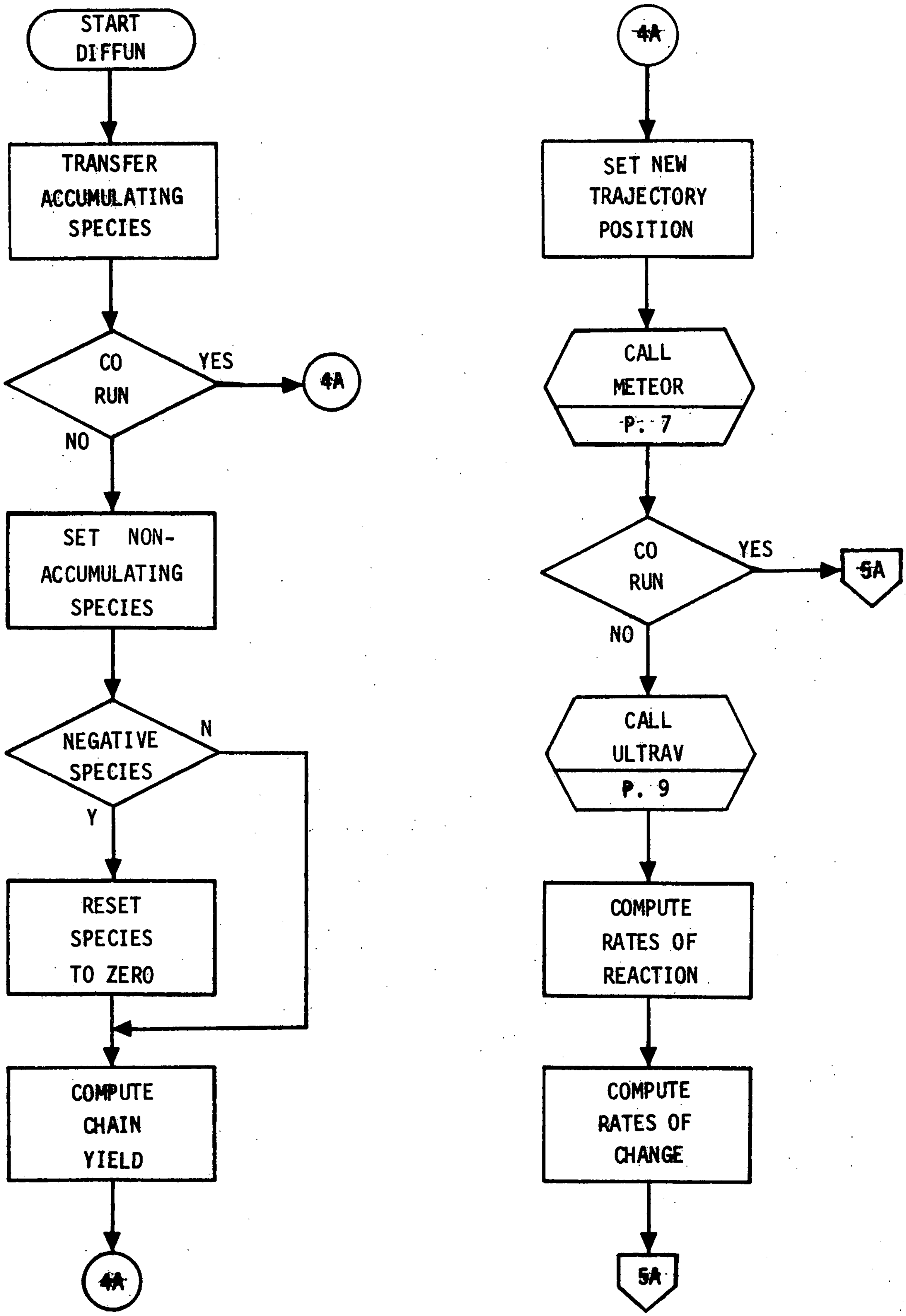
DIFSUB*

1. Called by MAIN

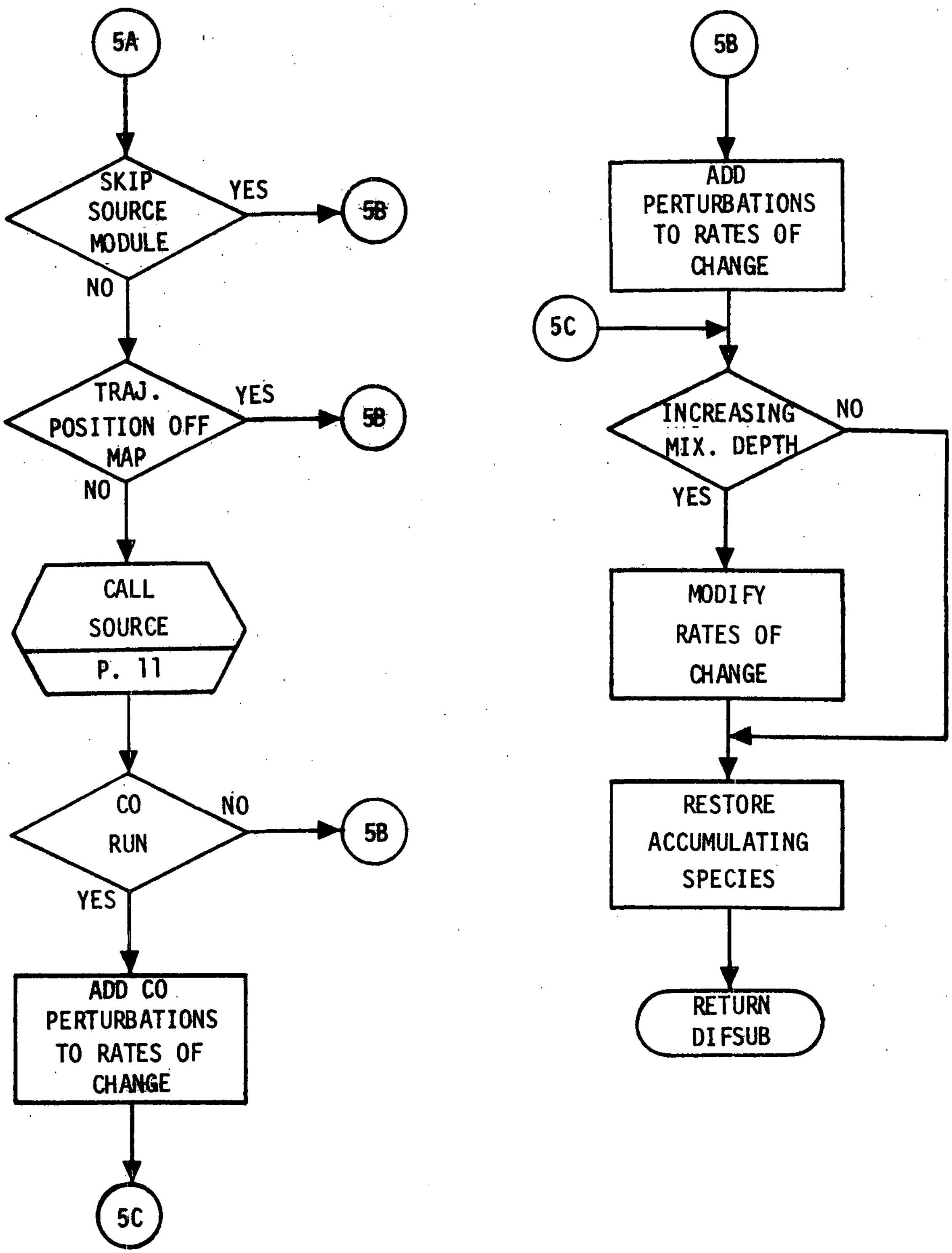
2. Calls DIFFUN

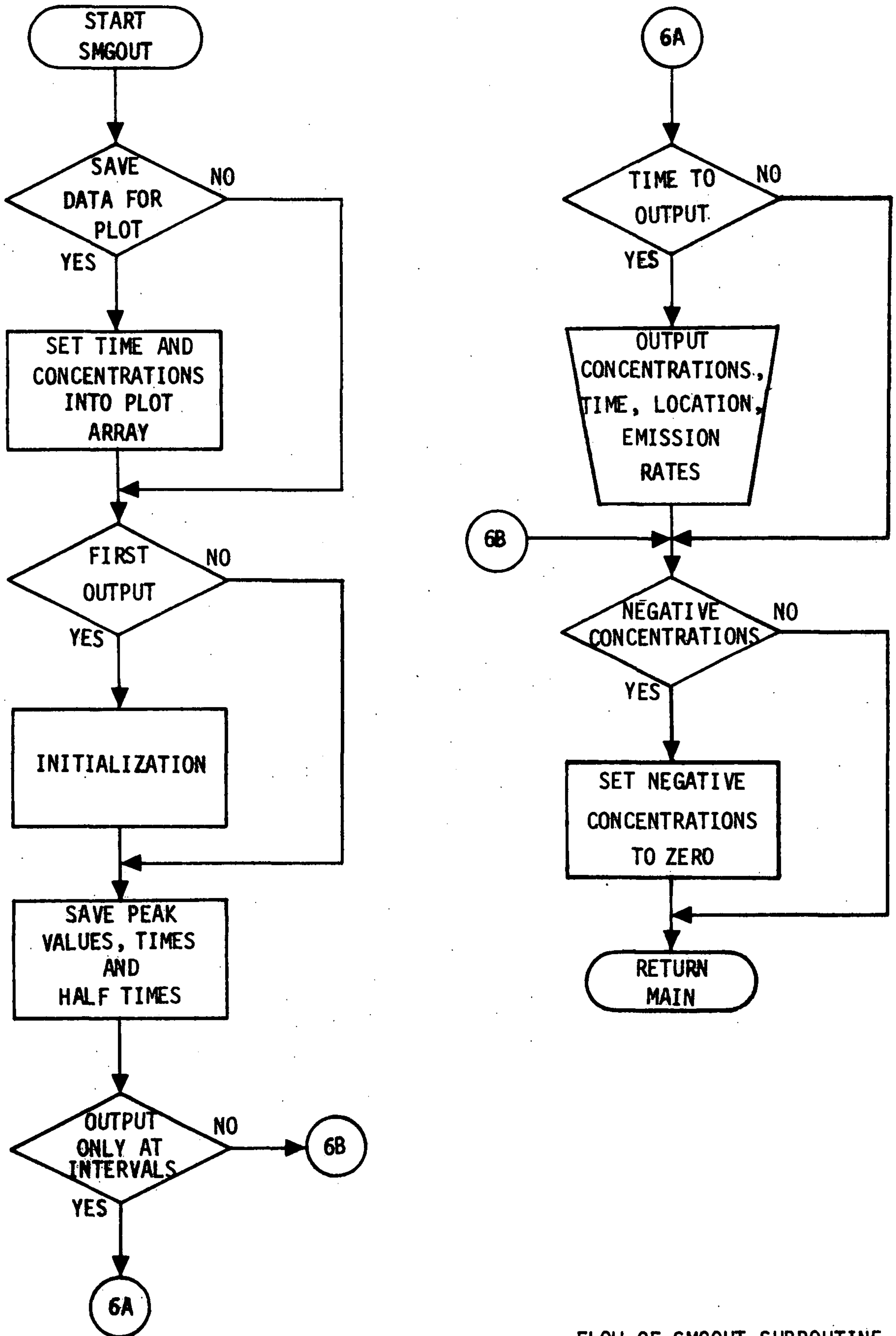
DIFSUB always returns to the calling program after completing its tasks.

*Flowchart of DIFSUB not provided since no programming was done on this routine by PES.

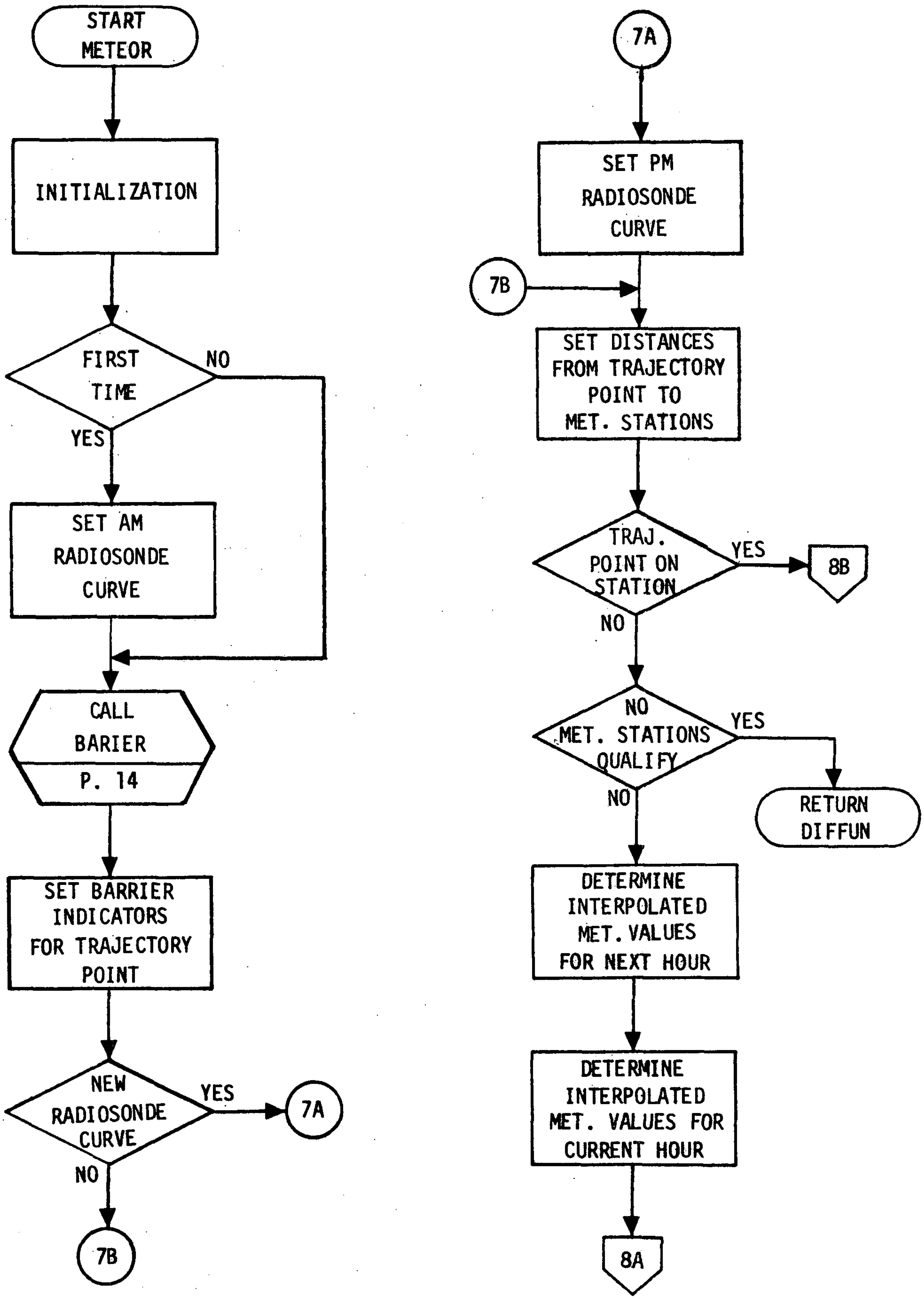



FLOW OF DIFFUN SUBROUTINE

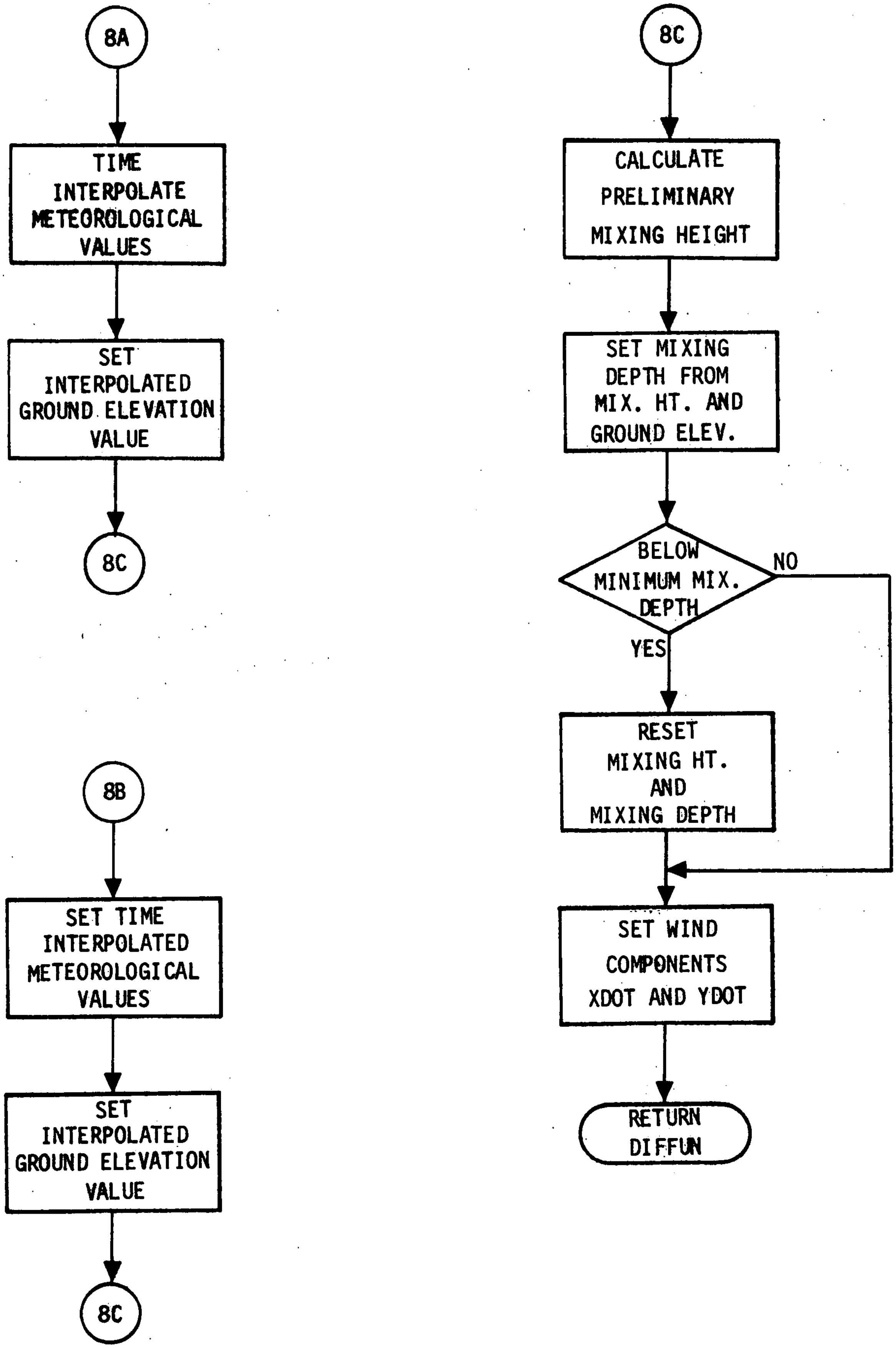

5A
SKIP SOURCE MODULE
YES
5B
NO
TRAJ. POSITION OFF MAP
YES
5B
NO
CALL SOURCE
P. 11
CO RUN
NO
5B
YES
ADD CO PERTURBATIONS TO RATES OF CHANGE
5C
5B
ADD PERTURBATIONS TO RATES OF CHANGE
5C
INCREASING MIX. DEPTH
NO
YES
MODIFY RATES OF CHANGE
RESTORE ACCUMULATING SPECIES
RETURN DIFSUB

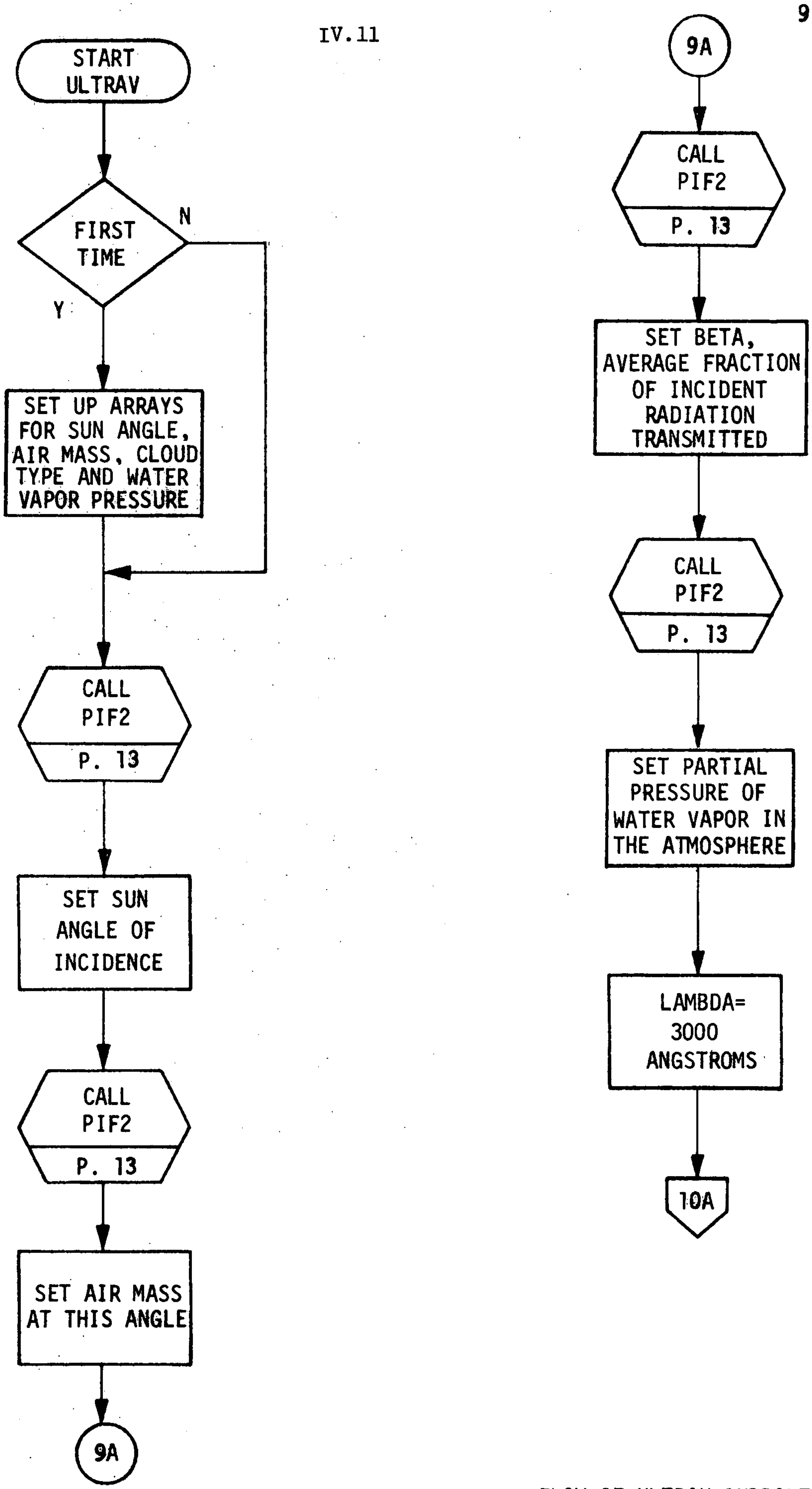



FLOW OF SMGOUT SUBROUTINE

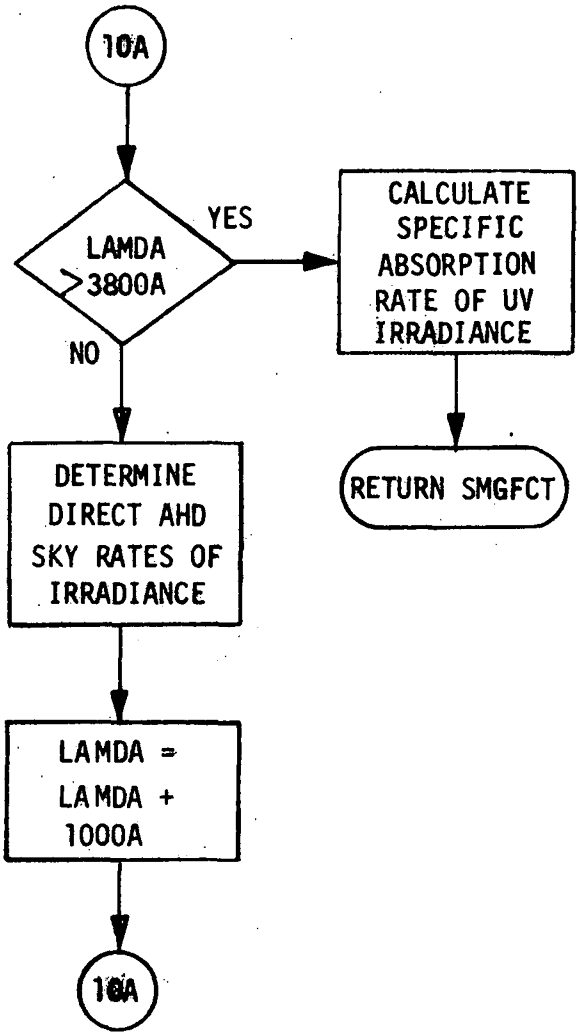


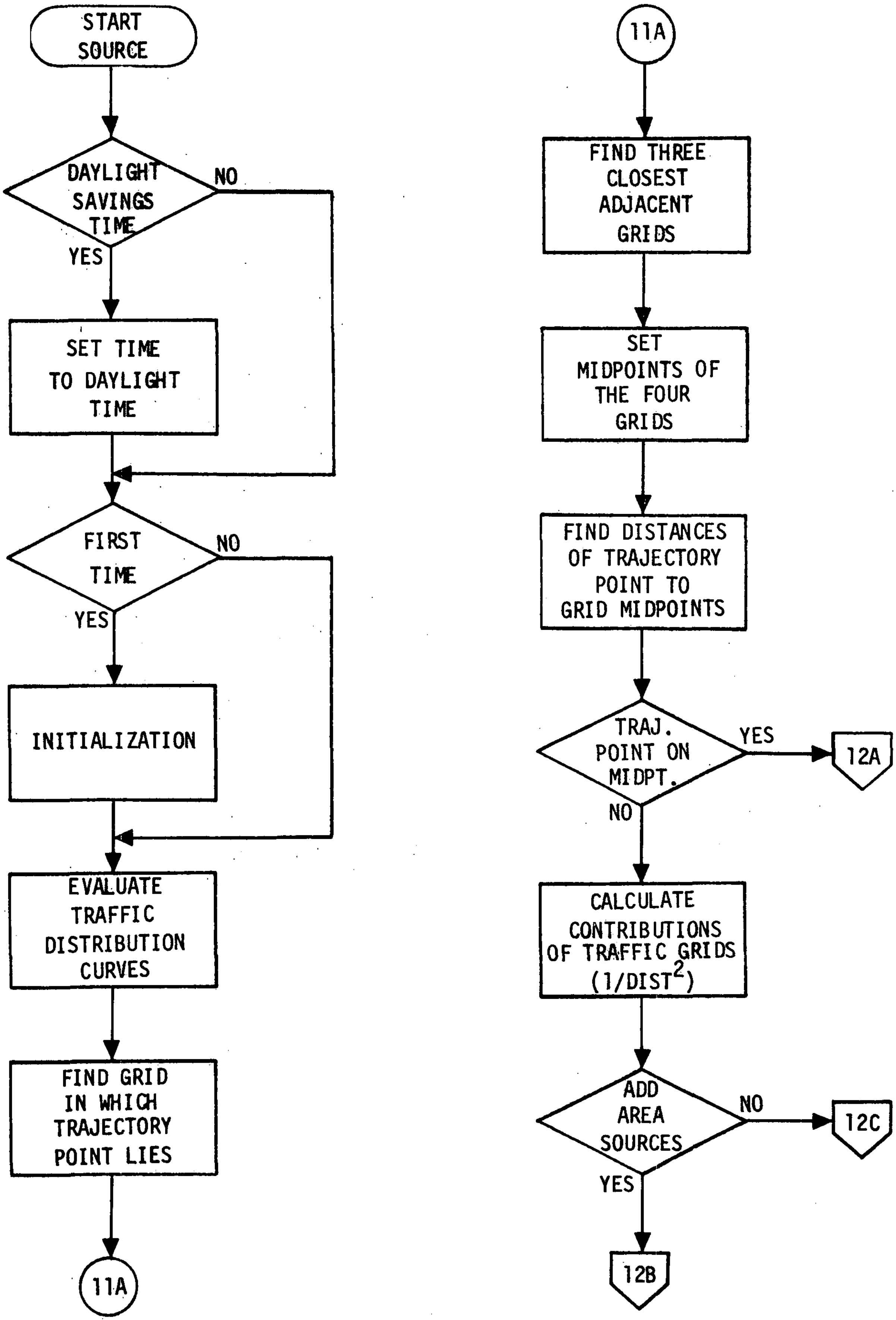

FLOW OF METEOR SUBROUTINE


8A
TIME INTERPOLATE METEOROLOGICAL VALUES
SET INTERPOLATED GROUND ELEVATION VALUE
8C
8B
SET TIME INTERPOLATED METEOROLOGICAL VALUES
SET INTERPOLATED GROUND ELEVATION VALUE
8C
8C
CALCULATE PRELIMINARY MIXING HEIGHT
SET MIXING DEPTH FROM MIX. HT. AND GROUND ELEV.
BELOW MINIMUM MIX. DEPTH
NO
YES
RESET MIXING HT. AND MIXING DEPTH
SET WIND COMPONENTS XDOT AND YDOT
RETURN DIFFUN

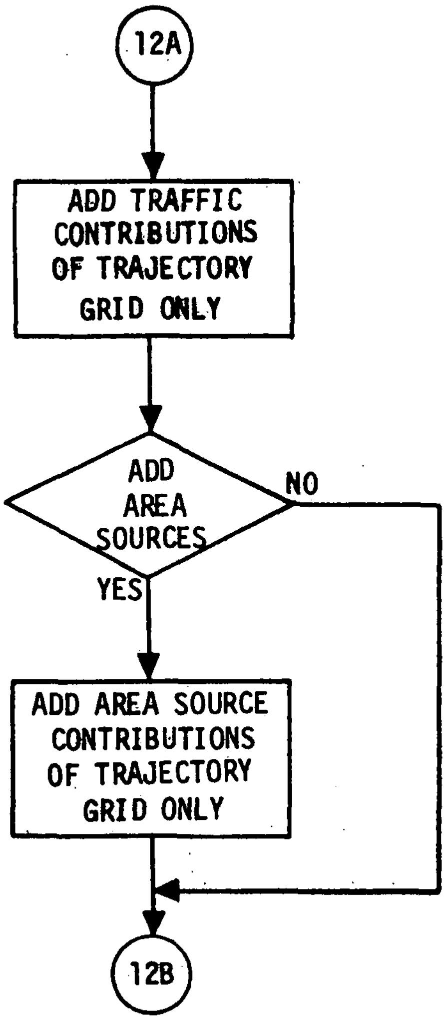


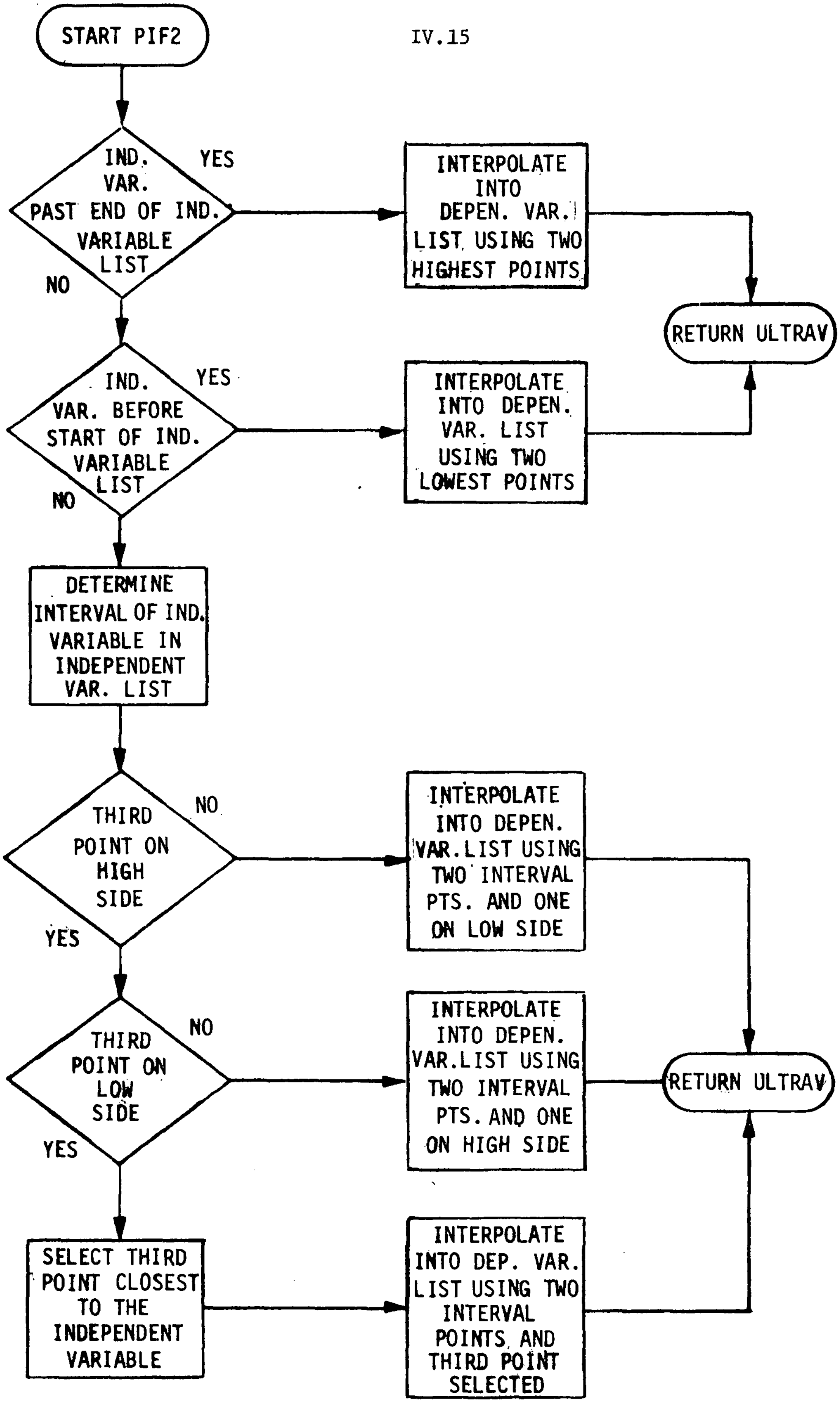

FLOW OF ULTRAV SUBROUTINE


10A
LAMDA
> 3800A
YES
NO
CALCULATE SPECIFIC ABSORPTION RATE OF UV IRRADIANCE
RETURN SMGFCT
DETERMINE DIRECT AHD SKY RATES OF IRRADIANCE
LAMDA = LAMDA + 1000A
10A

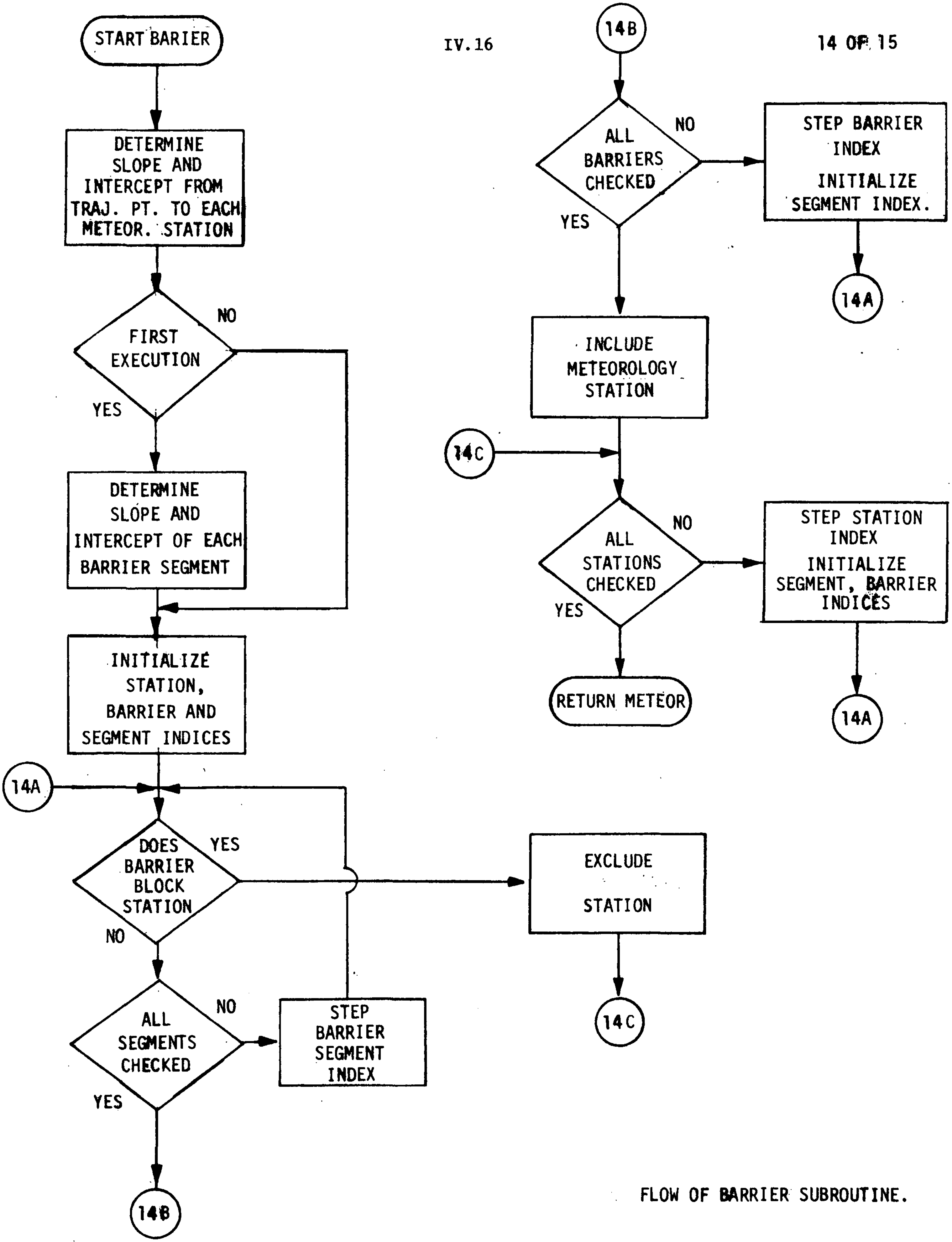



FLOW OF SOURCE SUBROUTINE

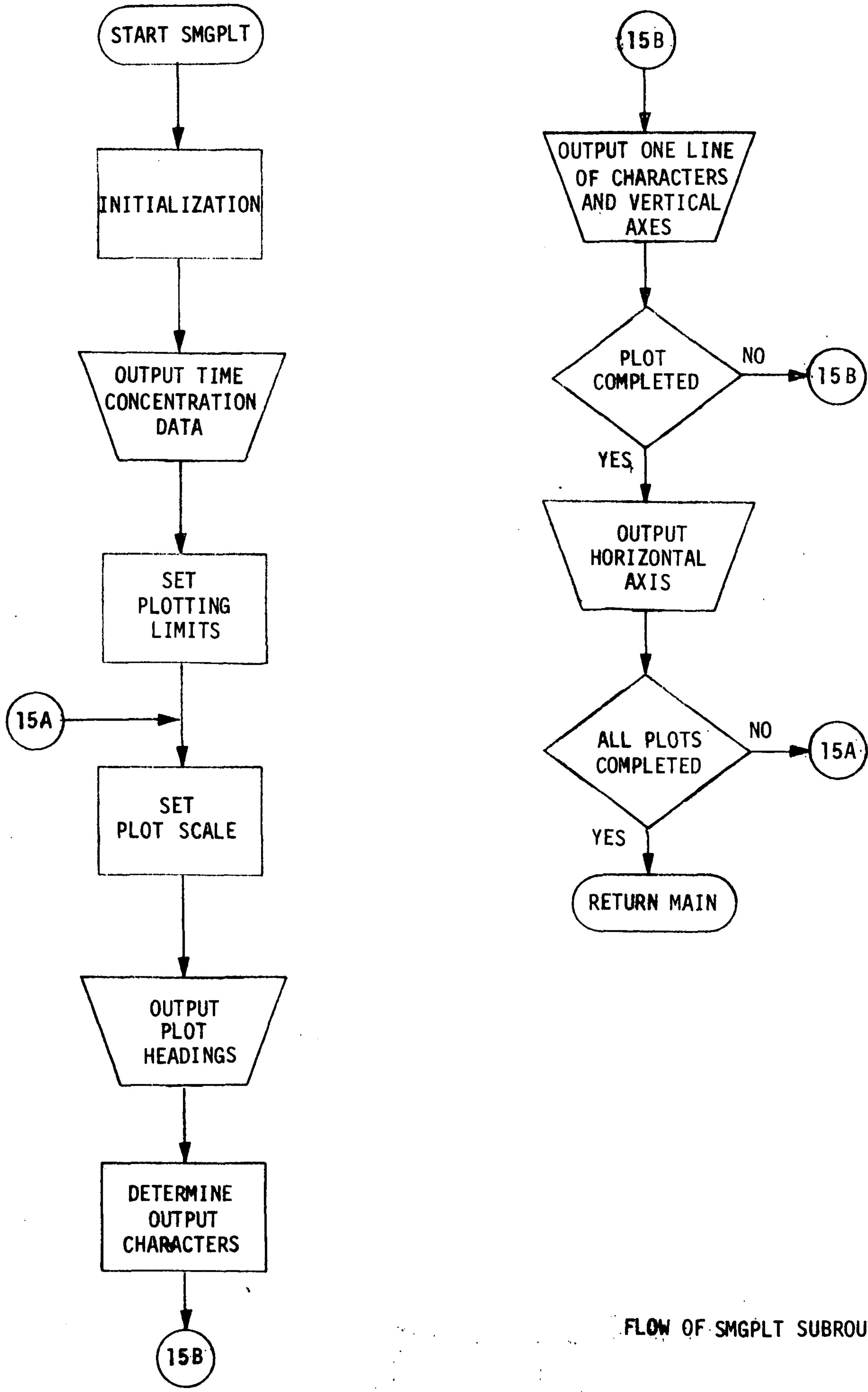

12A
ADD TRAFFIC CONTRIBUTIONS OF TRAJECTORY GRID ONLY
ADD AREA SOURCES
NO
YES
ADD AREA SOURCE CONTRIBUTIONS OF TRAJECTORY GRID ONLY
12B
12B
CALCULATE CONTRIBUTIONS OF SOURCE GRIDS (1/DIST$^2$)
12C
DAYLIGHT SAVINGS TIME
NO
YES
RESET TIME TO STANDARD TIME
RETURN DIFFUN




FLOW OF PIF2 SUBROUTINE.




FLOW OF BARRIER SUBROUTINE.




FLOW OF SMGPLT SUBROUTINE.

# Section V
## Model Inputs

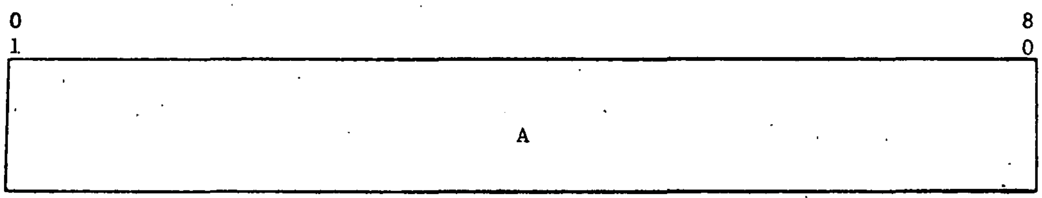
Model inputs must be prepared exactly as described. A complete sample input deck is shown in Section VI.

1. Card Type 1

   Heading data---1 array---4 cards.

   a. Alphanumeric data used as heading information. May be blank cards.

      FORMAT (20A4)




2. Card Type 2

   Starting data---4 items---1 card.

   XPOS - X coordinate of starting position in miles. Range: 17.0 to 67.0. Cols 1-10.

   YPOS - Y coordinate of starting position in miles. Range: 1.0 to 53.0. Cols 11-20.

   GOTIME - Simulation start time (local standard time) in hours and decimal fraction hours. Range: 7.000 to 18.999. Cols 21-30.

   XMIN - Minimum mixing depth in meters. Current value used is generally 50 meters. Cols. 31-40.

FORMAT (4F10.3)

| 0<br>1 | 11<br>01 | 22<br>01 | 33<br>01 | 44<br>01 | 8<br>0 |
|---|---|---|---|---|---|
| XPOS | YPOS | GOTIME | XMIN | | |

3. Card Type 3

Starting data---6 items---1 card.

PRMT (2) - Length of simulation in minutes and decimal fraction of minutes. Cols. 1-10.

PRMT (3) - Minimum step size for numerical integration in decimal fraction of minutes. Normal range is from .000001 to .001. Cols. 11-20.

PRMT (4) - Maximum step size for numerical integration in minutes and decimal fraction of minutes. Normal range is from 0.1 to 20.0 minutes. Cols. 21-30.

PRMT (5) - Initial value of step size for numerical integration in minutes and decimal fraction of minutes. Normal range is from .0001 to .01 minutes. Cols. 31-40.

PRMT (6) - Error criteria for numerical integration in decimal fraction of minutes. Normal range is from .0001 to .10 minutes. Cols. 41-50.

PRMT (7) - Indicator for plot routine. Determines how often data is to be saved for output in the plot. Reasonable value is usually .25*PRMT (2) in minutes. For example, if PRMT (2) is 300.0 minutes, then PRMT (7) would be 75.0. Cols. 51-60.

FORMAT (6F10.3)

| 0<br>1 | 11<br>01 | 22<br>01 | 33<br>01 | 44<br>01 | 55<br>01 | 66<br>01        8<br>           0 |
|---|---|---|---|---|---|---|
| PRMT(2) | PRMT(3) | PRMT(4) | PRMT(5) | PRMT(6) | PRMT(7) | |

4. Card Type 4

Starting data---14 items---1 card (all values <u>must</u> be right justified.

NDIM - Number of accumulating species. For CO simulation only, value must be 1. Cols. 1-5.

NC - Total number of species. For CO simulation only, value must be 3. Cols. 6-10.

NEQ - Number of elementary steps in mechanism. For CO simulation only, value must be 1. Cols. 11-15.

NLL - Number of lines to be used in plots, 0 gives 50 lines. Cols 16-20

NSTA - Number of meteorological stations. Cols. 21-25.

MF - Indicator for numerical integration method. Range: 0 to 2; values are:
- 0 - Adam's method
- 1 - Gear (matrix inversion) for less than 5 equations
- 2 - Gear (Gaussian elimination and back substitution) for 5 or more equations. Cols. 26-30.

MAXDER - Maximum number of derivatives calculated. Use MAXDER=12 if MF=0, or use MAXDER=6 if MF=1 or 2. Cols. 31-35.

ICLOUD - Index which defines seven different cloud types for ultraviolet radiation module.[1] Range: 2 to 8, values are:

[1] Leighton, Phillip A., Photochemistry of Air Pollution, Academic Press, New York, 1961, Page 40, Table 10.

2 - cirrus

3 - Cirrostratus

4 - Altocumulus

5 - Altrostratus

6 - Stratocumulus

7 - Stratus

8 - Fog

Cols. 36-40.

NRAD - Number of radiosonde points (maximum = 15) in the curve describing the mixing height. Cols. 41-45.

ITRAF - Traffic module operation indicator. 0 - module does not operate, 1 - module operates. Cols. 46-50.

ISOUR - Area source module operation indicator. 0 - module does not operate, 1 - module operates. Cols. 51-55.

IHT - Indicates if mixing height is entered by way of radiosonde data, or if it is input directly in meters. 0 - radiosonde data, 1 - input mixing height. Cols. 56-60.

IN - Indicates if model is to operate again with data from the previous run or a new set of data is necessary. 0 - a complete set of data is necessary for the run, 1 - return with the previous data. Must input only card types 1, 2, 3, 4, 5, 6 and 7. Need card type 6 only if IHT = 1. Cols. 61-65.

IPST - Time indicator. 0 - traffic module operates on daylight time, 1 - traffic module operates on standard time, Cols. 66-70.

FORMAT (14I5)

| | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 0 | 00 | 11 | 11 | 22 | 22 | 33 | 33 | 44 | 44 | 55 | 55 | 66 | 66 | 77 | 8 |
| 1 | 56 | 01 | 56 | 01 | 56 | 01 | 56 | 01 | 56 | 01 | 56 | 01 | 56 | 01 | 0 |
| NDIM | NC | NEQ | NLL | NSTA | MF | MAXDER | ICLOUD | NRAD | ITRAF | ISOUR | IHT | IN | IPST | | |

5. Card Type 5

Output data---1 item---1 array---1 card.

INTR - Integer. Positive value causes outputs at approximate times specified in array STEP. Zero or negative value causes outputs each time through. Cols. 1-2.

STEP - Array of up to 15 times for output in minuts. Output usually occurs within 1/2 minute of time specified. Cols. 6-80.

FORMAT (I2, 3X, 15F5.2)

| | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 000 | 00 | 11 | 11 | 22 | 22 | 33 | 33 | 44 | 44 | 55 | 55 | 66 | 66 | 77 | 77 | 8 |
| 123 | 56 | 01 | 56 | 01 | 56 | 01 | 56 | 01 | 56 | 01 | 56 | 01 | 56 | 01 | 56 | 0 |
| INTR | | STEP (1) | STEP (2) | STEP (3) | STEP (4) | STEP (5) | STEP (6) | STEP (7) | STEP (8) | STEP (9) | STEP (10) | STEP (11) | STEP (12) | STEP (13) | STEP (14) | STEP (15) |

6. Card Type 6

Mixing height data---1 array---1 card

XHITE - Array of up to 12 values of mixing height in meters. Cols. 1-72, optional (used only if IHT is set to 1; see IHT, card type 4). Represent hours 0700 to 1800, respectively.

FORMAT (12F6.0)

| 0<br>1 | 00<br>67 | 11<br>23 | 11<br>89 | 22<br>45 | 33<br>01 | 33<br>67 | 44<br>23 | 44<br>89 | 55<br>45 | 66<br>01 | 66<br>67 | 77<br>23 | 8<br>0 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| XHITE (1) | XHITE (2) | XHITE (3) | XHITE (4) | XHITE (5) | XHITE (6) | XHITE (7) | XHITE (8) | XHITE (9) | XHITE (10) | XHITE (11) | XHITE (12) | | |

7. Card Type 7

Species data--2 arrays--$\left[\frac{NC}{4}\right]^*$ + 1 cards, 4 species per card

LABEL - Alphanumeric array of NC** species names. Cols. 1-8, 21-28, 41-48, 61-68.

Y# - NC double precision values of initial species concentrations in pphm, except CO is in ppm. Cols. 9-20, 29-40, 49-60, 69-80.

| 0<br>1 | 00<br>89 | 22<br>01 | 22<br>89 | 44<br>01 | 44<br>89 | 66<br>01 | 66<br>89 | 8<br>0 |
|---|---|---|---|---|---|---|---|---|
| LABEL | Y | LABEL | Y | LABEL | Y | LABEL | Y | |

8. Card Type 8

Sun Angle Data---1 array---2 cards

ZENITH - Twelve pairs of an hour in standard time coupled with the sun angle at that time. Hour in cols. 1-5, 11-15, 21-25, 31-35, 41-45, 51-55, 61-65, 71-75. Sun angle in cols. 6-10, 16-20, 26-30, 36-40, 46-50, 56-60, 66-70, 76-80. Pairs carry

*[ ] means largest integer.

**See card type 4.

# $C_3H_6$ is set to .015 x CO in pphm

DUMHC is set to .15 x CO in pphm

over onto second card.

| | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 0 | 00 | 11 | 11 | 22 | 22 | 33 | 33 | 44 | 44 | 55 | 55 | 66 | 66 | 77 | 77 | 8 |
| 1 | 56 | 01 | 56 | 01 | 56 | 01 | 56 | 01 | 56 | 01 | 56 | 01 | 56 | 01 | 56 | 0 |
| Z (1,1) Hour | Z (1,2) Angle | Z (2,1) Hour | Z (2,2) Angle | Z (3,1) Hour | Z (3,2) Angle | Z (4,1) Hour | Z (4,2) Angle | Z (5,1) Hour | Z (5,2) Angle | Z (6,1) Hour | Z (6,2) Angle | Z (7,1) Hour | Z (7,2) Angle | Z (8,1) Hour | Z (8,2) Angle | |

**Z = array ZENITH**

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 0 | 00 | 11 | 11 | 22 | 22 | 33 | 33 | 44 | 8 |
| 1 | 56 | 01 | 56 | 01 | 56 | 01 | 56 | 01 | 0 |
| Z (9,1) Hour | Z (9,2) Angle | Z (10,1) Hour | Z (10,2) Angle | Z (11,1) Hour | Z (11,2) Angle | Z (12,1) Hour | Z (12,2) Angle | | |

**Z = array ZENITH**

9. Card Type 9

Meteorological data--2 arrays--maximum of 32 stations.

AIR - 3 cards per station, 4 hours per card, 12 hours per station. Cards are as follows:

IDNUM - column 1-3, station ID code

AIR - column 4-5, start hour of data, values are 7, 11 or 15

6, number of readings on card, max = 4

7-23
24-40
41-57
58-74

$\Bigg\}$ hourly data--17 columns

6 items in 17 columns in the following order:

3 columns - wind direction in degrees

3 columns - wind speed in miles/hour, last column is in tenths of a mile/hour

3 columns - temperature in °F

2 columns - dew point in °F

6 columns - blank

FORMAT (A3, 3X, 4(F3.0, F3.1, F3.0, F2.0, 6X), 6X)

Conversion: Wind speed and direction are converted to XDOT and YDOT, the X and Y components of the wind velocity at the column. Temperature is converted to °C. Relative humidity is determined from temperature and dew point. The station order on card types 8 and 9 must be exactly coincidental.

```
0 00000 01 11 1111      22 22 23 3333     44 44 44 4555     55566 66 6666     77    8
1 34567 90 23 5678      34 67 90 2345     01 34 67 9012     78901 34 6789     45    0
ID HOUR WDIR WSPD TEMP HUMID | WDIR WSPD TEMP HUMID | WDIR WSPD TEMP HUMID | WDIR WSPD TEMP HUMID | |
```

10. Card Type 10

Meteorological Stations--2 arrays--maximum of 8 cards, 4 stations per card

WPOS - Array of triplets, 4 stations per card, maximum of 32 stations. Cards are as follows:

IDMET - column 1-3, alphanumeric station ID code.

WPOS - column 4-8, X coordinate of station position in miles, last 2 columns in hundredths of miles. Column 9-13, Y coordinate of station position in miles, last 2 columns in hundredths of miles. Column 14-20, ground elevation of station in feet, last 2 columns in hundredths of feet. This 20 column grouping is repeated in columns 21-40, 41-60, 61-80 as required, and on additional cards if necessary.

FORMAT (4(A3, 2F5.2, F7.2))

The station order on card types 9 and 10 must be exactly coincidental.

| 0 1 | 00 34 | 00 89 | 11 34 | 22 01 | 22 34 | 22 89 | 33 34 | 44 01 | 44 34 | 44 89 | 55 34 | 66 01 | 66 34 | 66 89 | 77 34 | 8 0 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| ID | X | Y | ELEV | ID | X | Y | ELEV | ID | X | Y | ELEV | ID | X | Y | ELEV | |

11. Card Type 11

Traffic data---1 array---1 card

EMIT - Array of emission factors in grams per vehicle mile for chemical compounds in the following order:

1 - Propylene ($C_3H_6$). Cols. 1-5

2 - Nitric oxide (NO). Cols. 6-10

3 - Carbon monoxide (CO). Cols. 11-15

4 - Dummy hydrocarbons (DUMHC). Cols. 16-20

FORMAT (10F5.2)

| 0 1 | 00 56 | 11 01 | 11 56 | 22 01 | 8 0 |
|---|---|---|---|---|---|
| EMIT (1) $C_3H_6$ | EMIT (2) NO | EMIT (3) CO | EMIT (4) DUMHC | | |

12. Card Type 12

Omit if ITRAF is not set to 1 (see card type 4)

Vehicular mileage by 4-square mile grid---2 arrays---52 cards

FGRID - 650 values representing the freeway traffic mileage per grid in thousands of miles. 25 values at 3 columns each per card.

SGRID - 650 values representing the street traffic mileage per grid in thousands of vehicular miles. 25 values at 3 columns each per card.

FORMAT (25F3.0)

```
0 00 00 01 11 11 11 22 22 22 33 33 33 34 44 44 44 55 55 55 66 66 66 67 77 77    8
1 34 67 90 23 56 89 12 45 78 01 34 67 90 23 56 89 12 45 78 01 34 67 90 23 56    0
```

| | | | | | | | | | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| GRID | GRID | GRID | GRID | GRID | GRID | GRID | GRID | GRID | GRID | GRID | GRID | GRID | GRID | GRID | GRID | GRID | GRID | GRID | GRID | GRID | GRID | GRID | GRID | GRID | |

FGRID and SGRID have the same formats.

13. Card Type 13

Omit if ISOUR is not set to 1 (see card type 4)

Area source emissions by 4-square mile grid---3 arrays---78 cards

AGRID1 - 650 values representing distribution of reactive hydrocarbon (propylene) emissions by grid in units of kilograms per hour. 25 values at 3 columns each per card.

AGRID2 - 650 values representing distribution of nitric oxide (NO) emissions by grid in units of kilograms per hour. 25 values at 3 columns each per card.

AGRID4 - 650 values representing distribution of less reactive hydrocarbons (DUMHC) emissions by grid in units of kilograms per hour. 25 values at 3 columns each per card.

FORMAT (25F3.0)

| 0<br>1 | 00<br>34 | 00<br>67 | 01<br>90 | 11<br>23 | 11<br>56 | 11<br>89 | 22<br>12 | 22<br>45 | 22<br>78 | 33<br>01 | 33<br>34 | 33<br>67 | 34<br>90 | 44<br>23 | 44<br>56 | 44<br>89 | 55<br>12 | 55<br>45 | 55<br>78 | 66<br>01 | 66<br>34 | 66<br>67 | 67<br>90 | 77<br>23 | 77<br>56 | 8<br>0 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| AGRID | AGRID | AGRID | AGRID | AGRID | AGRID | AGRID | AGRID | AGRID | AGRID | AGRID | AGRID | AGRID | AGRID | AGRID | AGRID | AGRID | AGRID | AGRID | AGRID | AGRID | AGRID | AGRID | AGRID | AGRID | | |

AGRID1, AGRID2, AGRID4 have the same formats.

14. Card Type 14

Chemical mechanism data---3 arrays---NEQ* cards (see card type 3)

RCT - Alphanumeric array of NEQ chemical reactions. Cols. 1-24.

IR - 5 integer values per card of species designations. These values reflect the mechanism being used. Columns 25-39, 3 columns per number, right justified.

C - array of NEQ double precision reaction rate constants. Cols. 40-54.

FORMAT (3A8, 5I3, D15.8, 26X)

| 0<br>1 | 22<br>45 | 22<br>78 | 33<br>01 | 33<br>34 | 33<br>67 | 34<br>90 | 55<br>45 | 8<br>0 |
|---|---|---|---|---|---|---|---|---|
| RCT | IR (1) | IR (2) | IR (3) | IR (4) | IR (5) | C | | |

*See card type 4.

15. Card Type 15

Chemistry parameters---1 array---1 card

Z - Chain termination rate factors

Z(1) Combination of free radicats - current value used is 100.0

Z(2) Combination of radicals with NO - current value used is 0.05

FORMAT (2D20.8)

| 0<br>1 | 22<br>01 | 44<br>01          8<br>             0 |
|---|---|---|
| Z(1) | Z(2) | |

16. Card Type 16

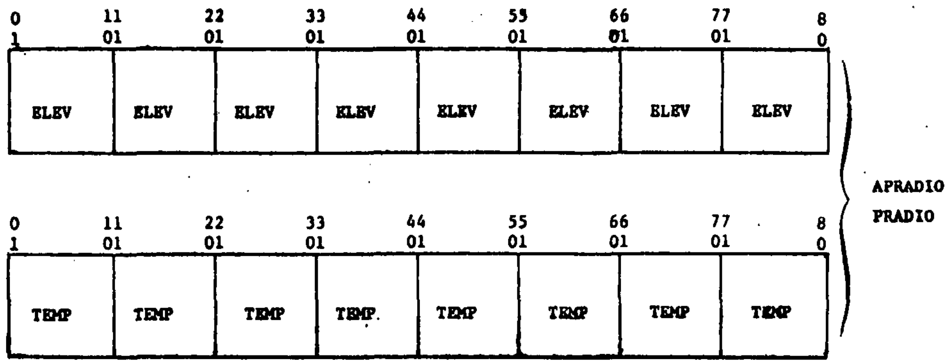
Omit if IHT is 1 (see card type 4)

Radiosonde data---2 arrays---maximum of 8 cards

ARADIO - AM radiosonde curve of NRAD (see card type 4) elevations in meters followed by NRAD temperatures in degrees centigrade. The first temperature is the temperature at the lowest elevation, the second temperature is the one at the next elevation etc. The temperatures must begin on a separate card. If NRAD is greater than 8, two cards must be used for elevation, followed by two for temperature. Ten columns are used for each elevation and temperature. The last column in each field is in tenths of a meter or degree.

PRADIO - PM radiosonde curve of NRAD elevations and temperatures. Data is identical to that for the array ARADIO. If only one radiosonde curve is available, the same one is used for both curves. If two curves are available, the model assumes they have the same number of points.

FORMAT (8F10.1)



# Section VI

## Sample Input Deck for REM

### Card Type 1

```
TRAJECTORY RUN ON SEPTEMBER 26, 1972
     SEPTEMBER 30, 1969                RUN TO POMONA AT 13:30
         390 MINUTE RUN
              25 METEOROLOGICAL STATIONS
```

### Card Type 2

```
57.5261   10.9335      7.01       50.0
```

### Card Type 3

```
390.0     .0001      0.1      .001      .01     100.0
```

### Card Type 4

```
12   25   33   0   25   0   12   2   6   1   1   0   0   0
```

### Card Type 5

```
15      0.   0.   30.   60. 100. 140. 180. 220. 260. 300. 330. 360. 380. 386. 389.
```

### Card Type 6*

```
80   200   260   220   260   300   315   450   500   460   400   300
```

### Card Type 7

```
NO2      0.106302D 02NO       0.364916D 0203       0.168827D 01C3H6     0.25      D 02
HNO3     0.0          CH3CHO  0.0         HCHO     0.0          CO (PPM)0.166638D 02
CH3ONO2  0.0          C2H3NO5 0.0         FIXED   020.0         DUMHC    0.25      D 03
         0.0          H       0.0         OH       0.0          HO2      0.0
CH3      0.0          CH3O    0.0         CH3O2    0.0          C2H3O    0.0
C2H3O2   0.0          C2H4O2  0.0         O        0.0          NO3      0.0
C2H3O3   0.0
```

### Card Type 8

```
 6   87    7   74    9   63    9   52   10   42   11   36   12   34   13   38
14   46   15   57   16   68   17   80
```

*Card type is shown only for illustrative purposes. As a result of inputs shown on Card Type 3, this data should be omitted.

Card Type 9

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| LAX07418 5 | 66621114 | 18 6 | 69641115 | 24 8 | 71651119 | 113 3 | | |
| LAX11422 8 | 76641111 | 24 9 | 78631103 | 25 12 | 79621095 | 25 13 | 76611089 | |
| LAX15423 13 | 76601084 | 25 10 | 75581074 | 24 12 | 73611074 | 21 8 | 70631070 | |
| BUR07428 3 | 7052 | 12 3 | 7753 | 9 9 | 8251 | 90 7 | | |
| BUR11415 7 | 9150 | 15 9 | 9158 | 15 9 | 9455 | 15 14 | 9345 | |
| BUR15414 9 | 9245 | 9 9 | 9448 | 10 9 | 8651 | 10 9 | 8153 | |
| LGB074 90 1 | 65571122 | 11 3 | 70601125 | 17 7 | 74591125 | 17 6 | 68581122 | |
| LGB11417 8 | 80591119 | 13 12 | 82571108 | 17 14 | 82581098 | 17 10 | 84591091 | |
| LGB15428 12 | 87531038 | 31 8 | 85521081 | 10 7 | 80611078 | 10 6 | 73611081 | |
| NTB07400 00 | 64621115 | 13 2 | 72621116 | 19 6 | 76201117 | 20 5 | 80621113 | |
| NTB11400 00 | 0000 | 22 8 | 81601104 | 20 12 | 82591095 | 20 13 | 80581087 | |
| NTB15420 13 | 78621083 | 20 7 | 78611075 | 00 00 | 0000 | 17 6 | 70621073 | |
| CAP07418 3 | | 18 3 | | 18 6 | | 18 5 | | |
| CAP11422 7 | | 22 8 | | 22 13 | | 27 11 | | |
| CAP15427 6 | | 22 6 | | 22 6 | | 22 6 | | |
| HOL074225 2 | | 225 2 | | 135 2 | | 225 2 | | 093019 |
| HOL114225 2 | | 225 2 | | 225 1 | | 180 2 | | 093020 |
| HOL154225 2 | | 225 6 | | 225 6 | | 225 2 | | 093021 |
| PIC07427 1 | | 22 2 | | 18 2 | | 18 2 | | |
| PIC11418 2 | | 18 2 | | 22 1 | | 18 1 | | |
| PIC15422 1 | | 18 1 | | 18 1 | | 22 1 | | |
| RLA074 45 1 | | 180 1 | | 45 1 | | 180 1 | | 093025 |
| RLA114180 1 | | 225 1 | | 180 1 | | 225 2 | | 093026 |
| RLA154225 1 | | 225 1 | | 225 1 | | 225 1 | | 093027 |
| VER074180 2 | | 180 3 | | 135 2 | | 135 7 | | 093028 |
| VER114180 9 | | 18010 | | 180 8 | | 18010 | | 093029 |
| VER15422514 | | 225 9 | | 225 7 | | 225 7 | | 093030 |
| WNT074 7 3 | | 11 3 | | 27 3 | | 24 5 | | |
| WNT11420 7 | | 22 9 | | 20 9 | | 20 8 | | |
| WNT15420 8 | | 18 6 | | 16 7 | | 16 5 | | |
| WLA07425 1 | | 18 1 | | 20 2 | | 20 1 | | |
| WLA11420 2 | | 20 3 | | 22 4 | | 22 5 | | |
| WLA15422 5 | | 22 3 | | 22 3 | | 22 1 | | |
| WHT074180 2 | | 158 2 | | 180 3 | | 180 3 | | 093037 |
| WHT114203 3 | | 203 6 | | 203 6 | | 180 7 | | 093038 |
| WHT154158 5 | | 180 4 | | 158 5 | | 158 3 | | 093039 |
| PAS07434 1 | | 13 1 | | 9 3 | | 11 2 | | |
| PAS11416 3 | | 18 3 | | 20 4 | | 22 7 | | |
| PAS15420 5 | | 20 3 | | 16 2 | | 16 1 | | |
| VEN07418 1 | | 16 2 | | 18 2 | | 18 5 | | |
| VEN11420 5 | | 25 5 | | 22 5 | | 25 6 | | |
| VEN15420 10 | | 22 5 | | 22 3 | | 13 1 | | |
| RVA074 45 2 | | 90 3 | | 90 5 | | 158 5 | | 093046 |
| RVA114158 5 | | 158 6 | | 203 8 | | 20310 | | 093047 |
| RVA154225 8 | | 225 6 | | 203 5 | | 203 5 | | 093048 |
| RES07427 1 | | 20 1 | | 20 1 | | 22 3 | | |
| RES11422 3 | | 27 3 | | 25 6 | | 25 8 | | |
| RES15427 8 | | 29 6 | | 31 2 | | 11 1 | | |
| RB 07418 5 | | 20 4 | | 20 2 | | 20 4 | | |
| RB 11422 5 | | 22 5 | | 22 7 | | 20 7 | | |
| RB 15420 7 | | 18 7 | | 20 9 | | 20 6 | | |
| CPK074315 1 | | 248 1 | | 225 1 | | 248 1 | | 093055 |
| CPK114225 2 | | 315 3 | | 293 6 | | 293 6 | | 093056 |
| CPK154315 4 | | 338 4 | | 338 3 | | 158 1 | | 093057 |
| KFI074180 1 | | 135 2 | | 203 3 | | 225 2 | | 093064 |
| KFI114225 5 | | 225 7 | | 225 9 | | 225 8 | | 093065 |
| KFI154203 8 | | 225 6 | | 225 7 | | 225 5 | | 093066 |
| ENC07422 3 | | 24 2 | | 34 2 | | 2 3 | | |
| ENC11416 4 | | 12 8 | | 18 8 | | 27 8 | | |

## Card Type 9 (continued)

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| ENC15427 9 | | 27 6 | | 29 5 | | 6 4 | | |
| ELM074315 1 | | 158 1 | | 180 1 | | 180 3 | | 093069 |
| ELM114225 4 | | 203 6 | | 18010 | | 22511 | | 093070 |
| ELM154180 8 | | 18012 | | 180 6 | | 180 8 | | 093071 |
| COM07416 2 | | 29 2 | | 22 3 | | 18 4 | | |
| COM11422 3 | | 27 7 | | 29 9 | | 29 12 | | |
| COM15429 14 | | 29 10 | | 29 7 | | 31 8 | | |
| POM074135 2 | | 180 2 | | 203 2 | | 270 2 | | 093082 |
| POM114270 5 | | 248 6 | | 270 6 | | 248 7 | | 093083 |
| POM154293 5 | | 270 5 | | 270 4 | | 293 3 | | 093084 |
| AZU07413 1 | | 13 2 | | 18 3 | | 18 3 | | |
| AZU11422 6 | | 22 8 | | 20 9 | | 20 12 | | |
| AZU15420 13 | | 20 7 | | 20 7 | | 20 3 | | |
| ONT07436 3 | 6949 | 17 5 | 7753 | 20 6 | 7952 | 27 6 | 8659 | |
| ONT11423 9 | 8553 | 28 12 | 9354 | 27 14 | 9344 | 00 00 | 0000 | |
| ONT15426 16 | 9161 | 26 16 | 8955 | 00 00 | 0000 | 27 9 | 8156 | |

## Card Type 10

| | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| LAX | 32 | 27 | 99 | BUR | 33 | 45 | 699 | LGB | 45 | 18 | 34 | NTB | 51 | 16 | 27 |
| CAP | 40 | 33 | 250 | HOL | 35 | 37 | 300 | PIC | 33 | 34 | 100 | RLA | 45 | 26 | 100 |
| VER | 41 | 31 | 180 | WNT | 63 | 30 | 950 | WLA | 29 | 34 | 200 | WHT | 51 | 28 | 250 |
| PAS | 47 | 42 | 870 | VEN | 26 | 30 | 5 | RVA | 48 | 29 | 180 | RES | 22 | 46 | 800 |
| RB | 31 | 21 | 10 | MSH | 28 | 48 | 850 | KFI | 53 | 23 | 100 | ENC | 24 | 43 | 800 |
| ELM | 51 | 35 | 300 | COM | 41 | 23 | 100 | POM | 69 | 34 | 850 | AZU | 59 | 41 | 600 |
| ONT | 72 | 35 | 916 | | | | | | | | | | | | |

## Card Type 11

2 4 80 16

## Card Type 12

```
                                                                               F01
                                                              18               F02
                                                              80  6            F03
                                                                  97 95 61 59  F04
                                                          115160163148     91  F05
                                                       153 78        67169 77  F06
                                11 22               181112183150    257131     F07
                               143 45107      529349213 144   25398156161      F08
                               131343545340323195            145 68    137     F09
                               625   236      278    59 83330251138108207  85  F10
                         391326217   241    56383102243253        15       16  F11
                      351 32   257   159131   314289104                        F12
                      348      305      302   527 30                           F13
                      404      366 _     281129444 33                           F14
                  295160       391      283332   265       12 59 42 21   3     F15
            101295511 51       531449623576      205263156 70           3  15  F16
               473141333426466795452585518224  79234285147                 16  F17
            242137           205436620257257297306311254362291214203170173159  F18
            356          215194290335193109                                    F19
            352      140275    423    13 90 28       41 74 66 65 43 11         F20
1692713111383890456426494178395190 51                                          F21
            222   126 17104150           37                                    F22
            242   156158109                                                    F23
            155 68144                                                          F24
 59          94119                                                             F25
```

Card Type 12 (continued)

```
            166                                                                F26
                                                                 5119 18       S01
                                                           7218196 52          S02
                                                       34104277 94114 10       S03
                                                    36125107248215100 29 15    S04
                             5  5                36 24133135116 74 80 11 26    S05
                    4  5 25176 88             33 48114195116166203190 98 19    S06
                   30 49 28142145 75157126153175 60125212200219249266182 32    S07
                   46121188266254157413386317162 75116209220255149168163 28    S08
                    1239304249175 94283192282165155173259228304169123109 11    S09
                    9360324231124 79204288430204138186305242323241113 31  6    S10
                  124215412322210121270312301 93 96104270179290197 82 48 30    011
                  189255328358176265293257298241230135114 62129114 95 57  4    S12
                22261296397285314254292255386263229234181240156103 21  9  7    S13
               106266413392331393273322305265253190295119 42 22  1 37  1  5    S14
             88305255255311473477364292273299198185 69 21 82 42 90 33 12       S15
         125476254338261412413512328324293264195127 43 39227121 45 53 27  5    S16
 47 64 99117231512346459478468642579290199186 75108173131180142 18 48 50 73    S17
    18     7 98283403549512572473226217229285243250242114190280244 71 10 99    S18
  9 25     2 30 70 32260478375259164116190236227236185160130155232143 66 77    S19
 25 30 17 12 59 63121155116 25245242191162318308241218183 77126149151 76 32    S20
139118107194182350268280247180204204 21173241212156 91 57  1  6  6  2          S21
239250249250264414328276212215  4131 58 91113 21  1  2           1  2          S22
137255238238266295251233 54 20 27157 50  4        1                 2          S23
 60155202223252221152 85 66 84 73  7  2        2                    2          S24
 35 12 34149146172135 43 28 17  1        4  2  1  2  2  1           2          S25
             60125 50                                                          S26
```

Card Type 13

```
                                                                 5             H01
                                                             10 11             H02
                                                        5 11 11 11             H03
                                                     5 11 11 11 11             H04
                             5                    5 11 11 11 11                H05
                   10 15 21 31 11              5 11 11 11 11 11 11 11          H06
                   25 30 32 33 18 18 18 18  3 14 11 11 11 11 11 11 11 11       H07
                   15 30 32 33 33 67 33 35 33 33 11 11 11 11 11 11 11 11       H08
                    1 31 39 47 50 78 34 34 34 34 32 13 11 11 11 11 11 10       H09
                    6 31 72 61 63 45 36 36 36 36 34 15 13 11 11 11 11  5       H10
                    6 31 46 61 61 36 36 39 36 36 34 34 13 11 11 11 11  2       H11
                   94 56 56 56 56 70 70 57 50 45 46 36 33 11 11 11  6          H12
                10 56 56 56 56 56 70 70 57 45 45 42 36 33 11 11  5             H13
                30 51 51 51 51 51 90 90 70 50 50 35 35 20  4  4                H14
             25 40 45 45 47 49 49110110 82 56 56 34 19 12 34  9  2  2  1       H15
          20 40 40 45 45 47 49 49110110 82 56 56 34  4 22 39 39 32 32  1       H16
 30 30 30 35 39 39 33 33 35 37 37 60 60 53 45 45 62 62 49 36 36  1  1  4 30    H17
           5 24 39 33 33 35 37 37 60 60 53 45 45 62 62 49 36 36 31 31  4 30    H18
              5 15 23 33 36 39 39 48 48 44 40 40 49 43 43 38 38 31 31 32 30    H19
     1  1    15 15 19 34 38 42 42 36 36 35 35 35 37 37 39 41 41 30 30 20 10    H20
 30 31 31 30 30 30 34 34 38 42 42 36  6 35 35 35 37 37 39 41 41 30 15          H21
 30 31 31 35 39 39 53 53 48 33 23 31 31 30 25 15                               H22
 30 31 31 35 39 39 53 53 48 13 13 31 16  5                                     H23
           3 36 36 42 42 40 37 27 10                                           H24
           1 32 32 31 31  1                                                    H25
                                                                               H26
                                                              1  3             N01
                                                           3 11 11             N02
```

Card Type 13 (continued)

```
                                                        5 11 11 11            N03
                                                     5 11 11 11 11            N04
                                                  5 11 11 11 11               N05
                    4  6 15 20  2              5 11 11 11 11 11 11 11         N06
                   14 18 21 23 25 37 37 30 22 13 11 11 11 11 11 11 11 11      N07
                   10 18 21 23 23480 35 55 21 21 11 11 11 11 11 11 11 11      N08
                      19 24 29 63603 30 26 22 22 13 11 11 11 11 11 11  8      N09
                    5 21371 34 61141 25 24 23 23 19 11 11 11 11 11 11  5      N10
                    6 21 27 34 34 25 25 24 23 23 19 19 11 11 11 11 11  2      N11
                  584 29 25 22 22 24 24 24 92 23162 27 23 11 11 11  8         N12
                 6 29 29 25 22 22 24 24 24 23 23106 27 23 11 11  5            N13
                13 25 25 22 20 20 31 31 26 22 22 22 18  7                     N14
             10 19 21 21 20 19 20 38 38 29 21 21 19  5  3  9  2  1  1         N15
           4  9 18 20 20 20 19 19 37 37 29 21 21  9  1  6 15 19 18 18  9  8   N16
  8  8  8  9 19 19 19 20 20 21 21 21 21 20 19 19 22 22 21 20 20  1  1  1 10   N17
           1  6 10 10 10 11 12 12 12 12 11 10 10 13 13 12 11 11  9  9  1 10   N18
           1  3  7  9 18 19 19 19 19 19 18 18 18 19 19 20 20 20 17 17  9  9   N19
              4  4  4  8  9 10 10  9  9 18 16  8 16 18 18 14 13  9  9  7      N20
  8  8 12 14 12  8  8  8  9 10 10  9  1  9 10 10 16 19 16 14 13  9  9  9  8   N21
  8  9 13 18 15 15 17 15 12  7  4  8  8  8  8  3                              N22
  8  9  9 18 17 15 15 15 12  1  1  8  4  1                                    N23
     1  1  1 10 10 12 12 11  9  7  2                                          N24
              9  9  9  9  1  1                                                N25
                                                                              N26
                                                                 15           L01
                                                              40 44           L02
                                                        20 44 44 44           L03
                                                     20 44 44 44 44           L04
                           10                    20 44 44 44 44               L05
                   11 26 72 95 26             20 44 44 44 44 44 44 44         L06
                   60 79 96111 63 91 91 91131 55 44 44 44 44 44 44 44 44      L07
                   40 79 96111111491156145 94 94 44 44 44 44 44 44 44 44      L08
                    3 78130182208576144122101101 86 51 44 44 44 44 44 40      L09
                   24 96433251271218131120108108 94 59 51 44 44 44 44 20      L10
                   54 96173251251131131152108108 94 94 51 44 44 44 44  5      L11
                  633233214193193245245197202150241137109 44 44 45 31         L12
                30233233214193193245245197150150196137109 44 44 23  1         L13
             10 90189189179175175333333277170170118118 68 19 19  1  1  1      L14
             71120145145150156156426426307189189 98 59 99108 38  7  7  4      L15
          41120121145145150156156426426307189189 98 19 69117117 86 86  4      L16
 79 79 79 99118118 90 90 98106106204204174143143212212158104104  6  6 21115   L17
          20 79118 90 90 98106106204204174143143212212158104104 85 85 21115   L18
    1  1 11 21 41 74 93105118118153153136122122159159137117117 82 82 90 97   L19
    2  2  2 41 41 57 96113129129103103102101101108106118128128 80 80 62 21   L20
 79 81 81 81 80 80 96 96113129129103 24102101101108108118129129 80 41  2  1   L21
 80 84 84105125125180180158116 76 81 81 80 70 30                              L22
 80 84 84105125125180180158 56 56 81 52 11                                    L23
    3  3  8108108123133101107 83 22  2  1                                     L24
           6 91 91 85 85  3                                                   L25
                                                                              L26
```

Card Type 14

```
NO2+HV       =NO+O          1  0  2 23  0 0.40       D 00
O+O2+M       =O3+M         23  0  3  0  0 0.14       D 07
O3+NO        =NO2+O2        3  2  1  0  0 0.4        0 00
NO2+O3       =NO3+O2        1  3 24  0  0 0.1        D-04
C2H3O3+O2 = C2H3O2+O3      25  0 21  3  0 0.2        D 02
NO3+NO       =2NO2         24  2  1  1  0 0.245      D 03
C3H6+OH = CH3CHO+CH3        4 15  6 17    0.1        D 04
NO+HO2       =NO2+OH        2 16  1 15  0 0.1        D 02
H+O2+M       =HO2+M        14  0 16  0  0 0.1        D 07
C2H3O + O2 = C2H3O3        20  0 25  0  0  .1        D 06

NO2+OH       =HNO3          1 15  5  0  0 0.1        D 03
OH+O3        =HO2+O2       15  3 16  0  0 0.1        D 02
OH+CO        =H+CO2        15  8 14  0  0 0.3        D 01
CH3+O2+M     =CH3O2+M      17  0 19  0  0 0.14       D 07
CH3O2+NO     =CH3O+NO2     19  2 18  1  0 0.2        D 01
CH3O+O2+NO =CH3O2+NO2      18  2 19  1  0 0.1        D 02
C2H3O3+NO = C2H3O2+NO2      2 25  1 21  0  .25       D 01
C2H3O2+NO    =C2H3O+NO2    21  2 20  1  0 0.2        D 02
C2H4O2+NO =CH3CHO+NO2      22  2  6  1  0 0.1        D 03
CH3O+O2      =HCHO+HO2     18  0  7 16  0 0.2        D 03
C3H6+O       =CH3+C2H3O     4 23 17 20  0 0.350      D 02
C3H6+O3      =HCHO+C2H4O2   4  3  7 22  0 0.5        D-04
C3H6+O+O2    =HCHO+C2H4O2   4 23  7 22  0 0.175      D 02
C2H4O2+O2 = C2H3O3+OH      22  0 15 25  0  .3        D 03
C3H6+HO2     =CH3O+CH3CHO   4 16 18  6  0 0.1        D 01
C3H6+MEO2=CH3+MEO+C2H3O     4 19 17 18 20 0.1        D-01
C2H3O+M      =CH3+CO+M     20  0 17  8  0 0.1        D 02
CH3O+NO2     =CH3ONO2      18  1  9  0  0 0.1        D 01
C2H3O3+NO2 = C2H3O3NO2      1 25 10  0  0  .2        D 00
DUMHC+O      =CH3+C2H3O    12 23 17 20  0 0.70       D 01
HCHO + HV = H + H + CO      7  0 14 14  8 0.3        D-02
NO2 +NO3 +H2O = HNO3+ "     1 24  5  5  0 0.1        D 03
```

Card Type 15

```
.1      D 03          .5      D-01
```

Card Type 16

```
33.5     97.5     289.6     591.3     1170.4    1517.9
17.7     18.9      23.0      27.7       25.5      22.4
50.0    100.6     149.4     359.7      640.1    1527.1
20.0     23.0      22.7      23.9       28.5      22.7
```

# Section VII
# Glossary

## A. COMMON REGIONS

### 1. KINCOM

A------Heading label
BB-----Numerical integration counter
C------Pollutant reaction rates
CC-----Plot data
D------Rates of reaction
DERY---Rates of change of species
INTR---Output list indicator
ITRAF--Execute traffic sources function indicator
KDIF---NDIF+2
LABEL--Species names
M------Page number of output
N------Temporary storage
NC-----No. of species
NDIF---No. of accumulating species
NEQ----No. of mechanism steps
NLL----No. of plot lines
NN-----No. of printouts
NNC----NC-NDIF
NNDIF--NDIF+1
PEAK1--Peak value of concentration 1
PEAK3--Peak value of concentration 3
PRMT---Parameter input list
RCT----Reaction list
STEP---Output list
TIM1---Half time of concentration 1
TIM2---Half time of concentration 2
TIM4---Half time of concentration 4
TIME1--Peak time of concentration 1
TIME3--Peak time of concentration 3
XPOS---X coordinate (miles)
YPOS---Y coordinate (miles)
YY-----Non-accumulating species
ZZ-----Chain yield

2. MYCOM

AIR----Meteorological data
AGRID1-Area source grid distribution of reactive hydrocarbons
AGRID2-Area source grid distribution of nitric oxide
AGRID4-Area source grid distribution of less reactive hydrocarbons
ARADIO-A.M. radiosonde curve
EMIT---Emission factors for vehicular sources
FGRID--Grid distribution of freeway traffic
ICLOUD-Type of clouds in sky
IDM----First time through METEOR module indicator
IDS----First time through SOURCE module indicator
IDU----First time through ULTRAV module indicator
IHT----Mixing height values input indicator
IPST---Pacific standard time indicator
NRAD---No. of radiosonde points
NSTA---No. of meteorological stations
POS----Stationary source position in meters
PRADIO-P.M. radiosonde curve
SGRID--Grid distribution of street traffic
TIME---Time of day
WPOS---Meteorological stations position and elevation
XDOT---X component of wind
XHITE--Array of input mixing height values
XMIN---Minimum mixing depth
YDOT---Y component of wind
ZENITH-12 hourly values of sun angle at Los Angeles

3. ALLCOM

ANS----Array of calculated meteorological values for the trajectory point
GOTIME-Simulation start time
GPOLL--Source inputs in gram-moles/minute
ISOUR--Execute source module indicator
POLL---Source inputs in pphm/minute
XDEPTH-Mixing depth
XDEPRV-Previous mixing depth

4. BARRR

IDB----First time through barrier check routine indicator

## B. MAIN

### 1. Arrays

CSAVE--Holds correction terms and derivatives for DIFSUB
ERROR--Contains estimated one step error
IDMET--Pollutant station names
IDNUM--Meteorological station names
IP-----Temporary storage space for pivots
PW-----Temporary storage space
SAVE---Saves matrix Y
Y------Dependent variables and their scaled derivatives
YMAX---Maximum values of Y
YSAVE--Temporary storage for Y

### 2. Scalars

ATEMP--Temporary temperature
BAROM--Barometric pressure
DEWPT--Dew point
IN-----Another simulation run indicator
KFLAG--DIFSUB completion code indicator
MAXDER-Maximum derivative number
MF-----Method indicator for Gear
NDIM---Order of set of ordinary differential equations

## C. SMGOUT

### 1. Arrays

Y------Dependent variables of differential equations (accumulating and non-accumulating species)

### 2. Scalars

H------Step size
HAL1---Half the current value of concentration 1
HAL2---Half the current value of concentration 2
HAL4---Half the current value of concentration 4
PREVY1-Previous value of concentration 1
PREVY2-Previous value of concentration 2
PREVY4-Previous value of concentration 4
PTIM1--Time when PREVY1 is saved
PTIM2--Time when PREVY2 is saved
PTIM4--Time when PREVY4 is saved
X------Time into simulation

D. DIFFUN

1. Arrays

DY-----First derivatives of accumulating species
Y------Set of accumulating and non-accumulating species
YSAVE--Temporary storage for Y

2. Scalars

STORE--Temporary rate of change of mixing depth
X------Time into simulation run
XPREV--Previous simulation time last step

E. METEOR

1. Arrays

DISINV-Sum of the square of the inverse distances from the air parcel location to the meteorological stations
DIST---Square of the distance from the air parcel point to a meteorological station
JBAR---Permissible station indicators
RADIO--Radiosonde curve in use
RSLOPE-Slopes of the line segments of RADIO
VAL1---Spatially interpolated meteorological values at first hour
VAL2---Spatially interpolated meteorological values at second hour

2. Scalars

HMIN---Minimum elevation point on the radiosonde curve
HOUR---Hour of the day
ITIME--Hour of the day minus 6
SLOPE--Adiabatic lapse rate
TIMEHR-Number of minutes into current hour
TMIN---Minimum temperature point on the radiosonde curve
X------X-coordinate position of the pollutant column
XPREV--Time previous cycle through routine
XTIME--Time into simulation run in minutes
XTIME1-Temporary storage of current time
XXDOT--X component of rate of change of wind
Y------Y-coordinate position of the pollutant column
YYDOT--Y-component of rate of change of wind

F. ULTRAV

1. Arrays

ABSORP-Absorption coefficients of $NO_2$ and $N_2O_4$
AIRMS--Air mass at various zenith angles
CLOUD--Average fractions of incident radiation transmitted by 7 cloud types
FLIST_-Dependent variable list corresponding to independent values in XLIST_
OZONE--Absorption coefficients of ozone in the ultraviolet region by wavelength, 3000A-4000A
SOLAR--Mean solar spectral irradiance outside the atmosphere for spectral bandwidths of 100A centered at wavelengths 3000A-4000A
VAPOR--Values of water vapor pressure for different temperatures
XLIST_-Independent variable interpolation list
XMOLE--Indices of refraction and molecular scattering coefficients for a homogeneous standard atmosphere at 3000A-4000A

2. Scalars

AIRMAS-Values of the air mass at various zenith angles
ALBEDO-Reflectively of the ground
ANGLE--Zenith angle of the sun
BETA---Value of air mass for given zenith angle
CANGLE-COS of zenith angle
C1-----Temporary storage
C2-----Temporary storage
DIRECT-Direct radiation from the sun in the smog layer
DUST---Dust content of the atmosphere; 1 near surface of urban areas, 0 in upper atmosphere
G------Parameter between 0 or 1 which is a function of the directional distribution of the scattered radiation and of the amount of multiple scattering
LAMDA--Wavelength in Angstroms
OZ3----Quantity of ozone in the atmosphere at standard temperature and pressure
PI-----3.14159
PRESS--Water vapor pressure
PZ-----Partial pressure of atmospheric water vapor
RATE---Specific ultraviolet absorpiton rate of $NO_2$
RATE1--Temporary storage
RATE2--Temporary storage
SCATOZ-Transmissivity with respect of ozone absorption
SCTMOL-Transmissivity relative to molecular scattering
SCTPAR-Transmissivity due to particle scattering
SKY----Radiation reflected from the sky into the smog layer

## G. SOURCE

### 1. Arrays

DIST---Square of the distance from the air parcel position to the midpoint of the three closest grid areas
EMITWT-Temporary storage
EPOS---Midpoints of three closest grid areas
FCURVE-Temporal distribution curve of freeway traffic
IBOX---Number of grid containing the air parcel
SCURVE-Temporal distribution curve of street traffic
WEIGHT-Molecular weight of major pollutants

### 2. Scalars

AREA1--Reactive hydrocarbon emissions in grid area containing parcel (kg./hr.)
AREA2--NO emissions in grid area containing parcel (kg./hr.)
AREA4--Less reactive hydrocarbon emission in grid area containing parcel (kg./hr.)
AX-----Value of diurnal area source usage curve at any time during the day
DISINV-Sum of the square of the inverse distance from the air parcel location to the midpoint of an adjoining grid square
FACTOR-Conversion factor inversely proportional to mixing depth
FWY----Daily freeway mileage in grid square containing air parcel
FX-----Value of diurnal curve for freeway traffic at any time during the day
GMIN---Minutes into current hour of the day
IHR----Current hour of the day
IPT----Grid square quadrant indicator
IXM----X-coordinate of midpoint of grid square containing air parcel
IYM----Y-coordinate of midpoint of grid square containing air parcel
STREET-Daily street traffic mileage in grid square containing air parcel
SX-----Value of diurnal curve for street traffic at any time during the day
X------X-coordinate of air parcel location
Y------Y-coordinate of air parcel location

# Section VIII

## Program Listing of Reactive Pollutant Environmental Simulation Model (REM)

OS/360 FORTRAN H

```
COMPILER OPTIONS - NAME=  MAIN,OPT=01,LINECNT=55,SIZE=0000K,
                   SOURCE,BCD,NOLIST,NODECK,LOAD,MAP,NOEDIT,ID,NOXREF
C     REACTIVE ENVIRONMENTAL MODEL          VERSION CB
C
      DIMENSION SAVE(13,40),CSAVE(40,3),YMAX(40),ERROR(40),PW(1600),
     1          IP(40),Y(13,40),YSAVE(40),IDNUM(32),IDMET(32),IR(50,5),
     2          DAIR(12,32,2),RSGRID(650),RFGRID(650),RGRID1(650),
     3          RGRID2(650),RGRID4(650)
      DOUBLE PRECISION C,D,Y,YY,ZZ,DERY,SAVE,CSAVE,YMAX,ERROR,YSAVE,
     1       POLL,PRMT,BB,Z
      REAL*8 LABEL,BLANK/'        '/,RCT
C
C
C     KINCOM---KINCOM---KINCOM---KINCOM---KINCOM
C
C     A-----HEADING LABEL
C     BB----SAVE PLOT DATA COUNTER
C     C-----POLLUTANT REACTION RATES
C     CC----PLOT DATA
C     D-----RATES OF REACTION
C     DERY--RATES OF CHANGE OF SPECIES
C     IDISP--TYPE OF DISPERSION CURVES
C     INTR--OUTPUT LIST INDICATOR
C     ISOUR-SOURCE EMISSIONS MODULE INDICATOR
C     ITRAF-TRAFFIC EMISSIONS MODULE INDICATOR
C     LABEL-SPECIES NAMES
C     N-----NO. OF COLUMNS FOR NUM. INT.
C     NC----NO. OF SPECIES
C     NDIF--NO. OF ACCUMULATING SPECIES
C     NEQ---NO. OF MECHANISM STEPS
C     NLL---NO. OF PLOT LINES
C     NN----NO. OF PRINTOUTS
C     NNC---NC-NDIF
C     NNDIF-NDIF+1
C     PEAK1-PEAK VALUE OF CONCENTRATION 1
C     PEAK3-PEAK VALUE OF CONCENTRATION 3
C     PRMT--PARAMETER INPUT LIST
C     RCT---REACTION LIST
C     STEP--OUTPUT LIST
C     TIM1--HALF TIME OF CONCENTRATION 1
C     TIM2--HALF TIME OF CONCENTRATION 2
C     TIM4--HALF TIME OF CONCENTRATION 4
C     TIME1-PEAK TIME OF CONCENTRATION 1
C     TIME3-PEAK TIME OF CONCENTRATION 3
C     XPOS--X COORDINATE (MILES)
C     YPOS--Y COORDINATE (MILES)
C     YY----NON-ACCUMULATING SPECIES
C     ZZ----CHAIN YIELD
C
C     NDIM--NO. OF ACCUMULATING SPECIES + 2
C     Y-----CONCENTRATIONS OF SPECIES
C
      COMMON /KINCOM/ ZZ(4),YY(40),LABEL(40),D(50),RCT(50,3),PRMT(8),
```

```
     1     DERY(40),C(50),BB,Z(2),N,NC,NEQ,NDIF,KDIF,M,NN,INTR,NNC,
     2     NNDIF,IUV,IM,IS,ITRAF,NLL,CC(16,100),A(80),STEP(15),TIM1,
     3     TIM2,TIM4,PEAK1,TIME1,PEAK3,TIME3,XPOS,YPOS
C
C
C
C
C
C     MYCOM---MYCOM---MYCOM---MYCOM---MYCOM---MYCOM
C
C     AGRID1-AREA SOURCE PROPYLENE EMISSIONS
C     AGRID1-AREA SOURCE NO        EMISSIONS
C     AGRID1-AREA SOURCE DUMHC     EMISSIONS
C     AIR----METEOROLOGICAL DATA
C     EMIT---TRAFFIC MODULE EMISSION RATES
C     ICLOUD-TYPE OF CLOUDS IN SKY
C     IDM----FIRST TIME THROUGH METEOR MODULE INDICATOR
C     IDS----FIRST TIME THROUGH SOURCE MODULE INDICATOR
C     IDU----FIRST TIME THROUGH ULTRAV MODULE INDICATOR
C     IHT----MIXING HEIGHT VALUES INPUT INDICATOR
C     IPST---PACIFIC STANDARD TIME INDICATOR
C     NRAD---NO. OF RADIOSONDE POINTS
C     NSTA---NO. OF METEOROLOGICAL STATIONS
C     NSTACK-NO. OF STATIONARY SOURCES
C     TIME---TIME OF DAY
C     WPOS---METEOROLOGICAL STATIONS POSITION AND ELEVATION
C     XDOT---X COMPONENT OF WIND
C     XHITE--ARRAY OF INPUT MIXING HEIGHT VALUES
C     XHT----MIXING HEIGHT
C     YDOT---Y COMPONENT OF WIND
C     ZENITH-12 HOURLY VALUES OF SUN ANGLE AT LOS ANGELES
C
      COMMON /MYCOM/ TIME,ICLOUD,IDM,IDU,IDD,IDS,IPST,NSTA,NSTACK,NRAD,
     1       AIR(12,32,6),WPOS(32,3),POS(32,3),SPOS(32,3),HS(12),
     2       DS(12),VS(12),TS(12),QS(12),SBAROM,STEMP,XDOT,YDOT,
     3       ARADIO(15,2),PRADIO(15,2),ZENITH(12,2),SGRID(650),
     4       FGRID(650),AGRID1(650),AGRID2(650),AGRID4(650),EMIT(10),
     5       XHITE(12),IHT,XMIN
C
      COMMON  /BARRR/ IDB
C     IDB----FIRST TIME THROUGH BARRIER CHECK INDICATOR
C
C
C     ALLCOM---ALLCOM---ALLCOM---ALLCOM---ALLCOM---ALLCOM
C
C     ANS----ARRAY OF CALCULATED METEOR. VALUES FOR THE TRAJ. PT.
C     GOTIME-SIMULATION START TIME
C     ISOUR--SOURCES MODULE INDICATOR
C     POLL---ARRAY OF CALCULATED TRAFFIC AND AREA SOURCES
C     XDEPTH-MIXING DEPTH AT TRAJECTORY POINT
C     XDEPRV-LAST CALCULATED MIXING DEPTH
C
      COMMON /ALLCOM/ POLL(4,3),GPOLL(4,3),ANS(8),GOTIME,XDEPTH,ISOUR,
```

```
     1                  XDEPRV
C
C
C
      EXTERNAL DIFFUN
      RH(ATEMP,DEWPT) = 10.**(7.5*(DEWPT/(DEWPT+237.3)
     1                   -ATEMP/(ATEMP+237.3)))
C
C     INITIALIZATION
C
C
C     INPUT HEADING INFORMATION
C
      IN = 0
    1 READ (5,1000,END=900) A
      JSTART = 0
      DO 10  I=1,40
      DO 5  J=1,13
    5 Y(J,I) = 0.D0
      YMAX(I) = 1.0D0
      YSAVE(I) = 0.D0
      LABEL(I) = BLANK
      D(I) = 0.0D0
   10 DERY(I) = 0.0D0
      DO 20  I=1,4
   20 ZZ(I) = 0.0D0
      N = 0
      M = 1
      NN = 1
      BB = 1.0E08
      IDB = 0
      IDD = 0
      IDM = 0
      IDS = 0
      IDU = 0
      IPST = 0
      IUV = 0
      IM = 0
      IS = 0
      DO 30  I=1,4
      DO 30  J=1,3
      SPOLL(I,J) = 0.
   30 POLL(I,J) = 0.D0
C
      BAROM = 1013.
      COVER = 0.
C
C     INPUT START POSITION, START TIME, MINIMUM XDEPTH
C     INPUT LENGTH OF SIMULATION, HMIN, HMAX, INITIAL STEP SIZE, ERROR
C           CRITERION, PLOT VALUE INDEX
C
      READ (5,1001) XPOS,YPOS,GOTIME,XMIN
      READ (5,1006) (PRMT(I),I=2,7)
```

```
      IF (PRMT(7))  70,70,75
   70 PRMT(7) = 2.D0*PRMT(2)
   75 PRMT(1) = 0.
      PRMT(8) = PRMT(1)
C
C     INPUT NO. OF ACCUMULATING SPECIES, TOTAL NO. OF SPECIES, NO. OF
C           MECHANISM STEPS, PLOT LINE PARAMETER, NO. OF METEOROLOGICAL
C           STATIONS, NUMERICAL INTEGRATION METHOD, NO. OF DERIVS, CLOUD
C           TYPES, NO. OF RADIOSONDE POINTS, TRAFFIC MODULE, SOURCE
C           MODULE, MIXING HEIGHT, SAME DAY FOR NEXT RUN, AND PACIFIC
C           STANDARD TIME INDICATORS
C
      READ (5,1002) NDIM,NC,NEQ,NLL,NSTA,MF,MAXDER,ICLOUD,NRAD,ITRAF,
     1  ISOUR,IHT,IN,IPST
C
C     INPUT OUTPUT INDICATOR AND LIST OF APPROXIMATE OUTPUT TIMES
C
      READ (5,1003) INTR,STEP
      NDIF = NDIM
      NDIM = NDIM+2
      KDIF = NDIM
      NNDIF = NDIF+1
C
C     INPUT MIXING HEIGHT
C
      IF (IHT .NE. 1)   GO TO 80
      READ (5,1020)  XHITE
C
C     INPUT SPECIES LIST AND INITIAL CONCENTRATIONS
C           CONCENTRATIONS ARE IN PPHM EXCEPT FOR CO IN PPM
C
   80 READ (5,1004)  (LABEL(I),Y(1,I),I=1,NC)
C
C     SAVE NON-ACCUMULATING SPECIES
C
      DO 85  I=NNDIF,40
      YY(I) = Y(1,I)
   85 Y(1,I) = 0.D0
C
C
C
C
C
C
C     CHECK FOR SECOND RUN
C
      IF (IN .EQ. 1)   GO TO 300
C
C     INPUT SUN ANGLE AT LOS ANGELES
C
      READ (5,1032) ((ZENITH(I,J),J=1,2),I=1,12)
C
C     INPUT METEOROLOGICAL DATA.
```

```
C
      DO 100  J=1,NSTA
      READ (5,1005)  IDNUM(J),((AIR(I,J,K),K=1,4),I=1,4)
      READ (5,1005)  IDNUM(J),((AIR(I,J,K),K=1,4),I=5,8)
  100 READ (5,1005)  IDNUM(J),((AIR(I,J,K),K=1,4),I=9,12)
C
C     INPUT METEOROLOGICAL STATION DATA
C
      WRITE (6,1013)
      READ (5,1014) (IDMET(I),(WPOS(I,J),J=1,3),I=1,NSTA)
C
C     CONVERT DATA TO METRIC UNITS
C
      DO 120  I=1,NSTA
      WPOS(I,3) = WPOS(I,3)*.3048
      DO 120  J=1,12
      IF (AIR(J,I,3) .EQ. 0)  GO TO 105
      AIR(J,I,3) = (AIR(J,I,3)-32.)*.55555
  105 IF (AIR(J,I,4) .EQ. 0)  GO TO 120
  107 AIR(J,I,4) = (AIR(J,I,4)-32.)*.55555
  120 CONTINUE
C
C     DETERMINE RELATIVE HUMIDITY.
C
  130 DO 150  I=1,12
      DO 150  J=1,NSTA
      IF (AIR(I,J,3) .NE. 0.)  GO TO 140
      AIR(I,J,4) = 0.
      GO TO 150
  140 IF (AIR(I,J,4) .EQ. 0.)  GO TO 150
      ATEMP = AIR(I,J,3)
      DEWPT = AIR(I,J,4)
      AIR(I,J,4) = RH(ATEMP,DEWPT)
  150 CONTINUE
C
C     OUTPUT METEOROLOGICAL DATA
C
  160 WRITE (6,1015) (IDMET(I),(WPOS(I,J),J=1,3),I=1,NSTA)
      IF (IHT .NE. 1)    GO TO 165
      WRITE (6,1021)  XHITE
  165 KOUT = 0
      WRITE (6,1007)
      DO 180  I=1,12
      IH = (I+6)*100
      DO 180  J=1,NSTA
      IF (KOUT .LE. 50)   GO TO 170
      KOUT = 0
      WRITE (6,1007)
      GO TO 180
  170 KOUT = KOUT+1
  180 WRITE (6,1008)  IDNUM(J),IH,(AIR(I,J,K),K=1,4)
C
C     SAVE  WIND DATA
```

```
C
      DO 200  J=1,12
      DO 200  I=1,NSTA
      DAIR(J,I,1) = AIR(J,I,2)
  200 DAIR(J,I,2) = AIR(J,I,1)
C
C     CONVERT WIND DATA TO RADIANS
C
      DO 230  J=1,12
      DO 230  I=1,NSTA
      AIR(J,I,1) = -DAIR(J,I,1)*SIN(DAIR(J,I,2)*3.14159/180.)
  230 AIR(J,I,2) = -DAIR(J,I,1)*COS(DAIR(J,I,2)*3.14159/180.)
C
C     INPUT TRAFFIC DATA.
C
      IF (ITRAF .EQ. 0)  GO TO 240
      READ (5,1027) EMIT
      READ (5,1009) FGRID,SGRID
      DO 232  I=25,650,25
      DO 232  J=1,25
      JJJ = J-I+650
      III = J+I-25
      RFGRID(JJJ) = FGRID(III)
  232 RSGRID(JJJ) = SGRID(III)
      WRITE (6,1029) RFGRID
      WRITE (6,1030) RSGRID
      DO 235  I=1,650
      FGRID(I) = FGRID(I)*1000.
  235 SGRID(I) = SGRID(I)*1000.
C
C     INPUT AREA SOURCES DATA
C
  240 IF (ISOUR .EQ. 0)  GO TO 260
      READ (5,1009) AGRID1,AGRID2,AGRID4
      DO 233  I=25,650,25
      DO 233  J=1,25
      JJJ = J-I+650
      III = J+I-25
      RGRID1(JJJ) = AGRID1(III)
      RGRID2(JJJ) = AGRID2(III)
  233 RGRID4(JJJ) = AGRID4(III)
      WRITE (6,1034) RGRID1
      WRITE (6,1035) RGRID2
      WRITE (6,1036) RGRID4
      DO 250  I=1,650
      AGRID1(I) = AGRID1(I)*1000.
      AGRID2(I) = AGRID2(I)*1000.
  250 AGRID4(I) = AGRID4(I)*1000.
      WRITE (6,1028)   (EMIT(I),I=1,4)
C
C     INPUT REACTION DATA
C
  260 READ (5,1011)  ((RCT(I,J),J=1,3),(IR(I,K),K=1,5),C(I),I=1,NEQ)
```

```
      READ (5,1038) Z
C
C     INPUT AM AND PM RADIOSONDE CURVES
C
      IF (IHT .EQ. 1)    GO TO 280
      READ (5,1022) (ARADIO(I,1),I=1,NRAD)
      READ (5,1022) (ARADIO(I,2),I=1,NRAD)
      READ (5,1022) (PRADIO(I,1),I=1,NRAD)
      READ (5,1022) (PRADIO(I,2),I=1,NRAD)
      WRITE (6,1023) (ARADIO(I,1),ARADIO(I,2),I=1,NRAD)
      WRITE (6,1024) (PRADIO(I,1),PRADIO(I,2),I=1,NRAD)
  280 WRITE (6,1033) ((ZENITH(I,J),J=1,2),I=1,12)
      IN = 1
  300 WRITE (6,1025) (PRMT(I),I=2,7),GOTIME,MF,MAXDER,A
      WRITE (6,1010)
      DO 320  I=1,NEQ
  320 WRITE (6,1012) I,(RCT(I,J),J=1,3),C(I),(IR(I,K),K=1,5)
      WRITE (6,1039) Z
      WRITE (6,1031)
      WRITE (6,1037) (I,LABEL(I),Y(1,I),DERY(I),I=1,NC)
C
C     SET UP POSITION FOR INTEGRATION
C
      Y(1,NDIF+1) = XPOS
      Y(1,NDIF+2) = YPOS
  400 CALL DIFSUB (NDIM,PRMT(1),Y,SAVE,CSAVE,PRMT(5),PRMT(3),PRMT(4),
     1             PRMT(6),MF,YMAX,ERROR,KFLAG,JSTART,MAXDER,PW,IP)
      IF (KFLAG .NE. 1)  GO TO 900
      DO 420  J=1,NC
  420 YSAVE(J) = Y(1,J)
      CALL SMGOUT (PRMT(1),YSAVE,PRMT(5))
      JSTART = 1
      IF (PRMT(1) .LT. PRMT(2))  GO TO 400
      IF (NEQ .EQ. 1)    GO TO 1
      CALL SMGPLT
      GO TO 1
  900 WRITE (6,1026) KFLAG
      STOP
 1000 FORMAT(20A4)
 1001 FORMAT(4F10.3)
 1002 FORMAT(14I5)
 1003 FORMAT(I2,3X,15F5.2)
 1004 FORMAT(4(A8,D12.8))
 1005 FORMAT(A3,3X,4(F3.0,F3.1,F3.0,F2.0,6X),6X)
 1006 FORMAT(6F10.3)
 1007 FORMAT(1H1,'STATION',6X,'DATA',6X,'WIND',6X,'WIND',16X,'REL.',
     1       /' ','NUMBER',6X,'HOUR',6X,'DIR.',5X,'SPEED',6X,'TEMP',
     25X,'HUM.',                    /' ',22X,'(DEG)',5X,'(MPH)',4X,
     3'(CENT)',         //)
 1008 FORMAT(' ',A7,6X,I4,6F10.3)
 1009 FORMAT(25F3.0)
 1010 FORMAT('0K-VALUES FOR REACTIONS'//)
 1011 FORMAT (3A8,5I3,D15.8,26X)
```

```
1012 FORMAT(' ',I4,5X,3A8,D20.8,5X,5I3)                                 00341000
1013 FORMAT(1H1,30X,'METEOROLOGICAL STATIONS',/1H0,21X,'X-COORD',11X,   00342000
    1'Y-COORD',10X,'ELEVATION',/' ',3X,'STATION',11X,'(MILES)',11X,     00343000
    2'(MILES)',11X,'(METERS)'/)                                         00344000
1014 FORMAT(4(A3,2F5.2,F7.2))                                           00345000
1015 FORMAT(' ',A10,2F18.3,F19.3)                                       00346000
1020 FORMAT(12F6.0)                                                     00347000
1021 FORMAT(//////' INPUT MIXING HEIGHTS---0700 HOURS TO 1800 HOURS',//00348000
    110X,12F9.1)                                                        00349000
1022 FORMAT(8F10.1)                                                     00350000
1023 FORMAT(1H1,20X,'AM RADIOSONDE CURVE',///1H ,23X,'HEIGHT',6X,'TEMP'00351000
    1,/1H ,21X,'(METERS)    (CENT.)',//(1H ,19X,2F10.1))                00352000
1024 FORMAT(1H0,20X,'PM RADIOSONDE CURVE',///1H ,23X,'HEIGHT',6X,'TEMP'00353000
    1,/1H ,21X,'(METERS)    (CENT.)',//(1H ,19X,2F10.1))                00354000
1025 FORMAT('1',D10.4,' MIN SIMULATION',4X,'HMIN=',D10.4,4X,'HMAX=',    00355000
    1 D10.4,4X,'INITIAL H=',D10.4/30X,'ERROR CRITERIA=',D10.4,13X,      00356000
    2 'BB=',D10.4//' START TIME IS',F8.4,' HOURS',21X,'MF=',I2,14X,     00357000
    3 'MAXDER=',I3//4(' ',20A4,/))                                      00357100
1026 FORMAT(//////' KFLAG= ',I3)                                        00358000
1027 FORMAT(10F5.2)                                                     00359000
1028 FORMAT(//////' TRAFFIC EMISSION RATES',//'  PROPYLENE=',F5.2,10X, 00360000
    1'NO=',F5.2,10X,'CO=',F5.2,10X,'DUMHC=',F5.2)                       00361000
1029 FORMAT(1H1,'GRID DISTRIBUTION OF FREEWAY TRAFFIC IN THOUSANDS OF V00362000
    1EHICLE MILES PER DAY',//(25F5.0))                                  00363000
1030 FORMAT(1H1,'GRID DISTRIBUTION OF STREET TRAFFIC IN THOUSANDS OF VE00364000
    1HICLE MILES PER DAY'//(25F5.0))                                    00365000
1031 FORMAT(1H1,'STARTING VALUES'///,8X,'  COMPOUND   CONCN PPHM    CHA00366000
    1NGE, PPHM/MIN'/)                                                   00367000
1032 FORMAT(8(2F5.1))                                                   00368000
1033 FORMAT('0',20X,'ANGLE OF THE SUN AT LOS ANGELES',//'0',25X,'HOUR',00369000
    1 5X,'ANGLE',//(1H ,19X,2F10.1))                                    00370000
1034 FORMAT    (1H1,'GRID DISTRIBUTION OF REACTIVE HYDROCARBONS (PROPYL00371000
    1ENE) IN KILOGRAMS PER HOUR',//(25F5.0))                            00372000
1035 FORMAT(1H1,'GRID DISTRIBUTION OF NO IN KILOGRAMS PER HOUR',//(25F500373000
    1.0))                                                               00374000
1036 FORMAT(1H1,'GRID DISTRIBUTION OF LESS REACTIVE HYDROCARBONS (DUMHC00375000
    1) IN KILOGRAMS PER HOUR',//(25F5.0))                               00376000
1037 FORMAT(' ',5X,I3,1X,A8,2D16.7)                                     00377000
1038 FORMAT (2D20.8)                                                    00377100
1039 FORMAT (//////10X,'Z(1)=',D10.4,10X,'Z(2)=',D10.4)                 00377120
     END                                                                00378000
```

```
COMPILER OPTIONS - NAME=  MAIN,OPT=01,LINECNT=55,SIZE=0000K,
                  SOURCE,BCD,NOLIST,NODECK,LOAD,MAP,NOEDIT,ID,NOXREF
      SUBROUTINE DIFSUB(N,T,Y,SAVE,CSAVE,H,HMIN,HMAX,EPS,MF,YMAX,
     1                 ERROR,KFLAG,JSTART,MAXDER,PW,IP)
      IMPLICIT REAL*8 (A-H,Q-Z)
C*********************************************************************
C*                                                                   *
C* THIS SUBROUTINE INTEGRATES A SET OF N ORDINARY DIFFERENTIAL FIRST  *
C* ORDER EQUATIONS OVER ONE STEP OF LENGTH H AT EACH CALL.  H CAN BE  *
C* SPECIFIED BY THE USER FOR EACH STEP, BUT IT MAY BE INCREASED OR    *
C* DECREASED BY DIFSUB WITHIN THE RANGE HMIN TO HMAX IN ORDER TO      *
C* ACHIEVE AS LARGE A STEP AS POSSIBLE WHILE NOT COMMITTING A SINGLE  *
C* STEP ERROR WHICH IS LARGER THAN EPS IN THE L-2 NORM, WHERE EACH    *
C* COMPONENT OF THE ERROR IS DIVIDED BY THE COMPONENTS OF YMAX.       *
C*                                                                   *
C* THE PROGRAM REQUIRES FOUR SUBROUTINES NAMED                       *
C*    DIFFUN(T,Y,DY)                                                 *
C*    DECOMP(N,M,PW,IP)                                              *
C*    SOLVE(N,M,PW,CSAVE(1,1),IP)                                    *
C*    PEDERV(T,Y,PW,M)                                               *
C* THE FIRST, DIFFUN, EVALUATES THE DERIVATIVES OF THE DEPENDENT      *
C* VARIABLES STORED IN Y(1,I) FOR I = 1 TO N, AND STORES THE          *
C* DERIVATIVES IN THE ARRAY DY.  THE NEXT TWO ARE CALLED ONLY IF THE  *
C* METHOD FLAG MF IS SET TO 1 OR 2 FOR STIFF METHODS.  DECOMP IS A    *
C* STANDARD LU DECOMPOSITION WITH PIVOTING THAT DECOMPOSES THE MATRIX *
C* PW, LEAVING THE PIVOTS IN THE INTEGER ARRAY IP.  M IS THE DECLARED *
C* SIZE OF PW.  IP(N) IS SET TO 0 IF PW IS SINGULAR   SOLVE PERFORMS  *
C* BACK SUBSTITUTION ON THE CONTENTS OF CSAVE(I,1), LEAVING THE       *
C* RESULTS THERE.  THE MATRIX IN BOTH SHOULD BE SINGLE PRECISION,     *
C* WHILE ALL FLOATING POINT VECTORS SHOULD BE DOUBLE PRECISION.       *
C* PEDERV IS USED ONLY IF MF IS 1, AND COMPUTES THE PARTIAL           *
C* DERIVATIVES OF THE DIFFERENTIAL EQUATIONS AS DESCRIBED UNDER THE   *
C* MF PARAMETER.                                                     *
C*                                                                   *
C* THE PROGRAM USES DOUBLE PRECISION ARITHMETIC FOR ALL FLOATING      *
C* POINT VARIABLES EXCEPT THOSE STARTING WITH P.  THE FORMER ARE      *
C* SINGLE PRECISION TO SAVE TIME AND SPACE.                           *
C*                                                                   *
C* THE TEMPORARY STORAGE SPACE IS PROVIDED BY THE CALLER IN THE       *
C* INTEGER ARRAY IP, THE SINGLE PRECISION ARRAY PW, AND THE DOUBLE    *
C* PRECISION ARRAYS SAVE AND CSAVE.  THE ARRAY PW IS USED ONLY TO HOLD *
C* THE MATRIX OF THE SAME NAME, AND SAVE IS USED TO SAVE THE VALUES   *
C* OF Y IN CASE A STEP HAS TO BE REPEATED, BUT CSAVE IS USED TO HOLD  *
C* SEVERAL ARRAYS.  THE REGIONS USED ARE                              *
C*    CSAVE(I,1)    IS USED MAINLY TO HOLD THE CORRECTION TERMS IN THE *
C*                  CORRECTOR LOOP, AND HOLDS THE DERIVATIVES DURING   *
C*                  JACOBIAN EVALUATIONS.                              *
C*    CSAVE(I,2)    IS USED TO SAVE THE VALUES OF THE SUMS OF ALL OF THE*
C*                  CORRECTION TERMS IN THE PREVIOUS STEP AFTER THEY   *
C*                  HAVE BEEN ACCUMULATED IN THE ARRAY ERROR IN THE    *
C*                  CURRENT STEP.  THIS ENABLES THE BACKWARDS DIFFERENCE*
C*                  OF ERROR TO BE FORMED.  IT IS USED TO ESTIMATE THE *
C*                  STEP SIZE FOR ONE ORDER HIGHER THAN CURRENT.       *
```

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C*     CSAVE(I,3)    IS USED TO STORE THE DERIVATIVES WHEN THEY ARE
C*                   COMPUTED BY DIFFUN.
C*
C* THE PARAMETERS TO THE SUBROUTINE DIFSUB HAVE
C* THE FOLLOWING MEANINGS..
C*
C*    N          THE NUMBER OF FIRST ORDER DIFFERENTIAL EQUATIONS.  N
C*                 MAY BE DECREASED ON LATER CALLS IF THE NUMBER OF
C*                 ACTIVE EQUATIONS REDUCES, BUT IT MUST NOT BE
C*                 INCREASED WITHOUT CALLING WITH JSTART = 0.
C*    T          THE INDEPENDENT VARIABLE.
C*    Y          A 13 BY N ARRAY CONTAINING THE DEPENDENT VARIABLES AND
C*                 THEIR SCALED DERIVATIVES.  Y(J+1,I) CONTAINS
C*                 THE J-TH DERIVATIVE OF Y(I) SCALED BY
C*                 H**J/FACTORIAL(J) WHERE H IS THE CURRENT
C*                 STEP SIZE. ONLY Y(1,I) NEED BE PROVIDED BY
C*                 THE CALLING PROGRAM ON THE FIRST ENTRY.
C*                   IF IT IS DESIRED TO INTERPOLATE TO NON MESH POINTS
C*                 THESE VALUES CAN BE USED.  IF THE CURRENT STEP SIZE
C*                 IS H AND THE VALUE AT T + E IS NEEDED, FORM
C*                 S = E/H, AND THEN COMPUTE
C*                                 NQ
C*                   Y(I)(T+E) =  SUM  Y(J+1,I)*S**J
C*                                 J=0
C*    SAVE       A BLOCK OF AT LEAST 13*N FLOATING POINT LOCATIONS.
C*    CSAVE      N*3 FLOATING POINT LOCATIONS USED BY THE SUBROUTINES.
C*    H          THE STEP SIZE TO BE ATTEMPTED ON THE NEXT STEP
C*                 H MAY BE ADJUSTED UP OR DOWN BY THE PROGRAM
C*                 IN ORDER TO ACHEIVE AN ECONOMICAL INTEGRATION.
C*                 HOWEVER, IF THE H PROVIDED BY THE USER DOES
C*                 NOT CAUSE A LARGER ERROR THAN REQUESTED, IT
C*                 WILL BE USED.  TO SAVE COMPUTER TIME, THE USER IS
C*                 ADVISED TO USE A FAIRLY SMALL STEP FOR THE FIRST
C*                 CALL.  IT WILL BE AUTOMATICALLY INCREASED LATER.
C*    HMIN       THE MINIMUM STEP SIZE THAT WILL BE USED FOR THE
C*                 INTEGRATION.  NOTE THAT ON STARTING THIS MUST BE
C*                 MUCH SMALLER THAN THE AVERAGE H EXPECTED SINCE
C*                 A FIRST ORDER METHOD IS USED INITIALLY.
C*    HMAX       THE MAXIMUM SIZE TO WHICH THE STEP WILL BE INCREASED
C*    EPS        THE ERROR TEST CONSTANT.  SINGLE STEP ERROR ESTIMATES
C*                 DIVIDED BY  YMAX(I)  MUST BE LESS THAN THIS
C*                 IN THE EUCLIDEAN NORM. THE STEP AND/OR ORDER IS
C*                 ADJUSTED TO ACHEIVE THIS.
C*    MF         THE METHOD INDICATOR. THE FOLLOWING ARE ALLOWED..
C*                         0    AN ADAMS PREDICTOR CORRECTOR IS USED.
C*                         1    A MULTI-STEP METHOD SUITABLE FOR STIFF
C*                                SYSTEMS IS USED. IT WILL ALSO WORK FOR
C*                                NON STIFF SYSTEMS.  HOWEVER THE USER
C*                                MUST PROVIDE A SUBROUTINE PEDERV WHICH
C*                                EVALUATES THE PARTIAL DERIVATIVES OF
C*                                THE DIFFERENTIAL EQUATIONS WITH RESPECT
C*                                TO THE Y'S.   THIS IS DONE BY CALL
C*                                PEDERV(T,Y,PW,M). PW IS AN N BY N ARRAY
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C*                              WHICH MUST BE SET TO THE PARTIAL OF         *00483000
C*                              THE I-TH EQUATION WITH RESPECT              *00484000
C*                              TO THE J DEPENDENT VARIABLE IN PW(I,J).     *00485000
C*                              PW IS ACTUALLY STORED IN AN M BY M          *00486000
C*                              ARRAY WHERE M IS THE VALUE OF N USED ON     *00487000
C*                              THE FIRST CALL TO THIS PROGRAM.             *00488000
C*                        2   THE SAME AS CASE 1, EXCEPT THAT THIS          *00489000
C*                              SUBROUTINE COMPUTES THE PARTIAL             *00490000
C*                              DERIVATIVES BY NUMERICAL DIFFERENCING       *00491000
C*                              OF THE DERIVATIVES. HENCE PEDERV IS         *00492000
C*                              NOT CALLED.                                 *00493000
C*    YMAX    AN ARRAY OF  N LOCATIONS WHICH CONTAINS THE MAXIMUM           *00494000
C*              OF EACH Y SEEN SO FAR.  IT SHOULD NORMALLY BE SET TO        *00495000
C*              1 IN EACH COMPONENT BEFORE THE FIRST ENTRY. (SEE THE        *00496000
C*              DESCRIPTION OF EPS.)                                        *00497000
C*    ERROR   AN ARRAY OF  N ELEMENTS WHICH CONTAINS THE ESTIMATED          *00498000
C*              ONE STEP ERROR IN EACH COMPONENT.                           *00499000
C*    KFLAG   A COMPLETION CODE WITH THE FOLLOWING MEANINGS..               *00500000
C*                       +1   THE STEP WAS SUCCESFUL.                       *00501000
C*                       -1   THE STEP WAS TAKEN WITH H = HMIN, BUT THE     *00502000
C*                              REQUESTED ERROR WAS NOT ACHIEVED.           *00503000
C*                       -2   THE MAXIMUM ORDER SPECIFIED WAS FOUND TO      *00504000
C*                              BE TOO LARGE.                               *00505000
C*                       -3   CORRECTOR CONVERGENCE COULD NOT BE            *00506000
C*                              ACHIEVED FOR H .GT. HMIN.                   *00507000
C*                       -4   THE REQUESTED ERROR IS SMALLER THAN CAN       *00508000
C*                              BE HANDLED FOR THIS PROBLEM.                *00509000
C*    JSTART  AN INPUT INDICATOR WITH THE FOLLOWING MEANINGS..              *00510000
C*                       -1   REPEAT THE LAST STEP WITH A NEW H             *00511000
C*                        0   PERFORM THE FIRST STEP.  THE FIRST STEP       *00512000
C*                              MUST BE DONE WITH THIS VALUE OF JSTART      *00513000
C*                              SO THAT THE SUBROUTINE CAN INITIALIZE       *00514000
C*                              ITSELF.                                     *00515000
C*                       +1   TAKE A NEW STEP CONTINUING FROM THE LAST.     *00516000
C*              JSTART IS SET TO NQ, THE CURRENT ORDER OF THE METHOD        *00517000
C*              AT EXIT.  NQ IS ALSO THE ORDER OF THE MAXIMUM               *00518000
C*              DERIVATIVE AVAILABLE.                                       *00519000
C*    MAXDER  THE MAXIMUM DERIVATIVE THAT SHOULD BE USED IN THE             *00520000
C*              METHOD.  SINCE THE ORDER IS EQUAL TO THE HIGHEST            *00521000
C*              DERIVATIVE USED, THIS RESTRICTS THE ORDER. IT MUST          *00522000
C*              BE LESS THAN 13 FOR ADAMS AND 7 FOR STIFF METHODS.          *00523000
C*    PW      A BLOCK OF AT LEAST N**2 FLOATING POINT LOCATIONS.            *00524000
C*************************************************************************00525000
      DIMENSION Y(13,1), YMAX(1), SAVE(13,1), ERROR(1), PW(1),           00526000
     1          A(13),PERTST(12,2,3),CSAVE(N,3),IP(1)                     00527000
C*************************************************************************00528000
C* THE COEFFICIENTS IN PERTST ARE USED IN SELECTING THE STEP AND        *00529000
C* ORDER, THEREFORE ONLY ABOUT ONE PERCENT ACCURACY IS NEEDED.          *00530000
C*************************************************************************00531000
      DATA PERTST/2.,4.5,7.333,10.42,13.7,17.15,1.,1.,1.,1.,1.,1.,        00532000
     1           12.,12.,24.,37.89,53.33,70.08,87.97,100.9,126.7,147.3,00533000
     2           2168.8,191.4,3.,6.,9.167,12.5,15.98,1.,1.,1.,1.,1.,1.,00534000
     3           1.,312.,24.,37.89,53.33,70.08,87.97,136.9,126.7,147.3,00535000
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     4            168.9,4191.4,211.,1.,1.,.5,.1667,.04167,.008333,
     5            1.,1.,1.,1.,1.,51.,1.,1.,2.,1.,.3157, .07407,.0139,
     6            .0021818,.00029,6.000035,.0000037,.00000035  /
      DATA A(2) / -1.0 /
      IRET = 1
      KFLAG = 1
      IF (JSTART.LE.0) GO TO 140
C***********************************************************************
C* BEGIN BY SAVING INFORMATION FOR POSSIBLE RESTARTS AND CHANGING      *
C* H BY THE FACTOR R IF THE CALLER HAS CHANGED H.  ALL VARIABLES       *
C* DEPENDENT ON H MUST ALSO BE CHANGED.                                *
C* E IS A COMPARISON FOR ERRORS OF THE CURRENT ORDER NQ. EUP IS        *
C* TO TEST FOR INCREASING THE ORDER, EDWN FOR DECREASING THE ORDER.    *
C* HNEW IS THE STEP SIZE THAT WAS USED ON THE LAST CALL.               *
C***********************************************************************
 100  DO 110 I = 1,N
        DO 110 J = 1,K
 110      SAVE(J,I) = Y(J,I)
      HOLD = HNEW
      IF (H.EQ.HOLD) GO TO 130
 120  RACUM = H/HOLD
      IRET1 = 1
      GO TO 750
  125 HOLD = H
 130  NQOLD = NQ
      TOLD = T
      RACUM = 1.0
      IF (JSTART.GT.0) GO TO 250
      GO TO 170
 140  IF (JSTART.EQ.-1) GO TO 160
C***********************************************************************
C* ON THE FIRST CALL, THE ORDER IS SET TO 1 AND THE INITIAL            *
C* DERIVATIVES ARE CALCULATED.                                         *
C***********************************************************************
      BR = 1.0
      NQ = 1
      N3 = N
      N4 = N**2
      CALL DIFFUN(T,Y,CSAVE(1,3))
      DO 150 I = 1,N
  150   Y(2,I) = CSAVE(I,3)*H
      HNEW = H
      K = 2
      GO TO 100
C***********************************************************************
C* REPEAT LAST STEP BY RESTORING SAVED INFORMATION.                    *
C***********************************************************************
 160  IF (NQ.EQ.NQOLD) JSTART = 1
      T = TOLD
      NQ = NQOLD
      K = NQ + 1
      GO TO 120
C***********************************************************************
```

```
C* SET THE COEFFICIENTS THAT DETERMINE THE ORDER AND THE METHOD        *
C* TYPE.  CHECK FOR EXCESSIVE ORDER.  THE LAST TWO STATEMENTS OF       *
C* THIS SECTION  SET IWEVAL .GT.0 IF PW IS TO BE RE-EVALUATED          *
C* BECAUSE OF THE ORDER CHANGE, AND THEN REPEAT THE INTEGRATION        *
C* STEP IF IT HAS NOT YET BEEN DONE (IRET = 1) OR SKIP TO A FINAL      *
C* SCALING BEFORE EXIT IF IT HAS BEEN COMPLETED (IRET = 2).            *
C***********************************************************************
 170  IF (MF.EQ.0) GO TO 180
      IF (NQ.GT.6) GO TO 190
      GO TO (221,222,223,224,225,226),NQ
  180 IF(NQ.GT.12) GO TO 190
      GO TO (205,206,207,208,209,210,211,212,213,214,215,216), NQ
 190  KFLAG = -2
      RETURN
C***********************************************************************
C* THE FOLLOWING COEFFICIENTS SHOULD BE DEFINED TO THE MAXIMUM         *
C* ACCURACY PERMITTED BY THE MACHINE.  THEY ARE, IN THE ORDER USED..   *
C*                                                                     *
C* -1                                                                  *
C* -1/2,-1/2                                                           *
C* -5/12,-3/4,-1/6                                                     *
C* -3/8,-11/12,-1/3,-1/24                                              *
C* -251/720,-25/24,-35/72,-5/48,-1/120                                 *
C* -95/288,-137/120,-5/8,-17/96,-1/40,-1/720                           *
C* -19087/60480,-49/40,-203/270,-49/192,-7/144,-7/1440,-1/5040         *
C*                                                                     *
C* METHODS TO CALCULATE FURTHER COEFFICIENTS CAN BE FOUND IN           *
C* HENRICI, DISCRETE VARIABLE METHODS IN ORDINARY D. E.                *
C*                                                                     *
C* -1                                                                  *
C* -2/3,-1/3                                                           *
C* -12/25,-7/10,-1/5,-1/50                                             *
C* -120/274,-225/274,-85/274,-15/274,-1/274                            *
C* -180/441,-58/63,-15/36,-25/252,-3/252,-1/1764                       *
C***********************************************************************
  205 A(1) = -1.0
      GO TO 230
  206 A(1) = -.50000000000
      A(3) = -0.500000000
      GO TO 230
  207 A(1) = -0.4166666666666667
      A(3) = -0.750000000
      A(4) = -0.1666666666666667
      GO TO 230
  208 A(1) = -0.3750000000000
      A(3) = -0.9166666666666667
      A(4) = -0.3333333333333333
      A(5) = -0.04166666666666667
      GO TO 230
  209 A(1) = -0.3486111111111111
      A(3) = -1.0416666666666667
      A(4) = -0.4861111111111111
      A(5) = -0.1041666666666667
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      A(6) = -0.0083333333333333
      GO TO 230
  210 A(1) = -0.3298611111111111
      A(3) = -1.1416666666666667
      A(4) = -0.625000000
      A(5) = -0.1770833333333333
      A(6) = -0.0250000000
      A(7) = -0.0013888888888889
      GO TO 230
  211 A(1) = -0.3155919312169312
      A(3) = -1.225000000
      A(4) = -0.7518518518518519
      A(5) = -0.2552083333333333
      A(6) = -0.0486111111111111
      A(7) = -0.0048611111111111
      A(8) = -0.0001984126984126984
      GO TO 230
  212 A(1) = -0.3042245370370370
      A(3) = -1.296428571428485
      A(4) = -0.8685185185185185
      A(5) = -0.3357638888888888
      A(6) = -0.0777777777777777
      A(7) = -0.0106481481481481815
      A(8) = -0.0007936507936507937
      A(9) = -0.0000248015873015718 9
      GO TO 230
  213 A(1) = -0.2948680004409171
      A(3) = -1.358928571428505
      A(4) = -0.9765542328041257
      A(5) = -0.41718750000
      A(6) = -0.1113541666666667
      A(7) = -0.0187450000
      A(8) = -0.0019345238095238 09
      A(9) = -0.0001116071428570911
      A(10) = -0.0000027557319223 9706
      GO TO 230
  214 A(1) = -0.2869754464285714
      A(3) = -1.414484126983951
      A(4) = -1.077215608465301
      A(5) = -0.4985670194001107
      A(6) = -0.148437500000
      A(7) = -0.0290605709876226
      A(8) = -0.0037202380952323
      A(9) = -0.0002996858465601941
      A(10) = -0.0000137786596 1195214
      A(11) = -0.0000002755731922 3878
      GO TO 230
  215 A(1) = -0.280189564439367
      A(3) = -1.464484126986034
      A(4) = -1.171514550268255
      A(5) = -0.5793581900385553
      A(6) = -0.1883228615536998
      A(7) = -0.0414303626548524 3
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      A(8) = -0.006211144180002914
      A(9) = -0.0006252066799084720
      A(10) = -0.00004041740152967666
      A(11) = -0.000001515652557372595
      A(12) = -.00000002505210838649 32
      GO TO 230
  216 A(1) = -0.274265540031599
      A(3) = -1.509938672424507
      A(4) = -1.260271163994607
      A(5) = -0.659234182076101
      A(6) = -0.2304580026342793
      A(7) = -0.05569724610169335
      A(8) = -0.009439484126243074
      A(9) = -0.001119274966826774
      A(10) = -0.00009093915342935554
      A(11) = -0.000004822530863610993
      A(12) = -0.0000001503126502923833
      A(13) = -0.000000002087675698479380
      GO TO 230
  221 A(1) = -1.000000000
      GO TO 230
  222 A(1) = -0.6666666666666667
      A(3) = -0.3333333333333333
      GO TO 230
  223 A(1) = - 0.5454545454545455
      A(3) = A(1)
      A(4) = -0.09090909090909091
      GO TO 230
  224 A(1) = -0.480000000
      A(3) = -0.700000000
      A(4) = -0.200000000
      A(5) = -0.020000000
      GO TO 230
  225 A(1) = -0.437956204379562
      A(3) = -0.8211678832116788
      A(4) = -0.3102189781021898
      A(5) = -0.05474452554744526
      A(6) = -0.003649635036496350 4
      GO TO 230
  226 A(1) = -0.4081632653061225
      A(3) = -0.9206349206349206
      A(4) = -0.4166666666666667
      A(5) = -0.0992063492063492
      A(6) = -0.0119047619047619
      A(7) = -0.0005668934240362 82
  230 K = NQ+1
      IDOUB = K
      MTYP = (4 - MF)/2
      ENQ2 = .5/FLOAT(NQ + 1)
      ENQ3 = .5/FLOAT(NQ + 2)
      ENQ1 = 0.5/FLOAT(NQ)
      PEPSH = EPS
      EUP = (PERTST(NQ,MTYP,2)*PEPSH)**2
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      E = (PERTST(NQ,MTYP,1)*PEPSH)**2
      EDWN =(PERTST(NQ,MTYP,3)*PEPSH)**2
      IF (EDWN.EQ.0) GO TO 780
      BND = (EPS*ENO3)**2
 240  IWEVAL = MF
      GO TO ( 250 , 680 ),IRET
C***********************************************************************
C* THIS SECTION COMPUTES THE PREDICTED VALUES BY EFFECTIVELY           *
C* MULTIPLYING THE SAVED INFORMATION BY THE PASCAL TRIANGLE            *
C* MATRIX.                                                             *
C***********************************************************************
 250  T = T + H
      DO 260 J = 2,K
        DO 260 J1 = J,K
          J2 = K - J1 + J - 1
          DO 260 I = 1,N
 260        Y(J2,I) = Y(J2,I) + Y(J2+1,I)
C***********************************************************************
C*   UP TO 2 CORRECTOR ITERATIONS ARE TAKEN.  CONVERGENCE IS TESTED BY *
C*   REQUIRING THE L2 NORM OF CHANGES TO BE LESS THAN BND WHICH IS     *
C*   DEPENDENT ON THE ERROR TEST CONSTANT.                             *
C*      THE SUM OF THE CORRECTIONS IS ACCUMULATED IN THE ARRAY         *
C*   ERROR(I).  IT IS EQUAL TO THE K-TH DERIVATIVE OF Y MULTIPLIED     *
C*   BY  H**K/(FACTORIAL(K-1)*A(K)), AND IS THEREFORE PROPORTIONAL     *
C*   TO THE ACTUAL ERRORS TO THE LOWEST POWER OF H PRESENT. (H**K)     *
C***********************************************************************
      DO 270 I = 1,N
 270    ERROR(I) = 0.0
      DO 430   L=1,2
          CALL DIFFUN (T,Y,CSAVE(1,3))
C***********************************************************************
C*   IF THERE HAS BEEN A CHANGE OF ORDER OR THERE HAS BEEN TROUBLE     *
C*   WITH CONVERGENCE, PW IS RE-EVALUATED PRIOR TO STARTING THE        *
C*   CORRECTOR ITERATION IN THE CASE OF STIFF METHODS.  IWEVAL IS      *
C*   THEN SET TO -1 AS AN INDICATOR THAT IT HAS BEEN DONE.             *
C***********************************************************************
      IF (IWEVAL.LT.1) GO TO 350
        IF (MF.EQ.2) GO TO 310
        CALL PEDERV(T,Y,PW,N3)
        R = A(1)*H
        DO 280 I = 1,N4
 280      PW(I) = PW(I)*R
C***********************************************************************
C* ADD THE IDENTITY MATRIX TO THE JACOBIAN AND DECOMPOSE INTO LU = PW  *
C***********************************************************************
 290    DO 300 I = 1,N
 300      PW(I*(N3+1)-N3) = 1.0 + PW(I*(N3+1)-N3)
        IWEVAL = -1
      CALL DECOMP(N,N3,PW,IP)
         IF  (IP(N) .NE. 0)  GO TO 350
        GO TO 440
C***********************************************************************
C* EVALUATE THE JACOBIAN INTO PW BY NUMERICAL DIFFERENCING.  R IS THE  *
```

```
C* CHANGE MADE TO THE ELEMENT OF Y.  IT IS EPS RELATIVE TO Y WITH      *
C* A MINIMUM OF EPS**2.  F STORES THE UNCHANGED VALUE OF Y.            *
C***********************************************************************
  310   DO 340 J = 1,N
      F = Y(1,J)
          R = EPS*DMAX1(EPS,DABS(F))
          Y(1,J) = Y(1,J) + R
          D = A(1)*H/R
          CALL DIFFUN(T,Y,CSAVE(1,1))
          DO 330 I = 1,N
 330        PW(I+(J-1)*N3) = (CSAVE(I,1) -CSAVE(I,3)) * D
 340       Y(1,J) = F
        GO TO 290
 350      DO 360 I = 1,N
 360       CSAVE(I,1) = Y(2,I) - CSAVE(I,3)*H
      IF(MF.EQ.0) GO TO 410
      CALL SOLVE(N,N3,PW,CSAVE(1,1),IP)
C***********************************************************************
C* CORRECT AND COMPARE DEL, THE L2 NORM OF CHANGE/YMAX, WITH BND.      *
C* ESTIMATE THE VALUE OF THE L2 NORM OF THE NEXT CORRECTION BY         *
C* BR*2*DEL AND COMPARE WITH BND.  IF EITHER IS LESS, THE CORRECTOR    *
C* IS SAID TO HAVE CONVERGED.                                          *
C***********************************************************************
  410 DEL = 0.0D0
        DO 420 I = 1,N
          Y(1,I) = Y(1,I) + A(1)*CSAVE(I,1)
          Y(2,I) = Y(2,I) - CSAVE(I,1)
          ERROR(I) = ERROR(I) + CSAVE(I,1)
      DEL = DEL + (CSAVE(I,1)/YMAX(I))**2
 420      CONTINUE
  426 IF(L.GE.2) BR = DMAX1(.9*BR, DEL/DEL1)
      DEL1 = DEL
      IF(DMIN1(DEL,BR*DEL*2.0)  .LE.  BND)  GO TO 490
 430    CONTINUE
C***********************************************************************
C* THE CORRECTOR ITERATION FAILED TO CONVERGE IN 2 TRIES.  VARIOUS     *
C* POSSIBILITIES ARE CHECKED FOR.  IF H IS ALREADY HMIN AND            *
C* THIS IS EITHER ADAMS METHOD OR THE STIFF METHOD IN WHICH THE        *
C* MATRIX PW HAS ALREADY BEEN RE-EVALUATED, A NO CONVERGENCE EXIT      *
C* IS TAKEN. OTHERWISE THE MATRIX PW IS RE-EVALUATED AND/OR THE        *
C* STEP IS REDUCED TO TRY AND GET CONVERGENCE.                         *
C***********************************************************************
 440  T = TOLD
      IF ((H.LE.(HMIN*1.00001)).AND.((IWEVAL - MTYP).LT.-1)) GO TO 460
      IF ((MF.EQ.0).OR.(IWEVAL.NE.0)) RACUM = RACUM*0.25D0
      IWEVAL = MF
      IRET1 = 2
      GO TO 750
 460  KFLAG = -3
      NQ = NQOLD
 470  DO 480 I = 1,N
        DO 480 J = 1,K
 480      Y(J,I) = SAVE(J,I)
```

```
      H = HOLD
      JSTART = NQ
      RETURN
C*********************************************************************
C* THE CORRECTOR CONVERGED AND CONTROL IS PASSED TO STATEMENT 520     *
C* IF THE ERROR TEST IS O.K.,  AND TO 540 OTHERWISE.                  *
C* IF THE STEP IS O.K. IT IS ACCEPTED. IF IDOUB HAS BEEN REDUCED      *
C* TO ONE,  A TEST IS MADE TO SEE IF THE STEP CAN BE INCREASED        *
C* AT THE CURRENT ORDER OR BY GOING TO ONE HIGHER OR ONE LOWER.       *
C* SUCH A CHANGE IS ONLY MADE IF THE STEP CAN BE INCREASED BY AT      *
C* LEAST 1.19  IF NO CHANGE IS POSSIBLE IDOUB IS SET TO 8 TO          *
C* PREVENT FUTHER TESTING FOR 8 STEPS.                                *
C* IF A CHANGE IS POSSIBLE, IT IS MADE AND IDOUB IS SET TO            *
C* NQ + 1    TO PREVENT FURTHER TESING FOR THAT NUMBER OF STEPS.      *
C* IF THE ERROR WAS TOO LARGE, THE OPTIMUM STEP SIZE FOR THIS OR      *
C* LOWER ORDER IS COMPUTED, AND THE STEP RETRIED.  IF IT SHOULD       *
C* FAIL TWICE MORE IT IS AN INDICATION THAT THE DERIVATIVES THAT      *
C* HAVE ACCUMULATED IN THE Y ARRAY HAVE ERRORS OF THE WRONG ORDER     *
C* SO THE FIRST DERIVATIVES ARE RECOMPUTED AND THE ORDER IS SET       *
C* TO 1.                                                              *
C*********************************************************************
 490  D = 0.0
      DO 500 I = 1,N
 500    D = D + (ERROR(I)/YMAX(I))**2
      IWEVAL = 0
      IF (D.GT.E) GO TO 540
      IF (K.LT.3) GO TO 520
C*********************************************************************
C* COMPLETE THE CORRECTION OF THE HIGHER ORDER DERIVATIVES AFTER A    *
C* SUCCESFUL STEP.                                                    *
C*********************************************************************
      DO 510 J = 3,K
        DO 510 I = 1,N
 510      Y(J,I) = Y(J,I) + A(J)*ERROR(I)
 520  KFLAG = +1
      HNEW = H
      IF (IDOUB.LE.1) GO TO 550
      IDOUB = IDOUB - 1
      IF (IDOUB.GT.1) GO TO 700
      DO 530 I = 1,N
 530    CSAVE(I,2) = ERROR(I)
      GO TO 700
C*********************************************************************
C* REDUCE THE FAILURE FLAG COUNT TO CHECK FOR MULTIPLE FAILURES.      *
C* RESTORE T TO ITS ORIGINAL VALUE AND TRY AGAIN UNLESS THERE HAVE    *
C* THREE FAILURES.  IN THAT CASE THE DERIVATIVES ARE ASSUMED TO HAVE  *
C* ACCUMULATED ERRORS SO A RESTART FROM THE CURRENT VALUES OF Y IS    *
C* TRIED. THIS IS CONTINUED UNTIL SUCCESS OR H = HMIN.                *
C*********************************************************************
 540  KFLAG = KFLAG - 2
      IF (H.LE.(HMIN*1.00001)) GO TO 740
      T = TOLD
      IF (KFLAG.LE.-5) GO TO 720
```

```
C***********************************************************************
C* PR1, PR2, AND PR3  WILL CONTAIN THE AMOUNTS BY WHICH THE STEP SIZE  *
C* CHOULD BE DIVIDED AT ORDER ONE LOWER, AT THIS ORDER, AND AT ORDER   *
C* ONE HIGHER RESPECTIVELY.                                            *
C***********************************************************************
 550  PR2 = (D/E)**ENQ2*1.2
      PR3 = 1.E+20
      IF ((NQ.GE.MAXDER).OR.(KFLAG.LE.-1)) GO TO 570
      D = 0.0
      DO 560 I = 1,N
 560    D = D + ((ERROR(I) - CSAVE(I,2))/YMAX(I))**2
      PR3 = (D/EUP)**ENQ3*1.4
 570  PR1 = 1.E+20
      IF (NQ.LE.1) GO TO 590
      D = 0.0
      DO 580 I = 1,N
 580    D = D + (Y(K,I)/YMAX(I))**2
      PR1 = (D/EDWN)**ENQ1*1.3
 590  CONTINUE
      IF (PR2.LE.PR3) GO TO 650
      IF (PR3.LT.PR1) GO TO 660
 600  R = 1.0/AMAX1(PR1,1.E-4)
      NEWQ = NQ - 1
  610 IDOUB = 8
      IF ((KFLAG.EQ.1).AND.(R.LT.(1.1))) GO TO 700
      IF (NEWQ.LE.NQ) GO TO 630
C***********************************************************************
C* COMPUTE ONE ADDITIONAL SCALED DERIVATIVE IF ORDER IS INCREASED.     *
C***********************************************************************
      DO 620 I = 1,N
 620    Y(NEWQ+1,I) = ERROR(I)*A(K)/DFLOAT(K)
 630  K = NEWQ + 1
      IF (KFLAG.EQ.1) GO TO 670
      RACUM = RACUM*R
      IRET1 = 3
      GO TO 750
 640  IF (NEWQ.EQ.NQ) GO TO 250
      NQ = NEWQ
      GO TO 170
 650  IF (PR2.GT.PR1) GO TO 600
      NEWQ = NQ
      R = 1.0/AMAX1(PR2,1.E-4)
      GO TO 610
 660  R = 1.0/AMAX1(PR3,1.E-4)
      NEWQ = NQ + 1
      GO TO 610
 670  IRET = 2
      R = DMIN1(R,HMAX/DABS(H))
      H = H*R
      HNEW = H
      IF (NQ.EQ.NEWQ) GO TO 680
      NQ = NEWQ
      GO TO 170
```

```
 680  R1 = 1.0
      DO 690 J = 2,K
        R1 = R1*R
        DO 690 I = 1,N
 690      Y(J,I) = Y(J,I)*R1
      IDOUB = K
 700  DO 710 I = 1,N
 710    YMAX(I) = DMAX1(YMAX(I),DABS(Y(1,I)))
      JSTART = NQ
      RETURN
 720  IF(NQ.GT.1) GO TO 725
      IF (H .LE. 2.D0*HMIN)  GO TO 780
      GO TO 550
  725 DO 730   I= 1,N
        Y(1,I) = SAVE(1,I)
        SAVE(2,I) = HOLD*CSAVE(I,3)
 730    Y(2,I) = SAVE(2,I)*R
      R = H/HOLD
      CALL DIFFUN (T,Y,CSAVE(1,3))
      NQ = 1
      KFLAG = 1
      GO TO 170
 740  KFLAG = -1
      HNEW = H
      JSTART = NQ
      RETURN
C***********************************************************************
C* THIS SECTION SCALES ALL VARIABLES CONNECTED WITH H AND RETURNS      *
C* TO THE ENTERING SECTION.                                            *
C***********************************************************************
 750  RACUM = DMAX1(DABS(HMIN/HOLD),RACUM)
      RACUM = DMIN1(RACUM,DABS(HMAX/HOLD))
      R1 = 1.0
      DO 760 J = 2,K
        R1 = R1*RACUM
        DO 760 I = 1,N
 760      Y(J,I) = SAVE(J,I)*R1
      H = HOLD*RACUM
      DO 770 I = 1,N
 770    Y(1,I) = SAVE(1,I)
      IDOUB = K
      GO TO ( 125 , 250 , 640 ),IRET1
 780  KFLAG = -4
      GO TO 470
      END
```

```
1PILER OPTIONS - NAME=  MAIN,OPT=01,LINECNT=55,SIZE=0000K,
                 SOURCE,BCD,NOLIST,NODECK,LOAD,MAP,NOEDIT,ID,NOXREF
      SUBROUTINE DECOMP(N,NDIM,A,IP)
      IMPLICIT REAL*8(B-H,O-Z)
C
C    MATRIX TRIANGULARIZATION BY GAUSSIAN ELIMINATION.
C
C   INPUT...
C     N = ORDER OF MATRIX
C     NDIM = DECLARED DIMENSION OF ARRAY A.
C     A = MATRIX TO BE TRIANGULARIZED. (FOR STIFF METHODS, A IS SINGLE
C                PRECISION;  ALL OTHER VARIABLE ARE DOUBLE PRECISION.)
C   OUTPUT...
C     A(I,J),  I.LE.J  = UPPER TRIANGULAR FACTOR, U.
C     A(I,J),    I.GT.J   = MULTIPLIERS  = LOWER TRIANGULAR FACTOR, I-L.
C     IP(K),   K.LT.N = INDEX OF K-TH PIVOT ROW.
C     IP(N)   = (-1)**(NUMBER OF INTERCHANGES) OR 0.
C   USE 'SOLVE' TO OBTAIN SOLUTION OF LINEAR SYSTEM.
C   DETERM(A) = IP(N)*A(1,1)*A(2,2)*...*A(N,N).
C   IF IP(N) = 0, A IS SINGULAR, SOLVE WILL DIVIDE BY ZERO.
C
      DIMENSION A(NDIM,NDIM),IP(NDIM)
      DIMENSION B(4,4)
      COMMON NFNS,NW,B
      NW = NW + 1
      IP(N) = 1
      DO 6  K=1,N
      IF(K.EQ.N) GO TO 5
      KP1 = K+1
      M = K
      DO 1  I=KP1,N
      IF(ABS(A(I,K)).GT.ABS(A(M,K)))    M=I
    1 CONTINUE
      IP(K) = M
      IF(M.NE.K)  IP(N) = -IP(N)
      T = A(M,K)
      A(M,K) = A(K,K)
      A(K,K) = T
      IF(T.EQ.0) GO TO 5
      DO 2  I=KP1,N
    2    A(I,K) = -A(I,K) / T
      DO 4  J=KP1,N
      T = A(M,J)
      A(M,J) = A(K,J)
      A(K,J) = T
      IF(T.EQ.0.) GO TO 4
      DO 3   I=KP1,N
    3     A(I,J) = A(I,J) + A(I,K)*T
    4  CONTINUE
    5 IF(A(K,K).EQ.0.) IP(N) = 0
    6 CONTINUE
      RETURN
      END
```

OS/360 FORTRAN H

```
COMPILER OPTIONS - NAME=  MAIN,OPT=01,LINECNT=55,SIZE=0000K,
                   SOURCE,BCD,NOLIST,NODECK,LOAD,MAP,NOEDIT,ID,NOXREF
      SUBROUTINE SOLVE(N,NDIM,A,B,IP)
      IMPLICIT REAL*8 (B-H,Q-Z)
C
C    SOLUTION OF LINEAR SYSTEM, A*X = B.
C
C    INPUT...
C      N = ORDER OF MATRIX.
C      NDIM = DECLARED DIMENSION OF ARRAY A.
C      A = TRIANGULARIZED MATRIX OBTAINED FROM 'DECOMP'.
C      B = RIGHT HAND SIDE VECTOR.
C      IP = PIVOT VECTOR OBTAINED FROM 'DECOMP'.
C    OUTPUT...
C      B = SOLUTION VECTOR, X.
      DIMENSION A(NDIM,NDIM), B(NDIM), IP(NDIM)
      IF(N.EQ.1) GO TO 9
      NM1 = N-1
      DO 7  K=1,NM1
         KP1 = K + 1
         M = IP(K)
      T = B(M)
      B(M) = B(K)
      B(K) = T
      DO 7  I=KP1,N
    7 B(I) = B(I) + A(I,K)*T
      DO 8   KB=1,NM1
      KM1 = N - KB
      < = KM1 + 1
      B(K) = B(K)/A(K,K)
      T = -B(K)
      DO 8  I=1,KM1
    8 B(I) = B(I) + A(I,K)*T
    9 B(1) = B(1)/A(1,1)
      RETURN
      END
```

OS/360 FORTRAN H

```
COMPILER OPTIONS - NAME=  MAIN,OPT=01,LINECNT=55,SIZE=0000K,
                   SOURCE,BCD,NOLIST,NODECK,LOAD,MAP,NOEDIT,ID,NOXREF
      SUBROUTINE PEDERV (T,Y,PW,N3)                                     01089300
      DIMENSION Y(13,40),PW(1600)                                       01089320
      DOUBLE PRECISION T,Y                                              01089340
      RETURN                                                            01089360
      END                                                               01089380
```

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                         OS/360  FORTRAN H

COMPILER OPTIONS - NAME=  MAIN,OPT=01,LINECNT=55,SIZE=0000K,
                   SOURCE,BCD,NOLIST,NODECK,LOAD,MAP,NOEDIT,ID,NOXREF
      SUBROUTINE SMGOUT (X,Y,H)
      DIMENSION Y(40)
      DOUBLE PRECISION X,Y,Z,DERY,D,ZZ,H,PRMT,YY,C,BB,POLL
      REAL*8 LABEL,RCT
      COMMON /KINCOM/ ZZ(4),YY(40),LABEL(40),D(50),RCT(50,3),PRMT(8),
     1       DERY(40),C(50),BB,Z(2),N,NC,NEQ,NDIF,KDIF,M,NN,INTR,NNC,
     2       NNDIF,IUV,IM,IS,ITRAF,NLL,CC(16,100),A(80),STEP(15),TIM1,
     3       TIM2,TIM4,PEAK1,TIME1,PEAK3,TIME3,XPOS,YPOS
C
      COMMON /ALLCOM/ POLL(4,3),GPOLL(4,3),ANS(8),GOTIME,XDEPTH,ISOUR,
     1                XDEPRV
C
      EQUIVALENCE (TEMP,ANS(3)),(HUMID,ANS(4)),(HT,ANS(7)),(XHT,ANS(8))
C
C
      IF (NN.EQ.1.AND.BB.EQ.0.1E02) GO TO 4
      IF (BB-PRMT(7))   400,4,4
C
C     SAVE VALUES FOR THE PLOTS.
C
    4 IF (NEQ .EQ. 1)    GO TO 110
      IF (NN .EQ. 101)   NN=100
      CC(1,NN) = X
      DO 10  I=1,NDIF
   10 CC(I+1,NN) = Y(I)
      IF (1.0E08-BB)110,20,30
C
   20 PEAK1 = Y(1)
      TIME1= X
      PEAK3= Y(3)
      TIME3= X
C
C     HAL1---HALF VALUE OF SPECIES 1
C     HAL2---HALF VALUE OF SPECIES 2
C     HAL4---HALF VALUE OF SPECIES 4
C
      HAL1=Y(1)/2.0
      HAL2=Y(2)/2.0
      HAL4=Y(4)/2.0
      PREVY1 = Y(1)
      PREVY2 = Y(2)
      PREVY4 = Y(4)
      TIM1 = 0.0
      TIM2 = 0.0
      TIM4 = 0.0
      PTIM1=0.0
      PTIM2=0.0
      PTIM4=0.0
C
      GO TO 110
C
```

```
C      SAVE PEAK VALUES, PEAK TIMES, AND HALF-TIMES.
C
   30 IF (Y(1).LT.PEAK1) GO TO 40
      PEAK1= Y(1)
      TIME1= X
   40 IF (Y(3).LT.PEAK3) GO TO 70
      PEAK3= Y(3)
      TIME3= X
   70 IF (Y(1)-PREVY1) 71, 71, 80
   71 IF (Y(1).GT.HAL1.OR.PREVY1.LT.HAL1) GO TO 73
      TIM1=PTIM1-(PTIM1-X)*((PREVY1-HAL1)/(PREVY1-Y(1)))
   73 PREVY1=Y(1)
      PTIM1=X
   80 IF (Y(2)-PREVY2) 81, 81, 90
   81 IF (Y(2).GT.HAL2.OR.PREVY2.LT.HAL2) GO TO 83
      TIM2=PTIM2-(PTIM2-X)*((PREVY2-HAL2)/(PREVY2-Y(2)))
   83 PREVY2=Y(2)
      PTIM2=X
   90 IF (Y(4)-PREVY4) 91, 91,110
   91 IF (Y(4).GT.HAL4.OR.PREVY4.LT.HAL4) GO TO 93
      TIM4=PTIM4-(PTIM4-X)*((PREVY4-HAL4)/(PREVY4-Y(4)))
   93 PREVY4=Y(4)
      PTIM4=X
C
C      CHECK IF OUTPUT THIS TIME.
C
  110 IF (INTR)  130,130,120
  120 IF (X .LT. (STEP(M)-0.5)) GO TO 170
  130 WRITE (6,1000) X,NN,XPOS,YPOS,H,M
      IF (ITRAF .EQ. 0 .AND. ISOUR .EQ. 0)   GO TO 145
      WRITE (6,1012)
      IF (ITRAF .EQ. 0)  GO TO 140
      WRITE (6,1013) (POLL(I,1),I=1,4),(GPOLL(I,1),I=1,4)
      WRITE (6,1007) (POLL(I,2),I=1,4),(GPOLL(I,2),I=1,4)
  140 IF (ISOUR .EQ. 0)  GO TO 145
      WRITE (6,1011) POLL(1,3),POLL(2,3),POLL(4,3),GPOLL(1,3),GPOLL(2,3)
     1               ,GPOLL(4,3)
  145 WRITE (6,1009)
      WRITE (6,1010) TEMP,HUMID,HT,XHT,XDEPTH
      WRITE (6,1001)
      WRITE (6,1002) (I,LABEL(I),Y(I),DERY(I),I=1,NDIF)
      DO 150  J=NNDIF,NC
      WRITE (6,1003)  J,LABEL(J),YY(J)
  150 CONTINUE
      IF (NEQ .EQ. 1)    GO TO 160
      WRITE (6,1005)
      WRITE (6,1006) (I,(RCT(I,J),J=1,3),D(I),I=1,NEQ)
  160 M = M+1
  170 IF (BB .EQ. 1.0E+08)  GO TO 180
      NN=NN+1
  180 BB = 0.0
C
C      CHECK FOR NEGATIVE CONCENTRATIONS OF SPECIES.
```

```
C
  400 DO 405  I=1,NDIF
      IF (Y(I))  401,405,405
  401 Y(I) = 0.
  405 CONTINUE
      DO 415  I=NNDIF,NC
      IF (YY(I))  411,415,415
  411 YY(I) = 0.
  415 CONTINUE
      BB=BB+1.0
      RETURN
 1000 FORMAT('1','TIME=',D15.8,' MINUTES',5X,'STEP=',I3,5X,'POSITION=',
     1F8.4,',',F8.4,6X,'STEP SIZE=',D15.8,6X,'PAGE',I4,///)
C
 1001 FORMAT(//'    COMPOUND   CONC PPHM    CHANGE, PPHM/MIN')
 1002 FORMAT(' ',I3,1X,A8,2D16.7)
 1003 FORMAT(' ',I3,1X,A8,D16.7)
 1005 FORMAT('1',16X,'RATES OF REACTION'/)
 1006 FORMAT(I4,4X,3A8,D16.5)
 1007 FORMAT('OFREEWAY TRAFFIC',4X,4D12.4,4X,4E12.4)
C
C
C
 1008 FORMAT ('ODIFFUSION EMISSIONS IN GRAMS/MIN',6X,'NO2=',E15.8,
     1 6X,'NO=',E15.8)
 1009 FORMAT(//1H0,16X,'RELATIVE'                              ,18X,'MIXING',
     16X,'MIXING',/'  TEMPERATURE    HUMIDITY',                          'E
     2LEVATION',6X,'HEIGHT',7X,'DEPTH',/6X,'(CENT.)                 ',
     3                 '  (METERS)    (METERS)    (METERS)')
 1010 FORMAT(1H0,5F12.4)
 1011 FORMAT('OAREA SOURCES',7X,2D12.4,12X,D12.4,4X,2E12.4,12X,E12.4///)
 1012 FORMAT(30X,'EXPECTED RATE OF CHANGE OF CONCENTRATIONS DUE TO EMISS
     1IONS FROM REGIONAL SOURCES'//40X,'PPHM/MIN',42X,'GRAM-MOLES/MIN'//
     222X,'PROPYLENE',7X,'NO',10X,'CO',8X,'DUMHC',9X,'PROPYLENE',7X,'NO'
     3,10X,'CO',8X,'DUMHC')
 1013 FORMAT('OSTREET TRAFFIC',5X,4D12.4,4X,4E12.4)
      END
```

OS/360 FORTRAN H

```
COMPILER OPTIONS - NAME=  MAIN,OPT=01,LINECNT=55,SIZE=0000K,
                SOURCE,BCD,NOLIST,NODECK,LOAD,MAP,NOEDIT,ID,NOXREF
      SUBROUTINE DIFFUN (X,YSAVE,DY)                                    01219000
      DIMENSION YSAVE(13,40),Y(40),DY(40)                               01220000
      DOUBLE PRECISION YSAVE,Y,DY,C,D,Z,X,YY,ZZ,BB,DERY,POLL,PRMT,XPREV 01221000
      REAL*8 LABEL,RCT                                                  01222000
      COMMON /KINCOM/ ZZ(4),YY(40),LABEL(40),D(50),RCT(50,3),PRMT(8),   01223000
     1       DERY(40),C(50),BB,Z(2),N,NC,NEQ,NDIF,KDIF,M,NN,INTR,NNC,   01224000
     2       NNDIF,IUV,IM,IS,ITRAF,NLL,CC(16,100),A(80),STEP(15),TIM1,  01225000
     3       TIM2,TIM4,PEAK1,TIME1,PEAK3,TIME3,XPOS,YPOS                01226000
C                                                                       01227000
      COMMON /ALLCOM/ POLL(4,3),GPOLL(4,3),ANS(8),GOTIME,XDEPTH,ISOUR,  01228000
     1                XDEPRV                                            01228200
      DO 2  I=1,NC                                                      01229000
    2 Y(I) = YSAVE(1,I)                                                 01230000
      IF (NEQ.EQ. 1)    GO TO 18                                        01230200
C                                                                       01231000
C     COMPUTE NON-ACCUMULAING SPECIES.                                  01232000
C                                                                       01233000
      IF (Y(2)) 6,6,8                                                   01234000
    6 Y(2) = (D(1)       )/(C(3)*Y(3)+C(6)*Y(24)            +C(8)*Y(16)+ 01235000
     1C(16)*Y(19) + C(17)*Y(18) + C(18)*Y(25) + C(19)*Y(21) +           01236000
     2C(20)*Y(22))                                                      01237000
      DERY(2) = 0.                                                      01238000
C                                                                       01238500
    8 YY(14) = (D(14)*100.D0+2.D0*D(32))/(C(9)+ZZ(3))                   01239000
C                                                                       01240000
      YY(15) = (D(8)+D(11)+D(25))/                                      01241000
     1         (C(7)*Y(4)+C(12)*Y(1)+C(13)*Y(3)+C(14)*100.D0*Y(8)+ZZ(3))01242000
C                                                                       01243000
      YY(16) = (D(9)+D(13)+D(21))/(C(8)*Y(2)+C(26)*Y(4)+ZZ(3))          01244000
C                                                                       01245000
      YY(17) = (D(7)+D(22)+D(27)+D(28)+D(31))/(C(15)+ZZ(3))             01246000
C                                                                       01247000
      YY(18) = (D(11)+D(16)+D(26)+D(27))/                               01248000
     1         (C(17)*Y(2)+C(21)+C(29)*Y(1)+ZZ(3))                      01249000
C                                                                       01250000
      YY(19) = (D(15)+D(17))/(C(16)*Y(2)+C(27)*Y(4)+ZZ(3))              01251000
C                                                                       01252000
      YY(20) = (D(19)+D(22)+D(27)+D(31))/(C(10)+C(28)+ZZ(3))            01253000
C                                                                       01254000
      YY(21) = (D(5)+D(18))/(C(19)*Y(2)+ZZ(3))                          01255000
C                                                                       01256000
      YY(22) = (D(23)+D(24))/(C(20)*Y(2)+C(25))                         01257000
C                                                                       01258000
      YY(23) = D(1)/(C(2)+C(22)*Y(4)+C(24)*Y(4)+C(31)*Y(12))            01259000
C                                                                       01260000
      YY(24) = D(4)/(C(6)*Y(2)+C(33)*Y(1))                              01261000
C                                                                       01262000
      YY(25) = (D(10)+D(25))/(C(18)*Y(2)+C(30)*Y(1)+C(5)+ZZ(3))         01263000
C                                                                       01264000
C     TEST FOR NEGATIVE SOLID STATE SPECIES                             01265000
C                                                                       01266000
```

```
      DO 10  I=NNDIF,NC
      IF (YY(I) .LT. 0.0)    YY(I) = 0.0
   10 CONTINUE
C
C     COMPUTE CHAIN YIELD.
C
      ZZ(2) = YY(14)+YY(15)+YY(16)+YY(17)+YY(18)+YY(19)+YY(20)+YY(21)+
     1        YY(25)
      ZZ(3) = ZZ(2)*Z(1)+Y(2)*Z(2)
C
C     SET TRAJECTORY POSITION
C
   13 XPOS = Y(NDIF+1)
      YPOS = Y(NDIF+2)
C
      CALL METEOR (XPOS,YPOS,0,X,XPREV,DERY(NDIF+1),DERY(NDIF+2))
      IF (NEQ .EQ. 1)    GO TO 40
C
      IF (IUV .NE. 0)    GO TO 20
      CALL ULTRAV (C(1))
   20 IUV = IUV+1
      IF (IUV .GT. 100)  IUV=0
C
C     COMPUTE RATES OF REACTION.
C
      D(1) = C(1)*Y(1)
      D( 2) = C( 2)*YY(23)
      IF (Y(2) .LE. 0.0)
     1 Y(2) = (D(1))/(C(3)*Y(3)+C(6)*YY(24)+C(8)*YY(16)+C(16)*YY(19)+
     2          C(17)*YY(18)+C(18)*YY(25)+C(19)*YY(21)+C(20)*YY(22))
C
      D( 3) = C( 3)*Y( 3)*Y(2)
      D( 4) = C( 4)*Y( 1)*Y(3)
      D( 5) = C( 5)*YY(25)
      D( 6) = C( 6)*YY(24)*Y(2)
      D( 7) = C( 7)*YY(15)*Y(4)
      D( 8) = C( 8)*YY(16)*Y(2)
      D( 9) = C( 9)*YY(14)
      D(10) = C(10)*YY(20)
      D(11) = 0.D0
      D(12) = C(12)*YY(15)*Y(1)
      D(13) = C(13)*YY(15)*Y(3)
      D(14) = C(14)*YY(15)*Y(8)
      D(15) = C(15)*YY(17)
      D(16) = C(16)*YY(19)*Y(2)
      D(17) = C(17)*YY(18)*Y(2)
      D(18) = C(18)*YY(25)*Y(2)
      D(19) = C(19)*YY(21)*Y(2)
      D(20) = C(20)*YY(22)*Y(2)
      D(21) = C(21)*YY(18)
      D(22) = C(22)*YY(23)*Y(4)
      D(23) = C(23)* Y( 4)*Y(3)
      D(24) = C(24)*YY(23)*Y(4)
```

```
      D(25) = C(25)*YY(22)
      D(26) = C(26)*YY(16)*Y(4)
      D(27) = C(27)*YY(19)*Y(4)
      D(28) = C(28)*YY(20)
      D(29) = C(29)*YY(18)*Y(1)
      D(30) = C(30)*YY(25)*Y(1)
      D(31) = C(31)*YY(23)*Y(12)
      D(32) = C(32)* Y( 7)
      D(33) = C(33)*YY(24)*Y(1)
C
C     COMPUTE RATES OF CHANGE.
C
       DERY( 1)=+D( 3)+D( 6)+D( 6)       +D( 8)       +D(16)+D(17)+D(18)
     1+D(19)+D(20)-D( 1)-D( 4)                -D(12)-D(29)-D(30) -D(33)
       DERY( 2)=+D( 1)       -D( 3)-D( 6)       -D( 8)       -D(16)-D(17)
     1-D(18)-D(19)-D(20)
      DERY(3) = D(2)-D(3)-D(4)+D(5)-D(13)-D(23)
      DERY( 4)=-D(22)-D(23)-D(24)-D(26)-D(27)-D(7)
       DERY( 5)=         + D(12)    + D(33) + D(33)
       DERY( 6)=+D(20)+D(26) + D(7)
      DERY(7)=+D(21)+D(23)+D(24)-D(32)
      DERY (8) = -D(14) + (D(28)+D(32))/100.D0
       DERY( 9)=+D(29)
       DERY(10)=+D(30)
      DERY(11) = 0.D0
C
C
      DERY(12) = -D(31)
C
   40 IF (ISOUR .EQ. 0 .AND. ITRAF .EQ. 0)   GO TO 65
      IF (XPOS .LE. 18. .OR. XPOS .GE. 66.)   GO TO 65
      IF (YPOS .LE. 2.  .OR. YPOS .GE. 52.)   GO TO 65
C
   45 CALL SOURCE (XPOS,YPOS)
C
   55 IF (NEQ .EQ. 1)    GO TO 60
      DERY(2) = DERY(2) + POLL(2,1)+POLL(2,2)+POLL(2,3)
      DERY(4) = DERY(4) + POLL(1,1)+POLL(1,2)+POLL(1,3)
      DERY(8) = DERY(8) + (POLL(3,1)+POLL(3,2))/100.D0
      DERY(12) = DERY(12) + POLL(4,1)+POLL(4,2)+POLL(4,3)
      GO TO 65
   60 DERY(1) = (POLL(3,1)+POLL(3,2))/100.D0
   65 IF (XDEPTH .LE. XDEPRV)   GO TO 80
      IF (X .EQ. XPREV)  GO TO 80
      STORE = ((XDEPRV-XDEPTH)*XDEPRV)/((X-XPREV)*XDEPTH*XDEPTH)
C
C     MODIFY CONCENTRATIONS DUE TO CHANGE IN MIXING DEPTH
C
      DO 70  I=1,NDIF
   70 DERY(I) = DERY(I)+Y(I)*STORE
C
   80 DO 131  I=1,KDIF
      DY(I) = DERY(I)
  131 YSAVE(1,I) = Y(I)
  200 RETURN
      END
```

OS/360 FORTRAN H

```
COMPILER OPTIONS - NAME=  MAIN,OPT=01,LINECNT=55,SIZE=0000K,
            SOURCE,BCD,NOLIST,NODECK,LOAD,MAP,NOEDIT,ID,NOXREF
      SUBROUTINE METEOR (X,Y,IIDD,XTIME,XPREV,XXDOT,YYDOT)
C
C     ARRAYS
C     AIR--12 HOURLY AVERAGES OF SIX VARIABLES FOR EACH STATION.
C            WIND SPEED AND DIRECTION, TEMPERATURE, HUMIDITY, BAROMETRIC
C            PRESSURE, AND CLOUD COVER.
C     ANS--METEOROLOGICAL DATA FOR AN INTERPOLATED POINT.
C     ARADIO--AM RADIOSONDE CURVE
C     DISINV--DISTANCE INVERSES, INTERPOLATED POINT TO STATIONS.
C     DIST--DISTANCES SQUARED FROM INTEPPOLATED POINT TO STATIONS.
C     JBAR--BARRIER CHECK INDICATORS, 1 MEANS ELIGIBLE STATION.
C     PRADIO--PM RADIOSONDE CURVE
C     RADIO--RADIOSONDE CURVE
C     RSLOPE--SLOPES OF RADIOSONDE CURVE SEGMENTS
C     WPOS--NSTA STATION LOCATIONS, THREE DIMENSIONS
C
C
      DIMENSION DIST(32),JBAR(32),RADIO(15,2),RSLOPE(14),JFUSE(32,32),
     1          DISINV(8),VAL1(8),VAL2(8)
C
      COMMON /MYCOM/ TIME,ICLOUD,IDM,IDU,IDD,IDS,IPST,NSTA,NSTACK,NRAD,
     1          AIR(12,32,6),WPOS(32,3),POS(32,3),SPOS(32,3),HS(12),
     2          DS(12),VS(12),TS(12),QS(12),SBAROM,STEMP,XDOT,YDOT,
     3          ARADIO(15,2),PRADIO(15,2),ZENITH(12,2),SGRID(650),
     4          FGRID(650),AGRID1(650),AGRID2(650),AGRID4(650),EMIT(10),
     5          XHITE(12),IHT,XMIN
      COMMON /ALLCOM/ POLL(4,3),GPOLL(4,3),ANS(8),GOTIME,XDEPTH,ISOUR,
     1                  XDEPRV
C
      EQUIVALENCE (TEMP,ANS(3)),(HT,ANS(7)),(XHT,ANS(8))
C
C     PRESET DATA
      DATA SLOPE/-.00986/
      DOUBLE PRECISION XTIME,XTIME1,XPREV,POLL
C
C     INITIALIZATION
C
      NPTS = 0
      DO 10  I=1,8
      ANS(I) = 0.
      DISINV(I) = 0.
      VAL1(I) = 0.
   10 VAL2(I) = 0.
      TIME = GOTIME + XTIME/60.
      ITIME = TIME - 6.
      HOUR = ITIME+6
      TIMEHR = TIME-HOUR
C
   20 IF (IDM .EQ. 1)  GO TO 75
      XDEPTH = 0.
      XTIME1 = 0.D0
```

```
C
C
C
C
C
C
C
C
C
   35 IF (IHT .EQ. 1)   GO TO 50
      ISONDE = 5
      NNRAD = NRAD-1
      IF (ITIME-ISONDE)  40,50,50
C
C     SET AM RADIOSONDE CURVE.
C
   40 DO 45  L=1,NRAD
      RADIO(L,1) = ARADIO(L,1)
   45 RADIO(L,2) = ARADIO(L,2)
      GO TO 60
C
C     SET PM RADIOSONDE CURVE.
C
   50 DO 55  L=1,NRAD
      RADIO(L,1) = PRADIO(L,1)
   55 RADIO(L,2) = PRADIO(L,2)
      ISONDE = 100
   60 DO 65  L=2,NRAD
   65 RSLOPE(L-1) = (RADIO(L,2)-RADIO(L-1,2))/(RADIO(L,1)-RADIO(L-1,1))
      GO TO 75
C
C     BARRIER CHECK POINT AGAINST ALL STATIONS.
C
   75 CALL BARIER (X,Y,WPOS,JBAR,NSTA)
      IF (ITIME-ISONDE) 100,80,80
C
C     SET PM RADIOSONDE CURVE.
C
   80 DO 85  K=1,NRAD
      RADIO(K,1) = PRADIO(K,1)
   85 RADIO(K,2) = PRADIO(K,2)
      ISONDE = 100
      DO 90  L=2,NRAD
   90 RSLOPE(L-1) = (RADIO(L,2)-RADIO(L-1,2))/(RADIO(L,1)-RADIO(L-1,1))
C
C     DETERMINE DISTANCES TO ALL USABLE POINTS.
C
  100 DO 120  I=1,NSTA
      IF (JBAR(I) .NE. 1)   GO TO 120
      GO TO 115
  115 NPTS = 1
      DIST(I) = (X-WPOS(I,1))**2 + (Y-WPOS(I,2))**2
      IF (DIST(I) .NE. 0.)   GO TO 120
```

```
C
C     INTERPOLATION POINT ON A STATION.
C
      IONE = I
      GO TO 250
  120 CONTINUE
C
C     NO STATIONS QUALIFY.
C
      IF (NPTS .EQ. 0)    RETURN
C
C     SUM CONTRIBUTIONS OF EACH STATION DIVIDED BY ITS DISTANCE TO THE
C         INTERPOLATED POINT SQUARED. DIVIDE RESULTS BY 1 OVER THE
C         SUM OF THE INVERSE DISTANCES. SET RESULTS INTO 'ANS'.
C
      DO 140  J=1,4
      DO 130  I=1,NSTA
      IF (JBAR(I) .NE. 1)   GO TO 130
      IF (AIR(ITIME+1,I,J) .EQ. 0.)   GO TO 130
      DISINV(J) = DISINV(J) + 1./DIST(I)
      VAL2(J) = VAL2(J)+AIR(ITIME+1,I,J)/DIST(I)
  130 CONTINUE
      IF (DISINV(J) .NE. 0)   GO TO 135
      VAL2(J) = 0.
      GO TO 140
  135 VAL2(J) = VAL2(J)/DISINV(J)
  140 CONTINUE
      DO 145  I=1,8
  145 DISINV(I) = 0.
      DO 160  J=1,4
      DO 150  I=1,NSTA
      IF (JBAR(I) .NE. 1)   GO TO 150
      IF (AIR(ITIME,I,J) .EQ. 0.)  GO TO 150
      DISINV(J) = DISINV(J) + 1./DIST(I)
      VAL1(J) = VAL1(J)+AIR(ITIME,I,J)/DIST(I)
  150 CONTINUE
      IF (DISINV(J) .NE. 0)    GO TO 155
      VAL1(J) = 0.
      GO TO 160
  155 VAL1(J) = VAL1(J)/DISINV(J)
  160 CONTINUE
      DO 170  J=1,4
  170 ANS(J) = VAL1(J)+(VAL2(J)-VAL1(J))*TIMEHR
      GO TO 190
C
C     SET GROUND ELEVATION
C
  190 DO 200  I=1,NSTA
      IF (JBAR(I) .NE. 1)     GO TO 200
      ANS(7) = ANS(7)+WPOS(I,3)/DIST(I)
      DISINV(7) = DISINV(7) + 1./DIST(I)
  200 CONTINUE
      HT = ANS(7)/DISINV(7)
```

```
      ANS(1) = ANS(1)/60.
      ANS(2) = ANS(2)/60.
      GO TO 400
C
C     TRAJECTORY POINT ON STATION.  SET ANS TO STATION VALUES.
C
C
  250 DO 270  J=1,6
      VAL2(J) = AIR(ITIME+1,IONE,J)
      VAL1(J) = AIR(ITIME,IONE,J)
  270 ANS(J) = VAL1(J)+(VAL2(J)-VAL1(J))*TIMEHR
      HT = WPOS(IONE,3)
C
C
C
C
C
C     DETERMINE MIXING HEIGHT AND MIXING HEIGHT DERIVATIVE.
C
  400 XDEPRV = XDEPTH
      XPREV = XTIME1
      IF (IHT .EQ. 1)    GO TO 480
      DO 420  I=1,NNRAD
      XHT = (ANS(3)-RADIO(I,2)+RSLOPE(I)*RADIO(I,1)-SLOPE*HT)/
     1      (RSLOPE(I)-SLOPE)
      IF ((XHT .GT. RADIO(I,1))   .AND.
     1    (XHT .LE. RADIO(I+1,1)) .AND.
     2    (XHT .GE. HT))           GO TO 450
  420 CONTINUE
      TMIN = 100.
      DO 425  I=1,NRAD
      IF ((HT .GT. RADIO(I,1)) .OR. (RADIO(I,2) .GE. TMIN))   GO TO 425
      TMIN = RADIO(I,2)
      HMIN = RADIO(I,1)
  425 CONTINUE
      IF ((TEMP+SLOPE*(HMIN-HT)) .GE. TMIN)    GO TO 450
  430 XDEPTH = AMAX1(XMIN,XDEPRV)
      XHT = XDEPTH+HT
      GO TO 500
  450 XDEPTH = XHT-HT
      XDEPTH = AMAX1(XMIN,XDEPTH)
      XHT = HT+XDEPTH
      GO TO 500
  480 XHT = XHITE(ITIME)
      XDEPTH = XHT-HT
  500 IDM = 1
      XTIME1 = XTIME
C
C
      XXDOT = ANS(1)
      YYDOT = ANS(2)
  620 RETURN
      END
```

```
COMPILER OPTIONS - NAME=  MAIN,OPT=01,LINECNT=55,SIZE=0000K,
                  SOURCE,BCD,NOLIST,NODECK,LOAD,MAP,NOEDIT,ID,NOXREF
          SUBROUTINE ULTRAV (RATE)
    C
    C                         ULTRAVIOLET RADIATION MODULE
          COMMON /MYCOM/ TIME,ICLOUD,IDM,IDU,IDD,IDS,IPST,NSTA,NSTACK,NRAD,
         1        AIR(12,32,6),WPOS(32,3),POS(32,3),SPOS(32,3),HS(12),
         2        DS(12),VS(12),TS(12),QS(12),SBAROM,STEMP,XDOT,YDOT,
         3        ARADIO(15,2),PRADIO(15,2),ZENITH(12,2),SGRID(650),
         4        FGRID(650),AGRID1(650),AGRID2(650),AGRID4(650),EMIT(10),
         5        XHITE(12),IHT,XMIN
    C
          DOUBLE PRECISION POLL
          COMMON /ALLCOM/ POLL(4,3),GPOLL(4,3),ANS(8),GOTIME,XDEPTH,ISOUR,
         1                 XDEPRV
          EQUIVALENCE (TEMP,ANS(3)),(HUMID,ANS(4)),(BAROM,ANS(5)),
         1            (COVER,ANS(6)),(HT,ANS(7)),(XHT,ANS(8))
    C
    C     DECLARE ARRAYS AND PRESET DATA
    C     ABSORP--11 VALUES OF ABSORPTION COEFFICIENTS OF NO2 AND N2O4
    C     AIRMS---12 VALUES OF THE AIR MASS AT VARIOUS ZENITH ANGLES
    C     CLOUD---4 AVERAGE FRACTIONS OF INCIDENT RADIATION TRANSMITTED BY
    C           7 CLOUD TYPES
    C     OZONE---11 ABSORPTION COEFFICIENTS OF OZONE IN THE ULTRAVIOLET
    C           REGION BY WAVELENGTH, 3000A-4000A
    C     SOLAR---11 MEAN SOLAR SPECTRAL IRRADIANCE OUTSIDE THE ATMOSPHERE
    C           FOR SPECTRAL BANDWIDTHS OF 100A CENTERED AT WAVELENGTHS
    C           3000A-4000A
    C     XMOLE---11 INDICES OF REFRACTION AND MOLECULAR SCATTERING COEFFI-
    C           CIENTS FOR A HOMOGENEOUS STANDARD ATMOSPHERE AT 3000A-4000A
    C     ZENITH--13 VALUES OF TIME OF DAY AND ANGLE OF SUN TO VERTICAL
    C     VAPOR---VALUES OF WATER VAPOR PRESSURE FOR DIFFERENT TEMPERATURES
    C     XLIST---INDEPENDENT VARIABLE INTERPOLATION LIST
    C     FLIST---DEPENDENT VARIABLE LIST CORRESPONDING TO INDEPENDENT
    C           VALUES IN FLIST
    C
          DIMENSION AIRMS(9,2),CLOUD(4,8),OZONE(11),SOLAR(11),XMOLE(11),
         1    VAPOR(9,2),ABSORP(11),
         2    XLISTZ(50),XLISTA(50),XLISTC(50),XLISTV(50),
         3    FLISTZ(50),FLISTA(50),FLISTC(50),FLISTV(50)
    C
    C     DECLARE PRESET CONSTANTS
    C
    C     DUST   == DUST CONTENT OF ATMOSPHERE
    C     OZ3    == OZONE CONTENT OF ATMOSPHERE
    C     G      == REFLECTION COEFFICIENT
    C     ALBEDO == FRACTION OF
    C     PI     == 3.14159
    C
    C     TIME          TIME OF DAY
    C     TEMP          HOURLY TEMPERATURE OF THREE CLOSEST WEATHER STATIONS
    C     BAROM         HOURLY BAROMETRIC PRESSURE OF 3 CLOSEST WEATHER STAS
    C     HUMID         HOURLY HUMIDITY OF THREE CLOSEST WEATHER STAS (PERCT)
```

```
C      COVER        HOURLY CLOUD COVER OF THE 3 CLOSEST WEATHER STATIONS
C      XHT         CALCULATED MIXING HEIGHT (M)
C      ZZ          INTERPOLATED ELEVATION AT BASE OF COLUMN (M)
C      TEMPD        RATE OF CHANGE OF TEMPERATURE
C      BAROMD                         BAROMETER
C      XHTD                           MIXING HEIGHT
C
       DOUBLE PRECISION RATE
       DATA  ALBEDO /0.0/
       DATA  DUST  /1.0/
       DATA  G  /0.5/
       DATA  OZ3  /2.2/
       DATA  PI  /3.14159/
C
       DATA
     &      ABSORP/37.,57.,78.,98.,119.,136.,149.,158.,163.,167.,171./,
     1      AIRMS/15.,20.,30.,40.,45.,60.,70.,80.,85.,1.03,1.06,1.15,
     2            1.30,1.41,2.00,2.90,5.60,10.39/,
     3      CLOUD/1.1,2.0,3.0,4.0,.85,.89,.82,.80,.84,.78,.71,.65,.52,
     4            .50,.47,.45,.41,.41,.41,.41,.35,.34,.32,.31,.25,.25,
     5            .24,.24,.17,.17,.18,.18/,
     1      OZONE/.44,.12,.032,.0085,.0020,.0005,5*0 /,
     &      SOLAR/.92,1.19,1.37,1.91,1.90,2.07,2.10,2.48,2.36,2.20,
     &            3.10/,
     5      XMOLE/.530,.461,.402,.353,.311,.275,.245,.218,.195,.175,
     1            .158/,
     &      VAPOR/0.,5.,10.,15.,20.,25.,30.,35.,40.,.4579,.6543,.9209,
     3            1.2788,1.7535,2.3756,3.1824,4.2175,5.5324/
C
C
C
C      CHECK FOR FIRST TIME THROUGH ULTRAV
C
       IF (IDU .EQ. 1)  GO TO 250
C      SET UP ARRAY ZENITH FOR INTERPOLATION (XLISTZ,FLISTZ)
C      SET UP ARRAY AIRMS FOR INTERPOLATION (XLISTA,FLISTA)
C      SET UP ARRAY CLOUD FOR INTERPOLATION (XLISTC,FLISTC)
C      SET UP ARRAY VAPOR FOR INTERPOLATION (XLISTV,FLISTV)
C
       DO 50 I=1,12
       XLISTZ(I) = ZENITH(I,1)
    50 FLISTZ(I) = ZENITH(I,2)
       DO 100  I=1,9
       XLISTA(I) = AIRMS(I,1)
   100 FLISTA(I) = AIRMS(I,2)
       DO 150 I=1,4
       XLISTC(I) = CLOUD(I,1)
   150 FLISTC(I) = CLOUD(I,ICLOUD)
       DO 200  I=1,9
       XLISTV(I) = VAPOR(I,1)
   200 FLISTV(I) = VAPOR(I,2)
       IDU = 1
C
```

```
C     DETERMINE ANGLE OF SUN
C              AIR MASS AT THIS ZENITH ANGLE
C              BETA (INCIDENT RADIATION) FOR THIS MASS AND A CLOUD TYPE
C              PARTIAL PRESSURE OF WATER VAPOR IN THE ATMOSPHERE
C
  250 ANGLE = PIF2(TIME,XLISTZ,12,FLISTZ)
      CANGLE = COS(ANGLE*PI/180.)
      AIRMAS = PIF2(ANGLE,XLISTA,9,FLISTA)
      BETA = PIF2(AIRMAS,XLISTC,4,FLISTC)
      PRESS = PIF2(TEMP,XLISTV,9,FLISTV)
      PZ = PRESS*HUMID
      W = 2.3*PZ*10.**(-HT/22000.)
      C1 = (1.-COVER)/CANGLE+2.0*BETA*COVER
      C2 = 2.0*(1.-COVER+BETA*COVER)
C
C
C     FOR EACH WAVELENGTH IN ANGSTROMS FROM 3000 TO 4000 (BY HUNDREDS),
C     DETERMINE THE FOLOWING VALUES
C          A   MOLECULAR SCATTERING COEFFICIENT (TABLE XMOLE)
C          B   TRANSMISSION DUE TO MOLECULAR SCATTERING
C          C   TRANSMISSION DUE TO PARTICLE SCATTERING
C          D   ABSORPTION COEFFICIENT OF OZONE (TABLE OZONE)
C          E   TRANSMISSION DUE TO OZONE
C          F   MEAN SOLAR SPECTRAL IRRADIANCE OUTSIDE THE ATMOSPHERE
C              (TABLE SOLAR)
C          G   DIRECT AND SKY RADIATION
C          H   CONTRIBUTION TO ULTRA VIOLET REACTANT RATE PARAMETER
C              FOR ONE WAVELENGTH
C     THEN SUM THE CONTRIBUTION TO GET THE SPECIFIC ABSORPTION RATE
C
C
      L = 1
      RATE1 = 0.
      RATE2 = 0.
      RATE  = 0.
      DO 300 LAMDA=3000,3800,100
C
C     A,B
      SCTMOL = -XMOLE(L)*BAROM*AIRMAS/1013.25
C
C     C
      XLAMD4 = 1.E+04/LAMDA
      SCTPAR = -(3.75E-03*W*XLAMD4*XLAMD4 +
     &        3.5E-02*DUST*XLAMD4**.75) *AIRMAS
C
C     D,E
      SCATOZ = -OZONE(L)*OZ3*AIRMAS
C     F,G
      DIRECT = 10.**(SCTMOL+SCTPAR+SCATOZ)*SOLAR(L)*CANGLE
      SKY = G*(1.-10.**(SCTMOL+SCTPAR))*10.**SCATOZ*SOLAR(L)*CANGLE
C
C     H
      RATE1 = RATE1+ABSORP(L)*DIRECT
      RATE2 = RATE2+ABSORP(L)*SKY
  300 L = L+1
      RATE = 2.303*6.0/(6.03E+04)*(1.+ALBEDO)*(C1*RATE1+C2*RATE2)
      RETURN
      END
```

OS/360 FORTRAN H

```
COMPILER OPTIONS - NAME=  MAIN,OPT=01,LINECNT=55,SIZE=0000K,
                   SOURCE,BCD,NOLIST,NODECK,LOAD,MAP,NOEDIT,ID,NOXREF
      SUBROUTINE SOURCE(X,Y)
C
C                         SOURCE EMISSIONS MODULE
C
      COMMON /MYCOM/ TIME,ICLOUD,IDM,IDU,IDD,IDS,IPST,NSTA,NSTACK,NRAD,
     1       AIR(12,32,6),WPOS(32,3),POS(32,3),SPOS(32,3),HS(12),
     2       DS(12),VS(12),TS(12),QS(12),SBAROM,STEMP,XDOT,YDOT,
     3       ARADIO(15,2),PRADIO(15,2),ZENITH(12,2),SGRID(650),
     4       FGRID(650),AGRID1(650),AGRID2(650),AGRID4(650),EMIT(10),
     5       XHITE(12),IHT,XMIN
C
      DOUBLE PRECISION POLL
      COMMON /ALLCOM/ POLL(4,3),GPOLL(4,3),ANS(8),GOTIME,XDEPTH,ISOUR,
     1              XDEPRV
C
C     DECLARE ARRAYS AND PRESET DATA
C     POLL----ARRAY OF 4 POLLUTANTS, 3 SOURCES
C     EMIT----EMISSION RATES OF POLLUTANTS
C     WEIGHT--GRAM MOLECULAR WEIGHTS OF POLLUTANTS
C     FCURVE--TEMPORAL DISTRIBUTION CURVE OF FREEWAY TRAFFIC
C     SCURVE--TEMPORAL DISTRIBUTION CURVE OF STREET TRAFFIC
C     IBOX----INDEX TO GRID POPULATION ARRAYS
C     EPOS----MIDPOINTS OF ADJACENT GRIDS TO TRAJECTORY POINT
C     FGRID---FREEWAY MILEAGE DISTRIBUTION BY GRID
C     SGRID---STREET MILEAGE DISTRIBUTION BY GRID
C     AGRID---AREA SOURCES USAGE DISTRIBUTION BY GRID
C
      DIMENSION WEIGHT(10),FCURVE(26),SCURVE(26),ACURVE(26),IBOX(4),
     1         EPOS(4,2),DIST(4),EMITWT(10)
C
C     ORDER OF MOLECULAR WEIGHTS--PROPYLENE,NO,CO,DUMHC
C
      DATA WEIGHT /42.,30.,28.,25.,6*0./
C
      DATA FCURVE /.03022,5*.00776,.0178,.0591,.0768,.0648,.0536,
     1          4*.049425,.0569,3*.0746,.0598,5*.03022,.00776/
C
      DATA SCURVE /.030775,6*.006783,.0293,2*.0651,2*.0502,5*.06088,
     1          2*.08195,2*.05405,4*.030775,.006783/
C
C     IF STANDARD TIME, DON'T RESET
C
      IF (IPST .EQ. 1)  GO TO 20
      TIME = TIME+1.0
C
C     CHECK FOR FIRST TIME THRU ROUTINE
C
   20 IF (IDS .EQ. 1)  GO TO 50
      AX = .0833
      POLL(3,3) = 0.
      DO 40 I=1,4
```

```
   40 EMITWT(I) = EMIT(I)/(WEIGHT(I)*60.)
      IDS = 1
   50 IHR = TIME+2.0
      GMIN = TIME+2.0-IHR
C
C     EVALUATE TEMPORAL DISTRIBUTION CURVES
C
      IF (GMIN .GT. 0.5)  GO TO 100
      FX = FCURVE(IHR-1)*(.5-GMIN) + FCURVE(IHR)*(.5+GMIN)
      SX = SCURVE(IHR-1)*(.5-GMIN) + SCURVE(IHR)*(.5+GMIN)
      GO TO 150
  100 FX = FCURVE(IHR)*(1.5-GMIN) + FCURVE(IHR+1)*(GMIN-0.5)
      SX = SCURVE(IHR)*(1.5-GMIN) + SCURVE(IHR+1)*(GMIN-0.5)
C
C     DETERMINE TRAJECTORY GRID EMISSION INDEX AND GRID MIDPOINT
C
  150 IX = (X+1)/2
      IY = (Y+1)/2-1
      IBOX(1) = IX+25*IY-8
      IXM = (X-1)/2
      IXM = 2*(IXM+1)
      IYM = (Y-1)/2
      IYM = 2*(IYM+1)
C
C     FIND QUADRANT OF GRID CONTAINING TRAJECTORY POINT
C     SET EMISSION INDICES FOR ADJACENT GRIDS
C
      IF (X .GE. IXM)  GO TO 200
      IF (Y .GE. IYM)  GO TO 250
C
C     X NEGATIVE, Y NEGATIVE
C
      IBOX(2) = IBOX(1)-25
      IBOX(3) = IBOX(1)-26
      IBOX(4) = IBOX(1)-1
      IPT = 1
      GO TO 400
  200 IF (Y .GE. IYM)  GO TO 300
C
C     X POSITIVE, Y NEGATIVE
C
      IBOX(2) = IBOX(1)-25
      IBOX(3) = IBOX(1)-24
      IBOX(4) = IBOX(1)+1
      IPT = 2
      GO TO 400
C
C     X NEGATIVE, Y POSITIVE
C
  250 IBOX(2) = IBOX(1)+25
      IBOX(3) = IBOX(1)+24
      IBOX(4) = IBOX(1)-1
      IPT = 3
```

```
      GO TO 400
C
C     X POSITIVE, Y POSITIVE
C
  300 IBOX(2) = IBOX(1)+25
      IBOX(3) = IBOX(1)+26
      IBOX(4) = IBOX(1)+1
      IPT = 4
C
C
C
C
C
C
C
C
C
C
C     SET MIDPOINTS OF ADJACENT GRIDS
C
  400 GO TO (420,440,460,480),IPT
  420 EPOS(2,2) = IYM-2
      EPOS(3,1) = IXM-2
      GO TO 500
  440 EPOS(2,2) = IYM-2
      EPOS(3,1) = IXM+2
      GO TO 500
  460 EPOS(2,2) = IYM+2
      EPOS(3,1) = IXM-2
      GO TO 500
  480 EPOS(2,2) = IYM+2
      EPOS(3,1) = IXM+2
  500 EPOS(2,1) = IXM
      EPOS(3,2) = EPOS(2,2)
      EPOS(4,1) = EPOS(3,1)
      EPOS(4,2) = IYM
C
C     CALCULATE EMISSION CONTRIBUTIONS TO THE COLUMN OF THE FOUR
C         ADJACENT GRIDS INVERSELY PROPORTIONAL TO THE SQUARE OF
C         THE DISTANCE FROM THE TRAJECTORY POINT TO THE GRID MIDPTS.
C
      DIST(1) = (X-IXM)**2 + (Y-IYM)**2
      IF (DIST(1) .EQ. 0.)  GO TO 600
      DISINV = 1/DIST(1)
      STREET = SGRID(IBOX(1))/DIST(1)
      FWY    = FGRID(IBOX(1))/DIST(1)
      IF (ISOUR .NE. 1)  GO TO 540
      AREA1  = AGRID1(IBOX(1))/DIST(1)
      AREA2  = AGRID2(IBOX(1))/DIST(1)
      AREA4  = AGRID4(IBOX(1))/DIST(1)
  540 DO 550  I=2,4
      IF (IBOX(I) .EQ. 0)  GO TO 550
      DIST(I) = (X-EPOS(I,1))**2 + (Y-EPOS(I,2))**2
```

```
      DISINV = DISINV+1/DIST(I)                                          01886000
      STREET = STREET + SGRID(IBOX(I))/DIST(I)                           01887000
      FWY    = FWY    + FGRID(IBOX(I))/DIST(I)                           01888000
      IF (ISOUR .NE. 1)  GO TO 550                                       01889000
      AREA1  = AREA1  + AGRID1(IBOX(I))/DIST(I)                          01890000
      AREA2  = AREA2  + AGRID2(IBOX(I))/DIST(I)                          01891000
      AREA4  = AREA4  + AGRID4(IBOX(I))/DIST(I)                          01892000
  550 CONTINUE                                                           01893000
      STREET = STREET/DISINV                                             01894000
      FWY    = FWY/DISINV                                                01895000
      IF (ISOUR .NE. 1)  GO TO 620                                       01896000
      AREA1  = AREA1/DISINV                                              01897000
      AREA2  = AREA2/DISINV                                              01898000
      AREA4  = AREA4/DISINV                                              01899000
      GO TO 620                                                          01900000
C                                                                        01901000
C     TRAJECTORY ON MIDPOINT OF GRID                                     01902000
C                                                                        01903000
  600 STREET = SGRID(IBOX(1))                                            01904000
      FWY    = FGRID(IBOX(1))                                            01905000
      IF (ISOUR .NE. 1)  GO TO 620                                       01906000
      AREA1  = AGRID1(IBOX(1))                                           01907000
      AREA2  = AGRID2(IBOX(1))                                           01908000
      AREA4  = AGRID4(IBOX(1))                                           01909000
C                                                                        01910000
C     CALCULATE EMISSIONS FROM SOURCES                                   01911000
C                                                                        01912000
  620 STTEMP = SX*STREET/10359386.                                       01913000
      FTEMP = FX*FWY/10359386.                                           01914000
      IF (ISOUR .NE. 1)  GO TO 640                                       01915000
      ATEMP1 = AX*AREA1/10359386.                                        01916000
      ATEMP2 = AX*AREA2/10359386.                                        01917000
      ATEMP4 = AX*AREA4/10359386.                                        01918000
  640 FACTOR = 4.0E6/XDEPTH                                              01918500
      DO 650  I=1,4                                                      01919000
      GPOLL(I,1) = STTEMP*EMITWT(I)                                      01920000
      GPOLL(I,2) = FTEMP*EMITWT(I)                                       01920200
      POLL(I,1) = GPOLL(I,1)*FACTOR                                      01921000
  650 POLL(I,2) = GPOLL(I,2)*FACTOR                                      01921200
      IF (ISOUR .NE. 1)  GO TO 680                                       01922000
      GPOLL(1,3) = ATEMP1*EMITWT(1)                                      01923000
      GPOLL(2,3) = ATEMP2*EMITWT(2)                                      01923200
      GPOLL(4,3) = ATEMP4*EMITWT(4)                                      01924000
      POLL(1,3)  = GPOLL(1,3)*FACTOR                                     01924200
      POLL(2,3)  = GPOLL(2,3)*FACTOR                                     01925000
      POLL(4,3)  = GPOLL(4,3)*FACTOR                                     01925200
  680 IF (IPST .EQ. 1)  GO TO 700                                        01926000
      TIME = TIME-1.0                                                    01927000
  700 RETURN                                                             01928000
      END                                                                01929000
```

```
                                OS/360  FORTRAN H

COMPILER OPTIONS - NAME=  MAIN,OPT=01,LINECNT=55,SIZE=0000K,
                   SOURCE,BCD,NOLIST,NODECK,LOAD,MAP,NOEDIT,ID,NOXREF
      FUNCTION PIF2 (X,XLIST,N,FLIST)
C
C     SECOND ORDER ONE VARIABLE INTERPOLATION
C
      DIMENSION XLIST(100), FLIST(100)
      BLI(FL0,FL1,FL2,FL3,FL4) = ((FL1-FL0)*(FL3-FL4)/(FL2-FL1)+FL3)
      IF (X-XLIST(N)) 2,1,1
C
C     PAST END OF INDEPENDENT VARIABLE LIST.
C
    1 I = N-1
      GO TO 5
    2 IF (X-XLIST(1)) 4,4,6
C
C     BEFORE START OF INDENDENT VARIABLE LIST.
C
    4 I = 1
    5 K = 1
      GO TO 30
    6 K = 2
C
C     DETERMINE INDEPENDENT VARIABLE INTERVAL.
C
    7 DO 8 I=1,N
      IF (X-XLIST(I)) 9,9,8
    8 CONTINUE
      I = N
    9 I = I-1
   30 BLIF1 = BLI(X,XLIST(I),XLIST(I+1),FLIST(I),FLIST(I+1))
   10 IF (K-1) 11,11,12
   11 PIF2 = BLIF1
      RETURN
C
C     FIND BEST THIRD POINT.
C
   12 IF ((I+2)-N) 13,13,16
   13 IF((I-1)-1) 15,14,14
   14 IF(ABS(XLIST(I-1)-X) - ABS(XLIST(I+2)-X)) 16,15,15
   15 L = I+2
      GO TO 17
   16 L = I-1
 17   BLIF2 = (BLI(X,XLIST(I),XLIST(L),FLIST(I),FLIST(L)))
      PIF2 = BLI(X,XLIST(I+1),XLIST(L),BLIF1,BLIF2)
   18 RETURN
      END
```

```
                              OS/360  FORTRAN H

COMPILER OPTIONS - NAME=  MAIN,OPT=01,LINECNT=55,SIZE=0000K,
               SOURCE,BCD,NOLIST,NODECK,LOAD,MAP,NOEDIT,ID,NOXREF
      SUBROUTINE BARIER (X,Y,WPOS,JBAR,NPOS)
C
C     DETERMINES IF INTERSECTION OF LINE SEGMENT CONNECTING TRAJECTORY
C     POINT AND STATION AND THE BARRIER LINE SEGMENT LIES ON THE BARRIER
C     ITSELF.  EVALUATE FUNCTIONS ALPHA AND BETA.  IF THEY ARE BOTH LESS
C     THAN 1 AND GREATER THAN 0, STATION IS ELIMINATED.
      COMMON  /BARRR/ IDB
C
      DIMENSION WPOS(32,3),JBAR(32),BAR(10,10),BSLOPE(10,10),
     1          TSLOPE(32,2)
C
C     NBAR IS NUMBER OF BARRIERS
C     ARRAY BAR---ODD COLUMNS CONTAIN X COORDINATES
C                 EVEN COLUMNS CONTAIN Y COORDINATES
C                 ROW 1 IN ODD COLUMNS CONTAIN NO. OF POINTS IN BARRIER
C     ARRAY BSLOPE--ODD COLUMNS CONTAIN M VALUES OF BARRIER LINE SEGMTS
C                 EVEN COLUMNS CONTAIN Y VALUES OF BARRIER LINE SEGMENTS
C     ARRAY TSLOPE--ODD COLUMN CONTAINS M VALUES OF TRAJECTORY POINT
C                       WEATHER STATION LINE SEGMENT
C                 EVEN COLUMN CONTAINS B VALUES OF TRAJECTORY POINT
C                       WEATHER STATION LINE SEGMENT
C
      DATA NBAR/ 2/, BAR/2.,16.,38.,8*0.,2*40.,7*0.,4.,53.,62.,66.,71.,
     1          6*0.,31.,27.,32.,23.,65*0./
C
C     DETERMINE SLOPE AND INTERCEPT FROM INTERPOLATION POINT TO EACH
C          STATION.
C
      DO 50  I=1,NPOS
      TSLOPE(I,1) = 0.
50    TSLOPE(I,2) = 0.
      DO 100  I=1,NPOS
      IF((WPOS(I,1)-X) .EQ. 0.)  GO TO 100
      TSLOPE(I,1) = (WPOS(I,2)-Y)/(WPOS(I,1)-X)
      TSLOPE(I,2) = Y-TSLOPE(I,1)*X
100   CONTINUE
C
C     DETERMINE SLOPE AND INTERCEPT OF EACH SEGMENT OF EACH BARRIER
C
      IF (IDB .EQ. 1)   GO TO 210
      DO 200  J=1,NBAR
      NNBAR = BAR(1,2*J-1)
      DO 200  K=2,NNBAR
      IF ((BAR(K+1,2*J-1)-BAR(K,2*J-1)) .EQ. 0.)  GO TO 200
      BSLOPE(K,2*J-1) = (BAR(K+1,2*J)-BAR(K,2*J))/
     1                        (BAR(K+1,2*J-1)-BAR(K,2*J-1))
      BSLOPE(K,2*J) = BAR(K,2*J)-BSLOPE(K,2*J-1)*BAR(K,2*J-1)
200   CONTINUE
      IDB = 1
C
C     DETERMINE INTERSECTION FUNCTIONS
```

```
C           IF VALUE OF INSECTION IS LE TO ZERO OR GE 1,
C           INCLUDE STATION.
C
  210 DO 400  I=1,NPOS
      DO 375  J=1,NBAR
      NNBAR = BAR(1,2*J-1)
      DO 375  K=2,NNBAR
      IF ((BAR(K+1,2*J-1)-BAR(K,2*J-1)) .EQ. 0.)  GO TO 220
      DENOM1 = BSLOPE(K,2*J-1)*(X-WPOS(I,1))-(Y-WPOS(I,2))
      IF (DENOM1 .EQ. 0.)   GO TO 350
      ALPHA = (WPOS(I,2)-BSLOPE(K,2*J-1)*WPOS(I,1)-BSLOPE(K,2*J))/
     &              DENOM1
      GO TO 240
220   DENOM2 = X-WPOS(I,1)
      IF (DENOM2 .EQ. 0.)   GO TO 350
      ALPHA = -WPOS(I,1)/DENOM2
240   IF (ALPHA .GE. 1.)  GO TO 350
      IF (ALPHA .LE. 0.)  GO TO 350
      IF ((WPOS(I,1)-X) .NE. 0.)  GO TO 250
      IF ((WPOS(I,2)-Y) .EQ. 0.)  GO TO 350
      GO TO 260
250   DENOM3 = TSLOPE(I,1)*(BAR(K,2*J-1)-BAR(K+1,2*J-1))
     &             -BAR(K,2*J)+BAR(K+1,2*J)
      IF (DENOM3 .EQ. 0.)    GO TO 350
      BETA = (BAR(K+1,2*J)-TSLOPE(I,1)*BAR(K+1,2*J-1)-TSLOPE(I,2))/
     &              DENOM3
      GO TO 280
260   DENOM4 = BAR(K,2*J-1)-BAR(K+1,2*J-1)
      IF (DENOM4 .EQ. 0.)   GO TO 350
      BETA = -BAR(K+1,2*J-1)/DENOM4
280   IF (BETA .GE. 1.)  GO TO 350
      IF (BETA .LE. 0.)  GO TO 350
      JBAR(I) = 0
      GO TO 400
  350 JBAR(I) = 1
375   CONTINUE
  400 CONTINUE
      RETURN
      END
```

```
COMPILER OPTIONS - NAME=  MAIN,OPT=01,LINECNT=55,SIZE=0000K,
                  SOURCE,BCD,NOLIST,NODECK,LOAD,MAP,NOEDIT,ID,NOXREF
      SUBROUTINE SMGPLT
      DIMENSION OUT(101),YPR(11)
      DOUBLE PRECISION C,D,Z,DERY,ZZ,PRMT,BB,POLL,YY
      COMMON /KINCOM/ ZZ(4),YY(40),LABEL(40),D(50),RCT(50,3),PRMT(8),
     1       DERY(40),C(50),BB,Z(2),N,NC,NEQ,NDIF,KDIF,M,NN,INTR,NNC,
     2       NNDIF,IUV,IM,IS,ITRAF,NLL,CC(16,100),A(80),STEP(15),TIM1,
     3       TIM2,TIM4,PEAK1,TIME1,PEAK3,TIME3,XPOS,YPOS
C
      COMMON /ALLCOM/ POLL(4,3),GPOLL(4,3),ANS(8),GOTIME,XDEPTH,ISOUR,
     1                XDEPRV
      REAL*8 LABEL, RCT
      REAL   BLANK/' '/,ANG(16)/'X','1','2','3','4','5','6','7','8','9',
     2'A','B','C','D','E','F'/,IB/'I'/
      YMIN = 0.
      DO 5  I=1,101
    5 OUT(I) = 0.
      DO 6  I=1,11
    6 YPR(I) = 0.
      MM=NDIF+1
      NN=NN-1
      WRITE(6, 9) NDIF,NN
      IF(CC(2,NN).NE.PEAK1.AND.CC(3,NN).NE.PEAK3) GO TO 10
      WRITE (6,115)
   10 WRITE (6,110) PEAK1,TIME1,PEAK3,TIME3
      IF(TIM1.NE.0.0) WRITE (6,120) TIM1
      IF(TIM2.NE.0.0) WRITE (6,130) TIM2
      IF(TIM4.NE.0.0) WRITE (6,140) TIM4
   11 NGRAPH=1
      IF(MM-9) 15, 15, 12
   12 NGRAPH=2
      IF (MM-14) 14,14,13
   13 NGRAPH=3
   14 JMAX=6
      GO TO 16
   15 JMAX=MM
   16 JMIN=2
      IF(NLL) 18,18,20
   18 NLL=51
   20 IF(NLL.LT.NN)NLL=NN+1
      AA=NLL-1
      XSCAL=(PRMT(2)-PRMT(8))/AA
      IF (PRMT(2) .GT. CC(1,NN)+5.0)  XSCAL=(CC(1,NN)-PRMT(8))/AA
      XSCLHF=XSCAL/2.0
      DO 95 K=1,NGRAPH
      IF(NGRAPH-K) 21,21,22
   21 JAX=MM
      GO TO 23
   22 JAX=K*5+1
   23 JIN=(K-1)*5+2
  125 YMAX=0.0
      DO 40 I=1,NN
```

```
      DO 40 J=JMIN,JMAX
      IF(CC(J,I)-YMAX) 40,40,30
   30 YMAX = CC(J,I)
   40 CONTINUE
      YSCAL=YMAX/100.
      XB=CC(1,1)
      L= 1
      I=1
      WRITE (6,1) PRMT(1),PRMT(7),PRMT(5),PRMT(6),A
      WRITE (6,7)
   45 F=I-1
      XPR=XB + F* XSCAL
   46 IF (XPR-CC(1,L)-1.0)  48,48,47
   47 L=L+1
      GO TO 46
   48 IF (CC(1,L)-XSCLHF-XPR)  50,50,70
   50 IF (L .GT. NN)  GO TO 70
      DO 55  IX=1,101
   55 OUT(IX)=BLANK
      OUT(1)=IB
      OUT(101)=IB
      DO 60 J=JIN,JAX
      JP =((CC(J,L)-YMIN)/YSCAL) +1.5
      IF(JP) 60,60,56
   56 IF(JP-101)57,57,60
   57 IF (OUT(JP).EQ.BLANK.OR.OUT(JP).EQ.IB) GO TO 59
      OUT(JP)= ANG(1)
      GO TO 60
   59 OUT(JP) = ANG(J)
   60 CONTINUE
      WRITE(6,2) XPR,(OUT(IZ),IZ=1,101),CC(1,L)
      L=L+1
      GO TO 80
   70 WRITE(6,3) XPR
   80 I=I+1
      IF (I-NLL)  45,45,86
   86 WRITE(6,7)
      YPR(1)= YMIN
      DO 90 KM=1,9
   90 YPR(KM+1)= YPR(KM) +YSCAL*10.0
      YPR(11)=YMAX
      WRITE(6,8)(YPR(IP),IP=1,11)
   95 CONTINUE
      JMIN=JMAX+1
      JMAX=MM
      JIN=6
      JAX=JMAX
      IF(JMAX-JMIN) 99,99,125
   99 RETURN
    1 FORMAT ('1',E10.4,' MIN SIMULATION  BB=',E10.4,'  PRMT(3)=',E10.4,
     1'  PRMT(4)=',E10.4,/,4(' ',20A4,/))
    2 FORMAT(1H ,F 8.1,2X,101A1,F7.2)
    3 FORMAT (1H ,F8.1,2X,'I',99X,'I')
```

```
  7 FORMAT(1H ,10X,10(10H*         ),1H*)
  8 FORMAT(1H ,3X,11F10.2)
  9 FORMAT('OTHERE ARE',I3,' DIF. CONCN. AND',I3,' STEPS IN THIS SET O
   1F DATA.',/////)
100 FORMAT(' ','MM WAS CHANGED TO 10, NN WAS CHANGED TO 50.')
110 FORMAT(' NO2 PEAK CONCN PPHM WAS ',E13.7,' AT TIME ',E9.3,' MIN,',
   1/,      ' O3 PEAK CONCN PPHM WAS ',E13.7,' AT TIME ',E9.3,' MIN.')
115 FORMAT(1H ,'BOTH PEAK VALUES NOT REACHED, HIGHEST VALUES WERE')
120 FORMAT('OHALF-TIME FOR NO2 IS ',F7.3,' MINUTES.')
130 FORMAT('OHALF-TIME FOR NO  IS ',F7.3,' MINUTES.')
140 FORMAT('OHALF-TIME FOR OLEFIN IS ',F7.3,' MINUTES.')
150 FORMAT(1H1)
    END
```

## Section IX
## Operation of the Reverse Trajectory Program

The reverse trajectory program calculates air parcel paths beginning with the terminal position. It uses hourly average wind information, and interpolates initial pollutant concentrations from hourly pollutant monitoring data. Starting values are computed for nitrogen dioxide, nitric oxide, ozone, and carbon monoxide. Trajectories may also be calculated in a forward direction with the pollutant interpolation occurring at the end point. In this case, the values computed for $NO_2$, NO, $O_3$ and CO amy be considered for validation purposes.

The program's operation, subroutine by subroutine follows:

1. MAIN

   a. Reads in all input data to the program.
   b. Converts all data to the metric system.
   c. Initialization function.
   d. Prints meteorological and pollutant data.
   e. Calls SMGDRV.
   f. Calls POLLUT.
   g. Outputs pollutant interpolation values.
   h. Checks for multiple runs.

2. SMGDRV

   a. Serves numerical integration function.
   b. Controls processing end time.
   c. Calls RWIND.
   d. Calls PUTOUT.

3. RWIND

   a. Calls BARIER.
   b. Determines wind velocity inputs for the particular trajectory point.

c. Determines wind velocity rates of change (derivatives) of wind velocity data.

4. BARIER

a. Determines if a natural barrier blocks a meteorological station or a pollutant monitoring station from the trajectory point in consideration. If so, the station is discounted.

5. PUTOUT

a. Prints trajectory positions, time into trajectory in minutes.

6. POLLUT

a. Calls BARIER

b. Determines interpolated concentrations of $NO_2$, NO, $O_3$, and CO at final trajectory point.

## Section X

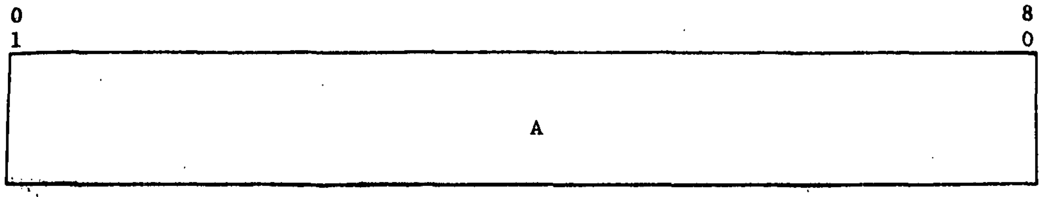
## Reverse Trajectory Inputs

Inputs must be prepared exactly as described. A sample input deck is shown in Section X.

1. Card Type 1

   Heading data---array A---4 cards

   Alphanumeric data used as heading information. May be blank cards.




2. Card Type 2

   Starting data--7 Items--1 Card

   XPOS - X coordinate of starting position in miles. Range: 17.0 to 67.0; cols. 1-10.

   YPOS - Y coordinate of starting position in miles. Range: 1.0 to 53.0; cols. 11-20.

   GOTIME - Simulation start time (local standard time) in hours and decimal fraction of hours. Range: 7.000 to 18.999; cols. 21-30.

   PRMT(2) - Length of simulation in minutes and decimal fraction of minutes. Cols 31-40. For backward trajectory, value must be negative. For forward trajectory, value must be positive.

   PRMT(3) - Initial value of step size for numerical integration in minutes and decimal fraction of minutes. For backward trajectory, value must be negative. For forward trajectory, value must be positive. Normal range in magnitude is from .001 to .5; cols. 41-50.

PRMT(4) - Upper bound of error in numerical integration. Determines allowable difference between predictor and corrector. Normal range is from .5 to .01; cols. 51-60.

TINT - Output interval. Specifies in minutes how often position print outs are to occur. Normal range is from 5.0 to 30.0 minutes; cols. 61-70.

FORMAT (4F10.3, 3F10.5)

0 11 22 33 44 55 66 77 8
1 01 01 01 01 01 01 01 0

| XPOS | YPOS | GOTIME | PRMT(2) | PRMT(3) | PRMT(4) | TINT | |
|---|---|---|---|---|---|---|---|

3. Card Type 3

Starting data--4 Items--1 Card (all values must be right justified)

NSTA - Number of meteorological stations; cols. 1-10.

NDIF - Number of accumulating species, usually 0; cols. 11-20.

NPOL - Number of pollutant monitoring stations; cols. 21-30.

IN - Indicates if program is to operate again with data from previous run or a new set of data is necessary.

0 - A complete set of data is necessary for the run.

1 - Rerun with previous data. Must input only card types 1, 2, and 3; cols. 31-40.

| 0<br>1 | 11<br>01 | 22<br>01 | 33<br>01 | 44<br>01 | 8<br>0 |
|---|---|---|---|---|---|
| NSTA | NDIF | NPOL | IN | | |

4. Card Type 4

Wind velocity data--1 array--maximum of 32 stations.

Use card type 9 from model, or set up cards as follows:

AIR - 3 cards per station, 4 hours per card, 12 hours per station.

IDNUM - Column 1-3, alphanumeric station ID

AIR - Column 4-5, start hour of data, values are 7, 11 or 15,

Column 6, number of readings on card, max = 4

Column 7-12<br>
Column 24-29<br>
Column 41-46<br>
Column 58-63

hourly data--6 columns

2 items in the 6 columns, 3 columns per item wind direction in degrees, wind speed in miles/hour, last column is in tenths of a mile/hour.

Conversion: wind speed and direction are converted into XDOT and YDOT, the X and Y components of wind velocity at the trajectory point.

FORMAT (A3, 3X, 4(F3.0, F3.1, 11X))

The station order on card types 4 and 5 must be exactly coincidental.

0 00000 01 11 22 22 23 44 44 44 55 66 66 8
1 34567 90 23 34 67 90 01 34 67 78 01 34 0

| | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| ID | HOUR | 4 | WDIR | WSPD | | WDIR | WSPD | | WDIR | WSPD | | WDIR | WSPD | | |

5. Card Type 5--(See Figure 4)

Meteorological Stations--2 arrays--maximum of 8 cards, 4 stations per card.

WPOS - Array of quadruplets, 4 stations per card, maximum of 32 stations.

Cards are as follows:

IDMET - Column 1-3, alphanumeric station ID code.

WPOS - Column 4-8, X coordinate of station position in miles, last 2 columns in hundreths of miles. Column 9-13, Y coordinate of station position in miles, last 2 columns in hundreths of miles. Column 14-20, ground elevation of station in feet, last 2 columns in hundreths of feet. This 20 column grouping is repeated in columns 21-40, 41-60, 61-80 as required, and on additional cards if necessary.

FORMAT (4(A3, 2F5.2, F7.2))

The station order on card types 4 and 5 must be exactly coincidental.

0 00 00 11 22 22 22 33 44 44 44 55 66 66 66 77 8
1 34 89 34 01 34 89 34 01 34 89 34 01 34 89 34 0

| | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| ID | X | Y | ELEV | ID | X | Y | ELEV | ID | X | Y | ELEV | ID | X | Y | ELEV |

6. Card Type 6

Pollutant monitoring data--2 arrays--maximum of 5 cards, 4 stations per card.

PPOS - Array of quadruplets, 4 stations per card, maximum of 20 stations.

Cards are as follows:

IDPOL - Column 1-3, alphanumeric station ID code.

PPOS - Column 4-8, X coordinate of station position in miles, last 2 columns in hundreths of miles.

Column 9 - 13, Y coordinate of station position in miles, last 2 columns in hundreths of miles.

Columns 14-20, blank.

This 20 column grouping is repeated in columns 21-40, 41-60, 61-80 as required, and on additional cards if necessary.

FORMAT (4(A3, 2F5.2, F7.2))

The station order card types 6 and 7 must be exactly coincidental.

```
0 00 00 11      22 22 22 33      44 44 44 55      66 66 66 77      8
1 34 89 34      01 34 89 34      01 34 89 34      01 34 89 34      0
|ID| X | Y |    |ID| X | Y |    |ID| X | Y |    |ID| X | Y |    |
```

7. Card Type 7

Pollutant monitoring data--2 arrays--maximum of 20 stations.

CONC - 4 cards per station, 3 hours per card, 12 hours per station.

Set up card as follows:

IDPOL - Column 1-3, alphanumeric station ID code.

CONC - Column 4-5, start hour of data, values are 7, 10, 13 or 16,

6, number of readings on card, max = 3.

7-27
28-48 } hourly data--21 columns, all values are in pphm
49-69

5 items in the 21 columns as follows:

4 columns - $NO_2$, last column is in parts/billion.

4 columns - NO, last column is in parts/billion.

4 columns - $O_3$, last column is in parts/billion.

4 columns - blank, field not used but has been set aside for input of hydrocarbon data or another pollutant of interest.

5 columns - CO, last column is in parts/billion.

| 01 | 03 04 05 | 06 | 07 10 | 11 14 | 15 18 | 19 22 | 23 27 | 28 31 | 32 35 | 36 39 | 40 43 | 44 48 | 49 52 | 53 56 | 57 60 | 61 64 | 65 69 | 70 80 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| ID | HOUR | 3 | $NO_2$ | NO | $O_3$ | | CO | $NO_2$ | NO | $O_3$ | | CO | $NO_2$ | NO | $O_3$ | | CO | |

FORMAT (A3, 3X, 3(3F4.1, 4X, F5.1), 11X)

The station order or card types 6 and 7 must be exactly coincidental.

# Section XI

## Reverse Trajectory Sample Input Deck

Card Type 1

```
SEPTEMBER 29, 1969   11 30 AM
TERMINATE AT PASADENA
29 METEOROLOGICAL STATIONS, 2 BARRIERS
12 POLLUTANT STATIONS
```

Card Type 2

```
      47.0      42.0      13.5    -300.0      -.25        .1      15.0
```

Card Type 3

```
        29                  12         0
```

Card Type 4

```
NTB074      67611114                                78611117               80621114
NTB114      86621111             90611105           88601099               92581095
NTB154      89561094             84541093           82521096               76521099
NZJ074      63631101                                77621113               84601113
NZJ114      88561107             92571101           92611096               92581091
NZJ154      90581091             88591093           86601093               77591093
CAP074 90 2 70          225 3    75        270 5    79          270 6      80
CAP114270 8 87          270 9    88        270 9    86          270 9      86
CAP154270 8 87          270 8    86        270 5    82          270 6      78
ONT074      6854                 7054                                      9047
ONT114      9542                 9745              10048                  10056
ONT154      9952                 9760               9248                   8638
LAX074350 5 65621113    350 5    69631118  240 9    72641121    240 9      74631119
LAX114240 9 80591116    26014    74621114  26014    73621109    26014      73621103
LAX15426016 72621100    26016    71601099  26016    71601096    230 8      70581096
BUR074     7 7151           1    7356          1    7756            1      8849
BUR114     1 9246           2    9839      180 3    9950        270 4      9950
BUR154315 4 10047       315 4    9642      338 2    9143        270 1      9038
LGB074315 2 67611122    270 3    71611125  270 4    77611125    293 7      84601125
LGB114270 5 87571119    270 8    91561112  27010    89581108    27010      86591105
LGB15427013 86571102    27010    81581102  270 7    77571102    270 3      72551105
ENC074113 2             158 2              293 3                293 3
ENC114293 3             293 5              293 7                293 6
ENC154293 6             270 6              270 5                270 3
ELM074120 3 7459        100 1    8055      140 2    8557        230 4      9055
ELM114220 7 9453        220 9    9752      22010    9846        22011      9643
ELM15424012 9539        25010    9334      200 6    8639        210 8      8850
```

Card Type 4 (Continued)

| | | | |
|---|---|---|---|
| COM074 45 3 | 315 3 | 293 4 | 293 9 |
| COM114293 9 | 29311 | 29314 | 29315 |
| COM15429315 | 27017 | 29316 | 29312 |
| CPK074203 1 | 135 1 | 180 1 | 135 1 |
| CPK114135 1 | 203 2 | 158 2 | 315 4 |
| CPK154338 6 | 338 6 | 338 4 | 315 2 |
| AZU074315 2 | 90 2 | 113 2 | 68 1 |
| AZU114203 5 | 203 7 | 225 7 | 203 9 |
| AZU15420310 | 20311 | 203 9 | 203 5 |
| WHT074338 4 | 293 2 | 180 2 | 248 2 |
| WHT114248 5 | 270 6 | 270 6 | 270 6 |
| WHT154270 6 | 270 6 | 270 4 | 248 3 |
| WLA074270 1 | 203 1 | 225 1 | 225 2 |
| WLA114225 4 | 225 5 | 225 4 | 225 3 |
| WLA154225 4 | 203 4 | 203 2 | 203 1 |
| WNT074 23 | 158 | 293 | 158 |
| WNT114248 | 248 | 203 | 203 |
| WNT154203 | 248 8 | 248 7 | 180 4 |
| VER074270 6 | 270 2 | 270 2 | 270 3 |
| VER114270 3 | 270 5 | 225 3 | 225 5 |
| VER15422511 | 270 5 | 270 9 | 27010 |
| VEN074293 1 | 248 2 | 270 5 | 248 3 |
| VEN114225 6 | 24810 | 24810 | 24811 |
| VEN15424811 | 248 8 | 225 6 | 203 7 |
| RVA074 23 3 | 338 3 | 23 3 | 180 4 |
| RVA114203 5 | 225 6 | 248 8 | 248 9 |
| RVA154248 7 | 225 7 | 248 6 | 225 5 |
| RSD074113 1 | 248 1 | 180 1 | 68 1 |
| RSD114203 1 | 68 2 | 135 2 | 90 2 |
| RSD154270 7 | 293 8 | 248 6 | 270 3 |
| RB 074293 3 | 248 3 | 248 4 | 225 3 |
| RB 114203 5 | 225 8 | 225 7 | 225 8 |
| RB 154225 8 | 203 7 | 203 5 | 203 6 |
| RLA074225 1 | 360 1 | 270 1 | 180 1 |
| RLA114225 1 | 225 1 | 270 1 | 225 1 |
| RLA154225 1 | 225 1 | 225 2 | 225 2 |
| POM074113 2 | 135 2 | 248 2 | 270 2 |
| POM114315 4 | 315 4 | 293 4 | 315 6 |
| POM154293 6 | 315 6 | 293 4 | 293 5 |
| PIC074315 1 | 360 1 | 225 1 | 225 1 |
| PIC114225 1 | 225 1 | | |
| PIC154180 1 | 180 1 | 225 1 | 180 1 |
| MAL074225 2 | 225 3 | 158 2 | 203 2 |
| MAL114225 5 | 225 7 | 225 5 | 225 8 |
| MAL15422510 | 225 8 | 90 2 | 90 3 |
| KFI074 23 1 | 270 1 | 225 1 | 293 2 |
| KFI114293 4 | 315 6 | 293 8 | 31510 |
| KFI15431510 | 315 9 | 293 7 | 293 5 |
| HOL074270 1 | 135 6 | 270 1 | 180 1 |
| HOL114225 1 | 180 1 | 225 9 | 225 5 |
| HOL154225 2 | 225 2 | 225 6 | 180 2 |

## Card Type 4 (Continued)

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| BKT074 90 5 | | 90 3 | | 90 4 | | 270 4 | |
| BKT114270 6 | | 270 7 | | 270 8 | | 27010 | |
| BKT15427011 | | 27012 | | 270 9 | | 270 7 | |
| PAS074338 2 | | 45 1 | | 225 1 | | 158 2 | |
| PAS114180 2 | | 203 3 | | 180 3 | | 225 4 | |
| PAS154225 6 | | 225 3 | | 225 2 | | 45 1 | |
| CMC074 60 3 | 7159 | 150 2 | 7957 | 190 5 | 8558 | 220 8 | 8955 |
| CMC114240 7 | 9355 | 26010 | 9450 | 26012 | 9152 | 26012 | 9148 |
| CMC15426011 | 8852 | 27010 | 8354 | 250 8 | 7854 | 230 5 | 7455 |

## Card Type 5

| | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| NTB | 51 | 16 | 27 | NZJ | 70 | 8 | 380 | CAP | 40 | 33 | 300 | ONT | 76 | 35 | 916 |
| LAX | 32 | 27 | 99 | BUR | 33 | 45 | 530 | LGB | 45 | 18 | 34 | ENC | 23 | 44 | 800 |
| ELM | 52 | 35 | 300 | COM | 39 | 22 | 100 | CPK | 19 | 46 | 800 | AZU | 59 | 41 | 600 |
| WHT | 51 | 30 | 250 | WLA | 30 | 34 | 200 | WNT | 63 | 30 | 950 | VER | 41 | 31 | 180 |
| VEN | 26 | 30 | 5 | RVA | 48 | 30 | 180 | RSD | 22 | 46 | 800 | RB | 31 | 21 | 10 |
| RLA | 45 | 26 | 100 | POM | 70 | 33 | 850 | PIC | 33 | 34 | 100 | MAL | 18 | 34 | 20 |
| KFI | 53 | 23 | 100 | HOL | 35 | 37 | 300 | BKT | 68 | 36 | 950 | PAS | 47 | 42 | 870 |
| CMC | 44 | 31 | 180 | | | | | | | | | | | | |

## Card Type 6

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| DLA | 40 | 35 | AZU | 59 | 41 | BUR | 33 | 45 | WLA | 30 | 34 |
| LGB | 45 | 18 | RSD | 22 | 46 | POM | 70 | 33 | LAX | 32 | 27 |
| PAS | 47 | 42 | WHT | 51 | 30 | CMC | 44 | 31 | ELM | 52 | 35 |

## Card Type 7

| | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| DLA073 | 3 | 28 | 2 | 17 | 11 | 36 | 5 | 18 | 19 | 30 | 8 | |
| DLA103 | 18 | 11 | 12 | | 10 | 5 | 9 | 6 | | | 8 | 3 |
| DLA133 | 5 | | 7 | 3 | | 2 | 5 | 2 | 6 | 3 | 3 | 6 |
| DLA163 | 7 | 5 | 2 | 6 | 7 | 6 | 1 | 5 | 5 | 8 | 1 | 4 |
| AZU073 | 13 | 4 | 3 | 10 | 16 | 3 | 9 | 11 | 11 | 1 | 16 | 10 |
| AZU103 | 8 | 1 | 22 | 8 | 5 | 1 | 24 | 6 | | | 28 | 7 |
| AZU133 | | | 38 | 9 | | | 25 | 6 | 5 | 1 | 14 | 6 |
| AZU163 | 7 | 1 | 7 | 4 | 7 | 1 | 2 | 5 | 11 | 1 | 1 | 7 |
| BUR073 | 17 | 34 | 2 | 18 | 25 | 27 | 4 | 17 | 29 | 14 | 7 | 9 |
| BUR103 | 28 | 7 | 11 | 11 | 19 | 3 | 14 | 10 | | | 21 | 11 |
| BUR133 | | | 14 | 7 | | | 11 | 7 | 11 | 1 | 5 | 5 |
| BUR163 | 10 | 2 | 3 | 5 | 11 | 3 | 2 | 6 | 17 | 12 | 2 | 12 |
| WLA073 | 12 | 35 | 1 | 17 | 21 | 38 | 3 | 17 | 19 | 6 | 5 | 8 |
| WLA103 | 14 | 3 | 10 | | | | 12 | 5 | | | 10 | 4 |
| WLA133 | 8 | 1 | 10 | 4 | 8 | 1 | 6 | 4 | 8 | 2 | 4 | 4 |
| WLA163 | 9 | 3 | 2 | 5 | 10 | 5 | 1 | 4 | 9 | 1 | 3 | 4 |
| LGB073 | 9 | 26 | 1 | 13 | 17 | 18 | 1 | 11 | 28 | 10 | 2 | 9 |
| LGB103 | 20 | 9 | 2 | 6 | 22 | 8 | 6 | 6 | | | 2 | 6 |
| LGB133 | 19 | 16 | 1 | 5 | 6 | 18 | 1 | 5 | 13 | 21 | 1 | 5 |
| LGB163 | 11 | 21 | 1 | 5 | 9 | 21 | 1 | 5 | 8 | 20 | 1 | 4 |

Card Type 7 (Continued)

| | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| RSD073 | 13 | 11 | 4 | 16 | 21 | 7 | 9 | 11 | 17 | 1 | 12 | 8 |
| RSD103 | 10 | 1 | 14 | 6 | 4 | 1 | 10 | 4 | | | 17 | 5 |
| RSD133 | | | 9 | 3 | | | 6 | 3 | 2 | 1 | 7 | 5 |
| RSD163 | 3 | 1 | 4 | 5 | 3 | 1 | 3 | 5 | 4 | 1 | 2 | 6 |
| POM073 | 18 | 6 | 3 | 9 | 21 | 4 | 9 | 9 | 15 | 1 | 16 | |
| POM103 | 10 | 1 | 19 | 6 | 10 | 1 | 14 | 5 | | | 15 | 4 |
| POM133 | | | 21 | 5 | 5 | 1 | 21 | 6 | 8 | 1 | 16 | 6 |
| POM163 | 13 | 2 | 6 | 6 | 13 | 2 | 6 | 5 | 14 | 3 | 3 | 6 |
| LAX073 | 10 | 20 | 2 | 9 | 13 | 9 | 2 | 5 | 10 | 6 | 3 | 5 |
| LAX103 | 11 | 4 | 4 | 6 | | | 10 | | | | 7 | 3 |
| LAX133 | | | 8 | 3 | 5 | 1 | 5 | 4 | 6 | 2 | 4 | 6 |
| LAX163 | 7 | 3 | 4 | 6 | 8 | 3 | 4 | 5 | 9 | 5 | 1 | 3 |
| PAS073 | 10 | 16 | 2 | | 9 | 2 | 9 | | 6 | 1 | 17 | |
| PAS103 | 6 | 1 | 26 | | 12 | 1 | 41 | | | | 32 | |
| PAS133 | 5 | 1 | 20 | | 8 | 2 | 12 | | 6 | 1 | 9 | |
| PAS163 | 5 | 1 | 6 | | 6 | 2 | 3 | | 9 | 5 | 2 | |
| WHT073 | 19 | 34 | 2 | 14 | 30 | 9 | 6 | 11 | 37 | 3 | 11 | 11 |
| WHT103 | 41 | 2 | 21 | 13 | 21 | 1 | 34 | | | | 30 | 2 |
| WHT133 | 10 | 1 | 19 | 1 | 9 | 1 | 12 | 1 | 10 | 1 | 7 | 1 |
| WHT163 | 12 | 2 | 4 | 1 | 9 | 1 | 5 | 1 | 11 | 1 | 3 | 1 |
| CMC073 | 16 | 32 | | 17 | 26 | 22 | | 15 | 32 | 15 | | 15 |
| CMC103 | 25 | 7 | | 9 | 14 | 6 | 9 | 6 | 10 | 3 | 5 | 4 |
| CMC133 | 9 | 9 | 2 | 3 | 7 | 6 | 2 | 3 | 7 | 9 | 1 | 4 |
| CMC163 | 4 | 8 | | 4 | 3 | | 2 | 3 | 5 | | | 3 |
| ELM073 | | | | | | | 2 | 8 | | | 6 | 6 |
| ELM103 | | | 13 | 6 | | 22 | | 9 | | | 23 | 5 |
| ELM133 | | | 14 | 3 | | 9 | | 2 | | | 5 | 2 |
| ELM163 | | | 2 | | | | | 4 | | | 3 | 5 |

# Section XII

# Reverse Trajectory Program Listing

```
C                                                                       BD0001
      DIMENSION Y(40),DERY(40),IDNUM(32),IR(50,5),DAIR(12,32,2),PRMT(6),BD0002
     1          A(80),IDMET(32),IDPOL(32)                               BE0003
      DOUBLE PRECISION AUX,C,D,DELT,DERY,H,X,Y,YY,Z,ZZ                  BD0004
      COMMON /RECOM/ TIME,ANS(8),DERIV(8), NSTA,NPOL,AIR(12,32,2),      BD0005
     1     WPOS(32,3),GOTIME                                            BD0006
C                                                                       BD0007
      COMMON /BARRR/ IDB                                                BD0008
      COMMON /OUTCOM/ TOUT,TINT                                         BD0009
      COMMON  /MILES/ COORD(2),DXY(2)                                   BD0010
      REAL*4 NO2,NO                                                     BD0011
      DIMENSION CONC(12,20,5),PPOS(32,3),ID(20)                         BE0012
C                                                                       BD0013
C     GOTIME--SIMULATION START TIME                                     BD0014
C                                                                       BD0015
      EXTERNAL RWIND,PUTOUT                                             BD0016
C                                                                       BD0017
C     INITIALIZATION                                                    BD0018
C                                                                       BD0019
C                                                                       BD0020
C     INPUT HEADING INFORMATION                                         BD0021
C                                                                       BD0022
    1 READ (5,1000,END=900) A                                           BD0024
      DO 10  I=1,40                                                     BD0025
      Y(I) = 0.0D0                                                      BD0026
   10 DERY(I) = 0.0D0                                                   BD0027
      TOUT = 0.0                                                        BD0028
      N = 0                                                             BD0029
      IDB = 0                                                           BD0030
C                                                                       BD0031
C           SIZE, UPPER BOUND ERROR LIMIT, AND OUTPUT INTERVAL          BD0033
C                                                                       BD0034
      READ (5,1001) XPOS,YPOS,GOTIME,PRMT(2),PRMT(3),PRMT(4),TINT       BD0035
C     INPUT START POSITION,START TIME, LENGTH OF SIMULATION, INTIAL STEPBD0032
   75 PRMT(1) = 0.                                                      BD0036
C     READ NO. METEOR. STATIONS, NO. OF EQUAT., NO. OF POLLUTANT STA.   BE003620
C                                                                       BE003640
C                                                                       BD0037
      READ (5,1002)  NSTA,NDIF,NPOL,IN                                  BE0038
C                                                                       BD0039
C                                                                       BD0040
C                                                                       BD0041
C     SET UP POSITION FOR INTEGRATION                                   BD0042
C                                                                       BD0043
      Y(NDIF+1) = XPOS*1609.3                                           BD0044
      Y(NDIF+2) = YPOS*1609.3                                           BD0045
C                                                                       BD0046
C     CHECK FOR SECOND RUN                                              BD0047
C                                                                       BD0048
      IF (IN .EQ. 1)   GO TO 300                                        BD0049
C                                                                       BD0051
C     INPUT METEOROLOGICAL DATA.                                        BD0052
C                                                                       BD0053
```

```
      DO 100  J=1,NSTA                                                  BD0054
      READ (5,1005)  IDNUM(J),((AIR(I,J,K),K=1,2),I=1,4)                BE0055
      READ (5,1005)  IDNUM(J),((AIR(I,J,K),K=1,2),I=5,8)                BE0056
  100 READ (5,1005)  IDNUM(J),((AIR(I,J,K),K=1,2),I=9,12)               BE0057
C                                                                       BD0058
C     INPUT METEOROLOGICAL STATION DATA                                 BD0059
C                                                                       BD0060
      WRITE (6,1013)                                                    BD0061
      READ (5,1014) (IDMET(I),(WPOS(I,J),J=1,3),I=1,NSTA)               BE0062
C                                                                       BD0063
C     CONVERT DATA TO METRIC UNITS                                      BD0064
C                                                                       BD0065
      DO 120  I=1,NSTA                                                  BD0066
  120 WPOS(I,3) = WPOS(I,3)*.3048                                       BD0067
C                                                                       BD0068
C     READ POLLUTANT STATION POSITIONS                                  BD0069
C                                                                       BD0070
      READ (5,1014) (IDPOL(I),(PPOS(I,J),J=1,3),I=1,NPOL)               BE0071
C                                                                       BD0072
C     READ POLLUTANT DATA                                               BD0073
C                                                                       BD0074
      DO 140  J=1,NPOL                                                  BD0075
      READ (5,1005)  ID(J),((CONC(I,J,K),K=1,4),I=1,3)                  BE0076
      READ (5,1006)  ID(J),((CONC(I,J,K),K=1,4),I=4,6)                  BE0077
      READ (5,1006)  ID(J),((CONC(I,J,K),K=1,4),I=7,9)                  BE007750
  140 READ (5,1006)  ID(J),((CONC(I,J,K),K=1,4),I=10,12)                BE0078
C                                                                       BD0079
C     OUTPUT METEOROLOGICAL DATA                                        BD0080
C                                                                       BD0081
      WRITE (6,1015) (IDMET(I),(WPOS(I,J),J=1,3),I=1,NSTA)              BE0082
      KOUT = 0                                                          BD0083
      WRITE (6,1007)                                                    BD0084
      DO 180  I=1,12                                                    BD0085
      IH = (I+6)*100                                                    BD0086
      DO 180  J=1,NSTA                                                  BD0087
      IF (KOUT .LE. 50)   GO TO 170                                     BD0088
      KOUT = 0                                                          BD0089
      WRITE (6,1007)                                                    BD0090
      GO TO 180                                                         BD0091
  170 KOUT = KOUT+1                                                     BD0092
  180 WRITE (6,1008)  IDNUM(J),IH,(AIR(I,J,K),K=1,2)                    BD0093
C                                                                       BD0094
C     WRITE POLLUTANT DATA                                              BD0095
C                                                                       BD0096
      WRITE (6,1009)                                                    BD0097
      WRITE (6,1016) (ID(I),PPOS(I,1),PPOS(I,2),I=1,NPOL)               CB0098
      KOUT = 0                                                          BD0100
      WRITE (6,1010)                                                    BD0101
      DO 150  I=1,12                                                    BD0102
      IH = (I+6)*100                                                    BD0103
      DO 150  J=1,NPOL                                                  BD0104
      IF (KOUT .LE. 50)  GO TO 145                                      BD0105
      KOUT = 0                                                          BD0106
```

```
      WRITE (6,1010)                                                    BD0107
      GO TO 150                                                         BD0108
  145 KOUT = KOUT+1                                                     BD0109
  150 WRITE (6,1011)  ID(J),IH,(CONC(I,J,K),K=1,4)                      BE0110
C                                                                       BD0111
C     SAVE  WIND DATA                                                   BD0112
C                                                                       BD0113
      DO 200  J=1,12                                                    BD0114
      DO 200  I=1,NSTA                                                  BD0115
      DAIR(J,I,1) = AIR(J,I,2)                                          BD0116
  200 DAIR(J,I,2) = AIR(J,I,1)                                          BD0117
C                                                                       BD0118
C     CONVERT WIND DATA TO RADIANS                                      BD0119
C                                                                       BD0120
      DO 230  J=1,12                                                    BD0121
      DO 230  I=1,NSTA                                                  BD0122
      AIR(J,I,1) = -DAIR(J,I,1)*SIN(DAIR(J,I,2)*3.14159/180.)           BD0123
  230 AIR(J,I,2) = -DAIR(J,I,1)*COS(DAIR(J,I,2)*3.14159/180.)           BD0124
C                                                                       BD0125
  300 WRITE (6,1025) PRMT(2),         PRMT(3),PRMT(4),GOTIME,A          BD0126
      CALL SMGDRV (PRMT,Y,DERY,2,2,IHLF,RWIND,PUTOUT)                   BD0127
      CALL POLLUT (TIME,COORD(1),COORD(2),CONC,NPOL,NO2,NO,O3,CO,PPOS)  BE0128
      WRITE (6,1012)  NO2,NO,O3,CO                                      BE0129
      WRITE (6,1026)  IHLF                                              BD0132
      GO TO 1                                                           BD0133
  900 STOP                                                              BD0134
 1000 FORMAT(20A4)                                                      BD0135
 1001 FORMAT(4F10.3,3F10.5)                                             BD0136
 1002 FORMAT(4I10)                                                      BE0137
 1005 FORMAT(A3,3X,4(F3.0,F3.1,11X))                                    BE0138
 1006 FORMAT(A3,3X,3(3F4.1,4X,F5.1),11X)                                BE0139
 1007 FORMAT(1H1,'STATION',5X,'DATA',6X,'WIND',6X,'WIND',/              BD0140
     1       ' ','NUMBER',6X,'HOUR',6X,'DIR.',5X,'SPEED',/              BD0141
     2       ' ',22X,'(DEG)',5X,'(MPH)',//)                             BD0142
 1008 FORMAT(' ',A7,6X,I4,2F10.3)                                       BE0143
 1009 FORMAT(1H1,20X,'POLLUTANT STATIONS',/1H0,'STATION',11X,'X-COORD', CB0144
     1 11X,'Y-COORD',/' ',18X,'(MILES)',11X,'(MILES)',/)                CB0145
 1010 FORMAT(1H1,'STATION',6X,'HOUR',7X,'NO2',8X,'NO',8X,'O3',8X,'CO',/ BD0146
     1  ' ',21X,'(PPHM)',4X,'(PPHM)',4X,'(PPHM)',4X,'(PPHM)',//)        BD0147
 1011 FORMAT(' ',A7,6X,I4,4F10.1)                                       BE0148
 1012 FORMAT(////'ONO2=',E15.8,10X,'NO=',E15.8,10X,'O3=',E15.8,10X,     BE014820
     1    'CO=',E15.8)                                                  BE014825
 1013 FORMAT(1H1,30X,'METEOROLOGICAL STATIONS',/1H0,21X,'X-COORD',11X,  BE0149
     1'Y-COORD',10X,'ELEVATION',/' ',3X,'STATION',11X,'(MILES)',11X,    BE0150
     2'(MILES)',11X,'(METERS)'/)                                        BE0151
 1014 FORMAT(4(A3,2F5.2,F7.2))                                          BE0152
 1015 FORMAT(' ',A10,2F18.3,F19.3)                                      BE0153
 1016 FORMAT(' ',A7,2F18.3)                                             CB015320
 1025 FORMAT ('1',E10.4,' MIN SIMULATION                   STEP SIZE=', BD0154
     1 E10.4,'    ERROR=',E10.4,/' STARTING TIME=',E10.4,/,4(' ',20A4,/))CA0155
 1026 FORMAT('OIHLF = ',I4)                                             CA0156
      END                                                               BD0157
```

```
      SUBROUTINE SMGDRV (PRMT,Y,DERY,NDIM,NSPEC,IHLF,SMGFCT,SMGOUT)
C
C
      DIMENSION PRMT(1),Y(1),DERY(1),AUX(16,50)
      DOUBLE PRECISION AUX,C,D,DELT,DERY,H,X,Y,YY,Z,ZZ
      N=1
      IHLF=0
      X=PRMT(1)
      DELT = 0.0D0
      H=PRMT(3)
      ISTEP = 0
      DO 1 I=1,NDIM
      AUX(16,I)=0.D0
      AUX(15,I)=DERY(I)
    1 AUX(1,I)=Y(I)
      IF(H*(PRMT(2)-X))3,2,4
C
C     ERROR RETURNS
    2 IHLF=12
      GOTO 4
    3 IHLF=13
C
C     COMPUTATION OF DERY FOR STARTING VALUES
    4 CALL SMGFCT (X,Y,DERY,-1)
C
C     RECORDING OF STARTING VALUES
      CALL SMGOUT (X,Y,DERY,DELT,H,IHLF)
    5 IF(IHLF)7,7,6
    6 RETURN
    7 DO 8 I=1,NDIM
    8 AUX(8,I)=DERY(I)
C
C     COMPUTATION OF AUX(2,I)
      ISW=1
      GOTO 100
C
    9 X=X+H
      DO 10 I=1,NDIM
   10 AUX(2,I)=Y(I)
C
C     INCREMENT H IS TESTED BY MEANS OF BISECTION
   11 IHLF=IHLF+1
      X=X-H
      DO 12 I=1,NDIM
   12 AUX(4,I)=AUX(2,I)
      H=.5D0*H
      N=1
      ISW=2
      GOTO 100
C
   13 X=X+H
      CALL SMGFCT (X,Y,DERY,1)
      N=2
```

```
      DO 14 I=1,NDIM
      AUX(2,I)=Y(I)
   14 AUX(9,I)=DERY(I)
      ISW=3
      GOTO 100
C
C     COMPUTATION OF TEST VALUE DELT
C     SET DELT TO MAX PREDICTOR-CORRECTOR DIFFERENCE
   15 DELT = DABS(Y(1)-AUX(4,1))
      DO 16  I=2,NSPEC
      IF (DABS(Y(I)-AUX(4,I)) .GT. DELT)    DELT = DABS(Y(I)-AUX(4,I))
   16 CONTINUE
      IF(DELT-PRMT(4))19,19,17
   17 IF(IHLF-10)11,18,18
C
C     NO SATISFACTORY ACCURACY AFTER 10 BISECTIONS. ERROR MESSAGE.
   18 IHLF=11
      X=X+H
      GOTO 4
C
C     THERE IS SATISFACTORY ACCURACY AFTER LESS THAN 11 BISECTIONS.
   19 X=X+H
      DO 20 I=1,NDIM
      AUX(3,I)=Y(I)
   20 AUX(10,I)=DERY(I)
      N=3
      ISW=4
      GOTO 100
C
   21 N=1
      X=X+H
      CALL SMGFCT (X,Y,DERY,1)
      X=PRMT(1)
      DO 22 I=1,NDIM
      AUX(11,I)=DERY(I)
  220Y(I)=AUX(1,I)+H*(.375D0*AUX(8,I)+.7916666666666667D0*AUX(9,I)
     1-.2083333333333333D0*AUX(10,I)+.04166666666666667D0*DERY(I))
   23 X=X+H
      N=N+1
      CALL SMGFCT (X,Y,DERY,-1)
      CALL SMGOUT (X,Y,DERY,DELT,H,IHLF)
   24 IF (N-4) 25,201,201
   25 DO 26 I=1,NDIM
      AUX(N,I)=Y(I)
   26 AUX(N+7,I)=DERY(I)
      IF (N-3) 27,29,201
C
   27 DO 28 I=1,NDIM
      DELT=AUX(9,I)+AUX(9,I)
      DELT=DELT+DELT
   28 Y(I)=AUX(1,I)+.3333333333333333D0*H*(AUX(8,I)+DELT+AUX(10,I))
      GOTO 23
C
```

```
   29 DO 30 I=1,NDIM
      DELT=AUX(9,I)+AUX(10,I)
      DELT=DELT+DELT+DELT
   30 Y(I)=AUX(1,I)+.375D0*H*(AUX(8,I)+DELT+AUX(11,I))
      GOTO 23
C
C
C     ******************************************************************
C     THE FOLLOWING PART OF SUBROUTINE DHPCG COMPUTES BY MEANS OF
C     RUNGE-KUTTA METHOD STARTING VALUES FOR THE NOT SELF-STARTING
C     PREDICTOR-CORRECTOR METHOD.
  100 DO 101 I=1,NDIM
      Z=H*AUX(N+7,I)
      AUX(5,I)=Z
  101 Y(I)=AUX(N,I)+.4D0*Z
C     Z IS AN AUXILIARY STORAGE LOCATION
C
      Z=X+.4D0*H
      CALL SMGFCT (Z,Y,DERY,1)
      DO 102 I=1,NDIM
      Z=H*DERY(I)
      AUX(6,I)=Z
  102 Y(I)=AUX(N,I)+.29697760924775360D0*AUX(5,I)+.15875964497103583D0*Z
C
      Z=X+.45573725421878943D0*H
      CALL SMGFCT (Z,Y,DERY,1)
      DO 103 I=1,NDIM
      Z=H*DERY(I)
      AUX(7,I)=Z
  103 Y(I)=AUX(N,I)+.21810038822592047D0*AUX(5,I)-3.0509651486929308D0*
     1AUX(6,I)+3.8328647604670103D0*Z
C
      Z=X+H
      CALL SMGFCT (Z,Y,DERY,1)
      DO 104 I=1,NDIM
  1040Y(I)=AUX(N,I)+.17476028226269037D0*AUX(5,I)-.55148066287873294D0*
     1AUX(6,I)+1.2055355993965235D0*AUX(7,I)+.17118478121951903D0*
     2H*DERY(I)
      GOTO(9,13,15,21),ISW
C     ******************************************************************
C
C
C     POSSIBLE BREAK-POINT FOR LINKAGE
C
C
C     STARTING VALUES ARE COMPUTED.
C     NOW START HAMMINGS MODIFIED PREDICTOR-CORRECTOR METHOD.
  201 IF(N-8)204,202,204
C
C     N>8 CAUSES THE ROWS OF AUX TO CHANGE THEIR STORAGE LOCATIONS
  202 DO 203 N=2,7
      DO 203 I=1,NDIM
      AUX(N-1,I)=AUX(N,I)
```

```
  203 AUX(N+6,I)=AUX(N+7,I)
      N=7
C
C     N LESS THAN 8 CAUSES NE1 TO GET N
  204 N=N+1
C
C     COMPUTATION OF NEXT VECTOR Y
      DO 205 I=1,NDIM
      AUX(N-1,I)=Y(I)
  205 AUX(N+6,I)=DERY(I)
      X=X+H
  206 DO 207  I=1,NDIM
     0DELT=AUX(N-4,I)+1.333333333333333300*H*(AUX(N+6,I)+AUX(N+6,I)-
     1AUX(N+5,I)+AUX(N+4,I)+AUX(N+4,I))
      Y(I)=DELT-.925619834710743800*AUX(16,I)
  207 AUX(16,I)=DELT
C     PREDICTOR IS NOW GENERATED IN ROW 16 OF AUX, MODIFIED PREDICTOR
C     IS GENERATED IN Y. DELT MEANS AN AUXILIARY STORAGE.
C
      CALL SMGFCT (X,Y,DERY,-1)
C     DERIVATIVE OF MODIFIED PREDICTOR IS GENERATED IN DERY
C
      DO 208 I=1,NDIM
     0DELT=.125D0*(9.D0*AUX(N-1,I)-AUX(N-3,I)+3.D0*H*(DERY(I)+AUX(N+6,I)
     1+AUX(N+6,I)-AUX(N+5,I)))
      AUX(16,I)=AUX(16,I)-DELT
  208 Y(I)=DELT+.074380165289256200D0*AUX(16,I)
C
C     TEST WHETHER H MUST BE HALVED OR DOUBLED
C   SET DELT TO MAX PREDICTOR-CORRECTOR DIFFERENCE
      DELT = DABS(AUX(16,1))
      DO 209  I=2,NSPEC
      IF (DABS(AUX(16,I)) .GT. DELT)     DELT = DABS(AUX(16,I))
  209 CONTINUE
      IF (DELT .GE. PRMT(4))   GO TO 222
      IHLF = 0
C
C     H MUST NOT BE HALVED. THAT MEANS Y(I) ARE GOOD.
  210 CALL SMGOUT (X,Y,DERY,DELT,H,IHLF)
  211 IF(IHLF-11)213,212,212
  212 RETURN
C
C     CHECK IF END TIME REACHED.
  213 IF(H*(X-PRMT(2)-0.1D 1)) 214,250,250
  214 IF(DABS(X-PRMT(2)-0.1D 1)-.1D0*DABS(H)) 250,215,215
  215 IF (DELT .LT. .01*PRMT(4))   GO TO 217
  216 ISTEP = 0
      GO TO 201
C
C     H COULD BE DOUBLED IF ALL NECESSARY PRECEEDING VALUES ARE
C     AVAILABLE.  CHECK FOR 8 CONSECUTIVE DELTS WITHIN LIMIT.
  217 IF (ISTEP-7)    218,219,219
  218 ISTEP = ISTEP+1
```

```
      GO TO 201                                                          BD0370
  219 IF (DABS(H)-17.0)  220,216,216                                     BD0371
  220 H=H+H                                                              BD0372
      ISTEP=0                                                            BD0373
      DO 221 I=1,NDIM                                                    BD0374
      AUX(N-1,I)=AUX(N-2,I)                                              BD0375
      AUX(N-2,I)=AUX(N-4,I)                                              BD0376
      AUX(N-3,I)=AUX(N-6,I)                                              BD0377
      AUX(N+6,I)=AUX(N+5,I)                                              BD0378
      AUX(N+5,I)=AUX(N+3,I)                                              BD0379
      AUX(N+4,I)=AUX(N+1,I)                                              BD0380
      DELT=AUX(N+6,I)+AUX(N+5,I)                                         BD0381
      DELT=DELT+DELT+DELT                                                BD0382
  2210AUX(16,I)=8.962962962962963D0*(Y(I)-AUX(N-3,I))                    BD0383
     1-3.3611111111111111D0*H*(DERY(I)+DELT+AUX(N+4,I))                  BD0384
      GOTO 201                                                           BD0385
C                                                                        BD0386
C                                                                        BD0387
C     H MUST BE HALVED                                                   BD0388
  222 IHLF=IHLF+1                                                        BD0389
      IF(IHLF-10)223,223,210                                             BD0390
  223 H=.5D0*H                                                           BD0391
      ISTEP=0                                                            BD0392
      DO 224 I=1,NDIM                                                    BD0393
     0Y(I)=.390625D-2*(8.D1*AUX(N-1,I)+135.D0*AUX(N-2,I)+4.D1*AUX(N-3,I)BD0394
     1+AUX(N-4,I))-.1171875D0*(AUX(N+6,I)-6.D0*AUX(N+5,I)-AUX(N+4,I))*H  BD0395
     0AUX(N-4,I)=.390625D-2*(12.D0*AUX(N-1,I)+135.D0*AUX(N-2,I)+         BD0396
     1108.D0*AUX(N-3,I)+AUX(N-4,I))-.0234375D0*(AUX(N+6,I)+              BD0397
     218.D0*AUX(N+5,I)-9.D0*AUX(N+4,I))*H                                BD0398
      AUX(N-3,I)=AUX(N-2,I)                                              BD0399
  224 AUX(N+4,I)=AUX(N+5,I)                                              BD0400
      X=X-H                                                              BD0401
      DELT=X-(H+H)                                                       BD0402
      CALL SMGFCT (DELT,Y,DERY,1)                                        BD0403
      DO 225 I=1,NDIM                                                    BD0404
      AUX(N-2,I)=Y(I)                                                    BD0405
      AUX(N+5,I)=DERY(I)                                                 BD0406
  225 Y(I)=AUX(N-4,I)                                                    BD0407
      DELT=DELT-(H+H)                                                    BD0408
      CALL SMGFCT (DELT,Y,DERY,1)                                        BD0409
      DO 226 I=1,NDIM                                                    BD0410
      DELT=AUX(N+5,I)+AUX(N+4,I)                                         BD0411
      DELT=DELT+DELT+DELT                                                BD0412
     0AUX(16,I)=8.962962962962963D0*(AUX(N-1,I)-Y(I))                    BD0413
     1-3.3611111111111111D0*H*(AUX(N+6,I)+DELT+DERY(I))                  BD0414
  226 AUX(N+3,I)=DERY(I)                                                 BD0415
      GOTO 206                                                           BD0416
  250 IHLF = 30                                                          BD0417
      GO TO 210                                                          BD0419
      END                                                                BD0420
```

```
      SUBROUTINE PUTOUT (TIME,Y,DERY,DELTA,SIZE,IHLF)                     BE0421
      DIMENSION Y(1),DERY(1)                                              BD0422
      DOUBLE PRECISION DELTA,DERY,SIZE,TIME,Y                             BD0423
      COMMON /OUTCOM/ TOUT,TINT                                           BD0424
      COMMON  /MILES/ COORD(2),DXY(2)                                     BD0425
      IF (IHLF .NE. 30)     GO TO 50                                      BE0426
      GO TO 100                                                           BD0428
   50 IF (DABS(TIME) .GE. TOUT)   GO TO 100                               BD0429
      GO TO 2000                                                          BD0430
  100 WRITE (6,1000) TIME,COORD(1),COORD(2),SIZE                          CB0431
      TOUT = TOUT+TINT                                                    BD0432
 1000 FORMAT('OTIME=',D15.8,15X,'POSITION=',2F15.4,15X,'SIZE=',D15.8)     CB0433
 2000 RETURN                                                              BD0436
      END                                                                 BD0437
```

```
      SUBROUTINE RWIND(XTIME,Y,DERY,NOT)                                BD0438
C                                                                       BD0439
      DIMENSION Y(1),DERY(1),DIST(32),JBAR(32),VAL1(8),VAL2(8),         CA0440
     1   DISINV(32)                                                     CA044010
      DOUBLE PRECISION  DERY,XTIME,Y                                    BD0441
      COMMON  /MILES/ COORD(2),DXY(2)                                   BD0442
      COMMON /RECOM/ TIME,ANS(8),DERIV(8), NSTA,NPOL,AIR(12,32,2),      BD0443
     1     WPOS(32,3),GOTIME                                            BD0444
C                                                                       BD0445
C     SET TIME AND POSITION                                             BD0446
C                                                                       BD0447
      TIME = GOTIME+XTIME/60.                                           BD0448
      ITIME = TIME-6                                                    BD0449
      COORD(1) = Y(1)/1609.3                                            BD0450
      COORD(2) = Y(2)/1609.3                                            BD0451
      DO 10  I=1,32                                                     BD0452
      DISINV(I) = 0.                                                    BD0453
   10 DIST(I) = 0.                                                      BD0454
      DO 15  I=1,8                                                      BD0455
      VAL1(I) = 0.                                                      CA045520
      VAL2(I) = 0.                                                      CA045540
   15 ANS(I) = 0.                                                       BD0456
C                                                                       BD0457
C     DETERMINE USABLE STATIONS AND SET STATION DISTANCES               BD0458
C                                                                       BD0459
      CALL BARIER (COORD(1),COORD(2),WPOS,JBAR,NSTA)                    BD0460
      DO 30  I=1,NSTA                                                   BD0461
      IF (JBAR(I) .NE. 1)   GO TO 30                                    BD0462
      DIST(I) = (COORD(1)-WPOS(I,1))**2 + (COORD(2)-WPOS(I,2))**2       BD0463
      IF (DIST(I) .NE. 0)   GO TO 30                                    BD0464
      IONE = I                                                          BD0465
      GO TO 100                                                         CA0466
   30 CONTINUE                                                          BD0467
C                                                                       BD0468
C     SET XDOT AND YDOT INTERPOLATED BETWEEN TWO SUCESSIVE HOURS        CA0469
C                                                                       BD0470
      DO 50  J=1,2                                                      BD0471
      DO 40  I=1,NSTA                                                   BD0472
      IF (JBAR(I) .NE. 1)   GO TO 40                                    BD0473
      IF (AIR(ITIME+1,I,J) .EQ. 0.)     GO TO 40                        CA0474
      DISINV(J) = DISINV(J)+1./DIST(I)                                  BD0475
      VAL2(J) = VAL2(J)+AIR(ITIME+1,I,J)/DIST(I)                        CA0476
   40 CONTINUE                                                          BD0477
      IF (DISINV(J) .NE. 0)   GO TO 45                                  BD0478
      VAL2(J) = 0.                                                      CA0479
      GO TO 50                                                          BD0480
   45 VAL2(J) = VAL2(J)/DISINV(J)                                       CA0481
   50 CONTINUE                                                          BD0482
      DO 60  I=1,2                                                      CA0483
   60 DISINV(I) = 0.                                                    CA048320
      DO 80 J=1,2                                                       CA048340
      DO 70 I=1,NSTA                                                    CA048360
      IF (JBAR(I) .NE. 1)  GO TO 70                                     CA048380
```

```
      IF (AIR(ITIME,I,J) .EQ. 0.)  GO TO 70                            CA0484
      DISINV(J) = DISINV(J) + 1./DIST(I)                               CA048420
      VAL1(J) = VAL1(J)+AIR(ITIME,I,J)/DIST(I)                         CA048440
   70 CONTINUE                                                         CA048460
      IF (DISINV(J) .NE. 0.)   GO TO 75                                CA048480
      VAL1(J) = 0.                                                     CA0485
      GO TO 80                                                         CA048520
   75 VAL1(J) = VAL1(J)/DISINV(J)                                      CA048540
   80 CONTINUE                                                         CA048560
      TIMEHR = TIME-(ITIME+6)                                          CA048580
      DO 90  J=1,2                                                     CA0486
   90 ANS(J) = VAL1(J)+(VAL2(J)-VAL1(J))*TIMEHR                        CA048620
      GO TO 120                                                        CA048640
C                                                                      CA048660
C     ONLY ONE STATION                                                 CA048670
C                                                                      CA048680
  100 DO 110  J=1,2                                                    CA0487
  110 ANS(J) = AIR(ITIME,IONE,J)                                       CA0488
  120 DO 130  I=1,2                                                    CA0489
      DXY(I) = ANS(I)/60.                                              BD0490
  130 DERY(I) = DXY(I)*1609.3                                          CA0491
      RETURN                                                           BD0492
      END                                                              BD0493
```

```
      SUBROUTINE POLLUT (TIME,X,Y,CONC,NPOL,A1,A2,A3,A4,PPOS)
C
C     CALCULATE POLLUTANT STARTING VALUES
C
      DIMENSION CONC(12,20,5),VAL(5),DISINV(32),DIST(32),JBAR(32),
     1    PPOS(32,3)
      ITIME = TIME-6
      DO 10  I=1,NPOL
      DISINV(I) = 0.
   10 DIST(I) = 0.
      DO 15  I=1,4
   15 VAL(I) = 0.
C
C     DETERMINE USABLE STATIONS AND SET STATION DISTANCES
C
      CALL BARIER (X,Y,PPOS,JBAR,NPOL)
      DO 30  I=1,NPOL
      IF (JBAR(I) .NE. 1)   GO TO 30
      DIST(I) = (X-PPOS(I,1))**2 + (Y-PPOS(I,2))**2
      IF (DIST(I) .NE. 0)   GO TO 30
      IONE = I
      GO TO 60
   30 CONTINUE
C
C     SET POLLUTANT VALUES
C
      DO 50  J=1,4
      DO 40  I=1,NPOL
      IF (JBAR(I) .NE. 1)   GO TO 40
      IF (CONC(ITIME,I,J) .EQ. 0)   GO TO 40
      DISINV(J) = DISINV(J)+1./DIST(I)
      VAL(J) = VAL(J)+CONC(ITIME,I,J)/DIST(I)
   40 CONTINUE
      IF (DISINV(J) .NE. 0)   GO TO 45
      VAL(J) = 0.
      GO TO 50
   45 VAL(J) = VAL(J)/DISINV(J)
   50 CONTINUE
      GO TO 80
   60 DO 70  J=1,4
   70 VAL(J) = CONC(ITIME,IONE,J)
   80 A1 = VAL(1)
      A2 = VAL(2)
      A3 = VAL(3)
      A4 = VAL(4)
      RETURN
      END
```

```
      SUBROUTINE BARIER (X,Y,WPOS,JBAR,NPOS)
C
C     DETERMINES IF INTERSECTION OF LINE SEGMENT CONNECTING TRAJECTORY
C     POINT AND STATION AND THE BARRIER LINE SEGMENT LIES ON THE BARRIER
C     ITSELF.  EVALUATE FUNCTIONS ALPHA AND BETA.  IF THEY ARE BOTH LESS
C     THAN 1 AND GREATER THAN 0, STATION IS ELIMINATED.
C
      DIMENSION WPOS(32,3),JBAR(32),BAR(10,10),BSLOPE(10,10),
     1          TSLOPE(32,2)
C
C     NBAR IS NUMBER OF BARRIERS
C     ARRAY BAR---ODD COLUMNS CONTAIN X COORDINATES
C                 EVEN COLUMNS CONTAIN Y COORDINATES
C                 ROW 1 IN ODD COLUMNS CONTAIN NO. OF POINTS IN BARRIER
C     ARRAY BSLOPE--ODD COLUMNS CONTAIN M VALUES OF BARRIER LINE SEGMTS
C                 EVEN COLUMNS CONTAIN Y VALUES OF BARRIER LINE SEGMENTS
C     ARRAY TSLOPE--ODD COLUMN CONTAINS M VALUES OF TRAJECTORY POINT
C                      WEATHER STATION LINE SEGMENT
C                 EVEN COLUMN CONTAINS B VALUES OF TRAJECTORY POINT
C                      WEATHER STATION LINE SEGMENT
C
      COMMON /BARRR/ IDB
      DATA NBAR/ 2/, BAR/2.,16.,38.,8*0.,2*40.,7*0.,4.,53.,60.,66.,71.,
     &          6*0.,31.,28.,32.,23.,65*0./
C
C     DETERMINE SLOPE AND INTERCEPT FROM INTERPOLATION POINT TO EACH
C           STATION.
C
      DO 50  I=1,NPOS
      TSLOPE(I,1) = 0.
50    TSLOPE(I,2) = 0.
      DO 100  I=1,NPOS
      IF((WPOS(I,1)-X) .EQ. 0.)  GO TO 100
      TSLOPE(I,1) = (WPOS(I,2)-Y)/(WPOS(I,1)-X)
      TSLOPE(I,2) = Y-TSLOPE(I,1)*X
100   CONTINUE
C
C     DETERMINE SLOPE AND INTERCEPT OF EACH SEGMENT OF EACH BARRIER
C
      IF (IDB .EQ. 1)   GO TO 210
      DO 200  J=1,NBAR
      NNBAR = BAR(1,2*J-1)
      DO 200  K=2,NNBAR
      IF ((BAR(K+1,2*J-1)-BAR(K,2*J-1)) .EQ. 0.)  GO TO 200
      BSLOPE(K,2*J-1) = (BAR(K+1,2*J)-BAR(K,2*J))/
     1                  (BAR(K+1,2*J-1)-BAR(K,2*J-1))
      BSLOPE(K,2*J) = BAR(K,2*J)-BSLOPE(K,2*J-1)*BAR(K,2*J-1)
200   CONTINUE
      IDB = 1
C
C     DETERMINE INTERSECTION FUNCTIONS
C           IF VALUE OF INSECTION IS LE TO ZERO OR GE 1,
C           INCLUDE STATION.
```

```
C
  210 DO 400  I=1,NPOS
      DO 375  J=1,NBAR
      NNBAR = BAR(1,2*J-1)
      DO 375  K=2,NNBAR
      IF ((BAR(K+1,2*J-1)-BAR(K,2*J-1)) .EQ. 0.)  GO TO 220
      DENOM1 = BSLOPE(K,2*J-1)*(X-WPOS(I,1))-(Y-WPOS(I,2))
      IF (DENOM1 .EQ. 0.)   GO TO 350
      ALPHA = (WPOS(I,2)-BSLOPE(K,2*J-1)*WPOS(I,1)-BSLOPE(K,2*J))/
     &              DENOM1
      GO TO 240
 220  DENOM2 = X-WPOS(I,1)
      IF (DENOM2 .EQ. 0.)   GO TO 350
      ALPHA = -WPOS(I,1)/DENOM2
 240  IF (ALPHA .GE. 1.)  GO TO 350
      IF (ALPHA .LE. 0.)  GO TO 350
      IF ((WPOS(I,1)-X) .NE. 0.)  GO TO 250
      IF ((WPOS(I,2)-Y) .EQ. 0.)  GO TO 350
      GO TO 260
 250  DENOM3 = TSLOPE(I,1)*(BAR(K,2*J-1)-BAR(K+1,2*J-1))
     &             -BAR(K,2*J)+BAR(K+1,2*J)
      IF (DENOM3 .EQ. 0.)    GO TO 350
      BETA = (BAR(K+1,2*J)-TSLOPE(I,1)*BAR(K+1,2*J-1)-TSLOPE(I,2))/
     &              DENOM3
      GO TO 280
 260  DENOM4 = BAR(K,2*J-1)-BAR(K+1,2*J-1)
      IF (DENOM4 .EQ. 0.)   GO TO 350
      BETA = -BAR(K+1,2*J-1)/DENOM4
 280  IF (BETA .GE. 1.)  GO TO 350
      IF (BETA .LE. 0.)  GO TO 350
      JBAR(I) = 0
      GO TO 400
  300 CONTINUE
      GO TO 400
  350 JBAR(I) = 1
 375  CONTINUE
  400 CONTINUE
      RETURN
      END
```