United States
Environmental Protection
Agency

Environmental Sciences Research
Laboratory
Research Triangle Park NC 27711

EPA-600/8-84-022a
November 1984

Research and Development

EPA

User's Guide for the Photochemical Box Model (PBM)

EPA-600/8-84-022a

USER'S GUIDE FOR THE PHOTOCHEMICAL BOX MODEL (PBM)

by

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NOTICE

AFFILIATION

Mr. Schere and Dr. Demerjian are on assignment to the Meteorology and Assessment Division, Environmental Sciences Research Laboratory, from the National Oceanic and Atmospheric Administration, U.S. Department of Commerce.

PREFACE

A significant area of research within the Meteorology and Assessment Division of the Environmental Sciences Research Laboratory is development, evaluation, validation, and application of models for air quality simulation, photochemistry, and meteorology. The models must be able to describe air quality and atmospheric processes affecting the dispersion of airborne pollutants on scales ranging from local to global. Within the Division, the Atmospheric Modeling Branch concentrates its activities on analytical and numerical air quality models for simulating the physical processes of transport and diffusion of pollutants in the atmosphere.

The Photochemical Box Model (PBM) is a relatively simple numerical model for simulating urban scale photochemical smog. Initial and boundary concentrations of relevant pollutant species must be provided by the user. Source emissions, wind speeds, and mixing heights must be also specified. Hourly averaged model results for O_3 and other species are optionally written to disk or tape for further analysis.

The first section of this user's guide is directed to managers and project directors who wish to evaluate the applicability of the model to their needs. Sections 2 and 3 are directed to engineers, meteorologists, and other scientists who will be required to become familiar with the details of the model. Sections 4 and 5 are directed to persons responsible for implementing and executing the programs.

Although attempts are made to thoroughly check computer programs with a wide variety of input data, errors are occasionally found. Revisions to the model may be obtained as they are issued by completing and returning the form on the last page of this guide. Comments and suggestions regarding this publication should be directed to:

Chief, Atmospheric Modeling Branch
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For technical questions regarding use of the model, call (919)541-4524. Users within the Federal Government may call FTS 629-4524. Copies of the user's guide are available from the National Technical Information Service (NTIS), Springfield, VA 22161. A magnetic tape containing the FORTRAN source code for the PBM will be available from Computer Products, NTIS, Springfield, VA 22161. The PBM will be included in the next release (Version 6) of EPA's UNAMAP series of dispersion models.

ABSTRACT

The User's Guide for the Photochemical Box Model (PBM) attempts to describe the structure and operation of the model and its preprocessors as well as provide the potential user with guidance in setting up input data. The PBM is a simple stationary single-cell model with a variable height lid designed to provide volume-integrated hour averages of O_3 and other photochemical smog pollutants of interest for an urban area for a single day of simulation. The PBM is most appropriate for application in air stagnation conditions with light and variable winds. Horizontal dimensions of the box are typically on the order of 10-50 km; the vertical dimension may vary between 0.1 and 2 km. Chemical reactions are simulated using a 63-step kinetic mechanism that includes diurnal variation of photolytic rate constants. The depth of the mixed layer, or depth of the PBM domain, also follows a diurnal pattern; it can be optionally specified as following a non-linear growth curve. The PBM assumes that emission sources are homogeneously distributed across the surface face of the box volume and that the volume is well mixed at all times. Atmospheric diffusion and wind shear are neglected.

The user must provide the PBM with initial species concentrations, hourly inputs of wind speed, source emission fluxes of CO, NO_x, THC, and hydrocarbon reactivity classes, and boundary species concentrations. Values of measured solar radiation and mixed layer depth may be specified at sub-hourly intervals throughout a simulation. The services of a qualified dispersion meteorologist, a chemist, and a computer programmer may be necessary to implement and apply the PBM and to interpret the results.

General information about the PBM system is contained in Section 1 of this User's Guide. A more technical description of the model and guidance for setting up input data are contained in Sections 2 and 3. Section 4 presents computer aspects of the modeling system, including an estimate of the resources needed to run the PBM. Section 5 presents an example problem.

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SECTION 1

OVERVIEW OF THE PBM

INTRODUCTION

The first section of the User's Guide for the Photochemical Box Model (PBM) provides a brief description of the model system and its basis along with the general data requirements, special features, and limitations of the model. This section is intended to provide the user with adequate information to decide whether the PBM is applicable to a particular situation.

The problem of assessing and controlling urban photochemical smog has been recognized for several decades. Much has been learned about the complex chemical and physical processses involved in smog formation and transport during that time. The emissions of nitrogen oxides (NO_x) and reactive hydrocarbons from area, point, and line sources interact with each other and with incoming solar radiation to produce a host of intermediate and secondary chemical species in the urban atmosphere. Many of these reactions are very rapid, occurring on time scales of several seconds to several minutes. The species of greatest interest generated by photochemical smog processes is ozone (O_3) because of its potentially harmful effects on human health and property. Air quality simulation models aid planners and managers in making decisions to control the primary emissions ultimately responsible for producing O_3.

The PBM is a complex model within a simple framework. Any model that describes urban smog reactions must address the complex non-linear chemical interactions among the reacting species. These coupled non-linear reactions and the disparate time scales among the reactions preclude the use of a statistically-based (e.g.-Gaussian) linear model and necessitate a mass-conservative approach that usually incorporates a numerical solution to time-dependent rate equations for the chemical species. The PBM encompasses this approach within the framework of a simple single-cell domain set over the urban area of interest. The domain is a variable-volume, well-mixed reacting cell within which the physical and chemical processes responsible for photochemical smog are simulated. These include the transport and dispersion of pollutant species through the cell, the injection of primary precursor species by emissions sources, and the chemical transformation of the reactive species into intermediate and secondary products. These processes are schematically illustrated in Figure 1.

Model simulation always begins at 0500h, local standard time (LST) and continues throughout the day, typically ending at or just before sunset. Model results are provided as hour averages of all species. Instantaneous results at selected time intervals are also available. The model domain is usually chosen such that the horizontal side of the box is of fixed length from 10^1 to 10^2 km and such that the domain encompasses most of the major emissions sources within the urban area. Model results are averaged over the entire box volume and may not coincide with a peak concentration at a single point within the volume. For this reason the PBM may be most useful as a screening tool as an aid in deciding whether a more spatially-resolved (and resource-intensive) grid model must be applied. Also, because the box volume is fixed in space, the most appropriate meteorological conditions for application are stagnation conditions with light and variable wind conditions. Depending on the size of the box, higher winds of persistent direction may transport emitted precursor species downwind of the urban area and out of the model domain within the simulation period. A photochemical trajectory model would be more appropriate for this situation.

Earlier versions of the PBM have been used in research studies by EPA's Meteorology Division to study photochemical smog in St. Louis, MO (Schere and Demerjian, 1977) and Houston, TX (Demerjian and Schere, 1979). Also, model evaluation exercises have been conducted with the PBM for O_3 air quality (Shreffler and Schere, 1982; Schere and Shreffler, 1982) and for NO_2

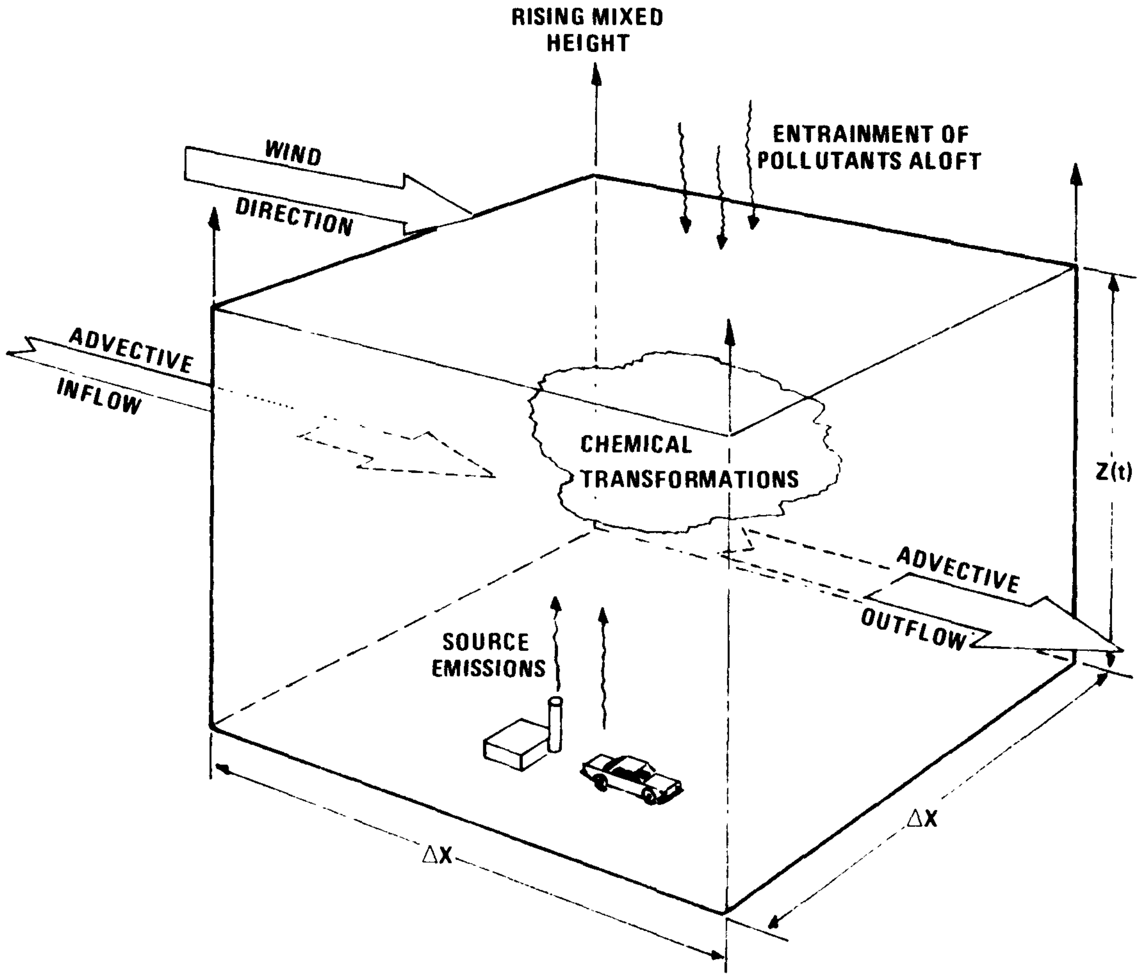

Figure 1. Schematic illustration of the PBM domain.

air quality (Schere and Shreffler, 1984) in St. Louis. The current version of the model includes several additional chemical reactions and revised reaction rate constants since the time of these earlier reports.

DATA REQUIREMENTS

The PBM system includes 3 components: a meteorological data preprocessor (PBMMET), an air quality and emissions data preprocessor (PBMAQE), and the air quality simulation model itself (PBM). Execution of the data preprocessors sets up card-image data read directly by the PBM. Complete instructions for preparing all data needed to run the system are included in Section 3. Required data are summarized below.

Meteorological Data:

- Date (month, day, year, Julian day)
- Location (latitude and longitude, degrees, and time zone)
- Wind speed, ms^{-1}, knots, or mi h^{-1}
- Mixing height, m
- Ambient air temperature, °C or °F (Optional)
- Total Solar (TSR) or Ultraviolet (UV) radiation, ly min^{-1} (Optional)
- Cloud layer amount and height, ft (Optional)

Commonly used meteorological data available from the National Climatic Center (NCC) in the form of Card Deck 144 (WBAN Hourly Surface Observations) and morning and afternoon mixing heights may be adapted as input for the PBM. However, either manual or computer processing of the NCC data will be required to scan for completeness and accuracy and to reformat the data for input to PBMMET. Use of the NCC data sets are discussed more fully in the User's Manual for CRSTER (EPA, 1977) and the Card Deck 144 WBAN Hourly Surface Observations Reference Manual (NCC, 1970).

Air Quality Data:

- Initial condition concentrations, ppm
- Boundary concentrations, ppm
- Observed concentrations, ppm (Optional)
- Hydrocarbon speciation factors for initial concentrations
- Hydrocarbon speciation factors for boundary concentrations
- Hydrocarbon speciation factors for observed concentrations (Optional)

Ambient concentrations of hydrocarbons in urban areas are frequently available as measures of non-methane hydrocarbons (NMHC). Since there are actually hundreds of specific compounds under this general heading, only several major structural categories or classes are chosen to simulate the range of all NMHC compounds. The speciation factors divide the gross measure of NMHC into these various categories for simulation in the air quality model.

Emissions Data:

- Source emission rate of CO from area and line sources, kg h^{-1}
- Source emission rate of CO from point sources, kg h^{-1}
- Source emission rate of NO_x from area and line sources, kg h^{-1}
- Source emission rate of NO_x from point sources, kg h^{-1}
- Source emission rate of total hydrocarbons (THC) from area and line sources, kg h^{-1}
- Source emission rate of THC from point sources, kg h^{-1}
- Source emission rates of hydrocarbon classes from area and line sources, moles h^{-1}
- Source emission rates of hydrocarbon classes from point sources, moles h^{-1}
- Ratio of NO_2/NO_x in area and line source NO_x emissions
- Ratio of NO_2/NO_x in point source NO_x emissions
- Ratio of CH_4/THC in area and line source THC emissions
- Ratio of CH_4/THC in point source THC emissions

Control Data:

Horizontal side of model domain, km
Number of hours of simulation
Time interval for printing and plotting instantaneous concentrations, min
Time interval for updating mixing height and photolytic rate constants, min
Numerical integration tolerance parameter
Values for selecting specific options

FEATURES AND LIMITATIONS

Several specific features of the PBM system are highlighted below. Also, the major assumptions invoked in the model's formulation and some of its limitations are explained.

The special features include:

(1) Mixing Height Growth - The PBM includes an option to interpolate between minimum and maximum specified mixing heights in a non-linear manner characteristic of the true growth rate in sunny, low-wind conditions ('characteristic curve').

(2) Photolytic Rate Constants - PBMMET generates values for the diurnal variation of the photolytic rate constants required for the photolysis reactions in the chemical kinetic mechanism. These rate constants are calculated from a theoretical clear-sky perspective with options to attenuate the values based on observed cloud conditions or measured solar radiation. These rate constants may be generated for the surface layer or as an integrated average through the depth of the mixed layer.

(3) Modular Chemical Kinetics - The default chemical kinetic mechanism in the PBM models the reactions of the HC-NO_x-O_3 urban photochemical smog system. It contains 63 reactions and 41 individual chemical species with 8 classes of hydrocarbons. The kinetics are modular and may be replaced with another mechanism with relatively few coding changes required by the user.

(4) Numerical Solution Scheme - A modified version of the Gear (1971) numerical solution technique is used to solve the coupled differential species rate equations. The solution scheme is very accurate and no steady-state approximations are needed.

The major assumptions contained in the PBM formulation include:

(1) The box volume is well mixed at all times and no spatial variations of concentration occur within it.

(2) Emissions sources are homogeneously distributed across the surface face of the box volume.

(3) Entrainment of outside air occurs laterally by advective transport and vertically by the rising mixed layer.

(4) Molecular and atmospheric diffusion are neglected.

(5) Horizontal and vertical wind shear are neglected.

These assumptions must be considered before applying the PBM to a particular situation. If, for example, the vast majority of hydrocarbons are emitted into the urban atmosphere from a single point source located near an edge of the domain, assumption (2) is probably violated and the model would not be appropriate for the application.

Care should be exercised in choosing the size and location of the PBM modeling domain for a given application. Because the domain is fixed in space, the locations of ambient monitoring stations and the spatial distribution of source emissions will aid in choosing the position of the domain. Major area and line sources within the urban area should be within the domain. Significant land areas without area or line sources should not be within the domain. Point sources should also be included within the domain to the extent that they are within an otherwise distributed emissions area and are not isolated outside of the area of interest. The following are rough guidelines for choosing the size of the horizontal side of the domain:

Small cities (population 10,000-100,000):	5-15 km
Medium cities (population 100,000-500,000):	15-30 km
Large cities (population >500,000):	30-50 km

The exact size for a particular application should be determined more by the spatial distribution of emissions and population rather than by the overall population. For very large cities distributed over considerable distances, the model domain may have to focus only on a portion of the urban area. Because the PBM is most aptly used in stagnation conditions, wind speeds are not a major factor in determining the domain size. The domain that is finally chosen should include at least one meteorological and air quality monitoring site that is representative of the area being modeled. Also, an upwind monitoring location outside of the domain is needed to provide boundary conditions.

The PBM is not applicable to the regional scale (500-1000 km) oxidant problem. Considerations of spatial inhomogeneities, large-scale meteorological processes, and multi-day chemistry that includes slow reactions preclude use of the simplistic modeling framework of the PBM. Lamb (1983) discusses some of the special needs in regional photochemical modeling and presents a framework for such a model.

Finally, the PBM provides a measure of air quality averaged over the entire volume of the domain. It does not show "hotspots" or single sites of National Ambient Air Quality Standards (NAAQS) exceedance. However, if the PBM application shows the volume-average concentration of O_3, for instance, to be in excess of the NAAQS, use of a more sophisticated model to help identify hotspots may be required.

SECTION 2

TECHNICAL DESCRIPTION OF THE PBM

The basic equation underlying the PBM is the atmospheric diffusion equation, simplified as a result of the assumptions listed in the previous section:

$$\frac{\partial \overline{c}_i}{\partial t} = \overline{u}\,\frac{\partial \overline{c}_i}{\partial x} + \frac{\partial z}{\partial t}\,\frac{\partial \overline{c}_i}{\partial z} + \frac{\overline{Q}_i}{z} + R_i(\overline{c}_i, \ldots, \overline{c}_n) \qquad (1)$$

where $\overline{c}_i$ = mean concentration of species i within the PBM domain,

$\overline{u}$ = mean wind speed within the domain,

$\overline{Q}_i$ = source emissions flux (mass time^{-1} length^{-2}) of species i into the domain,

R_i = rate of production and/or destruction of species i from chemical species,

x,z,t = length and time variables.

This equation embodies the principle of conservation of mass; it is solved numerically within the PBM for the concentrations c_i as a function of time. Hour-averaged concentrations are then formed. This section of the User's Guide discusses technical aspects of this formulation as implemented in the PBM system.

METEOROLOGY

The PBM requires values of specific meteorological parameters in order to solve Equation (1). These include hourly values of the wind speed $\bar{u}$, subhourly values of the mixing height growth $\partial z/\partial t$ and, optionally, solar radiation or observed cloud heights and amounts. Hourly ambient temperatures may also be required. These parameters are all processed by PBMMET, the meteorological preprocessor. Since the solar radiation and temperature values as well as the cloud parameters pertain to the calculation of chemical reaction rate constants, they will be discussed within the subsection on chemistry.

Ideally, the winds input to the model should be averaged through the depth of the mixed layer. Where such vertically resolved data are available they should be used. Otherwise, a representative sampling of surface wind speeds within the PBM domain will suffice. Wind speeds are needed within the PBM to help determine the advective transport term $\bar{u}\,\partial \bar{c}_i/\partial x$, providing a horizontal dilution rate of material within the box volume and entrainment from the upwind side. As mentioned previously, the PBM is most applicable under stagnation conditions where the wind speeds are light (generally under 2 ms^{-1}) and directions are variable. Winds with more persistent directions may also be used in the PBM, although the area of greatest interest for photochemical pollutant species may well be downwind of the box volume in this case.

Concentration predictions from the PBM are sensitive to changes in the volume of the modeling domain. It is therefore important to accurately specify the growth rate of the mixing height, $\partial z/\partial t$, since this term controls the vertical dilution and entrainment. Historically it has been frequent practice to linearly interpolate between the mixing height determined from a morning temperature sounding and an afternoon mixing height determined from a combination of sounding measurements and principles of atmospheric thermodynamics. The problem with this method is that the linear interpolation tends to overestimate the depth of the mixed layer at early times and to underestimate later. This error in the mixed layer depth, and hence in $\partial z/\partial t$, can introduce serious errors in the model predictions of pollutant species concentrations.

In an effort to produce a more realistic interpolation between morning minimum and afternoon maximum mixed layer depths, the following characteristic curve was developed along the lines of actual observed growth rates in clear sky, light wind conditions. If G represents the growth of the mixed layer (afternoon maximum depth minus morning minimum depth), and DL represents the day length or length of time between sunrise and sunset, the following points are postulated:

$$\begin{aligned} &Z(SR)=HMIN_0 \\ &Z(SR+0.07DL)=HMIN_0 + 0.02G \\ &Z(SR+0.14DL)=HMIN_0 + 0.10G \\ &Z(SR+0.33DL)=HMIN_0 + 0.58G \\ &Z(SR+0.50DL)=HMIN_0 + 0.85G \\ &Z(SR+0.70DL)=HMAX \end{aligned} \qquad (2)$$

where Z is the mixed layer depth, $HMIN_0$ and HMAX are the morning minimum and afternoon maximum depths, and SR is the time of sunrise. These node points represent percentages of the total growth occurring within corresponding percentages of elapsed daylight time. Intermediate depths are interpolated by cubic splines as often as every 10 minutes for frequent updates within the PBM. This produces smooth variations in $\partial z/\partial t$ during the period of fastest growth in the mixed layer depth. Beyond this time the following points are postulated:

$$\begin{aligned} &Z(SR+0.90DL)=HMAX \\ &Z(SS)=HMIN_0+0.50G \\ &Z(SS+0.50NL)=HMIN_1 \end{aligned} \qquad (3)$$

where $HMIN_1$ is the following morning minimum depth, SS is the time of sunset, and NL is the length of time between sunset and the following sunrise. The specification of these points accounts for the rapid drop in mixed layer depth as the surface layer becomes decoupled from the layer aloft when surface stabilities increase near sunset. Interpolation between the points shown by Equation set (3) is linear. Figure 2 shows the pattern of mixed layer growth (until time SS taken from Equation sets (2) and (3)) occurring during a typical PBM simulation period. Mixing depths and times have been normalized to HMAX and DL, respectively.

Alternatively, the PBM user may directly set up mixed layer height values for input to the PBM at subhourly intervals. Linear interpolation will be performed between input values if needed.

CHEMISTRY

The PBM contains a 63-step chemical kinetic mechanism, shown in Table 1, developed by Dr. Kenneth Demerjian of EPA. The reactions include 37 reactive species and 8 hydrocarbon classes. In Equation (1), the term representing the chemical interactions, $R_i(c_i,....,c_n)$, implies that the rate of change of species i is not only dependent upon the concentration of species i but also upon the concentrations of n other species. In this way the reaction set is coupled between species. Solution of the resulting set of 37 nonlinear differential equations is performed numerically by finite differences.

Most chemical kinetic mechanisms that simulate urban photochemical smog treat the relevant inorganic chemical reactions similarly. Differences between the mechanisms occur most often in the handling of the organic species chemistry where hundreds of different reactive hydrocarbon compounds have a role in the photochemical cycle. Limiting the number of these compounds in a kinetic mechanism requires the use of assumptions and approximations. The Demerjian mechanism uses the technique of generalized species lumping, in which an entire group of compounds is represented by a generalized species, the chemistry of which reflects the common features of that entire group. The rate constants for reactions that include these lumped groups, or

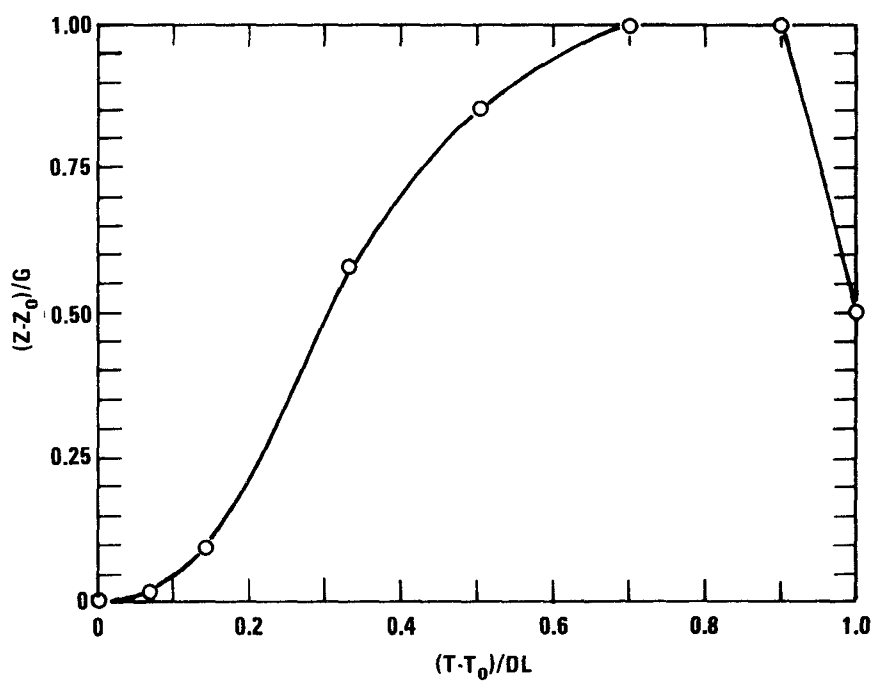

Figure 2. Normalized mixing height growth curve. T_0, Z_0 represents the time and mixing height at sunrise. DL, G represents the time between sunrise and sunset and the total mixing height growth.

TABLE 1. DEMERJIAN GENERALIZED CHEMICAL KINETIC MECHANISM.

REACTION NUMBER	REACTION			RATE CONSTANT (Units[a])
1	NO2 + $h\nu$	---->	NO + O	4.80E-01[b,d]
2	O + O2 + M	---->	O3 + M	2.25E-05[c]
3	O3 + NO	---->	NO2 + O2	2.68E+01
4	O3 + NO2	---->	NO3 + O2	4.76E-02
5	O3 + $h\nu$	---->	O1D + O2	1.96E-03[b,d]
6	O1D + M	---->	O + M	4.23E+04
7	O1D + H2O	---->	2.00HO	3.40E+05
8	NO3 + NO	---->	2.00NO2	2.96E+04
9	NO3 + NO2	---->	N2O5	1.78E+03
10	N2O5	---->	NO3 + NO2	3.11E+00[b]
11	N2O5 + H2O	---->	2.00HNO3	1.92E-05
12	HONO + $h\nu$	---->	HO + NO	9.58E-02[b,d]
13	HO + CO	---->	HO2 + CO2	4.14E+02
14	HO2 + NO2	---->	HONO + O2	4.40E+00
15	HO2 + NO	---->	HO + NO2	1.22E+04
16	HO2 + NO2 + M	---->	HO4N + M	1.52E-03[c]
17	HO4N	---->	HO2 + NO2	3.26E+00[b]
18	HO + HONO	---->	NO2 + H2O	9.75E+03
19	HO + NO2 + M	---->	HNO3 + M	1.43E-02[c]
20	HO + NO + M	---->	HONO + M	7.35E-03[c]
21	HO + HNO3	---->	H2O + NO3	1.97E+02
22	HO2 + O3	---->	HO + 2.00O2	2.96E+00
23	HO + O3	---->	HO2 + O2	1.01E+02
24	HO2 + HO2	---->	H2O2 + O2	3.73E+03
25	H2O2 + $h\nu$	---->	2.00HO	4.21E-04[b,d]
26	ETH + O3	---->	0.40RO2 + FORM + 0.10HO2	2.50E-03
27	ETH + HO	---->	FRO2 + FORM	1.20E+04
28	OLE + O	---->	RO2 + ALD + HO2	5.10E+03
29	OLE + O3	---->	0.75RO2 + 0.75ALD + 0.40HO2	9.50E-02
30	OLE + HO	---->	RO2 + 0.75ALD + 0.25FORM	5.50E+04
31	PAR + HO	---->	RO2	5.00E+03
32	FORM + $h\nu$	---->	CO	2.36E-03[b,d]
33	FORM + $h\nu$	---->	2.00HO2 + CO	1.62E-03[b,d]
34	FORM + HO	---->	HO2 + H2O + CO	1.60E+04
35	RO2 + NO	---->	RO + NO2	1.10E+04
36	RO + O2	---->	0.75ALD + HO2 + 0.25FORM	8.99E-01
37	ALD + $h\nu$	---->	RO2 + HO2 + CO	3.79E-04[b,d]
38	ALD + HO	---->	R1O2 + H2O	2.40E+04
39	FRO2 + NO	---->	FRO + NO2	1.10E+04
40	FRO + O2	---->	FORM + HO2	1.08E+00
41	R1O2 + NO2	---->	PAN	8.87E+03
42	PAN	---->	R1O2 + NO2	1.35E-01[b]
43	RO + NO2	---->	RNO3	1.00E+02

(continued)

TABLE 1. (CONTINUED)

REACTION NUMBER	REACTION								RATE CONSTANT (Units[a])
44	R02 + 03	---->	RO	+	2.0002				2.00E+00
45	R102 + NO	---->	R02	+	N02				2.07E+04
46	TOL + HO	---->	RT02	+	ALD	+	DCB1		8.70E+03
47	ARO + HO	---->	RX02	+	ALD	+	DCB1		3.40E+04
48	RT02 + NO	---->	RTO	+	N02				1.10E+04
49	RTO + 02	---->	DCB1	+	H02	+	CO		8.87E-01
50	RX02 + NO	---->	RXO	+	N02				1.10E+04
51	RXO + 02	---->	DCB2	+	H02	+	CO		8.87E-01
52	DCB1 + $h\nu$	---->	2.00CO	+	2.00H02				1.92E-03[b,d]
53	DCB1 + $h\nu$	---->	0.20FORM	+	1.80CO				1.92E-03[b,d]
54	DCB1 + HO	---->	H02	+	2.00CO				1.70E+04
55	DCB2 + $h\nu$	---->	R102	+	H02	+	2.00CO		4.56E-03[b,d]
56	DCB2 + $h\nu$	---->	0.50ALD	+	0.50FORM	+	0.50FR02		4.56E-03[b,d]
57	DCB2 + HO	---->	R102	+	CO				2.56E+04
58	RT02 + 03	---->	RTO	+	2.0002				2.00E+00
59	RX02 + 03	---->	RXO	+	2.0002				2.00E+00
60	R102 + 03	---->	R02	+	2.0002				2.00E+00
61	OLE + 03	---->	COOH	+	ALD				1.50E-03
62	NMHC	---->							0.00E+00[b]
63	NONR	---->							0.00E+00[b]

[a] Rate constant units are $ppm^{-1}\ min^{-1}$ unless otherwise noted

[b] Units of rate constant are min^{-1}

[c] Units of rate constant are $ppm^{-2}\ min^{-1}$

[d] Photolysis rate constant - Value shown is for clear-sky conditions, a solar zenith angle of 40 degrees, and integrated through a 1 km deep mixed layer

reactivity classes, should be calculated as averages of the rate constants for the reactions that involve the individual compounds within the given reactivity class.

An earlier version of the mechanism used in the PBM is described in McRae et al. (1983). This earlier version and the current version include the lumped hydrocarbon classes of non-reactives, olefins, paraffins, aldehydes, and aromatics. In the current version, however, several species have been separated from these generalized classes to be treated explicitly within the mechanism either because of significant reactivity differences or product distributions different from the mainstream of the class. These species include ethylene (separated from the olefins), toluene (separated from the aromatics), and formaldehyde (separated from the aldehydes). In addition, the photolysis of the dicarbonyls, predominantly glyoxal and methylglyoxal, was included in the current version. Separate reaction pathways for the new species were included in the mechanism. Reaction rate constants used are current literature values, and where ambient temperature changes may significantly affect these values the full temperature-dependent expressions are used to compute them.

Predicted concentrations of NMHC (ppmC) can not be simply formed from the sum of the predictions of the concentrations of the individual hydrocarbon classes (ppm). Therefore, the concentrations of ambient NMHC produced by the PBM using the Demerjian kinetic mechanism are estimates based on emissions, transport and dilution. Predicted NMHC concentrations are therefore only approximations. They should be most accurate when emissions and dilution are dominant processes, such as in the first few hours of simulation, or when transport is dominant.

The chemical kinetic mechanism requires that the photolytic rate constants for NO_2, $O_3 \rightarrow O(^1D)$, HONO, H_2O_2, formaldehyde (into molecular products), formaldehyde (into radical products), acetaldehyde (into radical products), and the dicarbonyl species glyoxal and methylglyoxal be specified. These rate constants correspond to reactions 1, 5, 12, 25, 32, 33, 37, 52, 53, 55, and 56, respectively, of the default kinetic mechanism (Table 1). Two photolysis reactions for each of the dicarbonyl species are shown. The photolytic rate constants are directly proportional to the amount of solar radiation received and, thus, vary over a diurnal cycle which changes with season and geographical location. While clear-sky and totally overcast days show smoothly varying functions of solar radiation, partly cloudy days are often characterized by more rapid fluctuations. Because the entire reaction mechanism is perturbed by the changes in the photolytic rate constants they are frequently updated during model simulation.

There are significant vertical variations in the values of some of the photolytic rate constants within the lowest 1-2 km of the atmosphere. A problem arises as to the choice of a vertical level for values of the photolytic rate constants because the PBM does not permit vertical resolution in its structure. The meteorological preprocessor, PBMMET, provides the user with a choice of surface-level rate constants or rate constants averaged through the depth of the mixed layer at any point in time. These two methods serve as lower and upper bounds on the probable value of the photolytic rate constants.

The rates at which a particular species photolyzes are dependent upon the particular wavelength band of radiation the species is sensitive to, the amount of radiation received within this band, the efficiency with which the species absorbs the radiation, and the yield of product species per unit of absorbed radiation. Demerjian et al. (1980) discuss the theoretical considerations involved in calculating photolytic rate constants for many species of interest to air pollution analysts and tabulate values of the rate constants over a range of zenith angles and vertical levels for clear-sky conditions. PBMMET uses these values, with some updates since the time of the article's publication, to generate surface-level or layer-averaged values of photolytic rate constants.

In real atmospheric situations, conditions often vary from clear skies. The clear sky theoretical rate constants may be reduced by an attenuation factor to account for the presence of clouds or other obscuring phenomena. This factor may be determined from measured values of solar radiation, either in the ultraviolet or total solar bands, or from cloud cover and height observations. For the case of measured radiation, the attenuation factor is formed from a ratio of the empirically determined surface layer value of the NO_2 photolysis rate constant (from radiation measurements) to the clear-sky theoretically determined value of the same parameter. For the case of cloud cover observations, the method of Jones et al. (1981) was used to calculate attenuation factors. These authors calculated the attenuation factors corresponding to various cloud amounts and heights (commonly reported from National Weather Service (NWS) observations) from empirical relationships based on measured NO_2 photolysis data.

Many of the remaining non-photolytic reactions in the chemical kinetic mechanism have rate constant values that are sensitive to temperature. When available, hourly ambient temperatures may be input to the PBM to adjust the temperature-dependent rate constants. This is done once for each hour of simulation for each such reaction. In the absence of input temperatures all temperature-dependent rate constants are calculated for 298°K (~77°F).

AIR QUALITY AND EMISSIONS

Air quality observations are required to compute values for certain $\bar{c}_i$'s in Equation (1). In particular, initial conditions are needed for the $\partial\bar{c}_i/\partial t$ term, lateral inflow boundary conditions for $\partial\bar{c}_i/\partial x$, and boundary conditions at the top of the model domain for $\partial\bar{c}_i/\partial z$. Also, air quality observations may be used to verify the results of the PBM simulation.

It is important to attempt to specify the initial species concentrations as accurately as possible because they determine the amount of mass with which the reactive system begins the simulation. Until the emissions terms have introduced sufficient mass into the system the simulation can be dominated by the initial condition specifications. At least one, and preferably several, air quality monitoring stations should be within the bounds of the model domain. Their average should provide a representative sampling of conditions within the area being modeled. Initial conditions existing at model simulation starttime (0500h, LST) must be specified for CO, NO, NO_2, and NMHC. The intermediate and termination species concentrations need not be specified.

A critical element in specifying initial conditions is apportioning the hydrocarbon concentration among the various organic reactivity classes. For the default chemical kinetic mechanism these include non-reactives (NONR), ethylene (ETH), olefins or all alkenes except ethylene (OLE), paraffins or all alkanes other than methane (PAR), formaldehyde (FORM), all other aldehyde species (ALD), toluene (TOL), and all other aromatic species (ARO). The preferred method for determining this apportionment is from a detailed analysis of a gas chromatograph-mass spectrometer (GC/MS) profile of the particular organic compounds and their fractional weights within a captured air sample taken in the urban area modeled during the period 0600-0900h, LST. These compounds and their weights are then assigned to the various reactivity classes; sums of each class are then calculated and proportional splitting factors are determined. McRae et al. (1983) provide a detailed example of how this apportionment is done using a detailed GC/MS analysis from a smog chamber air sample and 6 different chemical kinetic mechanisms. Alternatively, an option is available to the user of utilizing the urban splitting factors developed by the authors for application of the PBM to St. Louis. These factors are presented in Section 4 of the user's guide and are applied to the measured NMHC initial condition. The risk in using these factors is that the relative weighting of the reactivity classes in the user's area of application may be different from those in St. Louis. This is especially true for cities where the relative distribution of mobile and stationary sources differs appreciably from St. Louis.

Hourly values of upwind boundary species concentrations are also required for each hour of simulation. At least one monitoring station should be available for determining boundary concentrations of CO, NO, NO_2, NMHC, and O_3. Boundary concentrations for the speciated hydrocarbon classes are also required. As in the case of initial conditions, the preferred method for determining the splits between these classes is from a GC/MS analysis of upwind sampled air. Alternatively, the same splitting factors developed for the initial conditions may be applied to the boundary concentrations. The inherent problem in this approach is that the reactive splits of the more aged air moving into the urban area at the upwind boundary may be different from those representing urban air laden with fresh reactive organic emissions. In the absence of any analyzed samples the default factors for St. Louis may be used with the caution expressed above for default initial conditions. The PBM contains an option to calculate the upwind O_3 concentration from the given upwind NO and NO_2 concentrations and photostationary state assumptions. This is advisable when upwind O_3 measurements are not available, but NO and NO_2 are. Where upwind O_3 observations exist, they should be used. The relative importance of boundary conditions to the air quality simulation increases as wind speed increases.

In addition to lateral boundary conditions, hourly boundary concentrations at the top of the model domain may be input. If vertical profiles of species concentrations exist for the urban area, the top boundary concentrations may be determined from them. Without such profiles, tropospheric background concentrations may be assumed. Frequently, there is a significant concentration of O_3 aloft that is entrained into the rising mixing layer during the growth period. A technique is presented in Section 3 for estimating the O_3 concentration aloft at the top of the modeling domain in the absence of measured O_3 profiles.

Optionally, hourly concentrations of measured species within the PBM domain may be specified for comparison with model predictions. These observed concentrations are output by the PBM on time series plots and written off to disk/tape storage for later use in statistical analysis of model results. If desired, splitting factors for the observed hydrocarbon species may be specified here also, or the default factors can be used. Preparation of all air quality data for the PBM is handled by the air quality and emissions preprocessor, PBMAQE.

Source emissions are also prepared by PBMAQE for input to the PBM. For primary pollutant species i, source emissions enter the model formulation shown in Equation (1) through the flux term $\overline{Q}_i/z$.

The spatial and temporal variation in primary pollutant sources is a major influence for air pollutant patterns in a region. Temporal resolution of sources is an important parameter within the PBM; spatial resolution is not of concern because of the assumption of spatial homogeneity of sources. The PBM accepts hourly source emission rates that encompass the sum of all sources within the modeling domain. In reality, emissions originate from one of three distinct types of source configurations: area, line, or point. Although line sources, principally roadways, are not treated explictly by the PBM, they represent a major portion of the total emissions of primary reactive species emanating from an urban area. The temporal resolution of the line sources is apt to contain more structure than that of the other source types because of a twin-peaked diurnal traffic pattern. Some knowledge of this pattern for a potential modeling site is essential in order to form a representative temporal emissions pattern from the mobile sources. Point sources are not treated separately by the PBM. Total hourly emission rates from all point sources are calculated and added to the hourly rates from area and line sources to form a single emissions rate for each hour for each primary species.

The PBM requires partitioning of nitrogen oxides (NO_x) and total hydrocarbon (THC) emissions into their respective chemical components for the default chemical kinetic mechanism. Source emissions of NO_x are subdivided between the constituent species NO and NO_2. Estimates of NO_2/NO_x in auto exhaust tailpipe emissions range from 3 to 5%. However, there is a rapid period of thermal oxidation of NO to NO_2 due to Reaction (4) occurring in the early stages of exhaust dilution.

$$2NO + O_2 \rightarrow 2NO_2 \qquad (4)$$

The implicit consideration of this process in the model leads to the estimate of $NO_2/NO_x \approx 10\%$ for primary emissions of NO_x.

Hydrocarbon emissions are generally reported as THC and must be distributed among the reactive organic classes required by the generalized kinetic mechanism. This is accomplished through an approach similar to that outlined by Bucon et al. (1978), in which distributions are derived based on hydrocarbon composition analysis by source emissions processes. The splits between the various hydrocarbon classes: NONR, ETH, OLE, PAR, FORM, ALD, ARO, and TOL will vary with the distribution of source types in a given modeling domain. A concentration of petroleum refineries and storage tank facilities in a particular area, for instance, would cause the hydrocarbon distribution to differ from that found in a non-industrial metropolitan area with heavy automobile traffic.

Emission rates are typically reported as mass of material within a set time interval, such as kg h^{-1}. PBMAQE accepts emissions in these units for the species CO, NO_x, and THC. These emission rates along with the horizontal size of the model domain, ambient temperature, and molecular weight of the emitted species allow PBMAQE to compute corresponding volumetric flux rates for the PBM. Emission rates of the reactive organic classes are reported as moles/hr, according to the procedure of Bucon et al. (1978).

NUMERICAL SOLUTION

Each reactive species included in the chemical kinetic mechanism is represented in the model by a differential equation such as Equation (1). The equilibrium time constants among the various reactions can vary by orders of magnitude; this variation makes the system of equations "stiff" and difficult to solve by conventional numerical techniques used for ordinary differential equations. The technique chosen for the PBM is a modified version of Gear's method (1971), a variable-order method based on a backward differentiation multistep formula. Because the chemistry has the most stringent step size requirements of any of the components in the PBM, it is the rate-controlling step for the entire model. The Gear routine begins with a very small time step and subsequently adjusts the step size upward while concurrently seeking to maintain the solution within all specified tolerances. Concentrations of all simulated species are computed in this manner. Steady-state approximations are not invoked here, as the efficiency of the numerical solution obviates the need for such computationally time saving measures. Moreover, such approximations may introduce large numerical errors into the solution (Farrow and Edelson, 1974).

SECTION 3

TECHNICAL GUIDANCE FOR INPUT DATA

Section 4 of this user's guide provides a detailed description of the structure and format of the data needed to run the PBM and its preprocessors. The identification of many of the data items there will be sufficient description for users to correctly choose values. However,an expanded description, with guidance for making decisions on values for the data, is necessary for some of the input data items. This section provides these descriptions and guidance where necessary. Unless otherwise indicated, values for data input items should be volume averaged over the PBM domain.

METEOROLOGICAL DATA

Mixing Heights

The meteorological preprocessor, PBMMET, offers the user several options for choosing mixing height values to be input to the PBM. The major choice is between direct specification of the mixing heights or interpolation between the morning minimum and afternoon maximum heights via the characteristic curve method. Where detailed vertical temperature soundings are available more frequently than the usual twice daily NWS profile, the user may be able to accurately determine the temporal variation of mixing heights. When this is the case, the direct input method should be chosen with an input time increment as small as possible, but no larger than 60 minutes. The characteristic curve method should be used in other situations. The morning minimum mixing height (and the next morning's minimum) can usually be determined from the 12Z sounding at the closest NWS rawinsonde location. If this location is not representative of the urban terrain and displays a surface-based temperature inversion, a minimum default value of 100 m above ground level (agl) for 0500h, LST should be input to account for the urban influence. In no case should a specified or interpolated mixing height value be less than 100 m, agl. The afternoon mixing height depth may be determined either from the 00Z NWS sounding or from the maximum afternoon surface temperature and the morning sounding (Holzworth, 1972). The maximum specified mixing height should not exceed 2000 m, agl. Daily minimum and maximum mixed layer depths for NWS rawinsonde sites are also available from the NCC.

Photolytic Rate Constants

A number of choices must be made concerning the calculation method of the photolytic rate constants. The first is whether to use surface-based or mixed-layer average rate constants. This is an important decision because there can be substantial vertical variation in the values of the photolytic rate constants in the lowest 1-2 km of the atmosphere; PBM results for O_3 are sensitive to these rate constants. For a single simulation, the layer-average method should be used to produce an upper bound on model results. However, if resources permit, a second simulation using surface-based rate constants may be conducted in order to determine the lower bound, and hence the probable range, of predicted concentrations based on the expected variations in the photolytic rate constant values.

A choice of clear-sky or attenuated photolytic rate constants is also available. In the absence of sufficient observations of solar radiation or cloud amounts and heights, the clear-sky method should be chosen. This method is also most applicable for determining the maximum potential O_3 generated by the given emissions and ventilation conditions within an urban area. If attenuated rate constants are desired, the attenuation factors may be determined based on continuously monitored UV solar radiation (wavelengths less than 3850 A), continuously monitored TSR, or hourly NCC cloud layer reports of amount and height. When the radiation data are available, they should be specified in units of langleys min^{-1}, at intervals as small as possible, but not less than 10 min or more than 60 min. A value of 10 min is recommended. Also, if mixing heights or solar radiation values are directly input to PBMMET, the time increment at which these values are specified should not be less than the time increment for outputs from PBMMET.

AIR QUALITY AND EMISSIONS DATA

Speciation Factors for Ambient NMHC

Initial condition and, optionally, boundary condition and observed values of NMHC concentrations must be subdivided into 8 hydrocarbon reactivity classes. The air quality and emissions preprocessor, PBMAQE, allows the user to specify the factors with which to perform this operation. The specific reactivity classes include NONR, ETH, OLE, PAR, FORM, ALD, ARO, and TOL.

Laboratory analysis of captured ambient air samples can help determine the splitting factors. A detailed example of this procedure is illustrated in McRae et al. (1983) for an earlier version of the Demerjian (default) chemical kinetic mechanism reactivity classes. The current version of the mechanism has similar classes, except that ethylene is split from other olefins, formaldehyde is split from other aldehydes, and toluene is split from other aromatics. This modification is easily incorporated into the procedure illustrated in the McRae reference.

If detailed analyses of ambient air samples are not available, the user has the option to choose the default values provided by PBMAQE. These values were determined for the PBM application to the St. Louis, MO area. They are presented below in Equation set (5).

$$
\begin{aligned}
&\text{NONR (ppm)} = 0.0440\ \text{NMHC (ppmC)}\\
&\text{ETH (ppm)} = 0.0263\ \text{NMHC (ppmC)}\\
&\text{OLE (ppm)} = 0.0394\ \text{NMHC (ppmC)}\\
&\text{PAR (ppm)} = 0.0786\ \text{NMHC (ppmC)}\\
&\text{FORM (ppm)} = 0.0608\ \text{NMHC (ppmC)}\\
&\text{ALD (ppm)} = 0.0202\ \text{NMHC (ppmC)}\\
&\text{ARO (ppm)} = 0.0149\ \text{NMHC (ppmC)}\\
&\text{TOL (ppm)} = 0.0099\ \text{NMHC (ppmC)}
\end{aligned} \tag{5}
$$

In this set, ethylene is represented as 40% of total olefins, formaldehyde as 75% of total aldehydes, and toluene as 40% of total aromatics. The greater the source emissions distribution for hydrocarbons differs from the St. Louis case, the less appropriate these default factors will be.

Boundary Concentration Options

Typically, values of lateral upwind boundary concentrations will be specified by the user at hour intervals based on observations from at least one ambient monitoring station upwind of the PBM domain. If it is thought that the contribution to the local pollution burden is minimal from upwind transported ozone and precursors, the user has the option of choosing a relatively clean tropospheric profile for default values of lateral boundary concentrations. These values are: CO = 0.10 ppm, NO = 0.001 ppm, NO_2 = 0.002 ppm, NMHC = 0.05 ppm, and O_3 = 0.03 ppm. These default values should not, however, be used as a substitute for knowledge about inflow boundary concentrations.

Measured boundary concentrations at the top of the model domain are generally not commonly available to the user. Without such measurements the user has the option in PBMAQE to choose an alternative method of specifying the top boundary condition for O_3. This method involves averaging the values of the lateral upwind boundary concentrations for O_3 specified during the hours of 0900-1000 and 1000-1100 L.S.T. and using the result for the top boundary concentration. It is presumed that O_3 in upper air layers will be mixed to the surface after the morning low-level temperature inversion has eroded and broken; the concentration detected by upwind surface monitors at that time should be indicative of the concentration aloft. This method is applied only for O_3 and not for precursor species, which are not considered at the top boundary.

Source Emissions

At the user's option, all source emissions may or may not be included in a PBM simulation. If source emissions are included, point source emissions may or may not be specified. If source emissions are specified, the preprocessor allows input in units of kg h^{-1} for CO, NO_x, and THC and moles h^{-1} for the hydrocarbon classes HCO (NONR), HC1 (ETH and OLE), HC2 (PAR), HC3 (FORM and ALD), and HC4 (ARO and TOL). These units are converted to ppm-m min^{-1} for output to the PBM. Alternatively, the user may specify emissions directly to PBMAQE in these final units and no conversions will be performed.

The source emission inputs should be resolved to hourly rates in order to generate representative hourly average concentration estimates from the PBM. Quite often, only a monthly or annual emissions rate is available for the various source configurations. In the absence of any other data that might aid in temporally distributing these emissions, the area and point source emission rates can be subdivided equally into hourly rates. For line sources however, the total daily emissions, where possible, should be distributed according to a weekday/weekend hourly traffic pattern.

Emission splits of organic compounds in the above hydrocarbon classes for most residential, commercial, and industrial processes are shown in Bucon et al. (1978). They must be specified to PBMAQE as total moles h^{-1} (or ppm-m min^{-1}) of HCO, HC1, HC2, HC3, and HC4. The preprocessor creates the adjusted reactivity categories for the source emissions terms output to the PBM. HCO becomes NONR, HC1 becomes ETH and OLE according to a 40%/60% split (0%/100% for point sources), HC2 becomes PAR, HC3 becomes FORM and

ALD according to a 75%/25% split (80%/20% for point sources), and HC4 becomes ARO and TOL according to a 60%/40% split (50%/50% for point sources). These splits are estimations based on work done with the St. Louis Regional Air Pollution Study emissions inventory.

Additionally, users may specify the ratio, NO_2/NO_x, in area source emissions and point source emissions and the ratio, CH_4/THC, in area source emissions and point source emissions. Default values may also be used instead. These values are 0.10, 0.10, 0.00, and 0.06, respectively.

If emissions are specified, PBMAQE expects hourly emissions fluxes in the 8 categories: CO, NOX, THC, HCO, HC1, HC2, HC3, and HC4 for the combined area and line sources and also, optionally, for the combined point sources.

SIMULATION CONTROL DATA

Simulation Options

An array of options is available to control various aspects of a PBM simulation. Some of the options are self-evident and need no further discussion. Options requiring less obvious choices are discussed below.

Option 5: Changing number of simulation hours.

The default period of simulation has been designed to start near sunrise and end in the late afternoon/early evening period, after the O_3 maximum concentration has typically been reached. At the user's option, the period of simulation may be specified as longer than the default, but not to exceed 18 hours. Appropriate input data must be specified for the additional time period. This option may also be used to shorten the simulation period. For example, if an input file exists with 13 hours of data but the user desires to end simulation after 10 hours, Option 5 is invoked and the number of hours of simulation is specified as 13 with the ending time specified as 600 minutes. Simulation start time is fixed at 0500h, LST.

Option 6: Changing numerical integration tolerance parameter.

The numerical integration routine that solves the species equations in the PBM requires a tolerance parameter within which the solution must converge. An allowable error of 1% has been specified as the default (.01). Occasionally, this value will not be sufficient for a particular simulation and the numerical solution routine will not converge, causing the simulation to consume inordinate amounts of time. To guard against such instances, a maximum time limit (e.g., 2 minutes, for a machine comparable to the UNIVAC 1100) should be specified at execution time. In a non-convergence situation, the simulation can usually be made to proceed by invoking Option 6 and raising the tolerance parameter to a value in the range of .02-.05. The larger the value, however, the greater is the amount of numerical error that will be allowed to propagate in the solution.

Option 8: Reading hourly ambient temperatures.

When hourly ambient temperatures are not specified, the temperature-dependent rate constants are calculated using a default temperature of 298°K ($\sim$ 77°F). When actual ambient temperatures are considerably greater or less than this value, rate constants, and consequently PBM-predicted concentrations, can vary significantly from default conditions. Because ambient temperatures are usually available, it is recommended that this option always be used. For measured temperatures above 38°C (100°F), specified temperatures should indicate 38°C because the temperature-dependent rate constant expressions are not accurate above this level.

Option 9: O_3 boundary conditions via photostationary state.

When upwind concentrations of O_3 are missing or unavailable Option 9 can be used to calculate them when NO and NO_2 concentrations are specified at the boundary. Because this situation would probably not occur very often, the option would not commonly be used.

Option 10: Specified emissions.

With the exception of special cases or sensitivity studies, this option (explicitly specifying emissions) will always be invoked.

Domain Size

The length of a horizonal side of the fixed model domain should be chosen such that the majority of the major area and line source emissions lie within the model domain. Further guidance in choosing the proper domain size is given in the discussion of features and limitations in Section 1.

SECTION 4

COMPUTER ASPECTS OF THE PBM

SYSTEM OVERVIEW

The PBM system consists of the main simulation model and two data preprocessors as depicted in Figure 3. The preprocessors, PBMMET and PBMAQE, must be executed before the PBM. Input data for all components of the system are recorded on cards or card-images. Device numbers for the card reader and printer are assumed to be 5 and 6, respectively. The user has the option of reading portions of the input card-image data from disk or tape devices. Output card-image data may also be stored on disk or tape.

The programming language used throughout the system is FORTRAN. The subroutine structures of PBMMET and the PBM are shown in Figures 4 and 5, respectively. Brief descriptions of the main programs and their subroutines are given below. Definitions of variables and array names are provided in glossaries within most main programs and subroutines.

PBMMET - Main program: reads and analyzes control information, reads remaining input parameters, processes mixing height and solar radiation data, calculates photolytic rate constants, calls CLOUD, if necessary, to determine cloud transmissivity, writes output data to printer and other data storage device.

SOLAR - Subroutine that provides, among other parameters, solar elevation and optical air mass given inputs of time and location.

SPLNA - Subroutine that sets up coefficients for cubic spline interpolation given a discrete set of (x,y) data points.

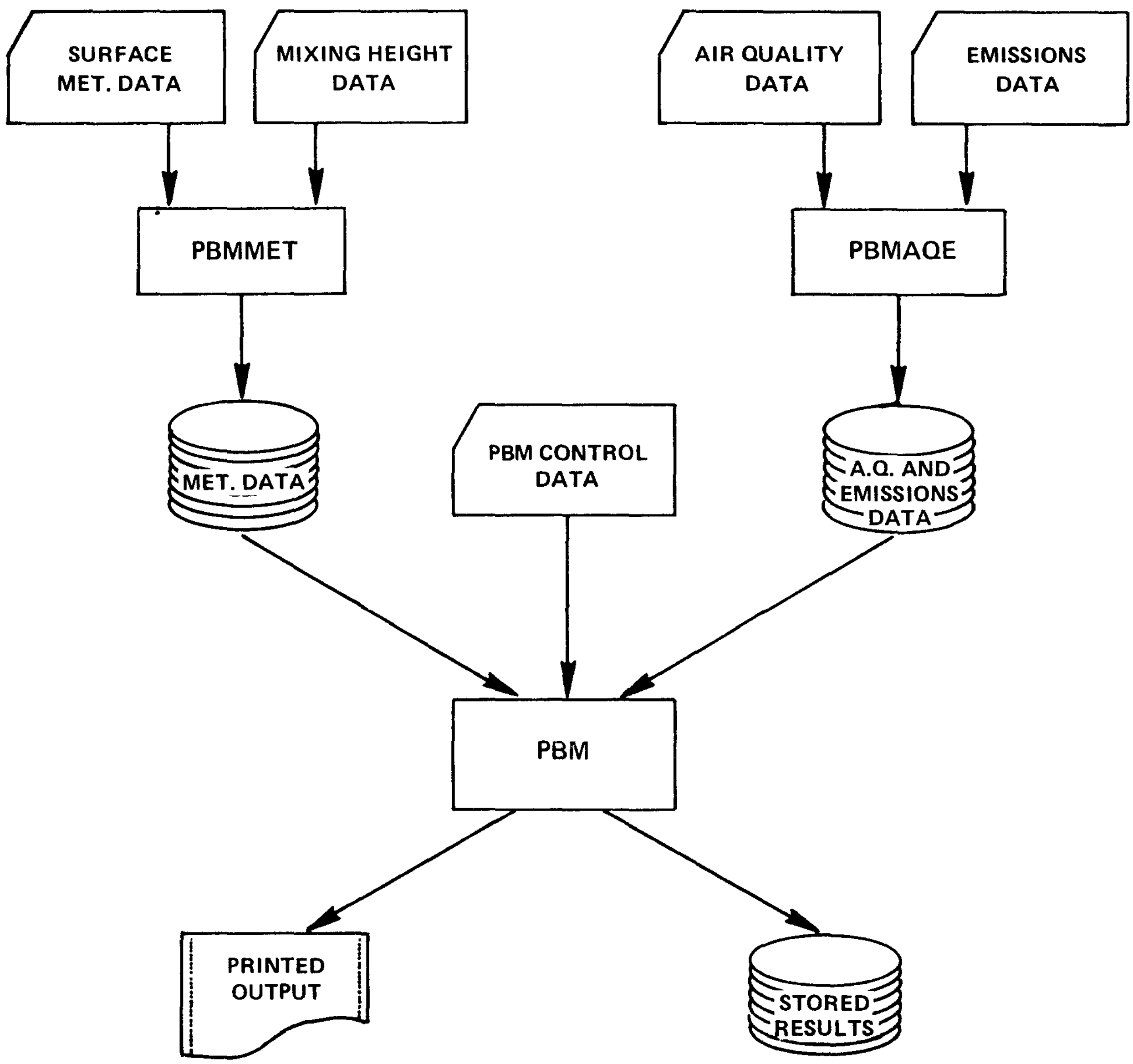

Figure 3. Schematic illustration of the PBM system.

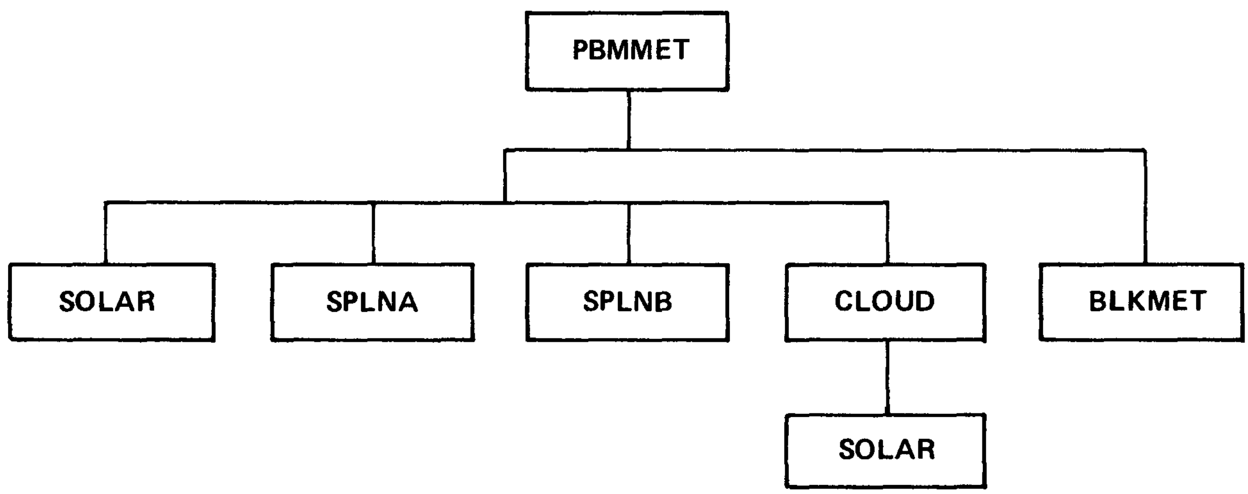

Figure 4. Subroutine structure of the PBMMET preprocessor.

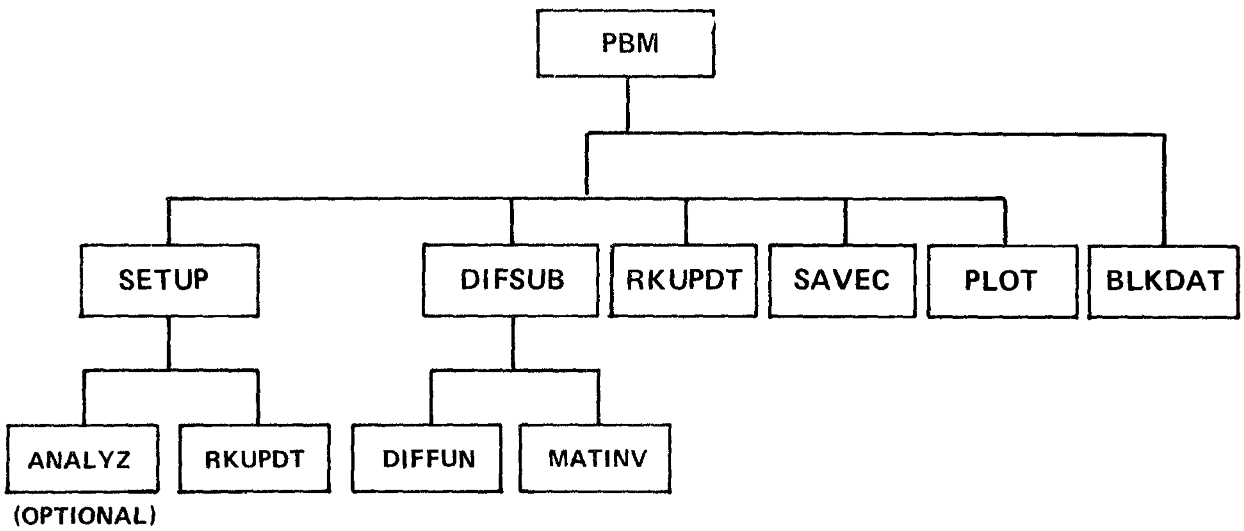

Figure 5. Subroutine structure of the PBM.

SPLNB - Subroutine that computes the interpolated value of y given any value of x within a prescribed range. It uses the cubic spline coefficients determined by SPLNA.

CLOUD - Subroutine that calculates a transmissivity factor used for attenuating photolytic rate constant values from cloud layer reports of height and sky coverage.

BLKMET - Block data that contains values of data arrays used by PBMMET, including the theoretical clear-sky values at various zenith angles of the photolytic rate constants used by the default chemical kinetic mechanism.

PBMAQE - Main program: reads and analyzes control information, processes initial concentrations, lateral and top boundary concentrations, combined area and line source emissions, combined point source emissions, and passes along species names for printer plots. (No subroutines called by PBMAQE).

PBM - Main program: Driving routine for the air quality simulation model, calls SETUP for initialization of variables, updates time and temperature-dependent rate constants and calls numerical integration routine, calls routines to do printer plots and save output data on disk/tape at end of simulation.

SETUP - Subroutine that performs initializations for the air quality simulation, reads and analyzes control options, reads all meteorological, air quality, and emissions data produced by the preprocessors, and prints out initial species concentrations.

DIFSUB - Subroutine that solves a system of differential equations using the Gear (1971) numerical method given data on initial conditions, step size, and convergence tolerance.

RKUPDT - Subroutine that calculates values of temperature-dependent reaction rate constants given the ambient temperature value.

SAVEC - Subroutine that writes out hourly values of predicted and observed (if available) concentrations of all species from the air quality simulation to disk/tape storage.

PLOT - Subroutine that produces printer plots of the time series of selected species from the air quality simulation.

BLKDAT - Block data that contains values of data variables and arrays used by PBM, including those arrays defining the structure of the default chemical kinetic mechanism.

ANALYZ - Subroutine (optionally used) that reads and analyzes a chemical kinetic mechanism other than the default mechanism for use in the PBM. (See Appendix A for further details.)

DIFFUN - Subroutine that provides the numerical solver (DIFSUB) with current rates of change of the reactive species concentrations, including the contributions from the components of chemistry, transport, vertical dilution, and source emissions.

MATINV - Subroutine that performs the matrix inversion step for DIFSUB.

INPUT DATA PREPARATION

Data input to the PBM preprocessors and the PBM as well as output data that will be archived are recorded on cards or card-images. The user may control the storage medium for data input/output through some of the control options available in the PBM system and the control language of the particular computer system used. For purposes of illustration, the nomenclature of cards will be used in this section describing the format of the data inputs. Tables 2 through 8 describe the input format for PBMMET, the meteorological preprocessor, and Figure 6 shows its input data deck setup. Tables 9 through 25 describe the input format for PBMAQE, the air quality and emissions preprocessor, and Figure 7 shows its input data deck setup. Finally, Tables 26 through 45 describe the input format for the PBM, and Figure 8 shows its input data deck setup.

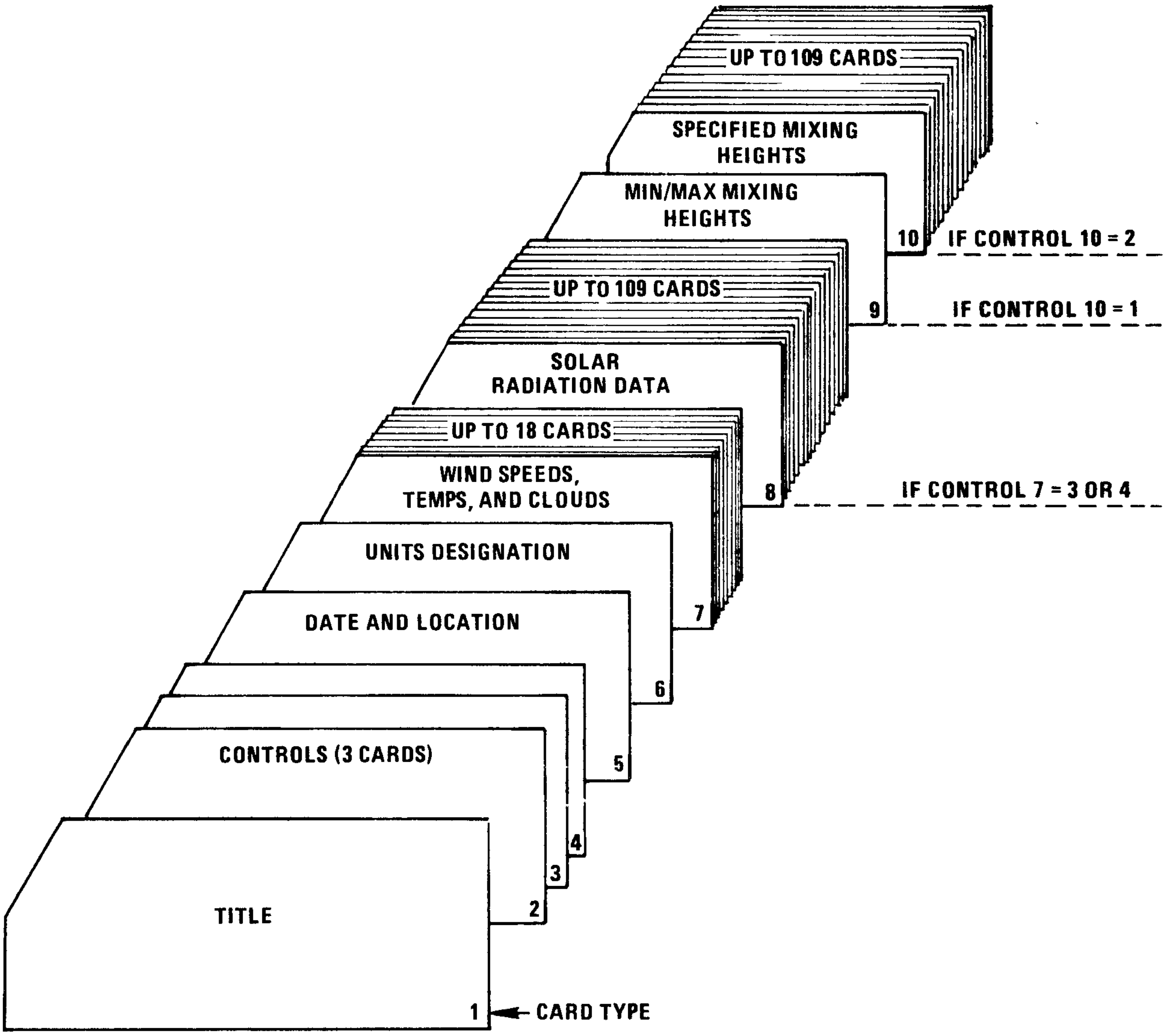

Figure 6. Input data deck setup for PBMMET.

TABLE 2. PBMMET CARD TYPE 1 - TITLE (1 card)

Variable	Format	Description	Units
ITIT	20A4	80 alphanumeric characters for title	-

TABLE 3. PBMMET CARD TYPES 2,3, AND 4 - CONTROLS (3 cards)

Variable	Format	Description	Units
		CARD TYPE 2 - GENERAL CONTROLS:	
ICON(1)	I5	Unit number for output device (card punch, disk, or tape) to receive and store card-image records from PBMMET.	-
ICON(2)	I5	Time increment for writing outputs of mixing height and photolytic rate constants; must match the update time increment in the PBM (variable = DELTIM). (Blank or 0 = DEFAULT = 10) (Otherwise: 15,20,30, or 60 are allowed)	minutes
ICON(3)	I5	Beginning of stop hour for processing of meteorological data, in Local Standard Time (L.S.T.) (Blank or 0 = DEFAULT = 17) (Maximum value allowed = 22)	hours, L.S.T.
ICON(4)	I5	Not currently used.	
		CARD TYPE 3 - SURFACE DATA AND SOLAR RADIATION CONTROLS:	
ICON(5)	I5	Unit number for input device for reading surface meteorological observations, including wind speed, temperature, solar radiation, and cloud report data.	-
ICON(6)	I5	Choice of mixed-layer average photolytic rate constants (control value = 1) or surface-based photolytic rate constants (control value = 2). (Blank or 0 = DEFAULT = 1)	

(continued)

TABLE 3 (continued)

Variable	Format	Description	Units
ICON(7)	I5	Photolytic rate constants are computed as follows: 1=Full value; clear-sky conditions 2=Attenuated; based on hourly cloud layer reports 3=Attenuated; based on measured total solar radiation every 'N' minutes (N=10,15,20,30, or 60) 4=Attenuated; based on measured ultraviolet radiation (wavelengths <3850A) every 'N' minutes (N=10,15,20,30, or 60). (Blank or 0 = DEFAULT = 1)	
ICON(8)	I5	'N' value described in ICON(7). Radiation values will be read with this time increment from unit number specified in ICON(5). (Specify value only if ICON(7) = 3 or 4)	minutes
		CARD TYPE 4 - MIXING HEIGHT CONTROLS:	
ICON(9)	I5	Unit number for input device for reading mixing height data.	
ICON(10)	I5	Mixing heights are calculated using the following: 1=Daily minimum and maximum, with 'characteristic curve' method. 2=Input values, every 'N' minutes (N=10,15,20,30 or 60) (Blank or 0=DEFAULT=1)	-
ICON(11)	I5	'N' value described in ICON(10). Mixing height values will be read with this increment from unit number specified in ICON(9). (Specify value only if ICON(10)=2)	minutes

TABLE 4. PBMMET CARD TYPES 5 AND 6 - LOCATION/UNITS (2 cards)

Variable	Format	Description	Units
		CARD TYPE 5 - DATE AND LOCATION:	
IMO	I5	Numerical designation of month (e.g., 07)	-
IDA	I5	Numerical designation of day (e.g., 13)	-
IYR	I5	Year (e.g., 1976)	-
JDA	I5,10X	Julian day number (e.g., 195)	-
LAT	F10.0	Latitude of model domain (negative for southern hemisphere)	degrees
LONG	F10.0	Longitude of model domain (negative for eastern hemisphere)	degrees
TZ	F10.0	Number of time zones away from Greenwich Mean Time (GMT), (e.g., E.S.T. = 5.0, C.S.T. = 6.0, M.S.T. = 7.0, P.S.T. = 8.0)	-
		CARD TYPE 6 - UNITS DESIGNATION:	
IUNW	I5	Input wind speed data units code: 1=m s^{-1} 2=knots 3=mi h^{-1}	-
IUNT	I5	Input temperature data units code: 1=degrees-Centigrade 2=degrees-Fahrenheit	-

TABLE 5. PBMMET CARD TYPE 7 - SURFACE METEOROLOGICAL DATA (up to 18 cards)

Variable	Format	Description	Units
IHR	I5	Beginning of hour during which surface meteorological data apply (e.g., 05)	hour, L.S.T.
WS	F10.0	Wind speed during the hour	m s^{-1}, knots, or mi h^{-1}
TEMPS	F10.0, 10X	Ambient temperature during the hour	deg-C or deg-F
The following variables are specified only if ICON(7)=2 on CARD TYPE 3:			
ICA(1)	A1,4X	Sky coverage, in tenths, of clouds in 1st reported layer during the hour. (Blank=no report or clear; 1 through 9; or '-'=10 are allowed)	-
ICH(1)	A3,2X	Height of 1st cloud layer (Blank=no report)	hundreds of ft, agl
ICA(2)	A1,4X	Cumulative sky coverage, in tenths, of clouds in 1st and 2nd reported layers, if given, during the hour.	-
ICH(2)	A3,2X	Height of 2nd cloud layer	hundreds of ft, agl
ICA(3)	A1,4X	Cumulative sky coverage, in tenths, of clouds in 1st , 2nd, and 3rd reported layers, if given, during the hour.	-
ICH(3)	A3	Height of 3rd cloud layer	hundreds of ft, agl

TABLE 6. PBMMET CARD TYPE 8 - SOLAR RADIATION DATA (up to 109 cards) (used with ICON(7) = 3 or 4)

Variable	Format	Description	Units
IT	I5	Time at which radiation value applies (e.g., 1040)	hours, L.S.T.
RAD	F10.0	Measured value of solar radiation data: Total solar radiation if ICON(7)=3 Ultraviolet radiation if ICON(7)=4 (Radiation values must be specified for the entire simulation period. Values of 0 should be entered for other than daytime conditions. Last specified value must be -1.0).	langleys min^{-1}

TABLE 7. PBMMET CARD TYPE 9 - MIN/MAX MIXING HEIGHTS (1 card) (used with ICON(10=1)

Variable	Format	Description	Units
HMINO	5X, F10.0	Height above ground of the morning minimum depth of the mixed layer. (For values < 100 m, use 100 m).	meters
HMAX	F10.0	Height above ground of the afternoon maximum depth of the mixed layer. (For values > 2000 m, use 2000 m).	meters
HMIN1	F10.0	Height above ground of the next morning minimum depth of the mixed layer. (For values < 100 m, use 100 m).	meters

TABLE 8. PBMMET CARD TYPE 10 - SPECIFIED MIXING HEIGHTS (up to 109 cards) (used with ICON(10)=2)

Variable	Format	Description	Units
IT	I5	Time at which mixing height value applies (e.g., 1040)	hours, L.S.T.
HEIGHT	F10.0	Depth of the mixed layer. ($100 < HEIGHT \leq 2000$) (Last specified value <u>must</u> be -1.0)	meters

TABLE 9. PBMAQE CARD TYPE 1 - TITLE (1 card)

Variable	Format	Description	Units
ITIT	20A4	80 alphanumeric characters for title	-

TABLE 10. PBMAQE CARD TYPE 2 - SIMULATION CONTROLS (1 card)

Variable	Format	Description	Units
WIDTH	F10.0	Size of horizontal edge of PBM domain	km
TEMP	F10.0	Average ambient temperature during simulation period	deg-C
NUMHR	I5	Number of hours of data to be processed by PBMAQE and simulated by the PBM (Blank or 0=DEFAULT=13)	-

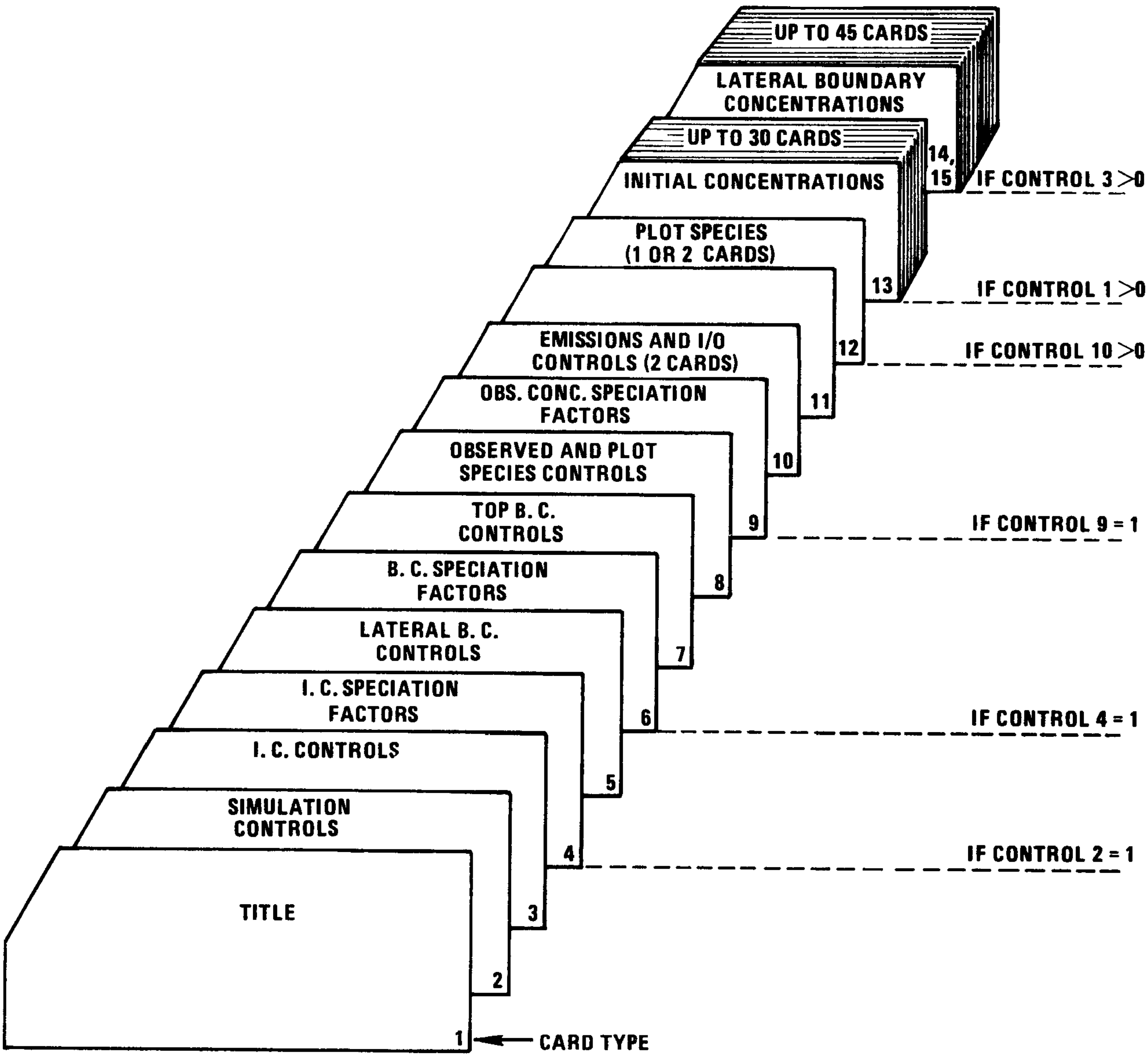

Figure 7. Input data deck setup for PBMAQE.

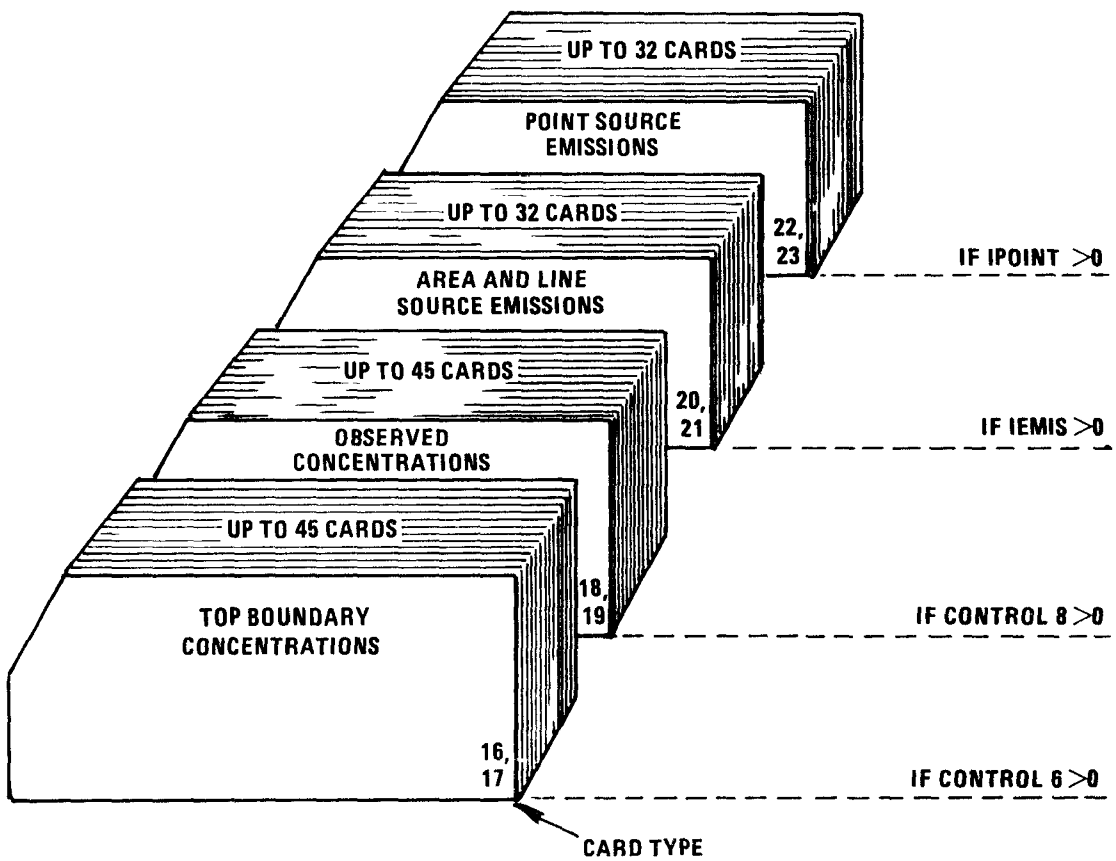

Figure 7. (continued)

TABLE 11. PBMAQE CARD TYPE 3 - I.C. CONTROLS (1 card)

Variable	Format	Description	Units
ICON(1)	I5	Number of initial species concentrations to be specified for 0500h, L.S.T. (Do not count hydrocarbon reactivity classes in the sum.)	-
ICON(2)	I5	Input values of hydrocarbon speciation factors for initial NMHC? (Blank or 0=DEFAULT=no; St. Louis default values will be used. 1=yes.)	

TABLE 12. PBMAQE CARD TYPE 4 - I.C. SPECIATION FACTORS (1 card) (used with ICON(2) = 1)

Variable	Format	Description	Units
SFIC	8F10.0	Hydrocarbon speciation factors to split initial NMHC concentration into 8 reactivity classes	-

TABLE 13. PBMAQE CARD TYPE 5 - LATERAL B.C. CONTROLS (1 card)

Variable	Format	Description	Units
ICON(3)	I5	Number of lateral boundary condition species to be specified (maximum=15)	-
ICON(4)	I5	Input values of hydrocarbon speciation factors for NMHC boundary concentrations (lateral and top)? (Blank or 0=DEFAULT=no; St. Louis default values will be used. 1=yes.)	-
ICON(5)	I5	Use 'clean troposphere' values for lateral boundary concentrations? (Blank or 0=DEFAULT=no; user will input hourly values of boundary concentrations. 1=yes; values will be set implicitly, ICON(3) must be set to 0.)	-

TABLE 14. PBMAQE CARD TYPE 6 - B.C. SPECIATION FACTORS (1 card) (used with ICON(4)=1)

Variable	Format	Description	Units
SFBC	8F10.0	Hydrocarbon speciation factors to split NMHC boundary concentrations (lateral and top) into 8 reactivity classes	-

TABLE 15. PBMAQE CARD TYPE 7 - TOP B.C. CONTROLS (1 card)

Variable	Format	Description	Units
ICON(6)	I5	Number of top boundary condition species to be specified. (maximum=15)	-
ICON(7)	I5	Top O_3 boundary concentration to be determined implicitly from lateral O_3 boundary concentrations? (Blank or 0=DEFAULT=no, 1=yes; do not count O_3 in total value of ICON(6))	

TABLE 16. PBMAQE CARD TYPE 8 - OBSERVED AND PLOT SPECIES CONTROLS (1 card)

Variable	Format	Description	Units
ICON(8)	I5	Number of observed species to be specified. (maximum=15)	-
ICON(9)	I5	Input values of hydrocarbon speciation factors for NMHC observed concentrations? (Blank or 0=DEFAULT=no; St. Louis default values will be used. 1=yes.)	-
ICON(10)	I5	Number of species to be plotted on printer during PBM simulation. (maximum=30)	-

TABLE 17. PBMAQE CARD TYPE 9 - OBS. CONC. SPECIATION FACTORS (1 card) (used with ICON(9)=1)

Variable	Format	Description	Units
SFOB	8F10.0	Hydrocarbon speciation factors to split NMHC observed concentrations into 8 reactivity classes.	-

TABLE 18. PBMAQE CARD TYPES 10 AND 11 - EMISSIONS AND I/O CONTROLS (2 cards)

Variable	Format	Description	Units
		CARD TYPE 10 - EMISSIONS CONTROLS:	
IEMIS	I5	Input emissions code: Blank or 0 = No emissions specified. 1=CO,NO_x,THC emissions specified in kg h^{-1}; HCO,HC1,...,HC4 emissions specified in moles h^{-1}. 2=CO,NO_x,THC,HCO,HC1,...,HC4 emissions specified in ppm-m min^{-1}.	-
IPOINT	I5	Point source flag: Blank or 0=no point emissions specified 1=point source emissions specified in same units indicated by IEMIS	-
RATIO(1)	2X, F8.0	Ratio of NO_2/NO_x in combined area and line source emissions	-
RATIO(2)	2X, F8.0	Ratio of NO_2/NO_x in point source emissions	-
RATIO(3)	2X, F8.0	Ratio of CH_4/THC in combined area and line source emissions	-
RATIO(4)	2X, F8.0	Ratio of CH_4/THC in point source emissions (If RATIO(1) and RATIO(3) are both blank, defaults of 0.10 and 0.00, respectively will be used. If RATIO(2) and RATIO(4) are both blank, defaults of 0.10 and 0.06, respectively will be used. Otherwise, specified values will be used.)	-
		CARD TYPE 11 - I/O CONTROLS:	
NAQ	I5	Input unit number for air quality values.	
NEM	I5	Input unit number for emissions values	-
NOUTD	I5	Output unit number for card, disk, or tape storage of card-image data for the PBM	-

TABLE 19. PBMAQE CARD TYPE 12 - PLOT SPECIES (1 or 2 cards) (used with ICON(10)>0)

Variable	Format	Description	Units
NPLOT	20A4	Alphanumeric names of species to be plotted on printer by the PBM.	-

TABLE 20. PBMAQE CARD TYPE 13 - INITIAL CONCENTRATIONS (up to 30 cards) (used with ICON(1)>0)

Variable	Format	Description	Units
ISPEC	A4	Alphanumeric name of i.c. species	-
CI	6X, F10.0	Species concentrations at 0500h, L.S.T.	ppm

TABLE 21. PBMAQE CARD TYPES 14 AND 15 - LATERAL BOUNDARY CONCENTRATIONS (up to 45 cards) (used with ICON(3)>0)

Variable	Format	Description	Units
	CARD TYPE 14 - SPECIES NAME: (1 card per species)		
ISPEC	A4	Alphanumeric name of lateral b.c. species	-
	CARD TYPE 15 - B.C. CONCENTRATIONS: (1 or 2 cards per species)		
CLAT	10F8.0	Hour-average lateral boundary concentrations of ISPEC for each hour of PBM simulation	ppm

TABLE 22. PBMAQE CARD TYPES 16 AND 17 - TOP BOUNDARY CONCENTRATIONS (up to 45 cards) (used with ICON(6)>0)

Variable	Format	Description	Units
		CARD TYPE 16 - SPECIES NAME: (1 card per species)	
ISPEC	A4	Alphanumeric name of top b.c. species	-
		CARD TYPE 17 - B.C. CONCENTRATIONS: (1 or 2 cards per species)	
C	10F8.0	Hour-average top boundary concentrations of ISPEC for each hour of PBM simulation	ppm

TABLE 23. PBMAQE CARD TYPES 18 AND 19 - OBSERVED CONCENTRATIONS (up to 45 cards) (used with ICON(8)>0)

Variable	Format	Description	Units
		CARD TYPE 18 - SPECIES NAME: (1 card per species)	
ISPEC	A4	Alphanumeric name of observed species	-
		CARD TYPE 19 - OBSERVED CONCENTRATIONS: (1 or 2 cards per species)	
C	10F8.0	Hour-average observed concentrations of ISPEC for each hour of PBM simulation. (-1.0 indicates missing data).	ppm

TABLE 24. PBMAQE CARD TYPES 20 AND 21 - AREA AND LINE SOURCE EMISSIONS (up to 32 cards) (used with IEMIS>0)

Variable	Format	Description	Units
	CARD TYPE 20 - SPECIES NAME: (1 card per species)		
ISPEC	A4	Alphanumeric name of emissions species	-
	CARD TYPE 21 - EMISSIONS: (up to 3 cards per species)		
C	8F10.0	Hourly emissions flux of ISPEC for combined area and line source emissions into PBM domain for each hour of simulation. Species must conform exactly to the 8 specified in Section 3.	Kg h^{-1} and moles h^{-1} (if IEMIS=1); ppm-m min^{-1} (if IEMIS=2)

TABLE 25. PBMAQE CARD TYPES 22 AND 23 - POINT SOURCE EMISSIONS (up to 32 cards) (used with IPOINT>0)

Variable	Format	Description	Units
	CARD TYPE 22 - SPECIES NAME: (1 card per species)		
ISPEC	A4	Alphanumeric name of emissions species	-
	CARD TYPE 23 - EMISSIONS: (up to 3 cards per species)		
CLAT	8F10.0	Hourly emissions flux of ISPEC for point source emissions into PBM domain for each hour of simulation. Species must conform exactly to the 8 specified in Section 3.	Kg h^{-1} and moles h^{-1} (if IEMIS=1); ppm-m min^{-1} (if IEMIS=2)

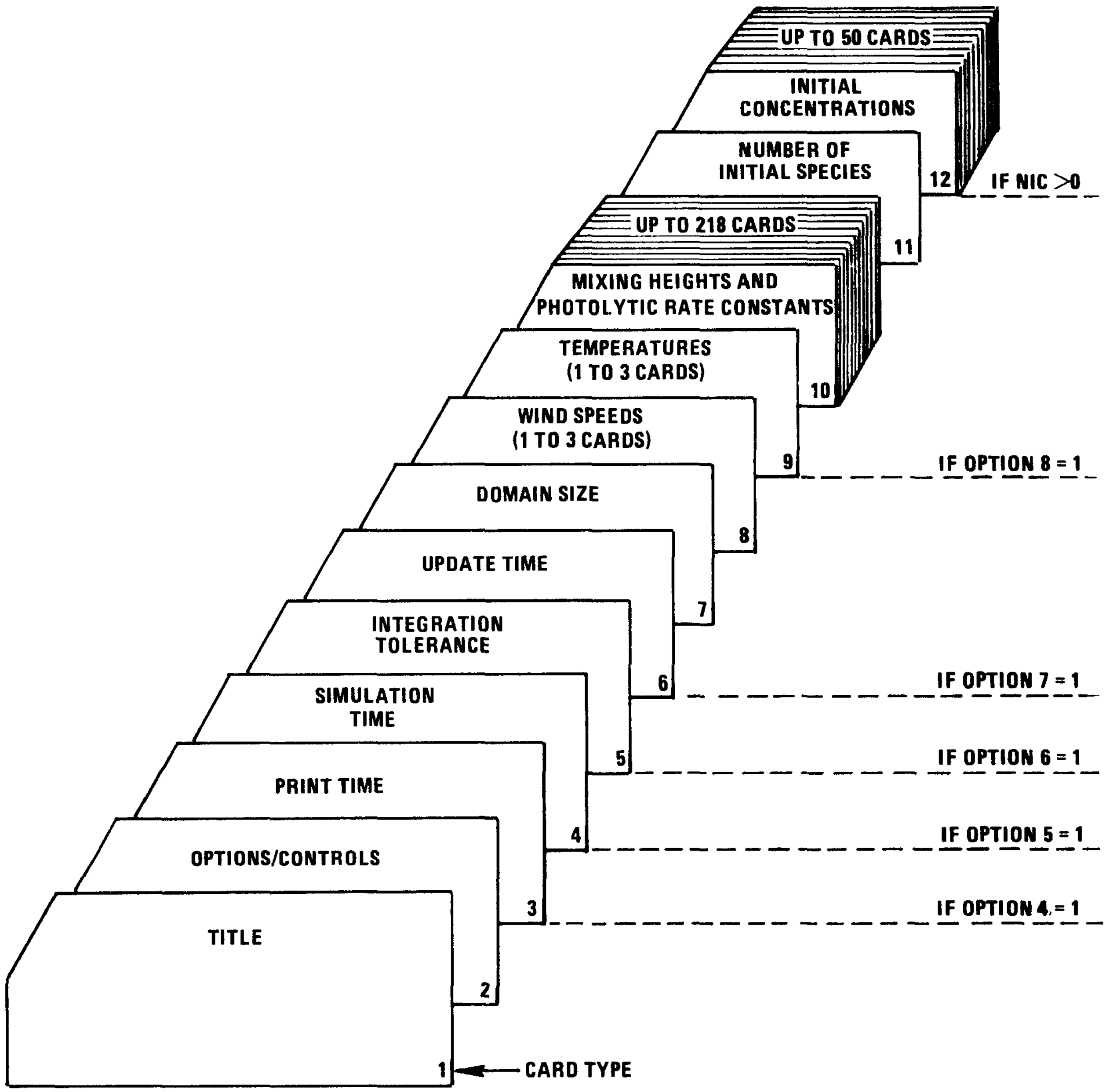

Figure 8. Input data deck setup for the PBM.

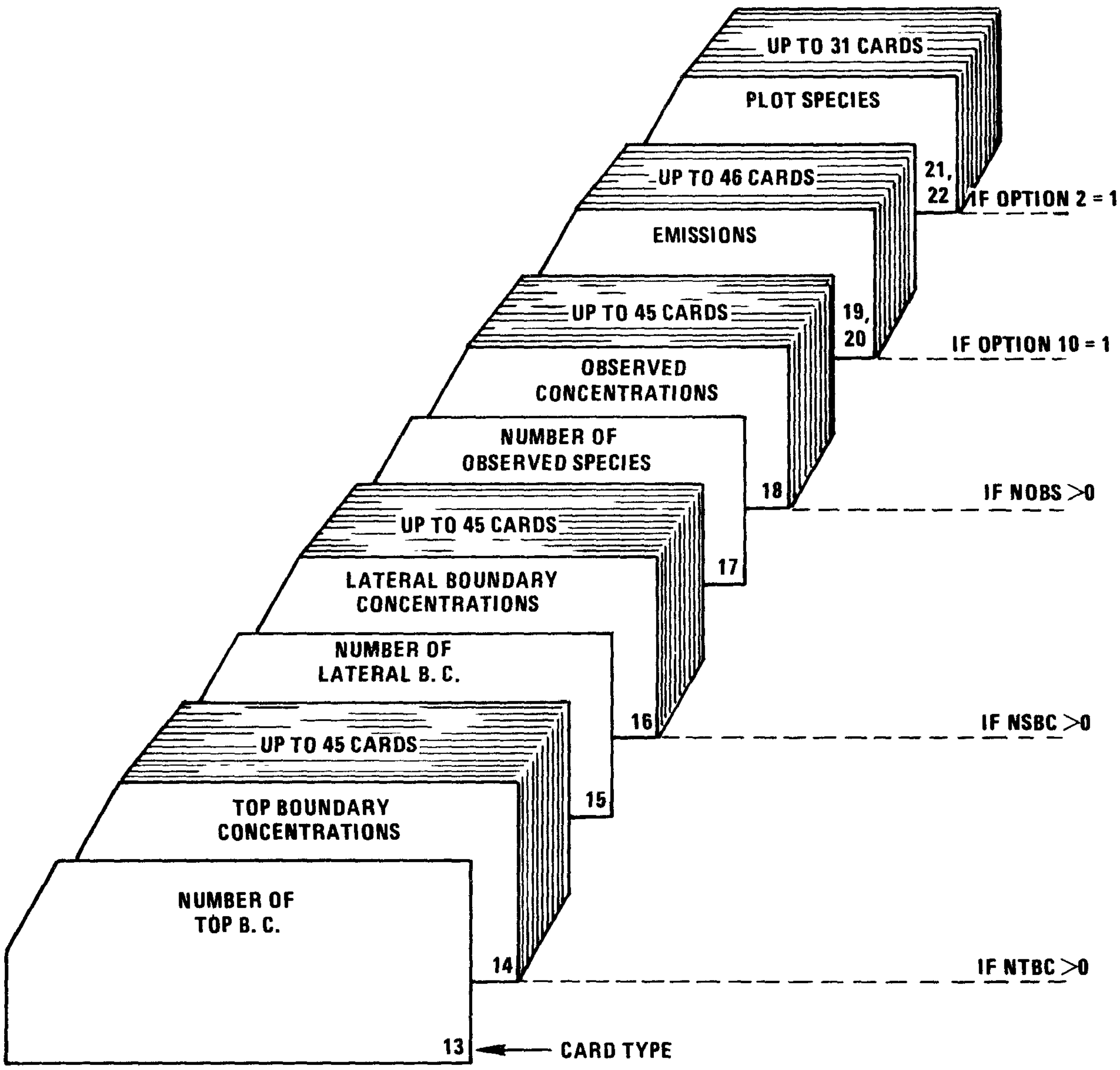

Figure 8. (continued)

TABLE 26. PBM CARD TYPE 1 - TITLE (1 card)

Variable	Format	Description	Units
NTIT	20A4	80 alphanumeric characters for title	-

TABLE 27. PBM CARD TYPE 2 - OPTIONS/CONTROLS (1 card)

Variable	Format	Description	Units
IOPT(1)	I5	Printed listing of concentrations at each time interval? (0=no, 1=yes)	-
IOPT(2)	I5	Printer plots of simulation results for selected species? (0=no, 1=yes)	-
IOPT(3)	I5	Save hour-average simulation results on card, disk, or tape storage? (0=no, 1=yes) (Note: If IOPT(3)=1, the storage device must be assigned unit number 8)	-
IOPT(4)	I5	Change time interval from default (10 min) to a larger value for printing and plotting of concentrations? (0=no, 1=yes)	-
IOPT(5)	I5	Change number of hours of simulation from default (13 hours)? (0=no, 1=yes)	-
IOPT(6)	I5	Change numerical integration tolerance parameter from default (0.01)? (0=no, 1=yes)	-
IOPT(7)	I5	Change time interval to a larger value for updating mixing heights and photolytic rate constants from default (10 min)? (0=no, 1=yes)	
IOPT(8)	I5	Read hourly ambient temperatures for temperature-dependent rate constant calculations? (0=no, 1=yes)	-
IOPT(9)	I5	Steady-state lateral boundary concentration for O_3? (0=no, 1=yes)	-
IOPT(10)	I5	Read emissions rates for simulation? (0=no, 1=yes)	-

TABLE 28. PBM CARD TYPE 3 - PRINT TIME (1 card)
(used with IOPT (4)=1)

Variable	Format	Description	Units
TINCR	F10.0	Time interval for printing and plotting of predicted concentrations. Allowable values are 10.,15.,20.,30., and 60. (Default=10.)	minutes

TABLE 29. PBM CARD TYPE 4 - SIMULATION TIME (1 card)
(used with IOPT(5)=1)

Variable	Format	Description	Units
NUMHR	I5	Number of hours of simulation data to be read in. (Default=13)(Must agree with NUMHR of PBMAQE - see Table 10)	-
TEND	F10.0	Stop time of simulation, in minutes after 0500h, L.S.T. (TEND is usually set to a value of 60.*NUMHR, but it may be set less than this value.)	minutes

TABLE 30. PBM CARD TYPE 5 - INTEGRATION TOLERANCE (1 card)
(used with (IOPT(6)=1)

Variable	Format	Description	Units
EPSF	F10.0	Numerical integration tolerance parameter. (Default=0.01)	-

TABLE 31. PBM CARD TYPE 6 - UPDATE TIME (1 card) (used with IOPT(7)=1)

Variable	Format	Description	Units
DELTIM	F10.0	Time interval for updating mixing heights and photolytic rate constants. Allowable values are 10.,20.,30., and 60. (Default=10.)(Must agree with ICON(2) of PBMMET - see Table 3)	minutes

TABLE 32. PBM CARD TYPE 7 - DOMAIN SIZE (1 card)

Variable	Format	Description	Units
WIDTH	F10.0	Size of horizontal edge of PBM domain.	km

Card-image input to the PBM described in Tables 26-32 must be prepared by the user for an execution of the PBM. Card-image input described in Tables 33-45 is prepared for the PBM by the preprocessors PBMMET and PBMAQE.

TABLE 33. PBM CARD TYPE 8 - WIND SPEEDS (up to 3 cards)

Variable	Format	Description	Units
WS	8F10.0	Average wind speed for each hour of simulation.	m s^{-1}

TABLE 34. PBM CARD TYPE 9 - TEMPERATURES (up to 3 cards) (used with IOPT(8)=1)

Variable	Format	Description	Units
TEMPS	8F10.0	Average ambient temperature for each hour of simulation.	deg-C

TABLE 35. PBM CARD TYPE 10 - MIXING HEIGHTS AND PHOTOLYTIC RATE CONSTANTS (up to 218 cards)

Variable	Format	Description	Units
ITIME	I5	Time at which data apply. (Time interval between data inputs must agree with DELTIM -- see Table 31.)	hours, L.S.T.
HTMIX	5X,F10.0	Depth of the mixed layer at current time (100<HTMIX<2000) (Last specified value must be = -1.0).	meters
PRC	6E10.0,/, 20X,6E10.0	Photolytic rate constants at current time for chemical species that participate in photolysis reactions.	$minute^{-1}$

TABLE 36. PBM CARD TYPE 11 - NUMBER OF INITIAL SPECIES (1 card)

Variable	Format	Description	Units
NIC	I5	Number of initial species concentrations to be specified for 0500h, L.S.T. (maximum=50)	-

TABLE 37. PBM CARD TYPE 12 - INITIAL CONCENTRATIONS (up to 50 cards) (used with NIC>0)

Variable	Format	Description	Units
ISPEC	A4	Alphanumeric name of i.c. species	-
CI	6X,E10.0	Species concentration at 0500h, L.S.T.	ppm

TABLE 38. PBM CARD TYPE 13 - NUMBER OF TOP B.C. (1 card)

Variable	Format	Description	Units
NTBC	I5	Number of top boundary condition species to be specified. (maximum=15)	-

TABLE 39. PBM CARD TYPE 14 - TOP BOUNDARY CONCENTRATIONS (up to 45 cards) (used with NTBC>0)

Variable	Format	Description	Units
ISPEC	A4	Alphanumeric name of top b.c. species	-
TPCONC	6X,7E10.0, /,(10X,7E10.0)	Hour-average top boundary concentrations of ISPEC for each hour of PBM simulation.	ppm

TABLE 40. PBM CARD TYPE 15 - NUMBER OF LATERAL B.C. (1 card)

Variable	Format	Description	Units
NSBC	I5	Number of lateral boundary condition species to be specified. (maximum=15)	-

TABLE 41. PBM CARD TYPE 16 - LATERAL BOUNDARY CONCENTRATIONS (up to 45 cards) (used with NSBC>0)

Variable	Format	Description	Units
ISPEC	A4	Alphanumeric name of lateral b.c. species	-
SDCONC	6X,7E10.0, /,(10X, 7E10.0)	Hour-average lateral boundary concentrations of ISPEC for each hour of PBM simulation	ppm

TABLE 42. PBM CARD TYPE 17 - NUMBER OF OBSERVED SPECIES (1 card)

Variable	Format	Description	Units
NOBS	I5	Number of observed species to be specified. (maximum=15)	-

TABLE 43. PBM CARD TYPE 18 - OBSERVED CONCENTRATIONS (up to 45 cards) (used with NOBS>0)

Variable	Format	Description	Units
ISPEC	A4	Alphanumeric name of observed species	-
OBS	6X,7E10.0, /,(10X, 7E10.0)	Hour-average observed concentrations of ISPEC for each hour of PBM simulation. (-1.0 indicates missing data)	ppm

TABLE 44. PBM CARD TYPES 19 AND 20 - EMISSIONS (up to 46 cards) (used with IOPT(10)=1)

Variable	Format	Description	Units
		CARD TYPE 19 - NUMBER OF EMISSIONS SPECIES: (1 card)	
NEMIS	I5	Number of emissions species to be specified. (maximum=15; NEMIS must equal 12 when using the default chemical mechanism in the PBM)	-
		CARD TYPE 20 - EMISSION FLUXES: (up to 3 cards per species)	
ISPEC	A4	Alphanumeric name of emissions species	-
EMIS	6X,7E10.0, /,(10X, 7E10.0)	Hourly emissions flux of ISPEC from all sources into PBM domain for each hour of simulation.	ppm-m min^{-1}

TABLE 45. PBM CARD TYPES 21 AND 22 - PLOT SPECIES (up to 31 cards) (used with IOPT(2)=1)

Variable	Format	Description	Units
		CARD TYPE 21 - NUMBER OF PLOT SPECIES: (1 card)	
NPLOT	I5	Number of species to be plotted on printer (maximum=30)	-
		CARD TYPE 22 - NAMES OF PLOT SPECIES: (up to 30 cards)	
ISPEC	A4	Alphanumeric name of species to be plotted on printer.	-

REQUIRED RESOURCES FOR THE PBM SYSTEM

Running the PBM and its preprocessors on a particular computer system requires some knowledge of the system resources needed for the procedure. The figures provided here are intended only as a rough guide since each computer system and model application will be different. The PBM system is installed on the EPA's UNIVAC 1110 computer; the following figures are taken from a model application to St. Louis, MO using that machine.

PBMMET (Meteorological Preprocessor)

- 25K words of memory required
- 8.5 s of computer time (88%-CPU, 12% - IO)
- 6-11 pages of printed output

PBMAQE (Air Quality and Emissions Preprocessor)

- 10K words of memory required
- 7.5 s of computer time (90%-CPU, 10%-IO)
- 9 pages of printed output

PBM (Photochemical Box Model)

- 45K words of memory required
- 30 - 90 s of computer time (90%-CPU, 10%-IO)
- 60 - 70 pages of printed output (all information printed)
- 10-30 pages of printed output (plots and concentrations summary only)

The actual amount of computer time required by the PBM and its preprocessors will, of course, depend on the length of the simulation. The figures cited above are for the standard 13h simulation, starting at 0500h, L.S.T. A failure of the numerical solution to converge will cause the PBM to consume a large amount of computer time without advancing the simulation.

To guard against this occurrence, a maximum time limit (90-120 s) should be specified for every execution of the PBM. If the solution fails to converge, the tolerance may be relaxed from the default (0.01) to a value between 0.01 and 0.05 until a convergence is reached. The appropriate parameter is EPSF in the simulation controls (see Table 30). The larger the value that EPSF is allowed to take the greater is the potential for numerical errors in the solution.

SECTION 5

EXAMPLE PROBLEM

DESCRIPTION

An example problem is shown here as an aid to the user in applying the PBM system. Input data and program output are given for the two preprocessors and the simulation model. The example illustrates the application of the PBM to the city of St. Louis, MO using the extensive RAPS data base (Schere and Shreffler, 1982). The model domain has 20-km horizontal sides and is centered on the downtown area. The scenario modeled occurred on Oct. 1, 1976, a day with light winds, subsidence aloft, and air stagnation near the surface. Locally generated products of photochemical activity were observed at considerably high concentrations.

Twelve surface-based meteorological and air quality monitors and one upper-air sounding location were available within the PBM domain for determining input data for the model and preprocessors. Data were averaged over all 12 monitors to determine PBM domain-average values. Nine monitors surrounding the domain were available for determining boundary concentrations. The RAPS data base also included a complete source emissions inventory for St. Louis.

The number of user-specified options among the inputs to the model and preprocessors is sufficiently large so that not all possibilities may be illustrated in the following example problem. However, the options chosen here probably represent some of the more commonly chosen ones within a large user group with a variety of applications.

Input data, UNIVAC runstream, and program output are presented. In the graphs shown in the example problem, the model-predicted instantaneous concentrations are represented by the '*'s, the predicted hour-average concentrations are represented by the 'H's, and the hour-average observed values are represented by the 'O's.

DATA INPUT AND PROGRAM OUTPUT

UNIVAC RUNSTREAM FOR EXAMPLE PROBLEM

```
@RUN ...
@
@
@ASG,A PBM.
@ASG,UP METDATA.
@USE 2.,METDATA.
@XQT PBM.PBMMET
@ADD PBM.PBMMET-INPUT
@
@
@ASG,UP AQEDATA.
@USE 3.,AQEDATA.
@XQT PBM.PBMAQE
@ADD PBM.PBMAQE-INPUT
@
@
@ASG,UP SAVERESULTS.
@USE 8.,SAVERESULTS.
@XQT PBM.PBM
PBM - DAY 76275 - 10/01/76  (EXAMPLE PROBLEM)
    0    1    1    0    0    0    0    1    0    1
      20.0
@ADD METDATA.
@ADD AQEDATA.
@
@
@FIN
```
**

INPUT DATA - PBMMET EXAMPLE PROBLEM

1	TEST OF PBMMET - 76275						
2	2						
3	5	1	3	10			
4	5	1					
5	10	01	1976	275	38.617	90.193	6.0
6	1	1					
7	5.0	1.583		11.1			
8	6.0	1.679		11.6			
9	7.0	1.513		14.5			
10	8.0	.862		17.8			
11	9.0	.391		20.8			
12	10.0	.386		23.5			
13	11.0	.805		25.5			
14	12.0	.086		26.9			
15	13.0	.479		27.8			
16	14.0	.709		28.5			
17	15.0	.792		28.7			
18	16.0	.888		28.2			
19	17.0	.896		26.1			
20	5.00	.0000					
21	5.17	.0000					
22	5.33	.0000					
23	5.50	.0000					
24	5.67	.0000					
25	5.83	.0000					
26	6.00	.0000					
27	6.17	.0059					
28	6.33	.0254					
29	6.50	.0556					
30	6.67	.0936					
31	6.83	.1308					
32	7.00	.1739					
33	7.17	.2178					
34	7.33	.2647					
35	7.50	.3086					
36	7.67	.3512					
37	7.83	.3954					
38	8.00	.4414					
39	8.17	.4872					
40	8.33	.5311					
41	8.50	.5671					
42	8.67	.6034					
43	8.83	.6390					
44	9.00	.6788					
45	9.17	.7141					
46	9.33	.7507					
47	9.50	.7825					
48	9.67	.8146					
49	9.83	.8374					
50	10.00	.8659					
51	10.17	.8933					
52	10.33	.9152					
53	10.50	.9388					
54	10.67	.9504					
55	10.83	.9689					
56	11.00	.9783					

INPUT DATA - PBMMET EXAMPLE PROBLEM

57	11.17	.9925		
58	11.33	1.0090		
59	11.50	1.0094		
60	11.67	1.0197		
61	11.83	1.0085		
62	12.00	1.0088		
63	12.17	.9914		
64	12.33	.9824		
65	12.50	.9796		
66	12.67	.9813		
67	12.83	.9764		
68	13.00	.9582		
69	13.17	.9374		
70	13.33	.9101		
71	13.50	.8843		
72	13.67	.8555		
73	13.83	.8301		
74	14.00	.7981		
75	14.17	.7607		
76	14.33	.7289		
77	14.50	.6871		
78	14.67	.6533		
79	14.83	.6162		
80	15.00	.5854		
81	15.17	.5471		
82	15.33	.5074		
83	15.50	.4684		
84	15.67	.4232		
85	15.83	.3774		
86	16.00	.3344		
87	16.17	.2957		
88	16.33	.2533		
89	16.50	.2163		
90	16.67	.1802		
91	16.83	.1406		
92	17.00	.1015		
93	17.17	.0642		
94	17.33	.0319		
95	17.50	.0083		
96	17.67	.0000		
97	17.83	.0000		
98	18.00	.0000		
99		-1.0		
100		100.0	532.0	100.0

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PBMMET -- METEOROLOGICAL PREPROCESSOR FOR THE PHOTOCHEMICAL BOX MODEL
**********************************************************************
TEST OF PBMMET  -  76275

SUMMARY OF CONTROLS:

  TIME INC. FOR OUTPUT OF MIX. HT. AND PHOTOLYTIC RATE CONST. =  10 MIN.

  OUTPUT DATA STORED ON UNIT NUMBER  2

  HOURLY SURFACE METEOROLOGICAL DATA READ FROM UNIT NUMBER  5

  MIXING HEIGHT DATA INPUT ON UNIT NUMBER  5

  MIXING HEIGHTS CALCULATED FROM CHARACTERISTIC CURVE METHOD

  PHOTOLYTIC RATE CONSTANTS (PRC'S) ARE AVERAGED THROUGH THE MIXED LAYER DEPTH

  PRC'S ARE ATTENUATED BASED ON MEASURED TOTAL SOLAR RADIATION

  RADIATION VALUES INPUT EVERY 10 MIN.
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HOURLY SURFACE METEOROLOGICAL DATA

HOUR	WIND SPEED (METERS/SEC)	TEMPERATURE (DEG.-C)
5- 6	1.58	11.10
6- 7	1.68	11.60
7- 8	1.51	14.50
8- 9	.86	17.80
9-10	.39	20.80
10-11	.39	23.50
11-12	.80	25.50
12-13	.09	26.90
13-14	.48	27.80
14-15	.71	28.50
15-16	.79	28.70
16-17	.89	28.20
17-18	.90	26.10

INPUT VALUES FOR 'CHARACTERISTIC CURVE' MIX. HT. CALCULATIONS:

HMIN1 = 100.00 HMAX = 532.00 HMIN2 = 100.00 METERS

INPUT VALUES OF TOTAL SOLAR RADIATION:

TIME (MIN. AFTER 0500 LST)	RAD. (LY/MIN)
0	.0000
10	.0000
20	.0000
30	.0000
40	.0000
50	.0000
60	.0000
70	.5900-002
80	.2540-001
90	.5560-001
100	.9360-001
110	.1308+000
120	.1739+000
130	.2178+000
140	.2647+000
150	.3086+000
160	.3512+000
170	.3954+000
180	.4414+000
190	.4872+000
200	.5311+000
210	.5671+000
220	.6034+000
230	.6390+000
240	.6788+000
250	.7141+000
260	.7507+000
270	.7825+000
280	.8146+000
290	.8374+000
300	.8659+000
310	.8933+000
320	.9152+000
330	.9388+000
340	.9504+000
350	.9689+000
360	.9783+000
370	.9925+000
380	.1009+001
390	.1009+001
400	.1020+001
410	.1008+001
420	.1009+001
430	.9914+000
440	.9824+000
450	.9796+000
460	.9813+000
470	.9764+000
480	.9582+000
490	.9374+000
500	.9101+000
510	.8843+000
520	.8555+000

530	.8301+000
540	.7981+000
550	.7607+000
560	.7289+000
570	.6871+000
580	.6533+000
590	.6162+000
600	.5854+000
610	.5471+000
620	.5074+000
630	.4684+000
640	.4232+000
650	.3774+000
660	.3344+000
670	.2957+000
680	.2533+000
690	.2163+000
700	.1802+000
710	.1406+000
720	.1015+000
730	.6420-001
740	.3190-001
750	.8300-002
760	.0000
770	.0000
780	.0000

```
INTERPOLATED MIXING HEIGHTS AND PHOTOLYTIC RATE  CONSTANTS:

TIME (LST)      MIX. HT (M)     RATE CONSTANTS :  K (ATTENUATED)       (/MIN)
                                              (K (CLEAR-SKY))
                                K( 1)       K( 2)       K( 3)       K( 4)       K( 5)       K( 6)
                                      K( 7)       K( 8)       K( 9)       K(10)       K(11)

 500.           100.00          .000        .000        .000        .000        .000        .000
                              (-.176+000) (-.183-003) (-.334-001) (-.132-003) (-.667-003) (-.361-003)
                                      .000        .000        .000        .000        .000
                                    (-.691-004) (-.706-003) (-.706-003) (-.168-002) (-.168-002)

 510.           100.00          .000        .000        .000        .000        .000        .000
                              (-.141+000) (-.130-003) (-.264-001) (-.859-004) (-.516-003) (-.274-003)
                                      .000        .000        .000        .000        .000
                                    (-.514-004) (-.566-003) (-.566-003) (-.134-002) (-.134-002)

 520.           100.00          .000        .000        .000        .000        .000        .000
                              (-.111+000) (-.892-004) (-.204-001) (-.511-004) (-.390-003) (-.202-003)
                                      .000        .000        .000        .000        .000
                                    (-.371-004) (-.442-003) (-.442-003) (-.105-002) (-.105-002)

 530.           100.00          .000        .000        .000        .000        .000        .000
                              (-.833-001) (-.583-004) (-.151-001) (-.261-004) (-.283-003) (-.143-003)
                                      .000        .000        .000        .000        .000
                                    (-.258-004) (-.333-003) (-.333-003) (-.792-003) (-.792-003)

 540.           100.00          .000        .000        .000        .000        .000        .000
                              (-.590-001) (-.357-004) (-.105-001) (-.920-005) (-.193-003) (-.964-004)
                                      .000        .000        .000        .000        .000
                                    (-.170-004) (-.236-003) (-.236-003) (-.561-003) (-.561-003)

 550.           100.00          .000        .000        .000        .000        .000        .000
                              (-.372-001) (-.198-004) (-.644-002) ( .112-005) (-.118-003) (-.588-004)
                                      .000        .000        .000        .000        .000
                                    (-.103-004) (-.149-003) (-.149-003) (-.353-003) (-.353-003)

 600.           100.00          .000        .000        .000        .000        .000        .000
                              (-.171-001) (-.900-005) (-.279-002) ( .648-005) (-.524-004) (-.283-004)
                                      .000        .000        .000        .000        .000
                                    (-.501-005) (-.686-004) (-.686-004) (-.163-003) (-.163-003)

 610.           100.00          .161-002    .000        .569-003    .850-005    .589-005    .000
                              ( .161-002) (-.164-005) ( .569-003) ( .850-005) ( .589-005) (-.250-005)
                                      .000        .644-005    .644-005    .153-004    .153-004
                                    (-.781-006) ( .644-005) ( .644-005) ( .153-004) ( .153-004)

 620.           100.29          .109-001    .217-005    .209-002    .486-005    .334-004    .115-004
                              ( .197-001) ( .392-005) ( .378-002) ( .878-005) ( .604-004) ( .208-004)
                                      .161-005    .436-004    .436-004    .103-003    .103-003
                                    ( .290-005) ( .787-004) ( .787-004) ( .187-003) ( .187-003)

 630.           101.24          .243-001    .601-005    .451-002    .575-005    .739-004    .283-004
                              ( .376-001) ( .929-005) ( .697-002) ( .889-005) ( .114-003) ( .437-004)
                                      .422-005    .973-004    .973-004    .231-003    .231-003
                                    ( .652-005) ( .150-003) ( .150-003) ( .357-003) ( .357-003)
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PBMMET OUTPUT

640.	102.96	.412-001	.118-004	.754-002	.765-005	.126-003	.504-004
		(.560-001)	(.161-004)	(.103-001)	(.104-004)	(.171-003)	(.685-004)
		.776-005	.165-003	.165-003	.391-003	.391-003	
		(.105-004)	(.224-003)	(.224-003)	(.532-003)	(.532-003)	
650.	105.54	.576-001	.197-004	.105-001	.113-004	.178-003	.745-004
		(.753-001)	(.257-004)	(.138-001)	(.148-004)	(.233-003)	(.973-004)
		.118-004	.230-003	.230-003	.547-003	.547-003	
		(.154-004)	(.301-003)	(.301-003)	(.715-003)	(.715-003)	
700.	109.11	.765-001	.317-004	.140-001	.187-004	.242-003	.105-003
		(.961-001)	(.398-004)	(.176-001)	(.235-004)	(.304-003)	(.132-003)
		.172-004	.306-003	.306-003	.727-003	.727-003	
		(.216-004)	(.384-003)	(.384-003)	(.913-003)	(.913-003)	
710.	113.77	.956-001	.480-004	.176-001	.303-004	.311-003	.140-003
		(.119+000)	(.597-004)	(.219-001)	(.377-004)	(.386-003)	(.174-003)
		.237-004	.382-003	.382-003	.908-003	.908-003	
		(.295-004)	(.475-003)	(.475-003)	(.113-002)	(.113-002)	
720.	119.64	.116+000	.696-004	.215-001	.457-004	.388-003	.181-003
		(.143+000)	(.859-004)	(.265-001)	(.564-004)	(.478-003)	(.224-003)
		.316-004	.463-003	.463-003	.110-002	.110-002	
		(.390-004)	(.572-003)	(.572-003)	(.136-002)	(.136-002)	
730.	126.85	.135+000	.954-004	.251-001	.624-004	.463-003	.224-003
		(.167+000)	(.119-003)	(.312-001)	(.777-004)	(.577-003)	(.279-003)
		.402-004	.538-003	.538-003	.128-002	.128-002	
		(.500-004)	(.670-003)	(.670-003)	(.159-002)	(.159-002)	
740.	135.50	.153+000	.126-003	.286-001	.794-004	.541-003	.270-003
		(.191+000)	(.158-003)	(.359-001)	(.995-004)	(.678-003)	(.338-003)
		.496-004	.611-003	.611-003	.145-002	.145-002	
		(.621-004)	(.765-003)	(.765-003)	(.182-002)	(.182-002)	
750.	145.74	.171+000	.164-003	.323-001	.962-004	.624-003	.321-003
		(.214+000)	(.205-003)	(.404-001)	(.120-003)	(.779-003)	(.400-003)
		.603-004	.686-003	.686-003	.163-002	.163-002	
		(.752-004)	(.856-003)	(.856-003)	(.203-002)	(.203-002)	
800.	157.56	.192+000	.211-003	.364-001	.113-003	.718-003	.379-003
		(.236+000)	(.259-003)	(.448-001)	(.139-003)	(.883-003)	(.467-003)
		.728-004	.768-003	.768-003	.182-002	.182-002	
		(.896-004)	(.945-003)	(.945-003)	(.224-002)	(.224-002)	
810.	170.80	.213+000	.266-003	.406-001	.130-003	.818-003	.443-003
		(.258+000)	(.322-003)	(.491-001)	(.157-003)	(.988-003)	(.536-003)
		.868-004	.853-003	.853-003	.202-002	.202-002	
		(.105-003)	(.103-002)	(.103-002)	(.245-002)	(.245-002)	
820.	185.25	.233+000	.328-003	.447-001	.147-003	.918-003	.510-003
		(.277+000)	(.390-003)	(.531-001)	(.174-003)	(.109-002)	(.605-003)
		.102-003	.934-003	.934-003	.222-002	.222-002	
		(.121-003)	(.111-002)	(.111-002)	(.263-002)	(.263-002)	
830.	200.69	.250+000	.392-003	.481-001	.162-003	.101-002	.571-003
		(.295+000)	(.462-003)	(.568-001)	(.191-003)	(.119-002)	(.674-003)

		.116-003	.100-002	.100-002	.238-002	.238-002	
		(.136-003)	(.118-002)	(.118-002)	(.281-002)	(.281-002)	
840.	216.92	.267+000	.461-003	.515-001	.177-003	.110-002	.634-003
		(.312+000)	(.539-003)	(.603-001)	(.207-003)	(.128-002)	(.742-003)
		.130-003	.107-002	.107-002	.254-002	.254-002	
		(.152-003)	(.125-002)	(.125-002)	(.296-002)	(.296-002)	
850.	233.73	.283+000	.535-003	.548-001	.193-003	.118-002	.698-003
		(.327+000)	(.619-003)	(.634-001)	(.223-003)	(.137-002)	(.807-003)
		.145-003	.113-002	.113-002	.269-002	.269-002	
		(.168-003)	(.131-002)	(.131-002)	(.311-002)	(.311-002)	
900.	250.91	.301+000	.617-003	.585-001	.210-003	.128-002	.767-003
		(.341+000)	(.700-003)	(.664-001)	(.238-003)	(.145-002)	(.870-003)
		.161-003	.120-002	.120-002	.286-002	.286-002	
		(.183-003)	(.137-002)	(.137-002)	(.324-002)	(.324-002)	
910.	268.26	.317+000	.700-003	.618-001	.226-003	.137-002	.832-003
		(.354+000)	(.782-003)	(.690-001)	(.253-003)	(.153-002)	(.930-003)
		.177-003	.127-002	.127-002	.301-002	.301-002	
		(.198-003)	(.142-002)	(.142-002)	(.336-002)	(.336-002)	
920.	285.57	.333+000	.788-003	.651-001	.243-003	.146-002	.899-003
		(.366+000)	(.865-003)	(.715-001)	(.267-003)	(.160-002)	(.987-003)
		.193-003	.133-002	.133-002	.316-002	.316-002	
		(.212-003)	(.146-002)	(.146-002)	(.347-002)	(.347-002)	
930.	302.64	.347+000	.874-003	.680-001	.259-003	.154-002	.960-003
		(.376+000)	(.947-003)	(.737-001)	(.280-003)	(.167-002)	(.104-002)
		.208-003	.139-002	.139-002	.330-002	.330-002	
		(.226-003)	(.150-002)	(.150-002)	(.357-002)	(.357-002)	
940.	319.24	.361+000	.962-003	.709-001	.274-003	.162-002	.102-002
		(.386+000)	(.103-002)	(.757-001)	(.293-003)	(.173-002)	(.109-002)
		.224-003	.145-002	.145-002	.343-002	.343-002	
		(.239-003)	(.154-002)	(.154-002)	(.366-002)	(.366-002)	
950.	335.19	.371+000	.104-002	.730-001	.286-003	.168-002	.107-002
		(.394+000)	(.111-002)	(.775-001)	(.304-003)	(.178-002)	(.114-002)
		.236-003	.149-002	.149-002	.353-002	.353-002	
		(.251-003)	(.158-002)	(.158-002)	(.374-002)	(.374-002)	
1000.	350.26	.384+000	.113-002	.756-001	.300-003	.175-002	.113-002
		(.402+000)	(.118-002)	(.791-001)	(.314-003)	(.183-002)	(.118-002)
		.251-003	.154-002	.154-002	.365-002	.365-002	
		(.262-003)	(.161-002)	(.161-002)	(.382-002)	(.382-002)	
1010.	364.30	.396+000	.121-002	.781-001	.314-003	.183-002	.118-002
		(.409+000)	(.125-002)	(.806-001)	(.324-003)	(.188-002)	(.122-002)
		.265-003	.158-002	.158-002	.376-002	.376-002	
		(.273-003)	(.163-002)	(.163-002)	(.388-002)	(.388-002)	
1020.	377.32	.406+000	.129-002	.802-001	.326-003	.188-002	.123-002
		(.416+000)	(.132-002)	(.821-001)	(.334-003)	(.193-002)	(.126-002)
		.277-003	.162-002	.162-002	.386-002	.386-002	
		(.284-003)	(.166-002)	(.166-002)	(.395-002)	(.395-002)	

1030.	389.41	.416+000	.137-002	.822-001	.338-003	.194-002	.128-002
		(.422+000)	(.139-002)	(.834-001)	(.342-003)	(.197-002)	(.130-002)
		.289-003	.166-002	.166-002	.395-002	.395-002	
		(.293-003)	(.169-002)	(.169-002)	(.401-002)	(.401-002)	
1040.	400.63	.421+000	.143-002	.833-001	.345-003	.198-002	.131-002
		(.427+000)	(.145-002)	(.845-001)	(.350-003)	(.201-002)	(.133-002)
		.297-003	.168-002	.168-002	.400-002	.400-002	
		(.302-003)	(.171-002)	(.171-002)	(.406-002)	(.406-002)	
1050.	411.06	.429+000	.149-002	.849-001	.354-003	.203-002	.135-002
		(.431+000)	(.150-002)	(.854-001)	(.356-003)	(.204-002)	(.136-002)
		.307-003	.172-002	.172-002	.407-002	.407-002	
		(.309-003)	(.173-002)	(.173-002)	(.410-002)	(.410-002)	
1100.	420.77	.433+000	.154-002	.858-001	.360-003	.205-002	.137-002
		(.435+000)	(.155-002)	(.862-001)	(.362-003)	(.207-002)	(.138-002)
		.314-003	.173-002	.173-002	411-002	.411-002	
		(.316-003)	(.174-002)	(.174-002)	(.413-002)	(.413-002)	
1110.	429.84	.438+000	.159-002	.869-001	.367-003	.209-002	.140-002
		(.438+000)	(.159-002)	(.869-001)	(.367-003)	(.209-002)	(.140-002)
		.321-003	.175-002	.175-002	.416-002	.416-002	
		(.321-003)	(.175-002)	(.175-002)	(.416-002)	(.416-002)	
1120.	438.33	.441+000	.162-002	.874-001	.370-003	.211-002	.141-002
		(.441+000)	(.162-002)	(.874-001)	(.370-003)	(.211-002)	(.141-002)
		.325-003	.176-002	.176-002	.419-002	.419-002	
		(.325-003)	(.176-002)	(.176-002)	(.419-002)	(.419-002)	
1130.	446.32	.443+000	.164-002	.878-001	.373-003	.212-002	.143-002
		(.443+000)	(.164-002)	(.878-001)	(.373-003)	(.212-002)	(.143-002)
		.328-003	.177-002	.177-002	.421-002	.421-002	
		(.328-003)	(.177-002)	(.177-002)	(.421-002)	(.421-002)	
1140.	453.88	.444+000	.165-002	.881-001	.375-003	.213-002	.143-002
		(.444+000)	(.165-002)	(.881-001)	(.375-003)	(.213-002)	(.143-002)
		.330-003	.178-002	.178-002	.422-002	.422-002	
		(.330-003)	(.178-002)	(.178-002)	(.422-002)	(.422-002)	
1150.	461.09	.445+000	.166-002	.883-001	.376-003	.213-002	.144-002
		(.445+000)	(.166-002)	(.883-001)	(.376-003)	(.213-002)	(.144-002)
		.331-003	.178-002	.178-002	.423-002	.423-002	
		(.331-003)	(.178-002)	(.178-002)	(.423-002)	(.423-002)	
1200.	468.02	.445+000	.166-002	.883-001	.376-003	.213-002	.144-002
		(.445+000)	(.166-002)	(.883-001)	(.376-003)	(.213-002)	(.144-002)
		.331-003	.178-002	.178-002	.423-002	.423-002	
		(.331-003)	(.178-002)	(.178-002)	(.423-002)	(.423-002)	
1210.	474.72	.441+000	.163-002	.875-001	.372-003	.211-002	.142-002
		(.445+000)	(.165-002)	(.882-001)	(.375-003)	(.213-002)	(.143-002)
		.327-003	.176-002	.176-002	.419-002	.419-002	
		(.330-003)	(.178-002)	(.178-002)	(.422-002)	(.422-002)	
1220.	481.17	.438+000	.161-002	.868-001	.368-003	.209-002	.141-002

		(.444+000)	(.163-002)	(.880-001)	(.373-003)	(.212-002)	(.143-002)
		.323-003	.175-002	.175-002	.416-002	.416-002	
		(.328-003)	(.177-002)	(.177-002)	(.421-002)	(.421-002)	
1230.	487.37	.437+000	.159-002	.868-001	.367-003	.209-002	.140-002
		(.442+000)	(.160-002)	(.877-001)	(.370-003)	(.211-002)	(.141-002)
		.321-003	.175-002	.175-002	.416-002	.416-002	
		(.324-003)	(.177-002)	(.177-002)	(.420-002)	(.420-002)	
1240.	493.28	.439+000	.157-002	.871-001	.366-003	.209-002	.140-002
		(.440+000)	(.157-002)	(.872-001)	(.367-003)	(.209-002)	(.140-002)
		.320-003	.176-002	.176-002	.417-002	.417-002	
		(.320-003)	(.176-002)	(.176-002)	(.418-002)	(.418-002)	
1250.	498.89	.437+000	.153-002	.867-001	.362-003	.207-002	.138-002
		(.437+000)	(.153-002)	(.867-001)	(.362-003)	(.207-002)	(.138-002)
		.315-003	.175-002	.175-002	.415-002	.415-002	
		(.315-003)	(.175-002)	(.175-002)	(.415-002)	(.415-002)	
1300.	504.18	.432+000	.147-002	.856-001	.355-003	.204-002	.135-002
		(.434+000)	(.148-002)	(.859-001)	(.357-003)	(.205-002)	(.136-002)
		.307-003	.173-002	.173-002	.410-002	.410-002	
		(.308-003)	(.174-002)	(.174-002)	(.412-002)	(.412-002)	
1310.	509.12	.424+000	.141-002	.840-001	.346-003	.199-002	.131-002
		(.430+000)	(.143-002)	(.851-001)	(.351-003)	(.202-002)	(.133-002)
		.297-003	.170-002	.170-002	.403-002	.403-002	
		(.301-003)	(.172-002)	(.172-002)	(.408-002)	(.408-002)	
1320.	513.69	.414+000	.133-002	.819-001	.334-003	.193-002	.127-002
		(.425+000)	(.136-002)	(.841-001)	(.343-003)	(.198-002)	(.130-002)
		.285-003	.166-002	.166-002	.393-002	.393-002	
		(.292-003)	(.170-002)	(.170-002)	(.404-002)	(.404-002)	
1330.	517.88	.404+000	.125-002	.798-001	.323-003	.187-002	.122-002
		(.420+000)	(.130-002)	(.829-001)	(.335-003)	(.194-002)	(.127-002)
		.272-003	.162-002	.162-002	.384-002	.384-002	
		(.283-003)	(.168-002)	(.168-002)	(.399-002)	(.399-002)	
1340.	521.66	.392+000	.116-002	.773-001	.309-003	.180-002	.116-002
		(.414+000)	(.123-002)	(.816-001)	(.326-003)	(.190-002)	(.123-002)
		.258-003	.157-002	.157-002	.372-002	.372-002	
		(.273-003)	(.165-002)	(.165-002)	(.393-002)	(.393-002)	
1350.	525.02	.381+000	.108-002	.751-001	.296-003	.174-002	.111-002
		(.407+000)	(.115-002)	(.802-001)	(.316-003)	(.185-002)	(.119-002)
		.245-003	.152-002	.152-002	.362-002	.362-002	
		(.261-003)	(.163-002)	(.163-002)	(.386-002)	(.386-002)	
1400.	527.92	.368+000	.989-003	.723-001	.281-003	.166-002	.105-002
		(.399+000)	(.107-002)	(.785-001)	(.305-003)	(.180-002)	(.114-002)
		.230-003	.147-002	.147-002	.349-002	.349-002	
		(.249-003)	(.160-002)	(.160-002)	(.379-002)	(.379-002)	
1410.	530.35	.352+000	.893-003	.691-001	.264-003	.157-002	.982-003
		(.390+000)	(.992-003)	(.766-001)	(.293-003)	(.174-002)	(.109-002)
		.213-003	.141-002	.141-002	.334-002	.334-002	

```
                              ( .237-003) ( .156-002) ( .156-002) ( .371-002) ( .371-002)

1420.          532.00        .338+000    .807-003    .663-001    .249-003    .149-002    .922-003
                            ( .381+000) ( .908-003) ( .746-001) ( .280-003) ( .168-002) ( .104-002)
                                 .198-003    .135-002    .135-002    .321-002    .321-002
                              ( .223-003) ( .152-002) ( .152-002) ( .362-002) ( .362-002)

1430.          532.00        .320+000    .713-003    .626-001    .231-003    .139-002    .849-003
                            ( .370+000) ( .824-003) ( .723-001) ( .267-003) ( .161-002) ( .980-003)
                                 .181-003    .128-002    .128-002    .304-002    .304-002
                              ( .209-003) ( .148-002) ( .148-002) ( .352-002) ( .352-002)

1440.          532.00        .306+000    .631-003    .596-001    .215-003    .131-002    .786-003
                            ( .358+000) ( .740-003) ( .698-001) ( .252-003) ( .153-002) ( .921-003)
                                 .165-003    .122-002    .122-002    .291-002    .291-002
                              ( .194-003) ( .143-002) ( .143-002) ( .340-002) ( .340-002)

1450.          532.00        .290+000    .551-003    .563-001    .199-003    .122-002    .720-003
                            ( .345+000) ( .656-003) ( .671-001) ( .237-003) ( .146-002) ( .858-003)
                                 .150-003    .116-002    .116-002    .275-002    .275-002
                              ( .178-003) ( .138-002) ( .138-002) ( .328-002) ( .328-002)

1500.          532.00        .277+000    .480-003    .536-001    .185-003    .114-002    .662-003
                            ( .331+000) ( .574-003) ( .641-001) ( .221-003) ( .137-002) ( .792-003)
                                 .136-003    .111-002    .111-002    .263-002    .263-002
                              ( .163-003) ( .133-002) ( .133-002) ( .315-002) ( .315-002)

1510.          532.00        .260+000    .408-003    .502-001    .168-003    .105-002    .597-003
                            ( .316+000) ( .495-003) ( .609-001) ( .204-003) ( .128-002) ( .724-003)
                                 .121-003    .104-002    .104-002    .247-002    .247-002
                              ( .146-003) ( .126-002) ( .126-002) ( .300-002) ( .300-002)

1520.          532.00        .243+000    .341-003    .466-001    .152-003    .961-003    .532-003
                            ( .299+000) ( .419-003) ( .574-001) ( .187-003) ( .118-002) ( .655-003)
                                 .106-003    .972-003    .972-003    .231-002    .231-002
                              ( .130-003) ( .120-002) ( .120-002) ( .284-002) ( .284-002)

1530.          532.00        .226+000    .280-003    .431-001    .136-003    .870-003    .471-003
                            ( .280+000) ( .348-003) ( .536-001) ( .169-003) ( .108-002) ( .584-003)
                                 .919-004    .903-003    .903-003    .215-002    .215-002
                              ( .114-003) ( .112-002) ( .112-002) ( .266-002) ( .266-002)

1540.          532.00        .206+000    .223-003    .391-001    .119-003    .770-003    .406-003
                            ( .260+000) ( .283-003) ( .494-001) ( .151-003) ( .975-003) ( .513-003)
                                 .777-004    .822-003    .822-003    .195-002    .195-002
                              ( .983-004) ( .104-002) ( .104-002) ( .247-002) ( .247-002)

1550.          532.00        .185+000    .174-003    .349-001    .102-003    .672-003    .344-003
                            ( .238+000) ( .224-003) ( .449-001) ( .132-003) ( .865-003) ( .443-003)
                                 .645-004    .739-003    .739-003    .176-002    .176-002
                              ( .830-004) ( .951-003) ( .951-003) ( .226-002) ( .226-002)

1600.          532.00        .165+000    .133-003    .310-001    .866-004    .582-003    .290-003
                            ( .213+000) ( .172-003) ( .400-001) ( .112-003) ( .752-003) ( .374-003)
                                 .530-004    .661-003    .661-003    .157-002    .157-002
                              ( .684-004) ( .853-003) ( .853-003) ( .203-002) ( .203-002)
```

1610.	532.00	.148+000	.101-003	.275-001	.724-004	.503-003	.242-003
		(.187+000)	(.128-003)	(.348-001)	(.918-004)	(.638-003)	(.307-003)
		.432-004	.591-003	.591-003	.140-002	.140-002	
		(.548-004)	(.749-003)	(.749-003)	(.178-002)	(.178-002)	
1620.	532.00	.128+000	.732-004	.236-001	.581-004	.421-003	.195-003
		(.160+000)	(.918-004)	(.296-001)	(.728-004)	(.527-003)	(.245-003)
		.339-004	.512-003	.512-003	.122-002	.122-002	
		(.425-004)	(.642-003)	(.642-003)	(.152-002)	(.152-002)	
1630.	532.00	.110+000	.521-004	.202-001	.460-004	.350-003	.156-003
		(.134+000)	(.630-004)	(.244-001)	(.557-004)	(.424-003)	(.189-003)
		.263-004	.442-003	.442-003	.105-002	.105-002	
		(.319-004)	(.535-003)	(.535-003)	(.127-002)	(.127-002)	
1640.	525.31	.927-001	.356-004	.168-001	.354-004	.284-003	.122-003
		(.108+000)	(.415-004)	(.196-001)	(.413-004)	(.332-003)	(.142-003)
		.198-004	.371-003	.371-003	.881-003	.881-003	
		(.232-004)	(.433-003)	(.433-003)	(.103-002)	(.103-002)	
1650.	494.34	.719-001	.227-004	.130-001	.256-004	.216-003	.888-004
		(.836-001)	(.263-004)	(.151-001)	(.297-004)	(.251-003)	(.103-003)
		.140-004	.288-003	.288-003	.683-003	.683-003	
		(.163-004)	(.335-003)	(.335-003)	(.795-003)	(.795-003)	
1700.	463.38	.512-001	.136-004	.928-002	.175-004	.152-003	.601-004
		(.606-001)	(.161-004)	(.110-001)	(.208-004)	(.180-003)	(.712-004)
		.917-005	.205-003	.205-003	.486-003	.486-003	
		(.109-004)	(.242-003)	(.242-003)	(.576-003)	(.576-003)	
1710.	432.42	.314-001	.735-005	.579-002	.112-004	.936-004	.353-004
		(.388-001)	(.907-005)	(.714-002)	(.138-004)	(.116-003)	(.436-004)
		.522-005	.126-003	.126-003	.298-003	.298-003	
		(.645-005)	(.155-003)	(.155-003)	(.368-003)	(.368-003)	
1720.	401.45	.145-001	.275-005	.282-002	.651-005	.448-004	.148-004
		(.178-001)	(.337-005)	(.346-002)	(.799-005)	(.550-004)	(.182-004)
		.202-005	.579-004	.579-004	.138-003	.138-003	
		(.248-005)	(.710-004)	(.710-004)	(.169-003)	(.169-003)	
1730.	370.49	.000	.000	.000	.000	.000	.000
		(-.275-002)	(-.275-005)	(-.159-003)	(.255-005)	(-.531-005)	(-.737-005)
		.000	.000	.000	.000	.000	
		(-.157-005)	(-.110-004)	(-.110-004)	(-.261-004)	(-.261-004)	
1740.	339.53	.000	.000	.000	.000	.000	.000
		(-.235-001)	(-.110-004)	(-.386-002)	(-.355-005)	(-.690-004)	(-.356-004)
		.000	.000	.000	.000	.000	
		(-.623-005)	(-.939-004)	(-.939-004)	(-.223-003)	(-.223-003)	
1750.	314.60	.000	.000	.000	.000	.000	.000
		(-.453-001)	(-.233-004)	(-.785-002)	(-.117-004)	(-.140-003)	(-.693-004)
		.000	.000	.000	.000	.000	
		(-.121-004)	(-.181-003)	(-.181-003)	(-.431-003)	(-.431-003)	
1800.	308.78	.000	.000	.000	.000	.000	.000
		(-.691-001)	(-.413-004)	(-.123-001)	(-.238-004)	(-.224-003)	(-.111-003)
		.000	.000	.000	.000	.000	
		(-.196-004)	(-.277-003)	(-.277-003)	(-.657-003)	(-.657-003)	

INPUT DATA - PBMAQE EXAMPLE PROBLEM

```
    AIR QUALITY AND EMISSIONS     ST. LOUIS  76275
        20.0      25.0
      6
      5
      1
      5         5
      1    1
      5    5    3
   CO  NO  NO2 O3  HO
   CO             1.6223
   NO              .1239
   NO2             .0391
   NMHC           1.1991
   O3              .0025
   H2O        7878.7730
   CO
     .66478  .94666  .88844  .80268  .81451  .80689  .06851  .27964  .31721  .42426
     .38884  .54567  .89854 2.20757 2.40522
   NO
     .04121  .03570  .03076  .01685  .01240  .00489  .00250  .00250  .00250  .00250
     .00255  .00261  .00298  .03592  .01368
   NO2
     .01933  .02250  .02729  .04307  .04161  .02248  .00979  .00783  .00936  .00342
     .02562  .02373  .03179  .05614  .06787
   NMHC
     .60496  .52997  .30059  .29770  .28063  .28063  .21800  .15500  .14700  .17874
     .27979  .27674  .40058  .44804  .81160
   O3
     .01018  .00505  .01328  .02404  .03312  .05421  .08282  .10150  .10375  .12857
     .13818  .14391  .11388  .10320  .09493
   O3
     .06300  .06300  .06300  .06300  .06300  .06300  .06300  .06300  .06300  .06300
     .06300  .06300  .06300  .06300  .06300
   CO
    1.77063 3.30528 4.01328 3.46760 2.69850 2.29946 2.12176 1.48728 1.36505 1.38847
    1.40420 1.62544 2.92169 5.76281 7.84034
   NO
     .12960  .18725  .16782  .10554  .03489  .01420  .00651  .00296  .00298  .00273
     .00276  .00380  .02440  .06017  .11055
   NO2
     .03824  .04084  .05692  .08629  .10230  .09985  .08254  .05818  .05340  .05142
     .05671  .06103  .10773  .16397  .16908
   NMHC
    1.20173 1.35853 1.48753 1.20917  .99288  .95591  .96199  .59593  .48726  .53084
     .53538  .58416 1.03837 2.28581 2.91273
   O3
     .00250  .00250  .00271  .00701  .03225  .06871  .10298  .13461  .15853  .18320
     .18078  .16096  .08373  .01287  .01084
   CO
     41741.79  72303.22  65620.24  37965.50  37311.44  39966.64  41547.18  40442.05
     43707.63  50127.14  61928.40  57936.70  36420.60
   NOX
      4924.99   7217.68   7270.63   6224.52   6057.58   6287.49   6465.04   6339.62
      6712.68   7449.48   7414.50   7067.02   3770.49
   THC
      9771.36  13836.15  14863.21  11771.58  11668.45  12069.51  12295.97  12143.83
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INPUT DATA - PBMAQE EXAMPLE PROBLEM

```
     12620.04  13714.90  15035.52   8548.48   6399.18
HC0
     58282.83  86591.98  78273.55  55688.74  53961.63  56016.37  57643.76  56539.04
     59870.05  66573.90  76041.83  56501.06  41390.16
HC1
     38788.37  62325.80  54292.58  36443.51  35828.05  38174.78  39541.86  38628.43
     41433.05  47186.80  55084.16  45865.09  32582.54
HC2
     52702.99  75766.95  81009.75  63490.92  63210.23  65640.60  66926.97  66066.33
     68787.98  75366.50  82637.54  46592.41  35838.98
HC3
     13972.26  19519.45  19183.75  14945.35  14764.24  15292.28  15616.36  15399.65
     16060.28  17382.19  19257.15  12828.51   9115.62
HC4
     15851.06  22445.79  26167.54  21256.50  21095.89  21769.87  22127.62  21887.91
     22645.74  24462.51  26629.47  13949.07  10513.27
CO
      7915.04   7922.14   7931.76   7940.81   7944.19   7932.51   7930.35   7934.00
      7941.62   7941.66   7933.38   7933.58   7934.12
NOX
      1367.89   1499.07   1671.33   1821.69   1845.21   1685.55   1645.74   1710.05
      1820.21   1828.15   1695.69   1701.91   1710.29
THC
      1902.87   1904.82   3365.71   3368.31   3368.95   3365.87   3365.22   3366.33
      3368.43   3368.38   3366.18   3343.57   3343.75
HC0
      7963.88   8034.24  10604.99  10698.35  10721.58  10610.57  10587.33  10627.30
     10702.67  10700.84  10622.01  10600.06  10606.53
HC1
      2238.85   2241.20   2413.33   2416.45   2417.22   2413.52   2412.74   2414.08
      2416.59   2416.53   2413.90   2413.92   2414.14
HC2
      8148.96   8151.30  16522.59  16525.70  16526.48  16522.78  16522.00  16523.33
     16525.85  16525.79  16523.07  16344.39  16344.60
HC3
        33.19     35.53     38.86     41.97     42.74     39.04     38.27     39.60
        42.11     42.05     39.43     39.45     39.66
HC4
      6677.94   6678.72  11800.71  11801.75  11802.01  11800.77  11800.52  11800.96
     11801.80  11801.78  11800.88  11776.00  11776.08
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PBMAQE -- AIR QUALITY/EMISSIONS PREPROCESSOR FOR THE PHOTOCHEMICAL BOX MODEL

****

AIR QUALITY AND EMISSIONS   ST. LOUIS 76275

SUMMARY OF CONTROLS:

NUMBER OF INITIAL CONDITION SPECIES SPECIFIED =   6

NUMBER OF TOP BOUNDARY CONDITION SPECIES SPECIFIED =   1

NUMBER OF LATERAL BOUNDARY CONDITION SPECIES SPECIFIED =   5

NUMBER OF OBSERVED SPECIES SPECIFIED =   5

NUMBER OF SPECIES SPECIFIED FOR PRINTER PLOTS =   5

DEFAULT HC SPECIATION FACTORS USED FOR INIT. NMHC =
.0440000 .0263000 .0394000 .0786000 .0608000 .0202000 .0149000 .0099000

DEFAULT HC SPECIATION FACTORS USED FOR BOUND. COND. NMHC =
.0440000 .0263000 .0394000 .0786000 .0608000 .0202000 .0149000 .0099000

DEFAULT HC SPECIATION FACTORS USED FOR OBSERVED NMHC =
.0440000 .0263000 .0394000 .0786000 .0608000 .0202000 .0149000 .0099000

SOURCE EMISSIONS ARE SPECIFIED

POINT SOURCES ARE SEPARATELY SPECIFIED

RATIO OF NO2/NOX IN AREA AND LINE SOURCES =   .1000

RATIO OF NO2/NOX IN POINT SOURCES =   .1000

RATIO OF CH4/THC IN AREA AND LINE SOURCES =   .0000

RATIO OF CH4/THC IN POINT SOURCES =   .0600

AIR QUALITY VALUES INPUT ON UNIT NUMBER 5

SOURCE EMISSIONS VALUES INPUT ON UNIT NUMBER 5

CARD-IMAGE OUTPUT DATA STORED ON UNIT NUMBER 3

SIZE OF HORIZONTAL SIDE OF PBM DOMAIN (KM) =   20.0000

AVERAGE AMBIENT TEMPERATURE DURING SIMULATION (DEG-C) =   25.0000

NUMBER OF HOURS OF DATA TO BE PROCESSED =   13

AIR QUALITY AND EMISSIONS ST. LOUIS 76275

SPECIFIED INITIAL CONCENTRATIONS (FOR 0500 L.S.T.):

SPECIES	CONCENTRATION (PPM)
CO	1.622300
NO	.123900
NO2	.039100
NMHC	1.199100
NONR	.052760
ETH	.031536
OLE	.047245
PAR	.094249
FORM	.072905
ALD	.024222
ARO	.017867
TOL	.011871
O3	.002500
H2O	7878.773010

AIR QUALITY AND EMISSIONS ST. LOUIS 76275

TOP BOUNDARY CONCENTRATIONS:

SPECIES CONCENTRATIONS (PPM) DURING SPECIFIED HOURS (L.S.T.)

SPECIES	5- 6	6- 7	7- 8	8- 9	9-10	10-11	11-12	12-13	13-14	14-15
O3	.6300-001	.6300-001	.6300-001	.6300-001	.6300-001	.6300-001	.6300-001	.6300-001	.6300-001	.6300-001

SPECIES	15-16	16-17	17-18
O3	.6300-001	.6300-001	.6300-001

LATERAL BOUNDARY CONCENTRATIONS:

SPECIES	CONCENTRATIONS (PPM) DURING SPECIFIED HOURS (L.S.T.) 5- 6	6- 7	7- 8	8- 9	9-10	10-11	11-12	12-13	13-14	14-15
CO	.6648+000	.9467+000	.8884+000	.8027+000	.8145+000	.8069+000	.6851-001	.2796+000	.3172+000	.4243+000
NO	.4121-001	.3570-001	.3076-001	.1685-001	.1240-001	.4890-002	.2500-002	.2500-002	.2500-002	.2500-002
NO2	.1933-001	.2250-001	.2729-001	.4307-001	.4161-001	.2248-001	.9790-002	.7830-002	.9360-002	.3420-002
NMHC	.6050+000	.5300+000	.3006+000	.2977+000	.2806+000	.2806+000	.2180+000	.1550+000	.1470+000	.1787+000
NONR	.2662-001	.2332-001	.1323-001	.1310-001	.1235-001	.1235-001	.9592-002	.6820-002	.6468-002	.7865-002
ETH	.1591-001	.1394-001	.7906-002	.7830-002	.7381-002	.7381-002	.5733-002	.4076-002	.3866-002	.4701-002
OLE	.2384-001	.2088-001	.1184-001	.1173-001	.1106-001	.1106-001	.8589-002	.6107-002	.5792-002	.7042-002
PAR	.4755-001	.4166-001	.2363-001	.2340-001	.2206-001	.2206-001	.1713-001	.1218-001	.1155-001	.1405-001
FORM	.3678-001	.3222-001	.1828-001	.1810-001	.1706-001	.1706-001	.1325-001	.9424-002	.8938-002	.1087-001
ALD	.1222-001	.1071-001	.6072-002	.6014-002	.5669-002	.5669-002	.4404-002	.3131-002	.2969-002	.3611-002
ARO	.9014-002	.7897-002	.4479-002	.4436-002	.4181-002	.4181-002	.3248-002	.2309-002	.2190-002	.2663-002
TOL	.5989-002	.5247-002	.2976-002	.2947-002	.2778-002	.2778-002	.2158-002	.1534-002	.1455-002	.1770-002
O3	.1018-001	.5050-002	.1328-001	.2404-001	.3312-001	.5421-001	.8282-001	.1015+000	.1037+000	.1286+000

	15-16	16-17	17-18
CO	.3888+000	.5457+000	.8985+000
NO	.2550-002	.2610-002	.2980-002
NO2	.2562-001	.2373-001	.3179-001
NMHC	.2798+000	.2767+000	.4006+000
NONR	.1231-001	.1218-001	.1763-001
ETH	.7358-002	.7278-002	.1054-001
OLE	.1102-001	.1090-001	.1578-001
PAR	.2199-001	.2175-001	.3149-001
FORM	.1701-001	.1683-001	.2436-001
ALD	.5652-002	.5590-002	.8092-002
ARO	.4169-002	.4123-002	.5969-002
TOL	.2770-002	.2740-002	.3966-002
O3	.1382+000	.1439+000	.1139+000

AIR QUALITY AND EMISSIONS ST. LOUIS 76275

OBSERVED CONCENTRATIONS:

SPECIES CONCENTRATIONS (PPM) DURING SPECIFIED HOURS (L.S.T.)

SPECIES	5- 6	6- 7	7- 8	8- 9	9-10	10-11	11-12	12-13	13-14	14-15
CO	.1771+001	.3305+001	.4013+001	.3468+001	.2699+001	.2299+001	.2122+001	.1487+001	.1365+001	.1388+001
NO	.1296+000	.1872+000	.1678+000	.1055+000	.3489-001	.1420-001	.6510-002	.2960-002	.2980-002	.2730-002
NO2	.3824-001	.4084-001	.5692-001	.8629-001	.1023+000	.9985-001	.8254-001	.5818-001	.5340-001	.5142-001
NMHC	.1202+001	.1359+001	.1488+001	.1209+001	.9929+000	.9559+000	.9620+000	.5959+000	.4873+000	.5308+000
NONR	.5288-001	.5978-001	.6545-001	.5320-001	.4369-001	.4206-001	.4233-001	.2622-001	.2144-001	.2336-001
ETH	.3161-001	.3573-001	.3912-001	.3180-001	.2611-001	.2514-001	.2530-001	.1567-001	.1281-001	.1396-001
OLE	.4735-001	.5353-001	.5861-001	.4764-001	.3912-001	.3766-001	.3790-001	.2348-001	.1920-001	.2092-001
PAR	.9446-001	.1068+000	.1169+000	.9504-001	.7804-001	.7513-001	.7561-001	.4684-001	.3830-001	.4172-001
FORM	.7307-001	.8260-001	.9044-001	.7352-001	.6037-001	.5812-001	.5849-001	.3623-001	.2963-001	.3228-001
ALD	.2427-001	.2744-001	.3005-001	.2443-001	.2006-001	.1931-001	.1943-001	.1204-001	.9843-002	.1072-001
ARO	.1791-001	.2024-001	.2216-001	.1802-001	.1479-001	.1424-001	.1433-001	.8879-002	.7260-002	.7910-002
TOL	.1190-001	.1345-001	.1473-001	.1197-001	.9830-002	.9464-002	.9524-002	.5900-002	.4824-002	.5255-002
O3	.2500-002	.2500-002	.2710-002	.7010-002	.3225-001	.6871-001	.1030+000	.1346+000	.1585+000	.1832+000

	15-16	16-17	17-18
CO	.1404+001	.1625+001	.2922+001
NO	.2760-002	.3800-002	.2440-001
NO2	.5671-001	.6103-001	.1077+000
NMHC	.5354+000	.5842+000	.1038+001
NONR	.2356-001	.2570-001	.4569-001
ETH	.1408-001	.1536-001	.2731-001
OLE	.2109-001	.2302-001	.4091-001
PAR	.4208-001	.4591-001	.8162-001
FORM	.3255-001	.3552-001	.6313-001
ALD	.1081-001	.1180-001	.2098-001
ARO	.7977-002	.8704-002	.1547-001
TOL	.5300-002	.5783-002	.1028-001
O3	.1808+000	.1610+000	.8373-001

AIR QUALITY AND EMISSIONS   ST. LOUIS 76275

INPUT AREA AND LINE SOURCE EMISSIONS:

SPECIES   EMISSION RATES (PPM-M / MIN) DURING SPECIFIED HOURS (L.S.T.)

SPECIES	5- 6	6- 7	7- 8	8- 9	9-10	10-11	11-12	12-13	13-14	14-15
CO	.1519+001	.2631+001	.2388+001	.1382+001	.1358+001	.1455+001	.1512+001	.1472+001	.1591+001	.1824+001
NOX	.1091+000	.1599+000	.1611+000	.1379+000	.1342+000	.1393+000	.1432+000	.1404+000	.1487+000	.1650+000
THC	.7112+000	.1007+001	.1082+001	.8568+000	.8493+000	.8785+000	.8950+000	.8839+000	.9186+000	.9983+000
HC0	.5939-001	.8824-001	.7976-001	.5675-001	.5499-001	.5708-001	.5874-001	.5761-001	.6101-001	.6784-001
HC1	.3953-001	.6351-001	.5532-001	.3714-001	.3651-001	.3890-001	.4029-001	.3936-001	.4222-001	.4808-001
HC2	.5371-001	.7721-001	.8255-001	.6470-001	.6441-001	.6689-001	.6820-001	.6732-001	.7010-001	.7680-001
HC3	.1424-001	.1989-001	.1955-001	.1523-001	.1504-001	.1558-001	.1591-001	.1569-001	.1637-001	.1771-001
HC4	.1615-001	.2287-001	.2667-001	.2166-001	.2150-001	.2218-001	.2255-001	.2230-001	.2308-001	.2493-001

	15-16	16-17	17-18
CO	.2254+001	.2109+001	.1325+001
NOX	.1642+000	.1566+000	.8353-001
THC	.1094+001	.6222+000	.4658+000
HC0	.7749-001	.5758-001	.4218-001
HC1	.5613-001	.4674-001	.3320-001
HC2	.8421-001	.4748-001	.3652-001
HC3	.1962-001	.1307-001	.9289-002
HC4	.2714-001	.1421-001	.1071-001

AIR QUALITY AND EMISSIONS   ST. LOUIS 76275

INPUT POINT SOURCE EMISSIONS:

SPECIES   EMISSION RATES (PPM-M / MIN) DURING SPECIFIED HOURS (L.S.T.)

SPECIES	5- 6	6- 7	7- 8	8- 9	9-10	10-11	11-12	12-13	13-14	14-15
CO	.2881+000	.2883+000	.2887+000	.2890+000	.2891+000	.2887+000	.2886+000	.2887+000	.2890+000	.2890+000
NOX	.3030-001	.3321-001	.3702-001	.4035-001	.4088-001	.3734-001	.3646-001	.3788-001	.4032-001	.4050-001
THC	.1385+000	.1386+000	.2450+000	.2452+000	.2452+000	.2450+000	.2449+000	.2450+000	.2452+000	.2452+000
HC0	.8115-002	.8187-002	.1081-001	.1090-001	.1093-001	.1081-001	.1079-001	.1083-001	.1091-001	.1090-001
HC1	.2281-002	.2284-002	.2459-002	.2462-002	.2463-002	.2459-002	.2459-002	.2460-002	.2463-002	.2462-002
HC2	.8304-002	.8306-002	.1684-001	.1684-001	.1684-001	.1684-001	.1684-001	.1684-001	.1684-001	.1684-001
HC3	.3382-004	.3621-004	.3960-004	.4277-004	.4355-004	.3978-004	.3900-004	.4035-004	.4291-004	.4285-004
HC4	.6805-002	.6806-002	.1203-001	.1203-001	.1203-001	.1203-001	.1202-001	.1203-001	.1203-001	.1203-001

	15-16	16-17	17-18
CO	.2887+000	.2887+000	.2887+000
NOX	.3756-001	.3770-001	.3789-001
THC	.2450+000	.2434+000	.2434+000
HC0	.1082-001	.1080-001	.1081-001
HC1	.2460-002	.2460-002	.2460-002
HC2	.1684-001	.1666-001	.1666-001
HC3	.4018-004	.4020-004	.4041-004
HC4	.1203-001	.1200-001	.1200-001

AIR QUALITY AND EMISSIONS ST. LOUIS 76275

TOTAL EMISSIONS OUTPUT:

SPECIES EMISSION RATES (PPM-M / MIN) DURING SPECIFIED HOURS (L.S.T.)

SPECIES	5- 6	6- 7	7- 8	8- 9	9-10	10-11	11-12	12-13	13-14	14-15
CO	.1807+001	.2920+001	.2677+001	.1671+001	.1647+001	.1743+001	.1801+001	.1761+001	.1880+001	.2113+001
NO	.1255+000	.1738+000	.1783+000	.1604+000	.1576+000	.1590+000	.1617+000	.1605+000	.1701+000	.1850+000
NO2	.1394-001	.1931-001	.1981-001	.1782-001	.1751-001	.1766-001	.1797-001	.1783-001	.1890-001	.2055-001
NMHC	.8414+000	.1137+001	.1312+001	.1087+001	.1080+001	.1109+001	.1125+001	.1114+001	.1149+001	.1229+001
NONR	.6751-001	.9643-001	.9057-001	.6765-001	.6591-001	.6789-001	.6953-001	.6844-001	.7191-001	.7874-001
ETH	.1581-001	.2540-001	.2213-001	.1485-001	.1460-001	.1556-001	.1612-001	.1575-001	.1689-001	.1923-001
OLE	.2600-001	.4039-001	.3565-001	.2474-001	.2437-001	.2580-001	.2663-001	.2608-001	.2780-001	.3131-001
PAR	.6201-001	.8551-001	.9939-001	.8154-001	.8125-001	.8373-001	.8504-001	.8416-001	.8694-001	.9364-001
FORM	.1071-001	.1495-001	.1469-001	.1146-001	.1132-001	.1172-001	.1197-001	.1180-001	.1231-001	.1332-001
ALD	.3566-002	.4980-002	.4895-002	.3816-002	.3770-002	.3904-002	.3986-002	.3931-002	.4100-002	.4437-002
ARO	.1309-001	.1713-001	.2201-001	.1901-001	.1891-001	.1932-001	.1954-001	.1940-001	.1986-001	.2097-001
TOL	.9863-002	.1255-001	.1668-001	.1468-001	.1461-001	.1489-001	.1503-001	.1493-001	.1524-001	.1598-001

SPECIES	15-16	16-17	17-18
CO	.2543+001	.2397+001	.1614+001
NO	.1816+000	.1748+000	.1093+000
NO2	.2018-001	.1943-001	.1214-001
NMHC	.1325+001	.8510+000	.6946+000
NONR	.8831-001	.6838-001	.5299-001
ETH	.2245-001	.1869-001	.1328-001
OLE	.3614-001	.3050-001	.2238-001
PAR	.1010+000	.6413-001	.5318-001
FORM	.1475-001	.9836-002	.6999-002
ALD	.4914-002	.3276-002	.2330-002
ARO	.2229-001	.1453-001	.1243-001
TOL	.1687-001	.1169-001	.1029-001

AIR QUALITY AND EMISSIONS ST. LOUIS 76275

SPECIES TO BE PLOTTED BY PBM:

CO
NO
NO2
O3
HO

INPUT DATA - PBM EXAMPLE PROBLEM

```
PBM - DAY 76275 - 10/01/76
    0   1   1   0   0   0   0   1   0   1
      20.0
      1.58      1.68      1.51       .86       .39       .39       .80       .09
       .48       .71       .79       .89       .90
     11.10     11.60     14.50     17.80     20.80     23.50     25.50     26.90
     27.80     28.50     28.70     28.20     26.10
 500.         100.00 .0000      .0000      .0000      .0000      .0000      .0000
                     .0000      .0000      .0000      .0000      .0000
 510.         100.00 .0000      .0000      .0000      .0000      .0000      .0000
                     .0000      .0000      .0000      .0000      .0000
 520.         100.00 .0000      .0000      .0000      .0000      .0000      .0000
                     .0000      .0000      .0000      .0000      .0000
 530.         100.00 .0000      .0000      .0000      .0000      .0000      .0000
                     .0000      .0000      .0000      .0000      .0000
 540.         100.00 .0000      .0000      .0000      .0000      .0000      .0000
                     .0000      .0000      .0000      .0000      .0000
 550.         100.00 .0000      .0000      .0000      .0000      .0000      .0000
                     .0000      .0000      .0000      .0000      .0000
 600.         100.00 .0000      .0000      .0000      .0000      .0000      .0000
                     .0000      .0000      .0000      .0000      .0000
 610.         100.00 .1610-002 .0000      .5685-003 .8500-005 .5892-005 .0000
                     .0000      .6439-005 .6439-005 .1529-004 .1529-004
 620.         100.29 .1089-001 .2170-005 .2094-002 .4862-005 .3343-004 .1151-004
                     .1606-005 .4358-004 .4358-004 .1035-003 .1035-003
 630.         101.24 .2432-001 .6009-005 .4505-002 .5751-005 .7391-004 .2828-004
                     .4215-005 .9727-004 .9727-004 .2310-003 .2310-003
 640.         102.96 .4118-001 .1182-004 .7544-002 .7646-005 .1257-003 .5043-004
                     .7759-005 .1647-003 .1647-003 .3912-003 .3912-003
 650.         105.54 .5762-001 .1971-004 .1053-001 .1131-004 .1785-003 .7445-004
                     .1181-004 .2305-003 .2305-003 .5474-003 .5474-003
 700.         109.11 .7652-001 .3172-004 .1401-001 .1870-004 .2422-003 .1051-003
                     .1722-004 .3061-003 .3061-003 .7269-003 .7269-003
 710.         113.77 .9557-001 .4800-004 .1760-001 .3031-004 .3108-003 .1403-003
                     .2374-004 .3823-003 .3823-003 .9079-003 .9079-003
 720.         119.64 .1158+000 .6957-004 .2145-001 .4571-004 .3875-003 .1814-003
                     .3163-004 .4631-003 .4631-003 .1100-002 .1100-002
 730.         126.85 .1345+000 .9537-004 .2509-001 .6244-004 .4634-003 .2244-003
                     .4019-004 .5381-003 .5381-003 .1278-002 .1278-002
 740.         135.50 .1526+000 .1262-003 .2864-001 .7939-004 .5406-003 .2700-003
                     .4956-004 .6105-003 .6105-003 .1450-002 .1450-002
 750.         145.74 .1714+000 .1640-003 .3234-001 .9622-004 .6239-003 .3207-003
                     .6025-004 .6856-003 .6856-003 .1628-002 .1628-002
 800.         157.56 .1920+000 .2109-003 .3642-001 .1133-003 .7179-003 .3793-003
                     .7281-004 .7679-003 .7679-003 .1824-002 .1824-002
 810.         170.80 .2131+000 .2661-003 .4064-001 .1303-003 .8182-003 .4434-003
                     .8680-004 .8526-003 .8526-003 .2025-002 .2025-002
 820.         185.25 .2335+000 .3280-003 .4472-001 .1469-003 .9184-003 .5096-003
                     .1015-003 .9338-003 .9338-003 .2218-002 .2218-002
 830.         200.69 .2502+000 .3915-003 .4812-001 .1617-003 .1007-002 .5708-003
                     .1156-003 .1001-002 .1001-002 .2377-002 .2377-002
 840.         216.92 .2669+000 .4609-003 .5153-001 .1771-003 .1096-002 .6341-003
                     .1303-003 .1067-002 .1067-002 .2535-002 .2535-002
 850.         233.73 .2831+000 .5348-003 .5485-001 .1927-003 .1185-002 .6977-003
                     .1452-003 .1132-002 .1132-002 .2689-002 .2689-002
 900.         250.91 .3010+000 .6172-003 .5851-001 .2101-003 .1281-002 .7669-003
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57			.1615-003	.1204-002	.1204-002	.2859-002	.2859-002	
58	910.	268.26	.3168+000	.7000-003	.6176-001	.2263-003	.1368-002	.8318-003
59			.1770-003	.1267-002	.1267-002	.3010-002	.3010-002	
60	920.	285.57	.3331+000	.7879-003	.6510-001	.2432-003	.1458-002	.8988-003
61			.1932-003	.1332-002	.1332-002	.3164-002	.3164-002	
62	930.	302.64	.3471+000	.8738-003	.6801-001	.2587-003	.1538-002	.9604-003
63			.2083-003	.1388-002	.1388-002	.3298-002	.3298-002	
64	940.	319.24	.3613+000	.9624-003	.7093-001	.2742-003	.1619-002	.1022-002
65			.2236-003	.1445-002	.1445-002	.3432-002	.3432-002	
66	950.	335.19	.3713+000	.1041-002	.7303-001	.2864-003	.1681-002	.1072-002
67			.2363-003	.1485-002	.1485-002	.3527-002	.3527-002	
68	1000.	350.26	.3838+000	.1128-002	.7561-001	.3005-003	.1754-002	.1129-002
69			.2506-003	.1535-002	.1535-002	.3646-002	.3646-002	
70	1010.	364.30	.3962+000	.1214-002	.7815-001	.3143-003	.1825-002	.1185-002
71			.2647-003	.1585-002	.1585-002	.3764-002	.3764-002	
72	1020.	377.32	.4059+000	.1293-002	.8015-001	.3260-003	.1885-002	.1232-002
73			.2770-003	.1624-002	.1624-002	.3856-002	.3856-002	
74	1030.	389.41	.4160+000	.1371-002	.8224-001	.3377-003	.1945-002	.1280-002
75			.2893-003	.1664-002	.1664-002	.3952-002	.3952-002	
76	1040.	400.63	.4209+000	.1428-002	.8327-001	.3449-003	.1979-002	.1310-002
77			.2975-003	.1684-002	.1684-002	.3998-002	.3998-002	
78	1050.	411.06	.4288+000	.1492-002	.8491-001	.3542-003	.2027-002	.1348-002
79			.3073-003	.1715-002	.1715-002	.4074-002	.4074-002	
80	1100.	420.77	.4328+000	.1538-002	.8576-001	.3599-003	.2054-002	.1372-002
81			.3138-003	.1731-002	.1731-002	.4112-002	.4112-002	
82	1110.	429.84	.4384+000	.1585-002	.8690-001	.3665-003	.2088-002	.1399-002
83			.3208-003	.1754-002	.1754-002	.4165-002	.4165-002	
84	1120.	438.33	.4409+000	.1615-002	.8744-001	.3702-003	.2105-002	.1414-002
85			.3250-003	.1764-002	.1764-002	.4188-002	.4188-002	
86	1130.	446.32	.4428+000	.1638-002	.8784-001	.3730-003	.2119-002	.1426-002
87			.3281-003	.1771-002	.1771-002	.4206-002	.4206-002	
88	1140.	453.88	.4441+000	.1652-002	.8812-001	.3748-003	.2127-002	.1433-002
89			.3302-003	.1776-002	.1776-002	.4219-002	.4219-002	
90	1150.	461.09	.4448+000	.1658-002	.8827-001	.3757-003	.2132-002	.1437-002
91			.3311-003	.1779-002	.1779-002	.4226-002	.4226-002	
92	1200.	468.02	.4450+000	.1656-002	.8831-001	.3757-003	.2133-002	.1437-002
93			.3310-003	.1780-002	.1780-002	.4227-002	.4227-002	
94	1210.	474.72	.4407+000	.1632-002	.8746-001	.3716-003	.2111-002	.1421-002
95			.3270-003	.1763-002	.1763-002	.4187-002	.4187-002	
96	1220.	481.17	.4376+000	.1606-002	.8682-001	.3681-003	.2092-002	.1406-002
97			.3232-003	.1750-002	.1750-002	.4157-002	.4157-002	
98	1230.	487.37	.4374+000	.1586-002	.8676-001	.3665-003	.2087-002	.1399-002
99			.3209-003	.1750-002	.1750-002	.4155-002	.4155-002	
100	1240.	493.28	.4394+000	.1567-002	.8712-001	.3664-003	.2090-002	.1397-002
101			.3196-003	.1758-002	.1758-002	.4174-002	.4174-002	
102	1250.	498.89	.4372+000	.1528-002	.8665-001	.3624-003	.2072-002	.1380-002
103			.3146-003	.1749-002	.1749-002	.4153-002	.4153-002	
104	1300.	504.18	.4320+000	.1474-002	.8557-001	.3554-003	.2038-002	.1351-002
105			.3069-003	.1728-002	.1728-002	.4104-002	.4104-002	
106	1310.	509.12	.4244+000	.1407-002	.8401-001	.3462-003	.1992-002	.1313-002
107			.2970-003	.1698-002	.1698-002	.4032-002	.4032-002	
108	1320.	513.69	.4140+000	.1329-002	.8187-001	.3344-003	.1931-002	.1265-002
109			.2847-003	.1656-002	.1656-002	.3933-002	.3933-002	
110	1330.	517.88	.4039+000	.1249-002	.7979-001	.3225-003	.1871-002	.1217-002
111			.2723-003	.1615-002	.1615-002	.3837-002	.3837-002	
112	1340.	521.66	.3917+000	.1162-002	.7730-001	.3088-003	.1800-002	.1162-002
113			.2582-003	.1567-002	.1567-002	.3721-002	.3721-002	

INPUT DATA - PBM EXAMPLE PROBLEM

```
1350.      525.02 .3812+000 .1079-002 .7511-001 .2962-003 .1736-002 .1111-002
                  .2450-003 .1525-002 .1525-002 .3621-002 .3621-002
1400.      527.92 .3677+000 .9888-003 .7233-001 .2811-003 .1658-002 .1050-002
                  .2299-003 .1471-002 .1471-002 .3493-002 .3493-002
1410.      530.35 .3517+000 .8935-003 .6905-001 .2641-003 .1569-002 .9824-003
                  .2132-003 .1407-002 .1407-002 .3341-002 .3341-002
1420.      532.00 .3383+000 .8073-003 .6628-001 .2491-003 .1491-002 .9217-003
                  .1982-003 .1353-002 .1353-002 .3214-002 .3214-002
1430.      532.00 .3203+000 .7132-003 .6257-001 .2307-003 .1393-002 .8486-003
                  .1806-003 .1281-002 .1281-002 .3042-002 .3042-002
1440.      532.00 .3059+000 .6315-003 .5960-001 .2152-003 .1310-002 .7860-003
                  .1654-003 .1224-002 .1224-002 .2906-002 .2906-002
1450.      532.00 .2900+000 .5508-003 .5631-001 .1988-003 .1222-002 .7201-003
                  .1498-003 .1160-002 .1160-002 .2755-002 .2755-002
1500.      532.00 .2770+000 .4801-003 .5360-001 .1847-003 .1145-002 .6623-003
                  .1359-003 .1108-002 .1108-002 .2631-002 .2631-002
1510.      532.00 .2604+000 .4080-003 .5019-001 .1685-003 .1054-002 .5970-003
                  .1207-003 .1041-002 .1041-002 .2474-002 .2474-002
1520.      532.00 .2430+000 .3408-003 .4664-001 .1521-003 .9605-003 .5322-003
                  .1059-003 .9720-003 .9720-003 .2309-002 .2309-002
1530.      532.00 .2259+000 .2804-003 .4314-001 .1364-003 .8701-003 .4706-003
                  .9193-004 .9035-003 .9035-003 .2146-002 .2146-002
1540.      532.00 .2056+000 .2234-003 .3906-001 .1192-003 .7702-003 .4058-003
                  .7771-004 .8224-003 .8224-003 .1953-002 .1953-002
1550.      532.00 .1849+000 .1739-003 .3491-001 .1023-003 .6722-003 .3444-003
                  .6452-004 .7394-003 .7394-003 .1756-002 .1756-002
1600.      532.00 .1653+000 .1333-003 .3100-001 .8660-004 .5825-003 .2896-003
                  .5301-004 .6613-003 .6613-003 .1571-002 .1571-002
1610.      532.00 .1477+000 .1011-003 .2747-001 .7245-004 .5033-003 .2422-003
                  .4324-004 .5908-003 .5908-003 .1403-002 .1403-002
1620.      532.00 .1280+000 .7324-004 .2359-001 .5808-004 .4207-003 .1954-003
                  .3392-004 .5118-003 .5118-003 .1216-002 .1216-002
1630.      532.00 .1105+000 .5205-004 .2018-001 .4598-004 .3503-003 .1564-003
                  .2632-004 .4419-003 .4419-003 .1050-002 .1050-002
1640.      525.31 .9269-001 .3556-004 .1681-001 .3542-004 .2844-003 .1219-003
                  .1983-004 .3708-003 .3708-003 .8806-003 .8806-003
1650.      494.34 .7192-001 .2266-004 .1301-001 .2557-004 .2157-003 .8879-004
                  .1398-004 .2877-003 .2877-003 .6833-003 .6833-003
1700.      463.38 .5116-001 .1361-004 .9284-002 .1755-004 .1517-003 .6007-004
                  .9173-005 .2046-003 .2046-003 .4860-003 .4860-003
1710.      432.42 .3140-001 .7347-005 .5787-002 .1118-004 .9362-004 .3533-004
                  .5225-005 .1256-003 .1256-003 .2983-003 .2983-003
1720.      401.45 .1448-001 .2745-005 .2819-002 .6515-005 .4480-004 .1484-004
                  .2019-005 .5791-004 .5791-004 .1375-003 .1375-003
1730.      370.49 .0000     .0000     .0000     .0000     .0000     .0000
                  .0000     .0000     .0000     .0000     .0000
1740.      339.53 .0000     .0000     .0000     .0000     .0000     .0000
                  .0000     .0000     .0000     .0000     .0000
1750.      314.60 .0000     .0000     .0000     .0000     .0000     .0000
                  .0000     .0000     .0000     .0000     .0000
1800.      308.78 .0000     .0000     .0000     .0000     .0000     .0000
                  .0000     .0000     .0000     .0000     .0000
 500.       -1.00 .0000     .0000     .0000     .0000     .0000     .0000
                  .0000     .0000     .0000     .0000     .0000
    14     INITIAL CONCENTRATIONS
CO         .1622+001
NO         .1239+000
```

171	NO2	.3910-001						
172	NMHC	.1199+001						
173	NONR	.5276-001						
174	ETH	.3154-001						
175	OLE	.4724-001						
176	PAR	.9425-001						
177	FORM	.7291-001						
178	ALD	.2422-001						
179	ARO	.1787-001						
180	TOL	.1187-001						
181	O3	.2500-002						
182	H2O	.7879+004						
183	1	TOP BOUNDARY CONCENTRATIONS						
184	O3	.6300-001	.6300-001	.6300-001	.6300-001	.6300-001	.6300-001	.6300-001
185		.6300-001	.6300-001	.6300-001	.6300-001	.6300-001	.6300-001	
186	13 LATERAL BOUNDARY CONCENTRATIONS							
187	CO	.6648+000	.9467+000	.8884+000	.8027+000	.8145+000	.8069+000	.6851-001
188		.2796+000	.3172+000	.4243+000	.3888+000	.5457+000	.8985+000	
189	NO	.4121-001	.3570-001	.3076-001	.1685-001	.1240-001	.4890-002	.2500-002
190		.2500-002	.2500-002	.2500-002	.2550-002	.2610-002	.2980-002	
191	NO2	.1933-001	.2250-001	.2729-001	.4307-001	.4161-001	.2248-001	.9790-002
192		.7830-002	.9360-002	.3420-002	.2562-001	.2373-001	.3179-001	
193	NMHC	.6050+000	.5300+000	.3006+000	.2977+000	.2806+000	.2806+000	.2180+000
194		.1550+000	.1470+000	.1787+000	.2798+000	.2767+000	.4006+000	
195	NONR	.2662-001	.2332-001	.1323-001	.1310-001	.1235-001	.1235-001	.9592-002
196		.6820-002	.6468-002	.7865-002	.1231-001	.1218-001	.1763-001	
197	ETH	.1591-001	.1394-001	.7906-002	.7830-002	.7381-002	.7381-002	.5733-002
198		.4076-002	.3866-002	.4701-002	.7358-002	.7278-002	.1054-001	
199	OLE	.2384-001	.2088-001	.1184-001	.1173-001	.1106-001	.1106-001	.8589-002
200		.6107-002	.5792-002	.7042-002	.1102-001	.1090-001	.1578-001	
201	PAR	.4755-001	.4166-001	.2363-001	.2340-001	.2206-001	.2206-001	.1713-001
202		.1218-001	.1155-001	.1405-001	.2199-001	.2175-001	.3149-001	
203	FORM	.3678-001	.3222-001	.1828-001	.1810-001	.1706-001	.1706-001	.1325-001
204		.9424-002	.8938-002	.1087-001	.1701-001	.1683-001	.2436-001	
205	ALD	.1222-001	.1071-001	.6072-002	.6014-002	.5669-002	.5669-002	.4404-002
206		.3131-002	.2969-002	.3611-002	.5652-002	.5590-002	.8092-002	
207	ARO	.9014-002	.7897-002	.4479-002	.4436-002	.4181-002	.4181-002	.3248-002
208		.2309-002	.2190-002	.2663-002	.4169-002	.4123-002	.5969-002	
209	TOL	.5989-002	.5247-002	.2976-002	.2947-002	.2778-002	.2778-002	.2158-002
210		.1534-002	.1455-002	.1770-002	.2770-002	.2740-002	.3966-002	
211	O3	.1018-001	.5050-002	.1328-001	.2404-001	.3312-001	.5421-001	.8282-001
212		.1015+000	.1037+000	.1286+000	.1382+000	.1439+000	.1139+000	
213	13	OBSERVED CONCENTRATIONS						
214	CO	.1771+001	.3305+001	.4013+001	.3468+001	.2699+001	.2299+001	.2122+001
215		.1487+001	.1365+001	.1388+001	.1404+001	.1625+001	.2922+001	
216	NO	.1296+000	.1872+000	.1678+000	.1055+000	.3489-001	.1420-001	.6510-002
217		.2960-002	.2980-002	.2730-002	.2760-002	.3800-002	.2440-001	
218	NO2	.3824-001	.4084-001	.5692-001	.8629-001	.1023+000	.9985-001	.8254-001
219		.5818-001	.5340-001	.5142-001	.5671-001	.6103-001	.1077+000	
220	NMHC	.1202+001	.1359+001	.1488+001	.1209+001	.9929+000	.9559+000	.9620+000
221		.5959+000	.4873+000	.5308+000	.5354+000	.5842+000	.1038+001	
222	NONR	.5288-001	.5978-001	.6545-001	.5320-001	.4369-001	.4206-001	.4233-001
223		.2622-001	.2144-001	.2336-001	.2356-001	.2570-001	.4569-001	
224	ETH	.3161-001	.3573-001	.3912-001	.3180-001	.2611-001	.2514-001	.2530-001
225		.1567-001	.1281-001	.1396-001	.1408-001	.1536-001	.2731-001	
226	OLE	.4735-001	.5353-001	.5861-001	.4764-001	.3912-001	.3766-001	.3790-001
227		.2348-001	.1920-001	.2092-001	.2109-001	.2302-001	.4091-001	

INPUT DATA - PBM EXAMPLE PROBLEM

PAR		.9446-001	.1068+000	.1169+000	.9504-001	.7804-001	.7513-001	.7561-001
		.4684-001	.3830-001	.4172-001	.4208-001	.4591-001	.8162-001	
FORM		.7307-001	.8260-001	.9044-001	.7352-001	.6037-001	.5812-001	.5849-001
		.3623-001	.2963-001	.3228-001	.3255-001	.3552-001	.6313-001	
ALD		.2427-001	.2744-001	.3005-001	.2443-001	.2006-001	.1931-001	.1943-001
		.1204-001	.9843-002	.1072-001	.1081-001	.1180-001	.2098-001	
ARO		.1791-001	.2024-001	.2216-001	.1802-001	.1479-001	.1424-001	.1433-001
		.8879-002	.7260-002	.7910-002	.7977-002	.8704-002	.1547-001	
TOL		.1190-001	.1345-001	.1473-001	.1197-001	.9830-002	.9464-002	.9524-002
		.5900-002	.4824-002	.5255-002	.5300-002	.5783-002	.1028-001	
O3		.2500-002	.2500-002	.2710-002	.7010-002	.3225-001	.6871-001	.1030+000
		.1346+000	.1585+000	.1832+000	.1808+000	.1610+000	.8373-001	
	12	EMISSIONS SPECIES						
CO		.1807+001	.2920+001	.2677+001	.1671+001	.1647+001	.1743+001	.1801+001
		.1761+001	.1880+001	.2113+001	.2543+001	.2397+001	.1614+001	
NO		.1255+000	.1738+000	.1783+000	.1604+000	.1576+000	.1590+000	.1617+000
		.1605+000	.1701+000	.1850+000	.1816+000	.1748+000	.1093+000	
NO2		.1394-001	.1931-001	.1981-001	.1782-001	.1751-001	.1766-001	.1797-001
		.1783-001	.1890-001	.2055-001	.2018-001	.1943-001	.1214-001	
NMHC		.8414+000	.1137+001	.1312+001	.1087+001	.1080+001	.1109+001	.1125+001
		.1114+001	.1149+001	.1229+001	.1325+001	.8510+000	.6946+000	
NONR		.6751-001	.9643-001	.9057-001	.6765-001	.6591-001	.6789-001	.6953-001
		.6844-001	.7191-001	.7874-001	.8831-001	.6838-001	.5299-001	
ETH		.1581-001	.2540-001	.2213-001	.1485-001	.1460-001	.1556-001	.1612-001
		.1575-001	.1689-001	.1923-001	.2245-001	.1869-001	.1328-001	
OLE		.2600-001	.4039-001	.3565-001	.2474-001	.2437-001	.2580-001	.2663-001
		.2608-001	.2780-001	.3131-001	.3614-001	.3050-001	.2238-001	
PAR		.6201-001	.8551-001	.9939-001	.8154-001	.8125-001	.8373-001	.8504-001
		.8416-001	.8694-001	.9364-001	.1010+000	.6413-001	.5318-001	
FORM		.1071-001	.1495-001	.1469-001	.1146-001	.1132-001	.1172-001	.1197-001
		.1180-001	.1231-001	.1332-001	.1475-001	.9836-002	.6999-002	
ALD		.3566-002	.4980-002	.4895-002	.3816-002	.3770-002	.3904-002	.3986-002
		.3931-002	.4100-002	.4437-002	.4914-002	.3276-002	.2330-002	
ARO		.1309-001	.1713-001	.2201-001	.1901-001	.1891-001	.1932-001	.1954-001
		.1940-001	.1986-001	.2097-001	.2229-001	.1453-001	.1243-001	
TOL		.9863-002	.1255-001	.1668-001	.1468-001	.1461-001	.1489-001	.1503-001
		.1493-001	.1524-001	.1598-001	.1687-001	.1169-001	.1029-001	
	5	PLOT SPECIES						
CO								
NO								
NO2								
O3								
HO								

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PBM - DAY 76275 - 10/01/76

TOTAL NUMBER OF REACTIONS =  63
NUMBER OF REACTIVE SPECIES =  37
NUMBER OF INERT OR CONSTANT SPECIES =   4
NUMBER OF SPECIES WITH TOP BOUNDARY CONDITIONS =   1
NUMBER OF SPECIES WITH SIDE BOUNDARY CONDITIONS =  13
NUMBER OF SPECIES WITH SOURCE EMISSIONS TERMS =  12
NUMBER OF SPECIES WITH OBSERVED CONCENTRATIONS =  13
NUMBER OF SPECIES TO BE PLOTTED =   5
NUMBER OF PHOTOLYZING SPECIES =  11
PHOTOLYSIS REACTION NUMBERS =      1     5    12    25    32    33    37    52    53    55    56
HOURS OF SIMULATION INPUT DATA TO BE READ =  13
ENDING TIME OF SIMULATION IN MINUTES FROM START =  780.00
STARTING TIME OF SIMULATION =  0500 L.S.T.
TIME INTERVAL FOR PRINTING/PLOTTING CONCENTRATIONS (MINUTES) =   10.00
TIME INTERVAL FOR UPDATING PHOTOLYTIC RATE CONSTANTS AND MIXING HEIGHTS (MINUTES) =   10.00
NUMERICAL CONVERGENCE TOLERANCE =   .0100
WIDTH OF SIMULATED BOX AREA (METERS) =   20000.00
HOURLY AMBIENT TEMPERATURES ARE SPECIFIED
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SPECIES CONTROL INFORMATION

SPECIE	TOP B.C.	SIDE B.C.	SOURCE EMISSIONS	OBS. CONC.	PLOT
CO		*	*	*	*
NO		*	*	*	*
NO2		*	*	*	*
NMHC		*	*	*	
NONR		*	*	*	
ETH		*	*	*	
OLE		*	*	*	
PAR		*	*	*	
FORM		*	*	*	
ALD		*	*	*	
ARO		*	*	*	
TOL		*	*	*	
O3	*	*		*	*
HONO					
HNO3					
PAN					
DCB1					
DCB2					
RNO3					
H2O2					
O					
O1D					
NO3					
N2O5					
HO					*
HO2					
HO4N					
RO					
RO2					
RTO					
RXO					
FRO2					
FRO					
R1O2					
RTO2					
RXO2					
COOH					
O2					
CO2					
M					
H2O					

LIST OF REACTIONS

	R. CONST. *	REACTANTS				PRODUCTS					
1	.0000			NO2	=	1.00	NO	1.00	O		
2	.0000	O	O2	M	=	1.00	O3	1.00	M		
3	.0000		O3	NO	=	1.00	NO2	1.00	O2		
4	.0000		O3	NO2	=	1.00	NO3	1.00	O2		
5	.0000			O3	=	1.00	O1D	1.00	O2		
6	.0000		O1D	M	=	1.00	O	1.00	M		
7	.3400+006		O1D	H2O	=	2.00	HO				
8	.2960+005		NO3	NO	=	2.00	NO2				
9	.1780+004		NO3	NO2	=	1.00	N2O5				
10	.0000			N2O5	=	1.00	NO3	1.00	NO2		
11	.1920-004		N2O5	H2O	=	2.00	HNO3				
12	.0000			HONO	=	1.00	HO	1.00	NO		
13	.4140+003		HO	CO	=	1.00	HO2	1.00	CO2		
14	.4400+001		HO2	NO2	=	1.00	HONO	1.00	O2		
15	.0000		HO2	NO	=	1.00	HO	1.00	NO2		
16	.0000	HO2	NO2	M	=	1.00	HO4N	1.00	M		
17	.0000			HO4N	=	1.00	HO2	1.00	NO2		
18	.9750+004		HO	HONO	=	1.00	NO2	1.00	H2O		
19	.0000	HO	NO2	M	=	1.00	HNO3	1.00	M		
20	.0000	HO	NO	M	=	1.00	HONO	1.00	M		
21	.0000		HO	HNO3	=	1.00	H2O	1.00	NO3		
22	.0000		HO2	O3	=	1.00	HO	2.00	O2		
23	.0000		HO	O3	=	1.00	HO2	1.00	O2		
24	.0000		HO2	HO2	=	1.00	H2O2	1.00	O2		
25	.0000			H2O2	=	2.00	HO				
26	.2500-002		ETH	O3	=	.40	RO2	1.00	FORM	.10	HO2
27	.1200+005		ETH	HO	=	1.00	FRO2	1.00	FORM		
28	.5100+004		OLE	O	=	1.00	RO2	1.00	ALD	1.00	HO2
29	.9500-001		OLE	O3	=	.75	RO2	.75	ALD	.40	HO2
30	.5500+005		OLE	HO	=	1.00	RO2	.75	ALD	.25	FORM
31	.5000+004		PAR	HO	=	1.00	RO2				
32	.0000			FORM	=	1.00	CO				
33	.0000			FORM	=	2.00	HO2	1.00	CO		
34	.1600+005		FORM	HO	=	1.00	HO2	1.00	H2O	1.00	CO
35	.1100+005		RO2	NO	=	1.00	RO	1.00	NO2		
36	.0000		RO	O2	=	.75	ALD	1.00	HO2	.25	FORM
37	.0000			ALD	=	1.00	RO2	1.00	HO2	1.00	CO
38	.2400+005		ALD	HO	=	1.00	R1O2	1.00	H2O		
39	.1100+005		FRO2	NO	=	1.00	FRO	1.00	NO2		
40	.1080+001		FRO	O2	=	1.00	FORM	1.00	HO2		
41	.8870+004		R1O2	NO2	=	1.00	PAN				
42	.0000			PAN	=	1.00	R1O2	1.00	NO2		
43	.1000+003		RO	NO2	=	1.00	RNO3				
44	.2000+001		RO2	O3	=	1.00	RO	2.00	O2		
45	.2070+005		R1O2	NO	=	1.00	RO2	1.00	NO2		
46	.8700+004		TOL	HO	=	1.00	RTO2	1.00	ALD	1.00	DCB1
47	.3400+005		ARO	HO	=	1.00	RXO2	1.00	ALD	1.00	DCB1
48	.1100+005		RTO2	NO	=	1.00	RTO	1.00	NO2		
49	.8870+000		RTO	O2	=	1.00	DCB1	1.00	HO2	1.00	CO
50	.1100+005		RXO2	NO	=	1.00	RXO	1.00	NO2		
51	.8870+000		RXO	O2	=	1.00	DCB2	1.00	HO2	1.00	CO
52	.0000			DCB1	=	2.00	CO	2.00	HO2		
53	.0000			DCB1	=	.20	FORM	1.80	CO		

54	.1700+005	DCB1	HO	=	1.00	HO2	2.00	CO			
55	.0000		DCB2	=	1.00	R1O2	1.00	HO2	2.00	CO	
56	.0000		DCB2	=	.50	ALD	.50	FORM	.50	FRO2	
57	.2560+005	DCB2	HO	=	1.00	R1O2	1.00	CO			
58	.2000+001	RTO2	O3	=	1.00	RTO	2.00	O2			
59	.2000+001	RXO2	O3	=	1.00	RXO	2.00	O2			
60	.2000+001	R1O2	O3	=	1.00	RO2	2.00	O2			
61	.1500-002	OLE	O3	=	1.00	COOH	1.00	ALD			
62	.0000		NMHC	=							
63	.0000		NONR	=							

* ONLY TEMPORALLY-FIXED RATE CONSTANT VALUES ARE GIVEN HERE.
VALUES OF OTHER RATE CONSTANTS ARE SHOWN AT EACH TIME STEP.

INITIAL SPECIES CONCENTRATIONS

REACTIVE (PPM)

SPECIES	VALUE	SPECIES	VALUE	SPECIES	VALUE	SPECIES	VALUE
CO	.1622+001	NO	.1239+000	NO2	.3910-001	NMHC	.1199+001
NONR	.5276-001	ETH	.3154-001	OLE	.4724-001	PAR	.9425-001
FORM	.7291-001	ALD	.2422-001	ARO	.1787-001	TOL	.1187-001
O3	.2500-002	HONO	.0000	HNO3	.0000	PAN	.0000
DCB1	.0000	DCB2	.0000	RNO3	.0000	H2O2	.1000-005
O	.0000	O1D	.0000	NO3	.0000	N2O5	.0000
HO	.0000	HO2	.0000	HO4N	.0000	RO	.0000
RO2	.0000	RTO	.0000	RXO	.0000	FRO2	.0000
FRO	.0000	R1O2	.0000	RTO2	.0000	RXO2	.0000
COOH	.0000						

INERT/CONSTANT (PPM)

O2	.2100+006	CO2	.3200+003	M	.1000+007	H2O	.7879+004

TIME = 782.969 MINUTES

PHOTOLYTIC RATE CONSTANTS:

RK(1) = .0000	RK(5) = .0000	RK(12) = .0000	RK(25) = .0000
RK(32) = .0000	RK(33) = .0000	RK(37) = .0000	RK(52) = .0000
RK(53) = .0000	RK(55) = .0000	RK(56) = .0000	

TEMPERATURE-DEPENDENT RATE CONSTANTS:

RK(2) = .2231-004	RK(3) = .2733+002	RK(4) = .4926-001	RK(6) = .4229+005
RK(10) = .3630+001	RK(15) = .1220+005	RK(16) = .1500-002	RK(17) = .3755+001
RK(19) = .1425-001	RK(20) = .7315-002	RK(21) = .1948+003	RK(22) = .2980+001
RK(23) = .1020+003	RK(24) = .3667+004	RK(36) = .9251+000	RK(42) = .1627+000

Z = 308.8 METERS WIND SPEED = 54.0 M/MIN TEMP = 299.3(K)

CONCENTRATIONS:

SPECIES	VALUE	SPECIES	VALUE	SPECIES	VALUE	SPECIES	VALUE
CO	.1961+001	NO	.4738-004	NO2	.5870-001	NMHC	.1001+001
NONR	.6276-001	ETH	.1367-001	OLE	.5080-002	PAR	.6810-001
FORM	.2787-001	ALD	.4971-001	ARO	.9295-002	TOL	.1040-001
O3	.1352+000	HONO	.8345-003	HNO3	.8336-001	PAN	.5363-002
DCB1	.5617-002	DCB2	.2221-002	RNO3	.2651-005	H2O2	.4314-003
O	.7333-014	O1D	.2191-021	NO3	.7410-004	N2O5	.2053-002
HO	.1293-007	HO2	.6179-004	HO4N	.1446-002	RO	.3125-009
RO2	.7533-004	RTO	.6189-011	RXO	.2157-010	FRO2	.4037-005
FRO	.9243-011	R1O2	.1703-005	RTO2	.1463-005	RXO2	.5101-005
COOH	.2559-003						

THIS SIMULATION ENDED WITH KFLAG = 1

HOUR-AVERAGE SIMULATION RESULTS FOR REACTIVE SPECIES:

HOUR-AVERAGES CENTERED AT 5.50 HRS, LOCAL STANDARD TIME

CO	.1999+001	NO	.1444+000	NO2	.4392-001	NMHC	.1355+001
NONR	.6811-001	ETH	.3388-001	OLE	.5138-001	PAR	.1054+000
FORM	.7113-001	ALD	.2366-001	ARO	.2034-001	TOL	.1384-001
O3	.1586-004	HONO	.4377-005	HNO3	.2284-005	PAN	.1804-006
DCB1	.3596-005	DCB2	.2692-005	RNO3	.4445-009	H2O2	.8690-006
O	.0000	O1D	.0000	NO3	.5220-011	N2O5	.5355-009
HO	.5142-010	HO2	.2506-009	HO4N	.3448-007	RO	.1892-011
RO2	.1645-009	RTO	.3297-013	RXO	.1896-012	FRO2	.1327-010
FRO	.9181-013	R1O2	.9610-011	RTO2	.3905-011	RXO2	.2247-010
COOH	.9313-007						

HOUR-AVERAGES CENTERED AT 6.50 HRS, LOCAL STANDARD TIME

CO	.2812+001	NO	.1853+000	NO2	.4872-001	NMHC	.1619+001
NONR	.9576-001	ETH	.3870-001	OLE	.5943-001	PAR	.1245+000
FORM	.6763-001	ALD	.2274-001	ARO	.2438-001	TOL	.1700-001
O3	.2905-003	HONO	.4830-004	HNO3	.2621-004	PAN	.1574-005
DCB1	.4012-004	DCB2	.2944-004	RNO3	.6290-008	H2O2	.6562-006
O	.2225-009	O1D	.8378-019	NO3	.8243-010	N2O5	.9196-008
HO	.2679-008	HO2	.1136-007	HO4N	.1304-005	RO	.9801-010
RO2	.6322-008	RTO	.2214-011	RXO	.1234-010	FRO2	.6019-009
FRO	.5689-011	R1O2	.3316-009	RTO2	.1924-009	RXO2	.1073-008
COOH	.4284-006						

HOUR-AVERAGES CENTERED AT 7.50 HRS, LOCAL STANDARD TIME

CO	.3099+001	NO	.1762+000	NO2	.6154-001	NMHC	.1601+001
NONR	.1020+000	ETH	.3599-001	OLE	.5429-001	PAR	.1222+000
FORM	.5381-001	ALD	.2145-001	ARO	.2413-001	TOL	.1741-001
O3	.2134-002	HONO	.5034-003	HNO3	.4750-003	PAN	.2476-004
DCB1	.5961-003	DCB2	.4234-003	RNO3	.1012-006	H2O2	.4102-006
O	.1549-008	O1D	.5050-017	NO3	.9600-009	N2O5	.1074-006
HO	.2184-007	HO2	.9343-007	HO4N	.1019-004	RO	.6522-009
RO2	.5150-007	RTO	.1752-010	RXO	.9438-010	FRO2	.5053-008
FRO	.4158-010	R1O2	.3127-008	RTO2	.1752-008	RXO2	.9431-008
COOH	.4531-005						

HOUR-AVERAGES CENTERED AT 8.50 HRS, LOCAL STANDARD TIME

CO	.2395+001	NO	.1064+000	NO2	.7914-001	NMHC	.1235+001
NONR	.7856-001	ETH	.2494-001	OLE	.3437-001	PAR	.9313-001
FORM	.3592-001	ALD	.2258-001	ARO	.1805-001	TOL	.1388-001
O3	.8195-002	HONO	.8082-003	HNO3	.2284-002	PAN	.1403-003
DCB1	.1877-002	DCB2	.1252-002	RNO3	.3669-006	H2O2	.2263-006
O	.3864-008	O1D	.7284-016	NO3	.8995-008	N2O5	.8983-006
HO	.5892-007	HO2	.3172-006	HO4N	.2958-004	RO	.1192-008

RO2	.1704-006	RTO	.3761-010	RXO	.1903-009	FRO2	.1683-007
FRO	.8242-010	R1O2	.1566-007	RTO2	.6326-008	RXO2	.3189-007
COOH	.1512-004						

HOUR-AVERAGES CENTERED AT 9.50 HRS, LOCAL STANDARD TIME

CO	.1816+001	NO	.5504-001	NO2	.8894-001	NMHC	.9673+000
NONR	.6064-001	ETH	.1737-001	OLE	.1953-001	PAR	.7153-001
FORM	.2630-001	ALD	.2698-001	ARO	.1293-001	TOL	.1094-001
O3	.2276-001	HONO	.5822-003	HNO3	.6103-002	PAN	.4727-003
DCB1	.3226-002	DCB2	.1952-002	RNO3	.7385-006	H2O2	.1970-006
O	.6211-008	O1D	.4357-015	NO3	.5624-007	N2O5	.4465-005
HO	.9346-007	HO2	.7615-006	HO4N	.5465-004	RO	.1349-008
RO2	.3929-006	RTO	.4755-010	RXO	.2190-009	FRO2	.3848-007
FRO	.9921-010	R1O2	.5598-007	RTO2	.1517-007	RXO2	.6952-007
COOH	.3451-004						

HOUR-AVERAGES CENTERED AT 10.50 HRS, LOCAL STANDARD TIME

CO	.1612+001	NO	.3137-001	NO2	.9235-001	NMHC	.8745+000
NONR	.5425-001	ETH	.1406-001	OLE	.1156-001	PAR	.6313-001
FORM	.2282-001	ALD	.3319-001	ARO	.1026-001	TOL	.9733-002
O3	.4654-001	HONO	.3640-003	HNO3	.1195-001	PAN	.1048-002
DCB1	.4436-002	DCB2	.2385-002	RNO3	.1181-005	H2O2	.4278-006
O	.7919-008	O1D	.1385-014	NO3	.2188-006	N2O5	.1323-004
HO	.1215-006	HO2	.1546-005	HO4N	.8199-004	RO	.1432-008
RO2	.7716-006	RTO	.5515-010	RXO	.2267-009	FRO2	.7446-007
FRO	.1106-009	R1O2	.1548-006	RTO2	.3054-007	RXO2	.1250-006
COOH	.6234-004						

HOUR-AVERAGES CENTERED AT 11.50 HRS, LOCAL STANDARD TIME

CO	.1517+001	NO	.1884-001	NO2	.9105-001	NMHC	.8451+000
NONR	.5194-001	ETH	.1234-001	OLE	.7069-002	PAR	.5949-001
FORM	.2161-001	ALD	.3849-001	ARO	.8577-002	TOL	.9125-002
O3	.7856-001	HONO	.2409-003	HNO3	.1893-001	PAN	.1792-002
DCB1	.5316-002	DCB2	.2545-002	RNO3	.1629-005	H2O2	.1328-005
O	.8538-008	O1D	.2827-014	NO3	.6317-006	N2O5	.2957-004
HO	.1424-006	HO2	.2813-005	HO4N	.1135-003	RO	.1476-008
RO2	.1384-005	RTO	.6065-010	RXO	.2226-009	FRO2	.1300-006
FRO	.1164-009	R1O2	.3447-006	RTO2	.5572-007	RXO2	.2036-006
COOH	.9125-004						

HOUR-AVERAGES CENTERED AT 12.50 HRS, LOCAL STANDARD TIME

CO	.1511+001	NO	.1221-001	NO2	.9019-001	NMHC	.8623+000
NONR	.5275-001	ETH	.1139-001	OLE	.4394-002	PAR	.5908-001
FORM	.2135-001	ALD	.4350-001	ARO	.7561-002	TOL	.8997-002
O3	.1150+000	HONO	.1756-003	HNO3	.2731-001	PAN	.2690-002
DCB1	.6077-002	DCB2	.2623-002	RNO3	.2115-005	H2O2	.3961-005
O	.8528-008	O1D	.4072-014	NO3	.1444-005	N2O5	.5687-004
HO	.1497-006	HO2	.4395-005	HO4N	.1472-003	RO	.1461-008
RO2	.2158-005	RTO	.6290-010	RXO	.2066-009	FRO2	.1948-006

FRO	.1144-009	R102	.6252-006	RTO2	.8800-007	RXO2	.2882-006
COOH	.1210-003						

HOUR-AVERAGES CENTERED AT 13.50 HRS, LOCAL STANDARD TIME

CO	.1579+001	NO	.8506-002	NO2	.9092-001	NMHC	.9040+000
NONR	.5528-001	ETH	.1088-001	OLE	.3053-002	PAR	.6043-001
FORM	.2151-001	ALD	.4766-001	ARO	.7026-002	TOL	.9143-002
O3	.1507+000	HONO	.1380-003	HNO3	.3628-001	PAN	.3526-002
DCB1	.6627-002	DCB2	.2614-002	RNO3	.2617-005	H2O2	.9144-005
O	.8032-008	O1D	.4281-014	NO3	.2786-005	N2O5	.9881-004
HO	.1403-006	HO2	.5953-005	HO4N	.1786-003	RO	.1366-008
RO2	.2948-005	RTO	.5990-010	RXO	.1800-009	FRO2	.2515-006
FRO	.1031-009	R1O2	.9209-006	RTO2	.1198-006	RXO2	.3592-006
COOH	.1477-003						

HOUR-AVERAGES CENTERED AT 14.50 HRS, LOCAL STANDARD TIME

CO	.1637+001	NO	.5691-002	NO2	.9036-001	NMHC	.9316+000
NONR	.5696-001	ETH	.1067-001	OLE	.2794-002	PAR	.6143-001
FORM	.2191-001	ALD	.4936-001	ARO	.6860-002	TOL	.9225-002
O3	.1768+000	HONO	.1178-003	HNO3	.4298-001	PAN	.4031-002
DCB1	.6695-002	DCB2	.2497-002	RNO3	.2922-005	H2O2	.1709-004
O	.6461-008	O1D	.2991-014	NO3	.4896-005	N2O5	.1589-003
HO	.1163-006	HO2	.7472-005	HO4N	.2041-003	RO	.1161-008
RO2	.3797-005	RTO	.5010-010	RXO	.1456-009	FRO2	.3022-006
FRO	.8290-010	R1O2	.1168-005	RTO2	.1493-006	RXO2	.4338-006
COOH	.1682-003						

HOUR-AVERAGES CENTERED AT 15.50 HRS, LOCAL STANDARD TIME

CO	.1730+001	NO	.3694-002	NO2	.9164-001	NMHC	.9761+000
NONR	.5976-001	ETH	.1124-001	OLE	.3210-002	PAR	.6432-001
FORM	.2346-001	ALD	.5093-001	ARO	.7321-002	TOL	.9595-002
O3	.1914+000	HONO	.1215-003	HNO3	.4830-001	PAN	.4454-002
DCB1	.6659-002	DCB2	.2452-002	RNO3	.3086-005	H2O2	.2869-004
O	.4635-008	O1D	.1351-014	NO3	.8188-005	N2O5	.2615-003
HO	.8873-007	HO2	.9198-005	HO4N	.2464-003	RO	.9552-009
RO2	.4834-005	RTO	.3970-010	RXO	.1182-009	FRO2	.3638-006
FRO	.6460-010	R1O2	.1325-005	RTO2	.1819-006	RXO2	.5428-006
COOH	.1932-003						

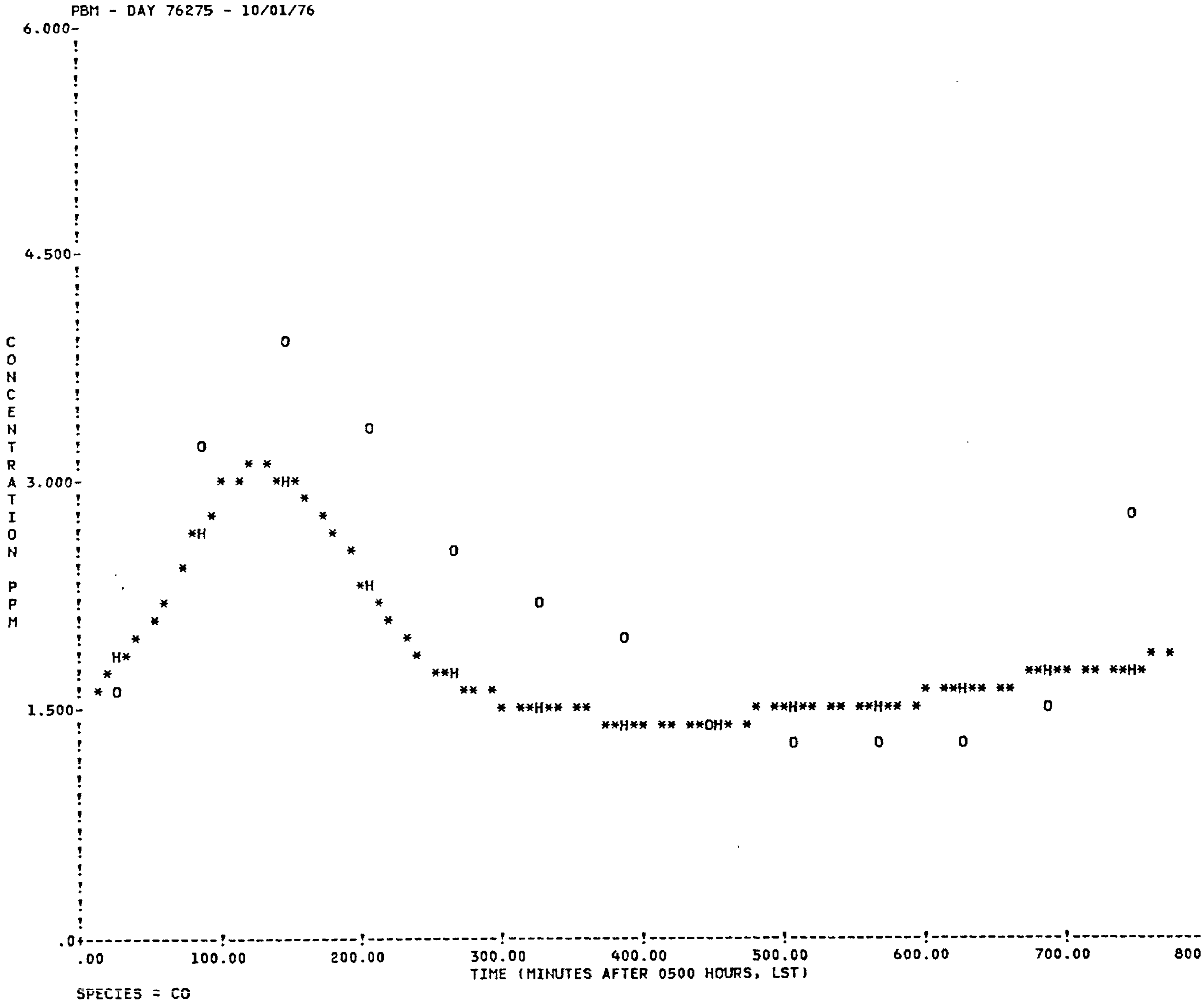
HOUR-AVERAGES CENTERED AT 16.50 HRS, LOCAL STANDARD TIME

CO	.1816+001	NO	.1849-002	NO2	.9121-001	NMHC	.9913+000
NONR	.6126-001	ETH	.1196-001	OLE	.3500-002	PAR	.6563-001
FORM	.2516-001	ALD	.5152-001	ARO	.7749-002	TOL	.9780-002
O3	.1903+000	HONO	.1688-003	HNO3	.5302-001	PAN	.4975-002
DCB1	.6484-002	DCB2	.2442-002	RNO3	.3069-005	H2O2	.4678-004
O	.2363-008	O1D	.2973-015	NO3	.1526-004	N2O5	.5071-003
HO	.5674-007	HO2	.1205-004	HO4N	.3363-003	RO	.6618-009
RO2	.6604-005	RTO	.2592-010	RXO	.8015-010	FRO2	.4745-006
FRO	.4193-010	R1O2	.1409-005	RTO2	.2360-006	RXO2	.7313-006

COOH .2206-003

HOUR-AVERAGES CENTERED AT 17.50 HRS, LOCAL STANDARD TIME

CO	.1893+001	NO	.2656-003	NO2	.7554-001	NMHC	.9867+000
NONR	.6159-001	ETH	.1281-001	OLE	.4145-002	PAR	.6621-001
FORM	.2676-001	ALD	.5045-001	ARO	.8432-002	TOL	.9976-002
O3	.1633+000	HONO	.4298-003	HNO3	.6650-001	PAN	.5391-002
DCB1	.6009-002	DCB2	.2338-002	RNO3	.2841-005	H2O2	.1468-003
O	.2971-009	O1D	.1564-016	NO3	.5679-004	N2O5	.1869-002
HO	.1796-007	HO2	.3385-004	HO4N	.9391-003	RO	.3382-009
RO2	.4386-004	RTO	.8187-011	RXO	.2667-010	FRO2	.1975-005
FRO	.1253-010	R1O2	.1419-005	RTO2	.7437-006	RXO2	.2483-005
COOH	.2436-003						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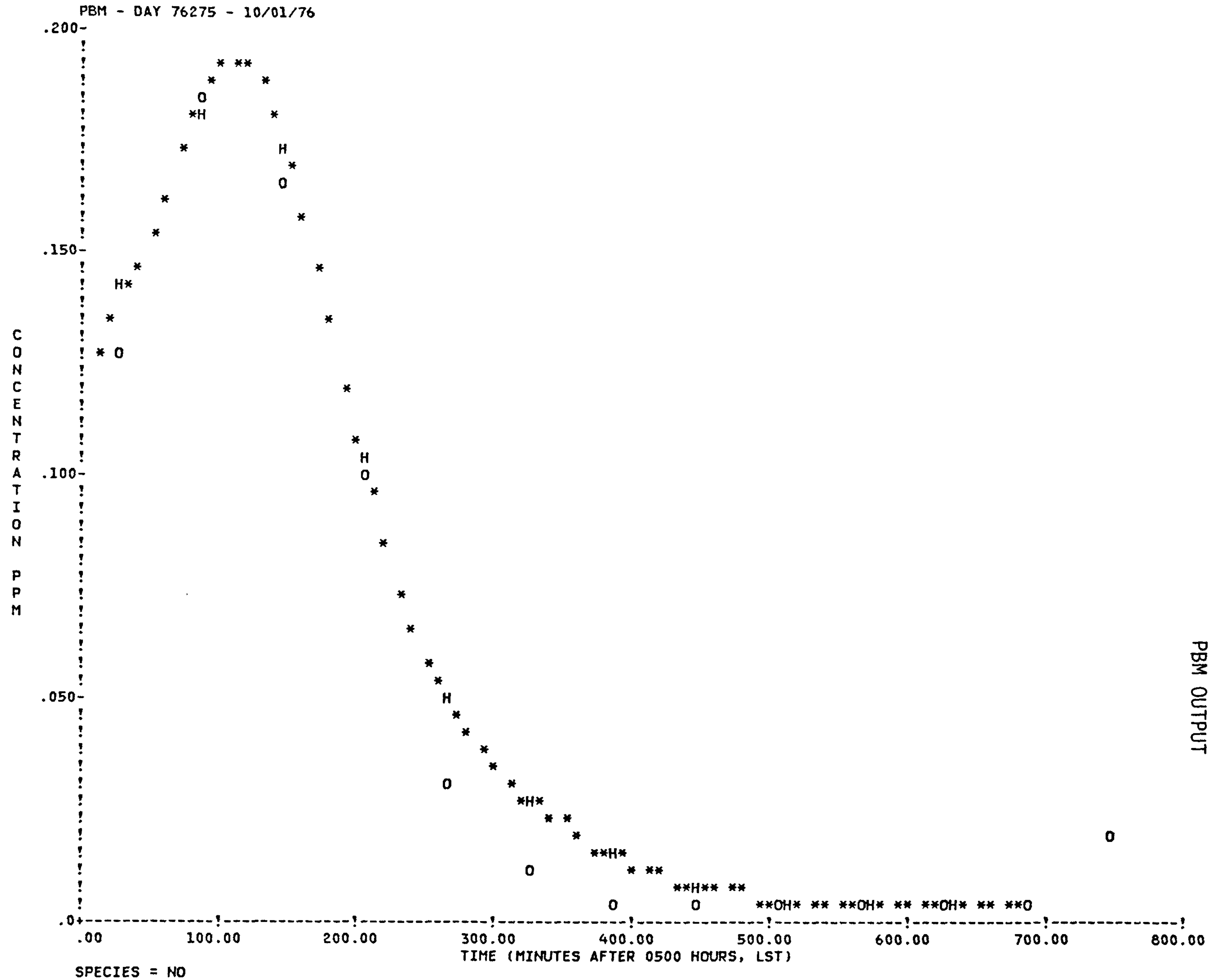
TIME (MINUTES AFTER 0500 HOURS, LST)
SPECIES = CO

PBM OUTPUT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TIME (MINUTES AFTER 0500 HOURS, LST)
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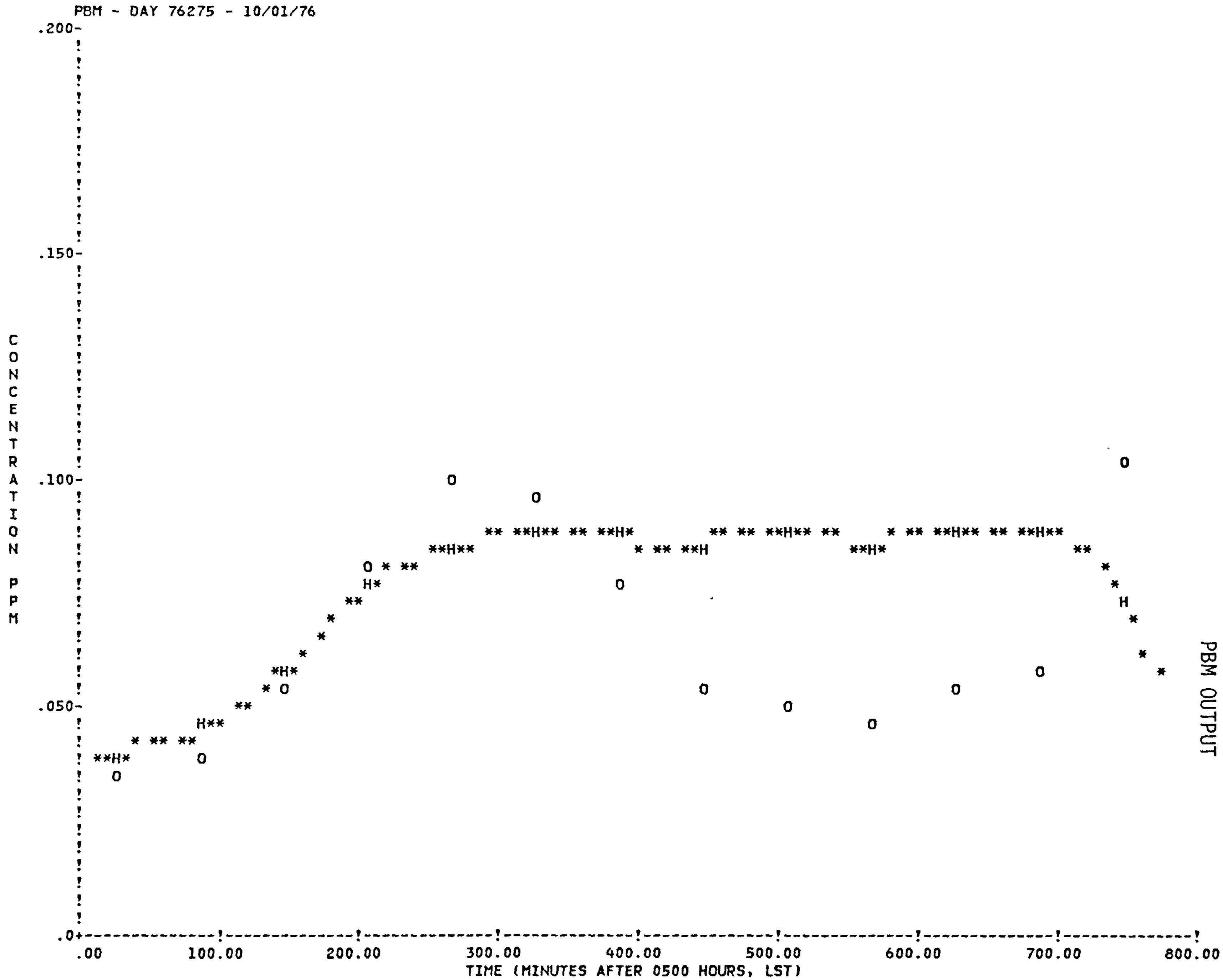

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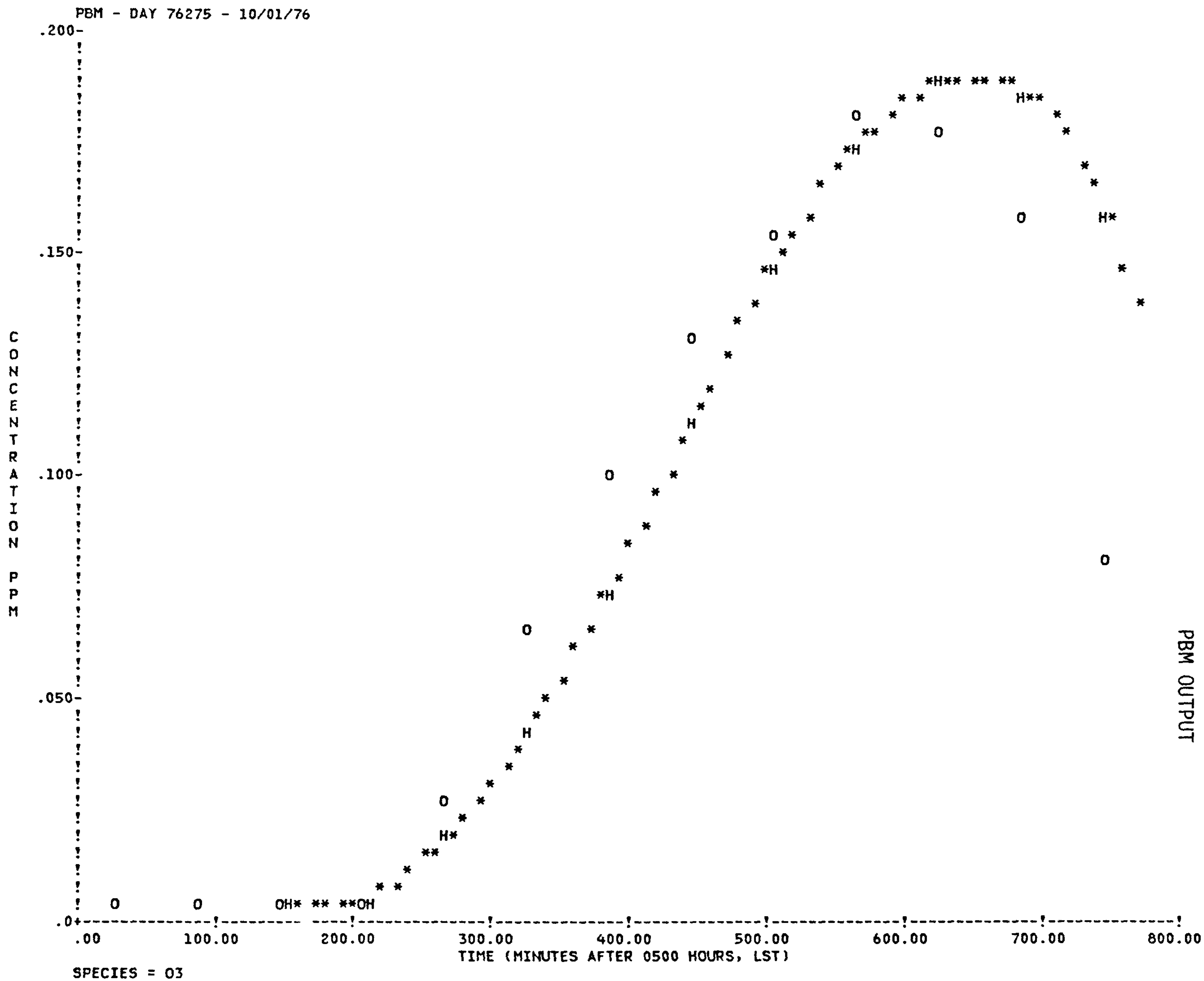
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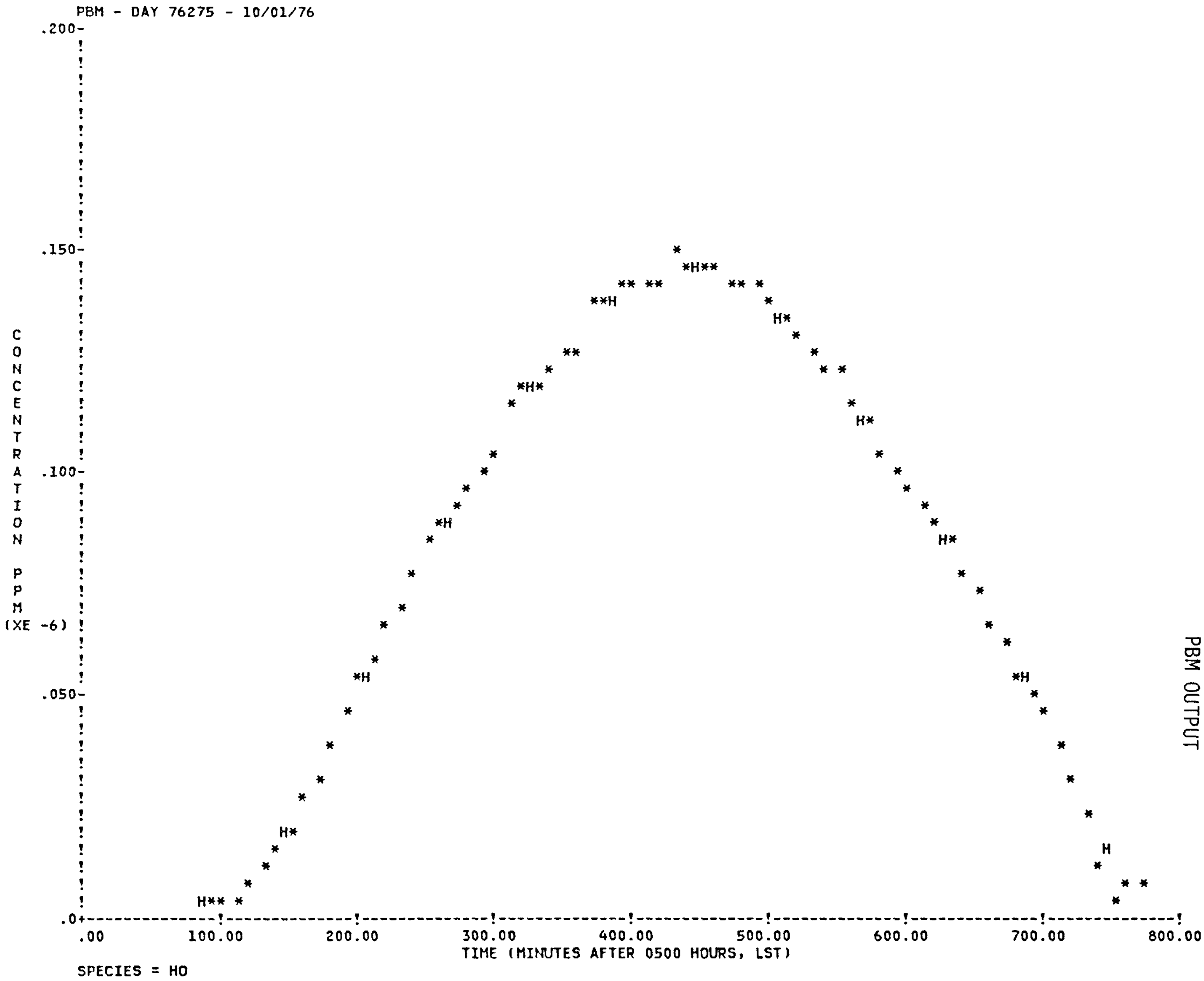
TIME (MINUTES AFTER 0500 HOURS, LST)
SPECIES = O3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TIME (MINUTES AFTER 0500 HOURS, LST)
SPECIES = HO

PBM OUTPUT

REFERENCES

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APPENDIX A

CONSIDERATIONS FOR USING ALTERNATIVE CHEMICAL KINETIC MECHANISMS

The default chemical kinetic mechanism included in the PBM system was developed by Dr. Kenneth Demerjian of the EPA. It simulates the urban photochemistry of the O_3-NO_x-HC reaction system and includes a temporal variation in the photolytic and temperature-dependent reaction rate constants. The Demerjian mechanism is one of several recognized photochemical smog mechanisms. Circumstances may exist where the user desires to employ an alternative chemical kinetic mechanism in the PBM system. This is relatively easy to do although the change may affect initial and boundary concentrations, emissions, and the diurnal variations in particular rate constants. It should not be attempted without the expert services of a chemist familiar with photochemical smog simulations and a computer programer familiar with simulation models. This appendix highlights the sections of code within the computer programs constituting the PBM system that may need revision if an alternative chemical kinetic mechanism is used and discusses effects on input data to the system. Line numbers referencing the computer programs are approximations and are intended only to guide the user to the general section of affected code.

PBMMET

Although the meteorological preprocessor would not seem to deal directly with the PBM chemistry, it does generate diurnally varying rate constants for the 11 photolysis reactions in the default kinetic mechanism. If the alternative mechanism contains photolysis reactions different in structure or order of appearance from those in the default mechanism, the following changes are needed.

In the main program PBMMET:

		Change Code*:
line 103	COMMON Z(10),...,RTCON(10,10,7)	A
line 107	......PRC(110,11),ARC(110,11),CRT(27,10,7)	A,B
line 366	DO 230 K=1,7	A
line 373	DO 250 K=1,11	B
line 390	DO 310 K=1,7	A
line 438	DO 350 K=1,11	B
line 443	DO 360 K=1,11	B
line 485	DO 440 K=1,11	B
line 493	DO 470 K=1,11	B
line 499	DO 490 K=1,11	B
line 550	WRITE (NOUT,2450) (ARC(I,K),...	B
line 551	WRITE (NOUTD,2500) TIME(I),...	B
line 554	DO 560 K=1,11	B
line 556	WRITE (NOUTD,2500) TIME(1),...	B
lines 414-417	Delete these lines. They are specific to the photolysis reactions of the default chemical kinetic mechanism.	

In the subroutine BLKMET:

line 5	COMMON Z(10),...,RTCON (10,10,7)	Change 7 to number of photolysis reactions with given clear-sky theoretical values if number is > 7.

---

*A = Change 7 to number of photolysis reactions with given clear-sky theoretical values if number is > 7.

B = Change 11 to total number of photolysis reactions.

lines 11-112 DATA ((RTCON)(I,J,1)),... Update this data array corresponding to the clear-sky theoretical values of the photolytic rate constants for zenith angles (I) of values Z and altitudes (J) of values HTRT. Rate constant units are minute $^{-1}$.

PBMAQE

The existing version of the air quality and emissions preprocessor is tied directly to the chemical species contained in the default chemical kinetic mechanism and will probably require a complete revision for a mechanism with different species, including different hydrocarbon reactivity classes. The purpose of this preprocessor is to set up data for the PBM for initial species concentrations, hourly lateral and top boundary species concentrations, hourly observed species concentrations, and hourly emissions. Most other mechanisms will include initial concentrations of CO, NO, and NO_2, but may differ in the reactivity splitting of the hydrocarbons. These splits should be consistent with the mechanism used. Boundary concentrations usually specify O_3 and may include precursor species as well. Emissions must include NO_x and THC and must be divided into NO, NO_2, and the hydrocarbon reactivity classes by the preprocessing program. If CO is a species in the mechanism, CO emissions must also be specified.

PBM

The PBM has been constructed to optionally read in an alternative chemical kinetic mechanism. The subroutine ANALYZ is invoked to do this. This subroutine is linked or mapped into the final executable program only when a mechanism other than the default mechanism is used. Other required code changes are outlined below. The PBM has been set up to accommodate up to 50 reactive species, 5 additional inert species, and 75 individual chemical reactions. If any of these limits are exceeded in an alternative mechanism, certain arrays in COMMON and DIMENSION must be expanded accordingly throughout the PBM. These arrays (and their current sizes) include: NAME(55), YAX(55), ICODE(3,50), Y(8,50), SAVCON(100,50), KOBS(50), KPLOT(50), AVCON(18,50), ERROR(50), SUM(50), YMAX(50), PSAVE(50^2), SAVE(12,50), RK(75), COEFF(3,75), NMPD(3,75), NMRC(4,75), KCOF(75,55), KPRD(3,75), KRCT(4,75), and KRXN(75,55). Some subroutines contain local arrays that also would need to be enlarged. They are not listed here, although they can be readily identified by the characteristic size of 50, 55, or 75.

In the subroutine SETUP:

line 325	CALL ANALYZ (LFLAG)	Remove 'C' from column 1 of line 325
line 326	IF (LFLAG.GT.0) GO TO 900	Remove 'C' from column 1 of line 326

In the subroutine DIFFUN:

line 75 DATA NUMNO/2/, NUMNO2/3/, NUMO3/13/

Change this data statement to show the position numbers in the species list of NO, NO_2, and O_3.

lines 110-111 +SDCONC(INDEX,I) = (RK(1)*SDCONC(INDEX,K))...

Change 1 in RK(1) corresponding to the reaction number for NO_2-->NO+O, and change 3 in RK(3) corresponding to the reaction number for NO+O_3-->NO_2+O_2.

In the subroutine RKUPDT:

This subroutine calculates the temperature-dependent rate constants for particular reactions in the default mechanism. The subroutine would need to be rewritten for an alternative kinetic mechanism.

In the subroutine BLKDAT:

line 34 DATA NIN/5/, NOUT/6/,...

Change 37 to the number of reactive species and 41 to the total number of species, including inert species.

lines 37-42 DATA NAME/...

Change this data statement to show the names of the species in the mechanism.

lines 49-51 DATA DELTIM/...

Change the data in IPHO to the numbers of the photolysis reactions. Change the data in YAX to specify the initial concentrations of species that will not be specified in the input data to the PBM.

lines 55-67 Change the rate constant array RK to the appropriate reaction rate constants for the alternative kinetic mechanism. Rate constants that are temperature-dependent or are for photolysis reactions are calculated elsewhere and can be set to zero here.

line 73 DATA MAXPRD/3/,...

Change MAXRXN to the maximum allowable reaction number. Change NRXN to the exact number of reactions in the alternative kinetic mechanism.

For the subroutine ANALYZ:

This subroutine must be compiled and linked into the PBM system. It reads and analyzes the new kinetic mechanism. The individual reactions are read, one to a card image, after all other inputs have been read by the PBM. The format for this data set is shown in Table A-1.

TABLE A-1. PBM CARD TYPE 23 - REACTIONS (1 card for each reaction) (used with subroutine ANALYZ)

Variable	Format	Description	Units
NMRC	4(A4,1X)	Alphanumeric names of reactant species (maximum=4) Coefficients of reactant species are set equal to 1.	-
COEFF	F6.0	Stoichiometric coefficient of product species.	-
NMPD	A4	Alphanumeric name of product species.	-

Note: A maximum of 3 COEFF,NMPD pairs may be specified on each card (i.e. 3(F6.0,A4)).

Date ____________________

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I would like to receive future revisions to the User's Guide for the Photochemical Box Model.

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Computer Characteristics (Optional):

Computer ______________________________

Compiler ______________________________

Operating System ______________________