

User's Guide for Executing OZIPR

by

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ABSTRACT

In this study a new trajectory-type, air quality simulation model called OZIPR was developed. OZIPR is based on EPA's Ozone Isopleth Plotting Program (OZIP) Model, but contains improved and expanded capabilities that make the model useful for research purposes. OZIPR serves the dual purpose of providing: (1) a simple trajectory model capable of utilizing complex chemical mechanisms, emissions, and various meteorological parameters, and (2) procedures through which the Empirical Kinetics Modeling Approach (EKMA) can be implemented for calculation of emission reductions needed to achieve compliance with the National Ambient Air Quality Standard for ozone. While these capabilities were included in earlier versions of OZIP, the new OZIPR contains major improvements that increase the program's ability to input, utilize, and output a much larger range of information.

The Project Report serves as a user's manual for OZIPR. It contains a description of the model, along with input and output requirements and options. The input and output files for nine examples are included. These examples employ three different chemical kinetics mechanisms and most of the major options available in OZIPR.

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Acknowledgements

We thank Professor Harvey Jeffries of the University of North Carolina for providing guidance concerning computer program design.

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1 Introduction

OZIPR is a research-oriented version of EPA's OZIP (Ozone Isopleth Plotting Package) computer modeling program. The OZIPR and OZIP programs employ a trajectory-based air quality simulation model, in conjunction with the Empirical Kinetics Modeling Approach (EKMA), to relate ozone concentrations to levels of organic and nitrogen oxide (NO_x) emissions. While the aim of earlier OZIP versions was to provide a rigid structure within which State Implementation Plans could be formulated, the goal of OZIPR is to furnish a comprehensive research tool that is of use to Agency planners and model developers.

This version, called OZIPR (R for research), is specifically enhanced to provide input of more parameters, but in a less rigid format. Output has been expanded and there are also significant improvements to all facets of the computer program. The structure of the program is similar to OZIPM-4, however, so the published user's guide (Hogo and Gery, 1988) for that program serves as a reference for the previous development and inherent structure of OZIPR.

Description of OZIPR

OZIPR simulates complex chemical and physical processes of the lower atmosphere through use of a trajectory model. The physical representation is a well-mixed column of air extending from the ground to the top of the mixed layer. This idealized air column moves with the wind (along the wind trajectory), but cannot expand horizontally. Emissions from the surface are included as the air column passes over different emission sources, and air from above the column is mixed in as the inversion rises during the day. Very complex chemical mechanisms may be input into OZIPR to describe the chemical processes that occur within the modeled air mass.

Besides individual trajectory simulations, the program can use the EKMA procedure to automatically estimate the amount and type of precursor emission reductions required to achieve a specified ozone level. The ozone level currently defaulted in EKMA is a one-hour

average maximum concentration of 0.12 ppm, the national ambient air quality standard. In the EKMA procedure, OZIPR performs multiple simulations with different levels of organic and NO_x precursor emissions to estimate the effect of reduced emissions on maximum ozone concentrations.

OZIPR can also perform a specified set of simulations to calculate ozone levels at fixed intervals. This allows for the plotting of fixed ozone concentration lines (isolines) as a function of initial precursors. A post-processor program called ISOPLOT is used to control isopleth dimensions, plot options, display results, and provide output to printers and data files.

Although the basic structure of the program is similar to earlier versions of OZIP, OZIPR was enhanced in this study to provide expanded yet simpler input capability, more calculation options, greater calculation speed, and enhanced output options. These improvements are described in the following sections. The next section provides an overview of OZIPR usage, Section 3 serves as a user's reference for the OZIPR commands and options, and Section 4 describes the ISOPLOT program and options. The fifth section provides examples of nine input files and the resulting output.

2 General Overview of OZIPR

Running OZIPR on a Personal Computer

The program is started by typing "OZIPR *filename*" for an input file called *filename*.INP. For this example, the program (ozipr.exe) and the input file are in the same subdirectory. However, it is also possible to use other directories as long as the path is designated. For example:

```
c:\ozipm\pgm\ozipr c:\ozipm\input\test1,
```

runs the OZIPR program in subdirectory c:\ozipm\pgm, using the input file test1.inp in subdirectory c:\ozipm\input.

Output files are created in the same sub-directory as the input files, if needed, using *filename* with different extensions. They are:

<i>filename</i> .OUT	The standard output file
<i>filename</i> .PRN	An ASCII file of selected time/concentration data suitable for importing into commercial spreadsheet programs.
<i>filename</i> .ISO	Output of isopleth results

The input file is a text file consisting of a series of OPTIONS and COMMANDS. In addition, the input file can contain the names of commonly used "include" files that are inserted into the text of the input file. This is done by inserting the character "@", followed by the complete filename of an include file at the location in the input file where the text of the include file is desired. More than one include file may be used, and they can also be used within the include files.

The general rules for the format of the input file and include files are:

- 1) The first 4 letters of a command are usually significant (in the following text, the actual significant letters are underlined);
- 2) Top level commands must be followed by ">", and commands end with a "<"

- 3) Upper case is currently mandatory;
- 4) Comments are allowed between { } and (), or on lines where the first character is "!";
- 5) The main input file (*filename*.INP) must terminate with "END."

Limits to Input

In previous versions of OZIPP, a fixed amount of input was allowed for a certain option, such as 20 photolysis reactions, or 24 hours of temperature, etc. These numbers were deeply buried in the computer code and could not be changed. One result of this study was to uncover these numbers and bring them to the top of the program so that they may now be easily changed if the user wishes to expand the program's capabilities.

In the following section many options allow up to n hours, species, reactions, etc. If the user attempts to input more than n values, the program will print a message and stop. The value n can be increased with minor alteration of the program, but possession of the source code and knowledge of FORTRAN compilation is required.

The parameters that can now be easily varied and their current limits are:

Simulation Hours =	24
Total Reactions =	160
Photolysis Reactions =	23
Reaction Products =	12
Total Species =	65
VOC Species =	20
Emitted Species =	10
Isopleth Species =	12
Deposition Species =	10
Print Species Names =	20
Average Species Names =	10
Dump Names =	12
Dump Rates =	12
File Species Names =	20

VOC, NMOC, and NMHC

Over the years a number of seemingly ambiguous methods to group volatile hydrocarbons have developed. In OZIPR any organic compound, including methane, may be entered as a species by including it in at least one reaction in the MECHANISM option. In addition, OZIPR and OZIPM allow grouping into one unique set of organics, the group named VOC (volatile organic compounds, which is usually used to describe those classes of anthropogenic emitted organics that are subject to control).

The group of individual organic species that comprise VOC is defined within the MECHANISM option; the species are named and the number of carbons in each is given. The BOUNDARY/REACTIVITY option allows the user to list the fractions of each species included in the VOC group that constitute emitted VOC, surface transported VOC, and aloft transported VOC. These three sets of information allow OZIPR to account for emissions and transport of the mass in the group VOC.

Most important, however, is the fact that this specific method of grouping facilitates the EKMA and ISOPLETH options. By lumping all organic species subject to emission control as VOC, it is a simple function for OZIPR to diminish VOC emissions in ozone attainment calculations. [Similarly, NO_x and CO are controlled in EKMA calculations, where NO_x is a combination of NO and NO_2 and CO represents carbon monoxide.]

Therefore, VOC is a specialized OZIPR subset of often-used organic compound groupings called non-methane organic compounds (NMOC) and non-methane hydrocarbon compounds (NMHC). VOC is reported in ppmC. The ratio of VOC to NO_x is not necessarily the ratio of all NMOC to NO_x . No effort is made in any OZIPP version to combine and count all organic species as NMOC.

3 User's Guide to Command Options

This section contains a list of the available command options that can appear in the input file. As noted, format is no longer column-oriented, but the conventions noted in the previous section must be followed. The options are first listed to indicate proper format. A brief discussion of each option follows this listing. The default values for each command are listed as "DF =". Most options are similar to those implemented in previous versions of OZIP, and the reader should consult the most recent OZIPM-4 report (Hogo and Gery, 1988) for more detail concerning the basis of various options.

Many options in OZIPR require data from a previous option. Therefore, the ordering of the options in the input file is important. In many cases, the program will terminate with a notice to check input if improper ordering could cause an otherwise undetectable error. It is suggested that the following order be maintained as the order of all input streams. However, note that it is possible to stack successive commands in one input stream. For instance, after input of various meteorological and boundary conditions, one can perform a CALC and EKMA, then change some earlier meteorological conditions and perform another EKMA.

The OZIPR options are:

ECHO of input file:

ECHO; or NOECHO;

ECHO allows the user to list the input file as it is read by the program. The NOECHO (or OFF) command terminates echoing of input (DF = NOECHO). These commands may appear anywhere in the input stream.

Program MODIFICATION commands:

MODIFY >

WIDTH = number;

ACCURACY = number;

TENSION = number;

< (MODIFY)

WIDTH is the column width of the device upon which the output file will be printed. The present options are for 80 or 132 columns (DF = 80).

ACCURACY is the error tolerance of the numerical integration routine, from 0.1 to 0.00001. Smaller values require more calculations at greater accuracy (DF = 0.003).

TENSION is the factor for the hyperbolic spline functions used in the EKMA routine when two ozone maxima occur in a single simulation (DF = 2) . If convergence is not achieved, changing this factor may help. However, the default is usually the best value and it is not recommended that this be to changed unless necessary.

Chemical Mechanism Listing command:

MLIST/(NOMECHLIST);

MLIST provides a listing of the chemical mechanism used, a list of rate constants at standard conditions, and a list of the kinetic expressions and rate parameters used (DF = NOMECHLIST).

NOMECHLIST disables chemical mechanism listing.

Chemical MECHANISM input:

MECHANISM [units] >

CNUMBERS = vocspecies1, C#,

vocspecies2, C#,

.

.

vocspeciesn, C#;

REACTIONS = (see below)
< (MECH)

MECHANISM is the **mandatory**, user-supplied chemical kinetics mechanism. Input is relatively free-format, although a certain order must be maintained as discussed next. *Units* refers to the type of units that the kinetic expressions and rates utilize (also below). At present, the default is "PPM" (ppm-min units) with the only option being "CM" (molec-cc-sec units). One unit format must be chosen per simulation. As noted, the previous top-level command, MLIST/NOMECHLIST can be used to provide a listing of the reactions and kinetic expressions in the output file.

CNUMBERS allows the **mandatory** naming of the non-methane organic species included in the "VOC" mixture, and tells OZIPR the number of carbon atoms in each species. The species named in CNUM must match the VOC species listed in the BOUN/REAC option. Also, this option must precede the REACTION listing on input.

The REACTION LISTING format follows these rules:

Immediately after the CNUM option, the text string "REACTIONS=" designates the beginning of free-format reaction listing input. This is followed by a listing of each consecutive reaction as described next. Species names have up to 4 significant characters, any extra are truncated. Legal characters to use in naming species are "A-Z", "a-z", "0-9", and ":". Tabs are not allowed (the space bar must be used to insert blank spaces).

Each reaction begins with the reactants (if there are any). Zero to 3 **Reactants** may be included, separated by "+". No stoichiometry is allowed for reactants. After the reactants, a "=" indicates that a list of products will follow. M, N₂ and O₂ may be used as reactants. The concentrations of these species have been coded into OZIPR and do not need to be specified by the user (DF: O₂ = 209,460 ppm, N₂ = 780,840 ppm, and M = 1,000,000 ppm). The rate constants given will be appropriately multiplied by the concentrations of these species to produce rate expressions.

Even if there are no products or no reactants, a "=" is mandatory for each reaction. Zero to twelve **products** and product coefficients are allowed. Products and their stoichiometric coefficients are joined by a "*". Products, or coefficient*product pairs, are linked by a "+". In the event of a negative coefficient, the "+" is still required prior to the "-" of the coefficient ("+" is a symbol linking entities while "-" is part of the coefficient).

After listing the reactions, a rate expression, initiated by either "#" or "%", must be included. There are many types of rate expressions, which are described below.

Further, the rate expression may be modified by a number of options, including dependence on the solar zenith angle (photolysis reactions) and dependence or equilibrium with other rates or reactions. These modifiers begin with the symbols "*" and "/", followed by symbolic language as described below.

Each reaction is terminated by ";".

Rate Expressions are of two types, standard and special. Most standard expressions, with the exception of falloff expressions, can be used when rate constants are expressed in either CM or PPM units. The input of standard rate expression parameters begins with "#". Following this, the "@", "^", and "&" are used to allow input of various parameters as follows:

<u>Standard Expression</u>	<u>Input Form</u>
$k = A$	#A
$k = A \times (T/300)^B$	#A^B
$k = A \times e^{(-C/T)}$ (where $C=E_a/R$)	#A@C
$k = A \times (T/300)^B \times e^{(-C/T)}$	#A^B@C

The **falloff expression** listed below requires the values of A, B, and C to be input in CM units even if all other reactions are listed in PPM units.

$$k = \left(\frac{k_o[M]}{1+k_o[M]/k_i} \right) F^G \qquad \#A_o^B_o@C_o\&A_i^B_i@C_i\&F\&n$$

where:

k_o and k_i are of the form $A \times (T/300)^B \times e^{(-C/T)}$, or any other standard format.

and,

$$G = \{1+[\log(k_o[M]/k_i)/n]^2\}^{-1}$$

[M] is known and automatically included in the falloff rate constant calculations. E_a is the activation energy in kcal/mole. The value included on input is $C = E_a/R$, where R is 0.0019872 in these units. **Be careful of the sign of C.**

The falloff parameters k_0 and k_i are input in one of the standard formats given above. k_0 always precedes k_i on input. F and n need not be included. If not specified, the defaults of 0.6 for F and 1.0 for n are used. Units of these falloff reactions are **always CM**.

Special rate expressions are fixed algebraic expressions of a non-standard type. These expressions begin with the character "%".

<u>Special Expression</u>	<u>Input Form</u>
$k = A \times (1.0 + 0.6 \times \text{Pressure})$	%1 #A
$k = k_0 + \left(\frac{k_3[M]}{1 + k_3[M]/k_2} \right)$	%2 #A ₀ @C ₀ &A ₂ @C ₂ &A ₃ @C ₃

where, k_0 , k_2 , and k_3 are of the form $A \times e^{(-C/T)}$, as in the standard expression above.

Special rate 1 is used for the OH + CO reaction where pressure is in atmospheres and the value for A is either in CM or PPM depending on the main **units** in the MECH option.

Special rate 2 is a Lindemann-Hinshelwood expression, primarily used for the OH + HNO₃ reaction. These parameters must **always** be in CM units.

Modifiers of rate expressions provide (1) dependence on another rate, (2) reverse equilibrium with a second-order forward reaction, or (3) dependence on a value that varies with zenith angle of the sun.

Linear dependence on another rate is of the form:

<u>Expression</u>	<u>Input Form</u>
$k = A \times Kn$	#A *Kn

where A is a linear factor and Kn is the *n*th reaction listed in the MECH option. This expression can be used in either rate format (CM or PPM).

A **reverse equilibrium rate** (only for first-order decomposition) can be calculated directly from the equilibrium constant (K_{eq}) by including the equilibrium constant data and the reaction number of the forward equilibrium reaction.

<u>Expression</u>	<u>Input Form</u>
-------------------	-------------------

$$k_r = k_f / A \times e^{(-C/T)} \quad \#A@C *En$$

where A@C is the equilibrium constant and n is the reaction number of the forward reaction. This expression can be used in either rate format (CM or PPM), with any type of forward rate expression, but the equilibrium expression must be in the "A@C" format and the reverse reaction must be a first-order process.

Photolysis reaction indicators follow the kinetic expressions for each reaction. The format is either "/Ln" or "/Rn", where L refers to a specific table (Ln) of absolute reaction rate factors vs. solar zenith angle in the ZENI option and R refers to table Rn of relative reaction rate factors in ZENI. The relative factors will be multiplied by the absolute factors listed for L1 in the ZENI option, after which, all relevant factors will be multiplied by the calculated rate of reaction. For this reason, in both the REACTION listing and the ZENI option, **the listing of L1 should precede the listing of any relative (R) reaction rates**. Note that first-order reaction rates are in min⁻¹ for PPM units and sec⁻¹ for CM units.

The rate modifiers operate under the following restrictions: (1) "*K" and "*E" cannot be used in the same reaction, (2) any "*" modification must precede "/" if in the same reaction, and (3) photolytic ("/L" or "/R") reactions are allowed with falloff rate expressions.

ZENITH Angle Dependence of Photolysis Rates

ZENITH >

L1: za0, za10, za20, za70, za78, za86,

R or Ln: za0, za10, za20, za70, za78, za86,

R or Ln: za0, za10, za20, za70, za78, za86,

R or Ln: za0, za10, za20, za70, za78, za86;

< (ZENI)

ZENITH allows the user to vary the rates of photolytic reactions relative to the angle of solar elevation (which is related to the spectral distribution of actinic flux). The values in these tables are input for 10 zenith angles (0 through 70 in increments of 10, and 78 and 86 degrees from zenith). A cubic spline interpolation is performed to find the factor value for the current zenith angle. The tables in this option are accessed by including "/Ln" or "/Rn" at the end of a reaction in MECH. Since all relative ("/R") factors are multiplied by the current value of L1, **the L1 listing must precede all R listings**.

Simulation TIME command:

TIME > *number1*, *number2* <

TIME controls the start and end times of simulations. *Number1* is the start time and *number2* is the end time. Both numbers are required (DF = 800 to 1800). The opening ">" may be substituted for by an "=" and the closing "<" may be substituted for by a ";".

TITLE of simulation:

TITLE > text(up to 72 characters) <

TITLE allows the user to insert a text string defining the simulations. The opening ">" may be substituted for by an "=" and the closing "<" may be substituted for by a ";".

PLACE of simulation

PLACE >

CITY = name;
LATITUDE = number,
LONGITUDE = number,
TZONE = number,
YEAR = number,
MONTH = number,
DAY = number;
< (PLACE)

PLACE is necessary to determine the zenith angle of the sun throughout the day.

CITY is the name of the location for the particular simulation. The city name can be up to 24 characters (DF = Los Angeles, CA).

LATITUDE is the latitude in degrees north (DF = 34.058).

LONGITUDE is the longitude in degrees west (DF = 118.250).

TZONE is the local time zone, Eastern Daylight Time = 4, Pacific Daylight Time = 7 (DF = 7).

YEAR is the year (DF = 1990).

MONTH is the month (DF = 6).

DAY is the day (DF = 21).

METEOROLOGICAL conditions:

METEOROLOGY >

DILUTION =

MHINIT = number,

MHFINAL = number,

TINIT = number,

TFINAL = number;

MIXING [*nmix*] = mh1, mh2, mh3, mhnmix;

TEMPERATURE [*ntemp,tunit*] = t1, t2, t3, ... *tntemp*;

PRESSURE [*punit*] = number;

WATER [*wnum*] = w1, w2, w3, ... *wwnum*;

RH [*wnum*] = w1, w2, w3, ... *wwnum*;

< (MET)

The METEOROLOGY command allows the user to input mixing heights, temperature, pressure and water vapor concentrations. This option must precede EMIS and MASS, as well as CALC, ISOP, and EKMA.

DILUTION activates the characteristic mixing height curve based on the following input information:

MHINIT is the initial mixing height **in meters** (DF = 510m).

MHFINAL is the final mixing height **in meters** (DF = 630m).

TINIT is the starting time of mixing height increase (DF = 800).

TFINAL is the ending time of mixing height increase (DF = 1500).

MIXING allows input of mixing height values (**in meters**) at the beginning and end of each simulation hour. *nmix* is the number of values input, if dilution occurs for *n* hours, the number of mixing height inputs should be *n*+1. (DF is to use DILU).

TEMPERATURE allows input of average column temperature values at the beginning and end of each simulation hour. *ntemp* is the number of values input, which is usually the number of hours+1 (DF = 303 K constant). *tunit* specifies the temperature scale used on input (DF = "K" for Kelvin; other options are "C" for Centigrade and "F" for Fahrenheit).

PRESSURE is the constant pressure to be used throughout the simulation. *punit* specifies the pressure scale used on input (DF = "AT" for atmosphere). Other options are "TO" for Torr (mm of Hg) and "IN" for inches of Hg (DF = 1 atm.).

WATER [*wnum*] allows input of average column water concentration in ppm at the beginning and end of each simulation hour. *wnum* is the number of values input,

which is usually the number of hours+1. If no water or RH values are input, DF = 20,000 ppm.

RH[*wnum*] allows input of relative humidity values at the beginning and end of each simulation hour. *wnum* is the number of values input, which is usually the number of hours+1. Because TEMP and PRES values are needed to calculate water concentrations from RH, this option must follow the TEMP and PRES options or an error will occur. There is no default for RH. If no option is used for water, water concentration is defaulted as described in the WATER option.

If the simulation time extends past the number of values entered for TEMP, WATER, or RH, the last value listed is extended to the end of the simulation. This makes it possible to perform simulations with constant values by merely including one initial value in a table.

BOUNDARY Conditions:

BOUNDARY >

REACTIVITY =
vocspecies1, init_reac, aloft_reac, surf_reac,
.
.
vocspeciesn, init_reac, aloft_reac, surf_reac;

IFRACTION NO2 = fraction;

EFRACTION NO2 = fraction;

TRANSPORT =
O3SURFACE = concentration,
O3ALOFT = concentration,
VOCSURFACE = concentration,
VOCALOFT = concentration,
NOXSURFACE = concentration,
NOXALOFT = concentration,
COSURFACE = concentration,
COALOFT = concentration;

ALOFT CONCENTRATIONS =
specie1 = concentration,
.
.
specien = concentration;

INITIAL CONCENTRATIONS =
specie1 = concentration,

```
. .  
. .  
specien = concentration;
```

```
DEPOSITION RATE PROFILES [numhours] =  
specie1 = ratehour1, ratehour2, ... ratehournum,  
. . . .  
specien = ratehour1, ratehour2, ... ratehournum;
```

```
CONSTANT DEPOSITION RATE =  
specie1 = rate,  
. . . .  
specien = rate;
```

< (BOUNDARY)

The BOUNDARY option controls the various concentrations, reactivities, and deposition rates that occur at the boundaries of the reacting column. This option must precede EMIS and MASS, as well as CALC, ISOP, and EKMA. It should be noted that the NO₂/NO_x fraction for transported surface and aloft NO_x is defaulted to 1.00 and cannot be changed.

REACTIVITY is mandatory. For each species of the VOC group listed in the MECHANISM option, the user must include the species name and the fraction of total VOC that each species represents in the initial mixture (resulting from controllable emissions), the aloft VOC, and the transported surface-layer VOC. These fractions should sum to 1.0 across all VOC species for each category. If this is not the case, the program assumes any missing mass is in non-reactive species, or stops with an error message if the total fraction exceeds unity.

IFRACTION is the NO₂/NO_x fraction for the NO_x that is present due to controllable emissions at the start of the simulation (DF = 0.25).

EFRACTION is the NO₂/NO_x fraction for the NO_x emissions throughout the simulation (DF = 0.05).

TRANSPORT controls the initial concentrations of **O₃, NO_x, VOC, and CO** in the surface and aloft layers that are due to transport. The SURFace concentrations are used to account for the initially present mass in the surface layer that is due to transport. In the simulation, this is added to the initial mass resulting from controllable emissions (input with the CALC, EKMA or ISOP options) and the non-controllable mass input with INIT option. The ALOFT mass is added into the surface layer as the mixing height rises. Default values are all 0.0.

ALOFT CONCENTRATIONS are constant upper-layer concentrations of **species other than the TRAN species**. Mixing height rise will entrain ALOFT concentrations into the surface layer. Only H₂O will not be diluted or enhanced with mixing height rise.

INITIAL CONCENTRATIONS are initial surface-layer concentrations of **species (other than the specific groups noted in the TRAN option)** at the start of a simulation. However, additional NO, NO₂, or specific VOCs can be added here. If specific VOCs are added, their concentration should be given in ppmV. Note that the INIT concentrations are not controlled in EKMA calculations. If a non-controlled species is emitted, which is only possible if the MASS option is used, the initial surface concentration from the MASS option is added to any INIT concentration to determine the total initial mass. Therefore, if the MASS option is being used, INIT should only be used for the same species if additional mass is needed. H₂O **cannot** be initialized with INIT. MET/WATER or MET/RH must be used for H₂O.

DEPOSITION allows input of hourly deposition velocity (cm/s) profiles for up to 10 species (the limit of 10 also includes the constant deposition velocity below).

CONSTANT DEPOSITION (or CDEP) allows the input of constant deposition velocities (cm/s) for up to 10 species (the limit of 10 also includes the species in the DEPOSITION option; thus, if DEPO is used for 6 species, only 4 species can be input using the CON option.)

Input of hourly EMISSIONS:

EMISSIONS [*numhrs*] >

VOC =
em1, em2, em*numhrs*,
NOX =
em1, em2, em*numhrs*,
CO =
em1, em2, em*numhrs*;

or

MASS [*numhrs*] >

VOC [mw] = *conc*,
em1, em2, em*numhrs*,
NOX [mw] = *conc*,
em1, em2, em*numhrs*,
CO [mw] = *conc*,
em1, em2, em*numhrs*,
specie3 [mw] = *conc*,
em1, em2, em*numhrs*,

specien [mw] = conc,
 em1, em2, emnumhrs;
< (MASS or EMIS)

To input emissions, the user has two optional methods: EMIS or MASS. Only one method may be used with each simulation. This option must follow MET and BOUN, and precede CALC, ISOP, and EKMA. Only 3 species (VOC, NO_x and CO) are allowed for EMIS but up to 10 may be used with the MASS option.

The differences between EMIS and MASS are described next. These options have in common the following:

In the option command line, the user must include the number of hours that values will be given for. All species must use the same number of hours.

VOC, NO_x and CO are unique groups because the emissions of these species are varied in EKMA and ISOP calculations. The species included in the VOC group and the fraction of total VOC that each comprises are input using the BOUN/REAC and MECH options. NO_x consists of NO and NO₂ and the ratio of NO-to-NO₂ for both the initial surface layer and the emissions can be given in BOUN/REAC.

An emission ratio table will be printed on output. Regardless of the method used, the output will show the ratio of emissions to initial concentration for all emitted species or groups. These ratios are calculated at the initial mixing height, a temperature of 298.15 K, and the specified simulation pressure. During simulation the program continuously accounts for changes in the volume of the column (changing mixing height) and air density (temperature) before the mass of emissions is added to the air column. A second table is also printed showing mass emission rates (kg/km² / hour).

EMIS allows the user to input hourly emission fractions that are directly ratioed to the initial surface concentrations of controllable VOC, NO_x and CO emissions (the initial concentrations are input in the CALC, EKMA or ISOP options). The emission fractions should be calculated at the same mixing height as the initial, controllable surface concentrations; the program will automatically account for later changes in mixing height. Since this is a direct ratio to initial values given elsewhere, *conc* is not used and *mw* is not needed for conversion.

MASS allows the user to input hourly emission mass for up to 10 species or groups in units of kg/km² per hour. An initial concentration (in units of ppm) that is used by the program to convert hourly emission densities into emission fractions, must be included on the species line. For VOC, NO_x and CO, OZIPR compares this value to the concentration input in CALC, EKMA or ISOP for consistency. A warning message will print if there is a mismatch, but in some cases a different value is useful so the program does not stop. For

species other than VOC, NO_x and CO, the initial concentration (*conc*) specified in the MASS option is used as the initial mass due to emissions and is added to any INIT mass (see BOUN/INIT). This mass is then converted to ppm ratios. As noted above, because the calculation of column concentration of emissions also depends on the molecular density of air and the volume of the column, the ppm emission ratio factors printed on output will differ if TEMP and mixing height values vary from 298.15 K and the initial mixing height.

conc is used in MASS only. The units are ppmC for VOC and ppmV for all other species, including individual organics that are part of the VOC group.

mw is the molecular weight of a species used for conversion of MASS units to ppm. MW is mandatory for all species except VOC, NO_x, and CO. Molecular weights for these species need not be entered if default values are desired; the defaults are: VOC = 14.5, NO_x = 46, and CO = 28. If a different value is desired for VOC, the user should note that mw is the molecular weight of a carbon unit (CH_{2.5}) since the calculation is in ppmC. The default NO_x is the molecular weight of NO₂ because emission inventories are given as 100% NO₂.

Since EKMA does not control species other than VOC, NO_x, and CO, any other emissions input with the MASS option, including specific VOC species, will not be reduced in attainment calculations.

Individual CALCULATIONS (single simulations)

CALCULATE >

VOC = concentration;

NOX = concentration;

CO = concentration;

PRINT [print control options] =

NAMES [number] = species1, species2, speciesX,

TINIT = number,

TSTEP = number,

AVG [number] = species1, species2, speciesX,

TAVG = number,

CDUMP [number] = species1, species2, speciesX,

RDUMP [number] = rxn#1, rxn#2, rxn#X,

NODUMP;

FILE [number] = species1, species2, speciesX;

< (CALCULATE)

VOC is mandatory. It is the concentration of VOC (ppmC) in the initial surface-layer mixture that is due to emissions and subject to control. This mass is added to any transported

or other uncontrollable VOC sources to total the actual concentration that a simulation will begin with (DF: VOC = 0.0 ppmC).

NOX is mandatory. It is the concentration of NO_x (ppm) in the initial surface-layer mixture that is due to emissions and subject to control. At the beginning of a simulation this mass is added to any uncontrollable NO or NO₂ (DF: NOX = 0.0 ppm).

CO is the concentration (ppm) in the initial surface-layer mixture that is due to emissions and subject to control. This mass is added to any transported or other uncontrollable CO sources to total the actual concentration that a simulation will begin with (DF: CO = 0.0 ppm).

The concentrations listed for VOC, NO_x, and CO in the output file represent all the initial mass of these species that is included in the calculation. That is, the values printed at each time step in the output file include the VOC, NO_x, and CO concentrations listed in the CALC option as well as any VOC, NO_x, and CO transported in the surface layer. In addition, it includes the initial surface-layer concentration of any individual VOC species specified with the INIT option. It also includes the concentration of individual VOC species included in the MASS option.

PRINT controls the standard CALC output.

TINIT is the first time (minutes from the beginning of the simulation) when concentration and rate information is to be printed (DF = 60).

TSTEP is the time step (in minutes) from TINIT until the end of the simulation that concentration and rate information is to be printed (DF = 60).

TAVG is the time interval (in hours!) that the running maximum average concentrations for species in the AVG option are calculated over (DF = 1).

NAMES [number] are the names of up to 20 species for which the concentrations at each time step will be printed along with information on the instantaneous mixing height, zenith angle and temperature. The format of the output generated when the NAME option is used is similar to the format used in the OZIPM-4 program. Inclusion of a delimiter (comma or semicolon) after the NAMES sub-command will print all species (DF = all species).

AVG [number] are the names of up to 10 species for which running averages will be calculated and the highest reported at the end of a simulation. This also controls the species whose concentration at each time step are listed on the screen during run time. Concentration-time information for up to 5 species are given on the screen for the default column width of 80. If the width of output is 132 columns, concentration-time information for 10 species is listed on the screen (DF = O3).

CDUMP [number] produces a tabular listing of the concentrations for up to 12 species at each TSTEP at the end of the listing (DF=NODUMP).

RDUMP [number] prints a listing of the instantaneous rates for up to 12 reactions at each TSTEP at the bottom of the listing after CDUMP (DF=NODUMP).

NODUMP disables the CDUMP and RDUMP options.

The print output control options are:

CONC/NOCONC toggles the printing of concentrations for species selected with the NAMES option and controlled with the TINIT and TSTEP options. If the CONC option is used without the NAMES option, the concentration of all species included in the mechanism will be printed (DF = print concentrations).

NET/NONET toggles the printing of net rates of change of species selected with the NAMES option and controlled with the TINIT and TSTEP options (DF = do not print net rates).

HVRATES/NOHVRATES toggles the printing of hourly photolysis rate information (DF = print the rate information).

RRATES/NORRATES toggles the printing of net rates for each reaction in the mechanism (DF = do not print net rates).

FULL/BRIEF selects all or none of the above options.

If the only print control option used is BRIEF, the output file will include a concentration-time listing of each species named in the AVG option. Therefore, under these conditions, it is not necessary to use the CDUMP option unless a tabular listing of concentration-time information is desired for species not named in the AVG option.

FILE [number] stores concentration-time information for up to 20 species in an ASCII file (filename.prn). This file is suitable for importing into LOTUS-123. The simulation time and the concentration for a maximum of 20 species are output on one line. The LOTUS-123 limit is 240 characters per line for importing.

EKMA Calculations

EKMA >

BASE =
O3 = concentration,
RATIO = number,
CO = concentration,
VOC (or HC) = concentration,
NOX = concentration;
FUTURE =
DELNOX = number,
DELCO = number,
O3SURFACE = concentration,
O3ALOFT = concentration,
VOCSURFACE = concentration,
VOCALOFT = concentration,
NOXSURFACE = concentration,
NOXALOFT = concentration,
COSURFACE = concentration,
COALOFT = concentration;
EXTRA OPTIONS =
VOCMEASURED = concentration,
NOXMEASURED = concentration,
VOCLEVEL = number,
VOCTABLE,
NOXTABLE,
COTABLE,
TRYS = number;

< (EKMA)

BASE controls the base condition simulations. The options are these:

O3 is the mandatory design (base case) ozone concentration.

RATIO is the design VOC/NO_x ratio (ppmC/ppm) for the initial controllable emissions in the base year. If the base year VOC and NO_x concentrations have been previously calculated, RATIO can be substituted for by the following two options. This eliminates the need to converge on the design O₃ along the RATIO (RATIO is calculated from these two option values).

VOC is the calculated level of controllable VOC (ppmC) emissions that yields the base case O₃.

NOX is the calculated level of controllable NO_x emissions that yields base case O₃.

CO is the mass (ppm) in the initial surface-layer that is due to emissions and can be controlled in EKMA. This mass is added to initial transported CO (given in BOUN

for the base case, and in FUTURE for the future case) to total the actual initial concentration. Surface transported CO (COSURFACE) is not controlled in EKMA calculations. (DF = 0.0)

FUTURE controls the future condition simulations. The options are these:

DELNOX allows the user to change future NO_x emissions by a fixed percent. For example, a 20 percent reduction would require input of "DELN = - 20" (DF = 0).

DELCO allows the user to change future CO emissions by a fixed percent (DF = 0). This replaces the old credit option used in OZIPM-4. Use of this option assumes that the user has included CO information in the EMIS or MASS option.

O3SURFACE is the future concentration of surface transported ozone (DF = base case value).

O3ALOFT is the future concentration of ozone aloft (DF = base case value).

VOCSURFACE is the future concentration of surface transported VOC (DF = base case value).

VOCALOFT is the future concentration of VOC aloft (DF = base case value).

NOXSURFACE is the future concentration of surface transported NO_x (DF = base case value).

NOXALOFT is the future concentration of aloft NO_x (DF = base case value).

COSURFACE is the future concentration of surface transported CO (DF = base case value).

COALOFT is the future concentration of CO aloft (DF = base case value).

EXTRA allows additional sub-commands that enable the user to control calculations and output.

VOCMEASURED and NOXMEASURED are used together. These values are the measured, initial VOC and NO_x concentrations. This information can be specified to allow the program to determine the location of the base year ozone should two base year ozone values occur along one VOC/NO_x design line.

TRYS tells the program how many simulations to attempt when trying to converge on a base or future year solution (DF = 8).

VOCLEVEL allows the user to specify one level of VOC control to be performed. The VOC level is expressed as a percent change from the base year level (use a minus sign for percent reduction, e.g., 60 percent reduction = -60). This calculation is performed in lieu of an attainment calculation.

VOCTABLE generates a tabular report of change in ozone as a function of change in VOC emissions. This is done in lieu of an attainment calculation. This calculation uses the **future conditions** of surface and aloft transported species, deltaCO, and deltaNO_x, and reduces the final base case VOC in 10 percent intervals. The ozone calculated for these conditions is compared to the calculated base case ozone. If base case VOC and NO_x are already known, these values are used in lieu of base case calculations.

NOXTABLE generates a tabular report of change in ozone as a function of change in NO_x emissions. This is done in lieu of an attainment calculation. This calculation uses the **future conditions** of surface and aloft transported species and deltaCO, and reduces the final base case NO_x in 10 percent intervals. The ozone calculated for these conditions is compared to the calculated base case ozone. If base case VOC and NO_x are already known, these values are used in lieu of base case calculations.

COTABLE generates a tabular report of change in ozone as a function of change in CO emissions. This is done in lieu of an attainment calculation. This calculation uses the **future conditions** of surface and aloft transported species and deltaNO_x, and reduces the final base case CO in 10 percent intervals. The ozone calculated for these conditions is compared to the final calculated base case ozone. If base case VOC and NO_x are already known, these values are used in lieu of base case calculations.

The concentrations of VOC, NO_x, and CO given in the output file for attainment calculations include only the mass of these species in the initial surface mix that is subject to control; it does not include any VOC, NO_x, or CO transported in the surface layer or any individual VOC species whose surface transport concentration may be given in the INIT option.

ISOPLETH Calculations

ISOP >

VOCMAX = concentration,

NOXMAX = concentration,

CO = concentration,

MAXT,

PLOT = species1, species2, ... speciesn,

NALR = number;

< (ISOP)

The ISOPLETH option performs the 121 CALC simulations necessary to provide data for constructing an isopleth diagram. The results of the simulations are printed in the output file and in a file named *filename.ISO*. The .ISO file is then used as input to the ISOPLOT program (see below) to draw isopleths of most species included in the .ISO file. Also, if the .ISO file is renamed *filename.ALR*, it can be used by OZIPR to save simulation time by including results of ISOP calculations already performed (see below).

Even though the ISOP option will generate data in a .ISO file for each species, it may not be possible to draw an isopleth using the ISOPLOT program for some species under some conditions. Limitations and possible recourse are discussed in the following ISOPLOT section.

VOCMAX refers to the maximum VOC concentration on the abscissa of the desired isopleth diagram (the minimum value is always 0). Simulations are performed at decade percentages of this value (DF = 2.0 ppmC).

NOXMAX refers to the maximum NO_x concentration on the ordinate of the desired isopleth diagram (the minimum value is always 0). Simulations are performed at decade percentages of this value (DF = 0.28 ppmC).

CO is the mass (ppm) in the 6-9 a.m. surface layer that is due to emissions and can be controlled. This mass is added to COSURF (the mass due to initial surface transport) to arrive at the total initial concentration (DF = 0.0).

MAXT is a flag that activates the printing of solar noon and the time of the center of the maximum average ozone concentration for each simulation.

PLOT designates the names of the species to include in the *filename.ISO* file. The ISOPLOT program can then draw isopleths for most of these species. It is not necessary to include the number of species as in other options (DF = O₃ only).

NALR indicates to the program that a file exists named *filename.ALR* which contains results from the *number* of simulations already performed and listed in that file. The results are read instead of calculations. Note that species to be plotted and plot scales in *filename.ALR* must be consistent with the current ISOP options.

Termination of Input

END;

4 The ISOPLOT Program - Drawing Isopleth Plots

Running ISOPLOT

Although the ISOP option of the OZIPR program is used to create a file containing the results of OZIPR isopleth simulations (*filename.ISO*), the isopleth plotting function has been removed from OZIPR and placed in a separate program, ISOPLOT. This allows direct manipulation of plot parameters without the requirement of re-entering the OZIPR program each time. Besides this data file, the user must also create a plotting information file (*filename.INF*) which lists the species to be plotted and other options (described below).

The ISOPLOT program is started by typing:

```
ISOPLOT filename.INF/s/s/s filename.ISO
```

The extensions .INF and .ISO may be omitted. The "/s" symbols refer to user-supplied plotter description switches:

```
/H Requests all plots to a HP LaserJet Printer  
/E Requests all plots to an Epson RX or FX Printer  
/11      Requests creation of a M11DRAW File.
```

If the switches are not used, each isopleth will appear on the screen. The user then has the option of typing <enter>, "H", or "E". The "H" and "E" commands are similar to those above for the two specified printers except that only the plot displayed on the screen is produced. If <enter> is typed the next isopleth appears on the screen.

In this simple example, it is assumed that the required program files (isoplot.exe and isplt.exe), the information (.INF), and the data (.ISO) files are all in the same directory. It is also possible to use other directories as long as the paths are correctly designated. For example:

```
c:\ozipr\pgm\isoplot info data
```

runs the ISOPLOT program in subdirectory c:\ozipr\pgm, using the information and data files in the current subdirectory. However, because the ISOPLOT program calls an intermediate processing program (isplt.exe) and might be requested to produce M11DRAW files, an additional configuration file called ISOPLOT.CFG must be created in either the current directory or the directory with the isoplot.exe file. The ISOPLOT.CFG file designates the

location of the intermediate program and the location where the M11DRAW files will be saved:

ISPLT=pathname

M11FILES=pathname

If the ISOPLOT.CFG file is not in the current directory or the ISOPLOT directory, an information message is displayed and the program continues.

As already noted, the ISOPLOT program actually calls on a second program, ISPLT (isplt.exe), that reads the .INF and .ISO files and prepares an output file with a .PRN extension. Control then reverts back to ISOPLOT for preparation of screen isopleths and plots. Upon completion, the .PRN file is deleted unless the user requests that it be saved (see below). The user may execute the ISPLT program directly, for example:

```
ISPLT TEST.INF EXAMPLE.ISO
```

Switches are not allowed on the command line. Executing ISPLT generates an EXAMPLE.PRN file. ISOPLOT can then be run with only the PRN as input:

```
ISOPLOT EXAMPLE.PRN/s/s/s
```

This two-step execution involves more work and is not recommended unless the .PRN file is already created and the user wishes to re-display or print an isopleth.

ISOPLOT Commands

The information file is a text file containing a series of COMMANDS. The general rules for the free format input files are similar to those used in OZIPR. The first four letters are significant and upper case is mandatory. Comment lines start with "!" and in-line comments can be inserted between "{" and "}". Commands may be given in any order but must end with a semicolon, and the .INF file must end with the END command. The only other required command is the PLOT command. Default settings will be used if other commands are not specified.

```
PLOT_SPECIES =  species1  units1  n1 n2 n3 . . . nn,  
                  species2  units2  n1 n2 n3 . . . nn,  
                  species3  units3  n1 n2 n3 . . . nn;
```

XMAX = xx;
YMAX = yy;
XTIC = nn;
YTIC = nn;
SAVE_PRN_FILE;
ONE_DIGIT;
END;

PLOT_SPECIES designates the species/units/concentrations values to be plotted. Plots can be requested for up to 12 species. Blank spaces are used to separate values and a comma appears at the end of each line. A semicolon ends the command. The input values are:

Species must be the name of a species appearing in the .ISO file (i.e., the species must have been included in the ISOP option in OZIPR).

Units specifies the concentration unit to be used in constructing the isopleth. The following units are accepted: PPM, PPHM, PPB, PPT, or CMS (molecules/cc). Default is PPB.

n1 n2 n3 . . . nn list the isopleth line concentrations in the units given. If default units are used, no concentrations can be specified. Up to 20 concentrations can be requested. If no concentrations are specified, the program will select default values. Remember to change concentrations if you change units. If no points are found in a plot region, no line is drawn.

XMAX and YMAX set the abscissa (VOC axis) and ordinate (NO_x axis) for the plots. ISOPLOT will calculate settings, but these options can be used to override calculated values.

XTIC and YTIC set the number of tic marks on the isopleth plots. Defaults are XTIC = 6 and YTIC = 10.

SAVE_PRN_FILE will disable deletion of the .PRN file created by the ISPLT program.

ONE_DIGIT prints one significant digit in line labels (DF=two digits).

END terminates the option list.

Diagram Problems and Improvements

The ISOPLOT graphics output is intended to provide draft quality plots. Some line-drawing anomalies may occur, and labels may be overwritten at times. High quality graphics output will usually require importing of either the .ISO or the M11DRAW files into a

graphics package. However, it is possible to obtain reasonably good results with ISOPLOT with some knowledge of the plotting algorithm. The following paragraphs contain suggestions for improving and interpreting ISOPLOT diagrams.

Because ozone is the principal species for which isopleth diagrams are used, the isoline generation procedure was optimized to provide smooth ozone lines under a variety of conditions. This algorithm generally provides adequate diagrams for other species. However, if anomalous lines (such as spikes or crossed lines) appear on a diagram, the user should question the result in that portion of the isopleth diagram (see ISOPLOT Example 9 in the following section). It may be possible to improve the diagram by changing the above options to include more points in the diagram region. In other cases it may be necessary to change the ISOP options is OZIPR and generate a new .ISO file with a larger data domain. Another option is to import the .ISO file into a spreadsheet program, or the M11DRAW file into a graphics package, and attempt to eliminate anomalies and utilize the line drawing capabilities in those programs.

Some species are very sensitive to VOC and NO_x changes and concentrations will vary over many orders of magnitude in the .ISO file. Peroxides often have such characteristics. The large differences in concentration cause the plotting algorithm to take an extremely long time to calculate the location of the proper isoline points and sometimes there is only one point in the entire diagram domain. This will lead to display of an error message on the screen (since the program cannot draw a line with only one point). One solution to this problem is to convert the concentrations in the .ISO file into logarithms, either by creating a program or importing the .ISO file into a spreadsheet program. The user can then either use the plotting package in the spreadsheet program or export a second .ISO file and rerun ISOPLOT.

5 Examples

This section provides descriptions of OZIPR and ISOPLOT examples, along with copies of the appropriate input and output files. The ISOPLOT examples also display and discuss isopleth diagrams.

{Note to online version: This document does not contain text of the example files. These files are available with the rest of the OZIPR input files.}

OZIPR Examples

Nine example input files that exercise most of the major OZIPR options are discussed. The output files (.OUT, .PRN., and .ISO) that are generated by OZIPR are also provided. The examples and options used are:

Example 1: Sample Calculation using cm RADM Mechanism

Options Used:

MLIST	PLACE
MODIFY/WIDTH=132	MET/DILU
MECH	MET/TEMP
ZENI	MET/PRES
BOUN/REAC	EMIS
BOUN/IFRAC	CALC/PRINT[BRIEF]
BOUN/TRAN	CALC/PRINT/TINIT
BOUN/DEPO	CALC/PRINT/TSTEP
TIME	CALC/PRINT/AVER
TITLE	

This is an example of an individual calculation using the RADM-II mechanism with rate constants expressed in CM (molec-cc-sec) units. The mechanism is entered with an include file (@meccm.rad). An include file (@zen.rad) is also used to provide information on photolysis rates as a function of zenith angle. The output file includes a listing of the mechanism. The width of the output is 132 columns. The PRINT/BRIEF option was used so the output file contains a concentration-time dump of the 10 specified AVG species.

Example 2: Test Calculation with Isoprene Emissions using a modified cm CB4 Mechanism

Options Used:

MLIST	PLACE
MECH	MET/DILU
ZENI	MET/TEMP
BOUN/REAC	MET/PRES
BOUN/TRAN	MET/RH
BOUN/DEPO	MASS
TIME	CALC/PRINT[FULL]
TITLE	CALC/PRINT/AVG

This is an example of an individual calculation using a modified CB4 mechanism with rate constants expressed in CM units (some inorganic rates are updated). The MASS option is used to input emissions of VOC, NO_x, CO and ISOP. The initial concentration included for ISOP in the MASS option is 0.001 ppmV. Note that the VOC concentration listed in the output file at the first time step is 0.685 ppm. This includes the 0.680 ppmC specified for VOC in the CALC option and 0.005 ppmC isoprene (0.001 ppmV x 5). In an attainment calculation, the ISOP would not be subject to control.

Example 3: Sample Calculation Using a modified cm CB4 Mechanism

Options Used:

NOECHO	TITLE
MLIST	PLACE
MECH	MET/DILU
ZENI	MET/TEMP
MODIFY/WIDTH=132	MET/PRES
MODIFY/ACCU=0.001	MET/WATER
BOUN/REAC	EMIS
BOUN/IFRAC	CALC/PRINT[CONC,NOHV]
BOUN/EFRAC	CALC/PRINT/AVG
BOUN/TRAN	CALC/PRINT/TAVG
BOUN/INIT	CALC/PRINT/CDUMP
TIME	CALC/PRINT/RDUMP

This is an example of an individual calculation using a modified CB4 mechanism with rate constants expressed in CM units (some inorganic rates are updated). Unlike Examples 1 and 2, however, all photolytic rate constants are expressed as absolute rate factors instead of relative rate factors (i.e., the modifier /L instead of /R is used for all photolytic reactions). In this example, include files are used for BOUN/REAC (@reac.cb4) as well as for the MECH and ZENI options. EFRACtion in this example is also changed from its default value

of 0.05 to 0.10. The output file includes the 8-hour average maximum concentration for O₃. A concentration-time dump is included for 6 species and a reaction rate-time dump is included for four reactions.

Example 4: CALC and EKMA using cm CAL Mechanism

Options Used:

ECHO	PLACE
MLIST	MET/DILU
MECH	MET/TEMP
ZENI	MET/PRES
BOUN/REAC	MET/RH
BOUN/IFRAC	MASS
BOUN/TRAN	CALC/PRINT[CONC]
BOUN/INIT	CALC/PRINT/NAMES
BOUN/DEPO	CALC/PRINT/AVG
TIME	CALC/PRINT/FILE
TITLE	EKMA/BASE

This is an example of a single calculation and an attainment calculation using the CAL mechanism expressed in CM units. Note that reaction 21 in the MECH option contains a product with a negative coefficient and, therefore, the product is entered as "+ -1 * NO2". The INIT option is used to provide for the surface transport of HONO. The MASS option is used to input emissions of VOC, NO_x, CO and PRPE. The initial concentration of PRPE included in the MASS option is 0.001 ppmV. Note that the 0.001 ppmV of PRPE and the emissions of this species added with the MASS option are not controlled in the attainment calculation. The output file for the CALC simulation lists a value for VOC at the first time step of 0.363 ppmC. This includes the 0.36 ppmC of VOC that is given in the CALC option and the 0.003 ppmC of PRPE included in the MASS option. Note that the PRINT/FILE option is used so the output files for this example consist of EX8.out and EX8.prn, where the .prn file contains the simulation times and concentrations of the named species; this file is suitable for importing into LOTUS-123. In the EKMA calculation, the future concentrations of surface and aloft transported species are identical to the base case concentrations and, therefore, it was not necessary to use the EKMA/FUTURE option.

Example 5: CALC and EKMA using a modified cm CB4 Mechanism

Options Used:

ECHO	PLACE
MLIST	TITLE
MECH	MET/MIXING
ZENI	MET/PRES
BOUN/REAC	MET/RH
BOUN/INIT	EMIS
BOUN/TRAN	CALC/PRINT[BRIEF,HV]
BOUN/ALOFT	CALC/PRINT/AVG
BOUN/DEPO	CALC/PRINT/CDUMP
BOUN/CON	EKMA/BASE
TIME	EKMA/FUTURE

This is an example of an individual calculation and an attainment calculation using a modified CB4 mechanism with rate constants expressed in CM units (some inorganic rates are updated). This example includes the use of the BOUN/CON option to express constant deposition velocities (i.e., deposition rates that do not change from hour to hour). Note that RH values are only given for 5 hours although the length of the simulation is 12 hours. The last value of 50% for the relative humidity is extended to the end of the simulation. The CALC output is similar to Example 1 except that it includes a listing of the photolytic rate constants (i.e., PRINT[BRIEF,HV] in contrast to PRINT[BRIEF] of Example 1). Because this example requested a listing of photolysis rates, the output file does not include a concentration-time dump of the five AVG species. To obtain such a dump in this case, the option CDUMP was included. In the EKMA calculation, the FUTURE option was used to reduce the concentration of VOCSurface, VOCALOFT and O3ALOFT used in the attainment calculation.

Example 6: CALC and EKMA using ppm CB4 Mechanism

Options Used:

MLIST	MET/DILU
MECH	MET/PRES
ZENI	MASS
BOUN/REAC	CALC/PRINT[NOHV]
BOUN/IFRAC	CALC/PRINT/NAMES
BOUN/TRAN	CALC/PRINT/AVG
PLACE	EKMA/BASE
TITLE	EKMA/FUTURE

This example includes an individual simulation and an attainment calculation using the CB4 mechanism with rate constants expressed in ppm-min (PPM) units. The option FUTURE is used in the attainment calculation to reduce the concentrations of transported species and to reduce future emissions of NO_x and CO by 10 and 35%, respectively. Note that the concentrations of initial surface-layer NO_x and CO that is due to emissions is also reduced by 10 and 35%..

Example 7: EKMA using Extra Option

Options Used:

MLIST	TITLE
MECH	MET/DILU
ZENI	MET/PRES
BOUN/REAC	MASS
BOUN/IFRAC	EKMA/BASE
BOUN/TRAN	EKMA/EXTRA
PLACE	

This example, which is very similar to Example 6, demonstrates the use of the option EXTRA. Note that the initial conditions are the same as for Example 6. In that example, the initial VOC and NO_x concentrations that generate the base case ozone were determined. These concentrations are entered in Example 7 under EKMA/BASE in lieu of listing the VOC/NO_x ratio. The EXTRA options included here specify generating VOC, NO_x and CO tables and calculating the percent decrease in O₃ that would result from a 15% decrease in VOC. The tables and the VOCLevel calculation are performed in lieu of an attainment calculation.

Example 8: ISOP using a modified cm CB4 Mechanism

Options Used:

MLIST	TITLE
MECH	MET/DILU
ZENI	MET/TEMP
BOUN/REAC	MET/PRES
BOUN/IFRAC	MET/RH
BOUN/TRAN	MASS
PLACE	ISOP
TIME	

This is an example of the Isopleth option. Execution of this input file generates the output file ex8.iso which includes the results of the 121 CALC simulations that were conducted to provide the data needed for constructing isopleth diagrams for O₃, PAN, HNO₃, FORM, OH, HO₂, and H₂O₂.

Example 9: ISOP using RADM Mechanism

Options Used:

MODIFY/WIDTH=132	TIME
MECH	TITLE
ZENI	PLACE
BOUN/REAC	MET/DILU
BOUN/IFRAC	MET/TEMP
BOUN/TRAN	EMIS
BOUN/DEPO	ISOP

This is an example of the Isopleth option using the RADM-II mechanism with rate constants expressed in CM (molec-cc-sec) units. The example is similar to Example 1 above. However, execution of this input file generates the output file ex9.iso which includes the results of the 121 CALC simulations that were conducted to provide the data needed for constructing isopleth diagrams for O₃, PAN, HNO₃, HCHO, HO, HO₂, and H₂O₂. The demonstration of the ISOPLOT program using the ex9.ISO file is given below.

ISOPLOT Examples

Two examples of the ISOPLOT program are given next. The following examples include the .INF files and the isopleths drawn from above Examples 8 and 9. The options used are similar, except that the ONE option was used in Example 8 to provide output with fewer significant digits.

Some plotting anomalies are evident in Example 9. The crossed lines in the HNO₃ plot are probably due to the lack of a low concentration point on the 5 ppb line. That line should be ignored along the straight line segment that crosses the 10 ppb line. In the HCHO and HO plots, the line labels must be carefully scrutinized. For HCHO, the 30 and 35 ppb labels are displaced from the lines, while for HO the .40 and .45 ppt labels are superimposed. Finally, for the HO₂ isopleth, the plotting algorithm could not fit lower left region with the existing .ISO data. Probably, a smaller plotting range must be given in OZIPR to generate more detail in the .ISO file for HO₂.

5 References

Hogo, H. and M.W. Gery, Users Guide for Executing OZIPM-4 with CBM-IV or Optional Mechanisms. Volume 1. Description of the Ozone Isopleth Plotting Package–Version 4, EPA/600/8-88/073a, U.S. EPA, Research Triangle Park, NC (1988).