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Environmental
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Agency

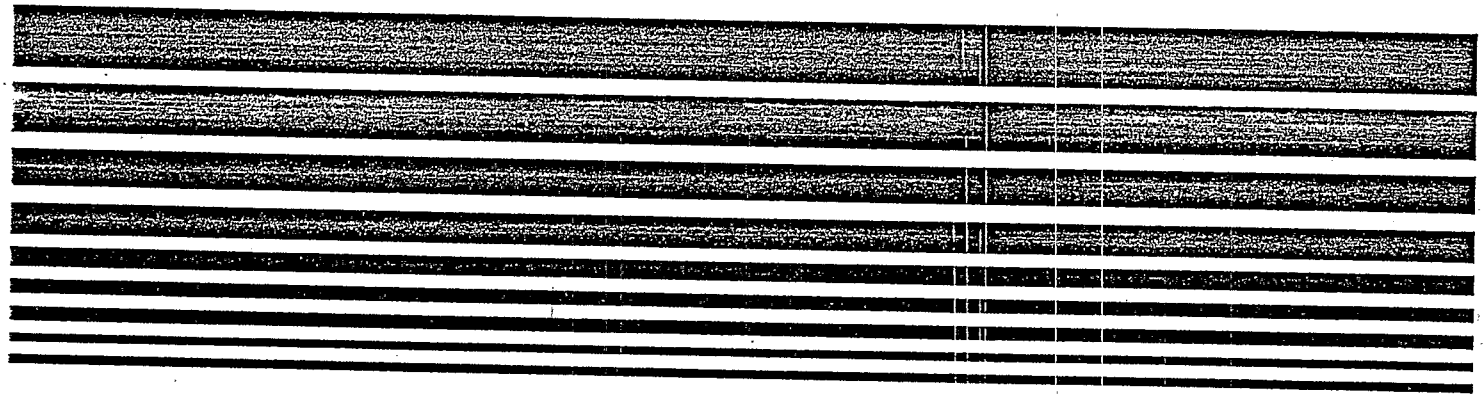
Office of Air Quality
Planning and Standards
Research Triangle Park, NC 27711

EPA-450/4-88-016
NOVEMBER 1988

AIR

EPA

# A PC BASED SYSTEM FOR GENERATING EKMA INPUT FILES



EPA-450/4-88-016

# A PC BASED SYSTEM FOR GENERATING EKMA INPUT FILES

By

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OFFICE OF AIR QUALITY PLANNING AND STANDARDS
U. S. ENVIRONMENTAL PROTECTION AGENCY
RESEARCH TRIANGLE PARK, NC 27711

NOVEMBER 1988

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## PREFACE

This document is one of five related to application of EKMA and the use of OZIPM-4 (Ozone Isopleth Plotting with Optional Mechanisms), the computer program used by EKMA. Listed below are the titles of the five documents and a brief description of each.

"Procedures for Applying City-specific EKMA", EPA-450/4-89-012, July 1989

- Describes the procedures for using the Empirical Kinetic Modeling Approach (EKMA). The major focus is on how to develop needed inputs for OZIPM-4. In addition this document describes how to determine a control target once OZIPM-4 has been run.

"A PC Based System for Generating EKMA Input Files", EPA-450/4-88-016, November 1988

- Describes a program that creates EKMA input files using a menu driven program. This sofware is only available for an IBM-PC or compatible machine. Files built using this system can be uploaded to a mainframe computer.

"User's Manual for OZIPM-4 (Ozone Isopleth Plotting with Optional Mechanisms)-Volume 1", EPA-450/4-89-009a, July 1989

- Describes the conceptual basis behind OZIPM-4. It describes the chemical mechanism, Carbon Bond 4, and each of the options available in OZIPM-4. Formats for each of the options are outlined so that a user can create input files using any text editor.

"User's Manual for OZIPM-4 (Ozone Isopleth Plotting with Optional Mechanisms)-Volume 2: Computer Code", EPA-450/4-89-009b, July 1989

- Describes modifications to the computer code that are necessary in order to use OZIPM-4 on various machines. A complete listing of OZIPM-4 is also found in this publication.

"Consideration of Transported Ozone and Precursors and Their Use in EKMA", EPA-450/4-89-010, July 1989

- Recommends procedures for considering transported ozone and precursors in the design of State Implementation Plans to meet national ambient air quality standards for ozone. A computerized (PC) system for determining whether an ozone exceedance is due to overwhelming transport is described. This document is necessary, only if an area is suspected of experiencing overwhelming transport of ozone or ozone precursors.

EKMA may be used in several ways: (1) as a means for helping to focus more resource-intensive photochemical grid modeling analyses on strategies most likely to be successful in demonstrating attainment; (2) as a procedure to assist in making comparisons between VOC and NOx controls; (3) in non-SIP applications, such as in helping to make national policy evaluations assessing cost/benefits associated with various alternatives and (4) for preparation of control estimates consistent with limitations/provisions identified in Clean Air Act Amendments.

## ABSTRACT

The OZIPM-4 computer program associated with the Empirical Kinetics Modeling Approach (EKMA) is an acceptable modeling approach for ozone air quality analyses. The OZIPM-4 computer program was developed for use on large mainframe computers. With the advancements in computer technology, many mainframe computer codes such as OZIPM-4 can now be executed on personal desktop computers. This report describes the use of a menu-driven version of the OZIPM-4 designed to run on an IBM PC/XT/AT or true compatible personal computers. Such a system provides an efficient method to develop input files required to execute the OZIPM-4 code. This report serves as a user's guide showing how to use the interactive system. The methods of developing the input variables are discussed elsewhere and are not presented in this document.

## ACKNOWLEDGEMENTS

The OZIPM-4 input file generator was developed using Turbo Prolog by Borland, Inc. Special thanks are given to Dr. Harvey Jeffries of the University of North Carolina for his guidance and recommendations in the development of the program.

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## FIGURES

# 1. INTRODUCTION

This computer program is intended to assist users in developing input files needed to run OZIPM-4 (Ozone Isopleth Plotting with Optional Mechanisms). It has been written for use on an IBM-PC or compatible machine. A menu driven system allows the user to select options, fill in the blanks and create input files. This program has on screen help features for nearly all input fields. In addition, the system can view input or output files and plot isopleth diagrams to the screen or to a compatible plotter.

An earlier version of this program could also make OZIPM-4 runs by accessing the RUN option from the menu. This feature is no longer supported. The OZIPM-4 code utilized in the earlier version contained some proprietary software which allowed intermediate results to be displayed to the screen. In order to provide an uncompiled version of OZIPM-4 to users, it was necessary to modify OZIPM-4 and to disable the RUN option. Users must now run OZIPM-4 in batch mode as described in Chapter 5.

This manual is divided into five chapters. The second chapter describes the hardware requirements, startup procedures, and moving around within the OZIPM-4 system. Chapter 3 provides quick-start procedures for users familiar with setting up input files for OZIPM-4. Chapter 4 describes the primary options available in the OZIPM-4 system. Chapter 5 describes methods for running OZIPM-4 and the plotting software in batch mode.

# 2. INSTALLATION AND STARTUP

System hardware requirements and procedures for installing the OZIPM-4 distribution disks onto the personal computers are presented in this chapter. This chapter also provides a general overview of the OZIPM-4 system and a summary of commonly used keys.

## SYSTEM REQUIREMENTS

This program is designed to run on any IBM PC/XT/AT or true compatible with a minimum of 512KB RAM memory. The OZIPM-4 system has been run under MS-DOS 3.1 and greater. The OZIPM-4 system requires a hard disk with at least 1MB of free disk space. (The software provided on the two distribution disks occupies about 720KB of disk space.) A math coprocessor is strongly recommended although it is not needed to run the OZIPM-4 system. A system with a math coprocessor will run approximately five times faster than a system without the coprocessor. The OZIPM-4 system will run under any of the four common screen displays (monochrome display adapter, MDA; Hercules-compatible monochrome graphics, MGA; color graphics adapter, CGA; and enhanced graphics adapter, EGA). The OZIPM-4 system will also run in several of the video graphics array (VGA) modes. A line printer and/or plotter is desirable, but not necessary to generate hard copy output of OZIPM-4 calculations.

## INSTALLATION

Note: The subdirectory containing the OZIPM-4 software must be called "OZIPM-4" and must be located directly under the ROOT directory.

To invoke the OZIPM-4 system from any place on the hard disk, edit the existing PATH statement in the AUTOEXEC.BAT file and append "\OZIPM-4". If the PATH statement is not used, simply type "PATH = \OZIPM-4". Refer to the DOS User's Guide for further information on the use of the PATH statement and AUTOEXEC.BAT. To complete the installation of the OZIPM-4 system, a "FILES=20" and "BUFFERS=20" specification must be set in the CONFIG.SYS file. If a CONFIG.SYS file already exists (this file can be found at the root directory), then edit the file and include the above statements. If a "CONFIG.SYS" files does not exist, then one must be created in order to use the OZIPM-4 system. To create this file, simply type the following statements:

```
CD \
TYPE CON CONFIG.SYS
FILES=20
BUFFERS=20
^Z      (NOTE:  this is control-Z)
```

Installation of the OZIPM-4 system is now completed.

## STARTUP

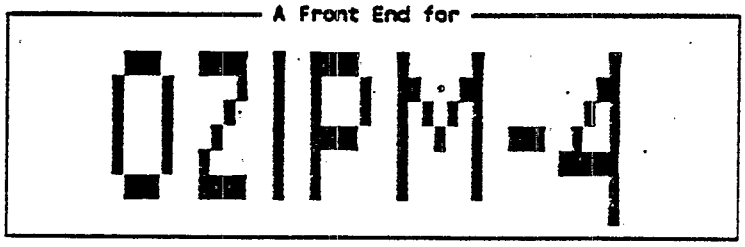
To access the program, type "**OZACCESS**" from any location of the hard disk. It is recommended that separate subdirectories be created to store the input and output files developed for OZIPM-4. The program will configure itself to access the input and output files in the current subdirectory when the "Directory" option is specified. (See Chapter 4 for more information on the Directory option.)

The OZIPM-4 front-end banner (Figure 2-1) will appear on the screen while the program is loaded into memory. After the program is loaded into memory, the primary option menu will appear on the screen.

## MOVING AROUND IN THE PROGRAM

The primary option menu (shown in Figure 2-2) consists of six options:

| | |
|---|---|
| Edit | Edit an existing or create a new input file |
| Load/save | Load or save an input file |
| Run | Execute the OZIPM-4 program (HAS BEEN DISABLED) |
| Plot | Plot isopleth diagrams onto the screen or on a plotter |
| Directory | Setting the working directory as the default directory |
| Quit | Exiting the OZIPM-4 system |




Written for the Environmental Protection Agency by
Systems Applications, Inc., San Rafael, California

Loading program files

Figure 2-1. Example screen display of the OZIPM-4 front-end banner page.

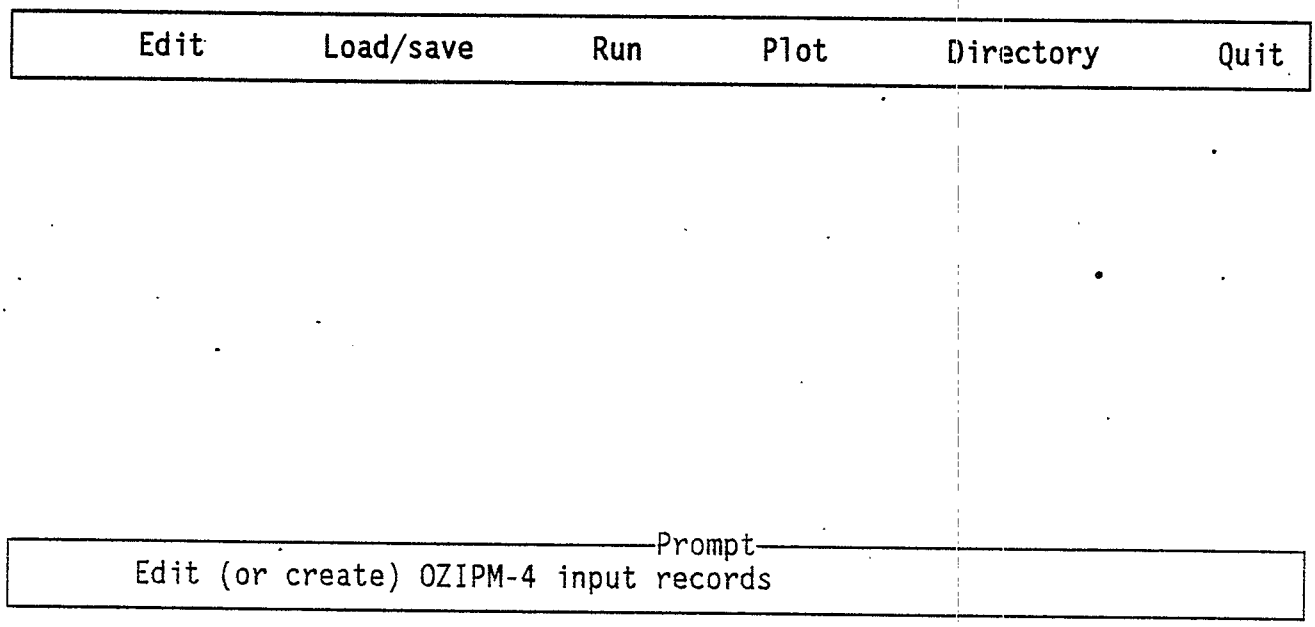



Figure 2-2. Example screen display of the primary option menu.

Access any of the six options by typing the first letter of the option or by using the left and right arrow keys (found on the numeric pad of the keyboard) to position on the desired option and hitting the **ENTER** key.

In order to provide a computer program that will run on many systems, the RUN option has been disabled. The procedure for making OZIPM-4 simulations is discussed in Chapter 5.

In general, first-time users of the program will perform the following tasks:

1. Create an input file for the OZIPM-4 main program.

2. Edit the existing input file to perform further simulations.

3. Save the input file.

As seen in Figure 2-2, the primary option menu consists of two banners. The top banner contains the six options. The bottom banner (the Prompt banner) shows a brief message describing the option. With the left and right arrow keys, you can move back and forth between the six options. As you do so, the message on the bottom banner will change accordingly. A reminder of the keys one can use to move around in the program is shown at the very bottom of the screen.

## KEY DEFINITIONS

The program relies on several keys to perform many of its basic functions. This section describes all special keys used by the program. Each key is defined as follows.

**↑↓←→** The up, down, left, and right arrows are used extensively to position the cursor to different locations of the screen.

**TAB** The TAB key operates in a similar fashion as the arrow keys within the OZIPM-4 submenus. Use of the TAB key is generally more efficient to move around the various input parameters. Hitting the TAB key will move the cursor forward. Hitting the SHIFT+TAB keys will move the cursor backwards.

**ENTER** The ENTER key is used to store an input value in OZIPM-4. The ENTER key **must** be hit to save the entered value.

**ESC** The ESC (Escape) key is used to leave a submenu of the program. Hitting the ESC key **will** discard any entry made in a submenu.

**F1** The F1 key activates the help message system. Help messages will appear on the screen. All help messages can be removed by hitting the SPACEBAR.

**F9** The F9 key is used to clear an input option from future use. For example, this key provides a way to erase the EKMA input option if the user wishes to run another option such as the ISOP input option. Use the F9 key only to clear an input option. Do not use this key when an option has not been declared with the F10 key.

**F10** The F10 key **must** be pressed after an input option is created or edited. The entered values will be saved within OZIPM-4 for later processing (either to be saved to a file or to be used in the execution of OZIPM-4).

## HELP MESSAGES AND ERROR MESSAGES

The program provides on-line help messages for nearly all the different options and parameters within the interactive system. The parameter options are those found in Appendix A. Error messages which may occur are FORTRAN errors which are recorded by the program and displayed on the monitor. Most FORTRAN error messages are self-explanatory. The most common error message will be:

**execution error U2253: command failed**

This error message indicates that there is not enough memory to execute the program. The user should check to see if enough memory is available to use the OZIPM-4 system by typing **"CHKDSK"**. The amount of free memory must be at least 460KB in order to execute the OZIPM-4 program. Usually memory-resident programs are using the RAM memory and must be unloaded from memory in order to use the program. Some memory-resident programs may be unloaded by the user, others are unloaded when the system is powered-off or rebooted. Check the manuals provided with the memory-resident program to determine how to unload the program from memory. An alternate approach is to boot the system from a system floppy diskette which does not contain an **AUTOEXEC.BAT** file which invokes the memory-resident program nor a **CONFIG.SYS** file which contains additional device driver specifications.

# 3. QUICK START PROCEDURES

This chapter describes several general steps in performing OZIPM-4 calculations. This chapter is intended for users familiar with the mainframe version of OZIPM-4 and serves as a summary of the procedures to follow in performing simple tasks in this program. This chapter is not recommended for first-time users. First-time users should read Chapter 4 and explore the various menus provided in the program before performing actual EKMA calculations. It is recommended that all users read Chapters 4 and 5 to receive maximum benefits from the program. This chapter is divided into six sections. Each section is presented in a step by step manner.

## SETTING THE WORKING DIRECTORY

1. Change directory location to the subdirectory containing the OZIPM-4 input files using the DOS "CD" command.

2. Invoke the program by typing "**OZACCESS**". (Make sure the **PATH** statement is used.)

3. In the primary option menu, either hit the **D** key or with the left and right arrow keys move the cursor to the **Directory** option and hit the **ENTER** key.

4. Chose the **Working** option by hitting the **ENTER** key.

5. Type in the name of the current subdirectory. **NOTE:** The full pathname including the drive letter should be entered (e.g., C:\MYWORKDR). Hit **ENTER** to set the working directory.

6. In order for the program to use the current subdirectory as the default directory, choose the **Save** option by hitting the **S** key or by using the down arrow to position on the **Save** option and hitting the **ENTER** key. The program will create a file called "WHIZ.SYS" in the current subdirectory. When the program is invoked in the current subdirectory, all pathnames will be defaulted to the current directory. **NOTE:** A "WHIZ.SYS" file can be created in every subdirectory which the user desires to perform OZIPM-4 simulations.

## CREATING AN INPUT FILE

1. Change directory location to the subdirectory containing the OZIPM-4 input files using the DOS "CD" command.

2. Invoke the program by typing "OZACCESS". (Make sure the PATH statement is used.)

3. In the primary option menu, either hit the E key or with the left and right arrow keys move the cursor to the Edit option and hit the ENTER key.

4. Chose one of the 18 available OZIPM-4 input option to create by hitting the appropriate letter (A-R) or by using the up and down arrow keys to position on the desired input option and hitting the ENTER key.

5. Enter the desired values for the input option. Be sure to hit the ENTER key after entering each value. Hit the F10 key when done.

6. Repeat steps 4 and 5 for each input option.

7. After all input options are entered, hit the ESC key to access the primary options.

8. Choose the Load/save option to save the input file.

## EDITING AN EXISTING INPUT FILE

1. Change directory location to the subdirectory containing the OZIPM-4 input files using the DOS "CD" command.

2. Invoke the program by typing "OZACCESS". (Make sure the PATH statement is used.)

3. In the primary option menu, either hit the L key or with the left and right arrow keys move the cursor to the Load/save option and hit the ENTER key.

4. Enter the filename of the input file to be edited or hit the ENTER key to choose the input file to be edit using the arrow keys. Note that the input filename should have the extension ".INP" appended in order to be recognized in the program. Also, the OZIPM-4 Load/save and Edit option can only operate on the 18 input options. All other input options are not recognized by the program will produce erroneous input formats for the OZIPM-4 program.

5. Hit the ESC key to access the six primary options. Choose the Edit option by hitting the E key or by using the left and right cursor keys to position to the Edit option and hitting the ENTER key.

6. Chose one of the 18 available OZIPM-4 input option to edit (or create) by hitting the appropriate letter (A-R) or by using the up and down arrows to position on the desired input option and hitting the ENTER key.

7. To remove this option from further use, hit the F9 key. To modify an existing value, enter the desired value for the input option. Be sure to erase any trailing nonzero value of the original data before hitting the ENTER key to accept the value. Hit the F10 key when done to accept all values set for the desired input option.

8. Repeat steps 6 and 7 for each input option.

9. After all input options are edited, hit the ESC key to access the primary options.

10. Choose the Load/save option to save the input file.

## RUNNING OZIPM-4

In order to provide a computer program that will run on many systems, the RUN option has been disabled. The procedure for making OZIPM-4 simulations is discussed in Chapter 5.

## RUNNING THE PLOT OPTION

WARNING

The OZIPM-4 code does not contain a graphics package needed to write plotter output to a metafile. The user must supply a graphics package and compile/link it with OZIPM-4 in order to produce metafiles that can be plotted.

1. Change directory location to the subdirectory containing the OZIPM-4 input files using the DOS "CD" command.

2. Invoke the program by typing "OZACCESS". (Make sure the PATH statement is used.)

3. In the primary option menu, either hit the P key or with the left and right arrow keys move the cursor to the Plot option and hit the ENTER key.

4. Choose the **Display** option to display isopleth diagrams on the monitor or the **Plotter** option to generate a hardcopy of the isopleth diagrams. Use the up or down arrow keys (or hit the **D** or **P** key) to choose the desired option.

5. If the **Display** option is chosen, type the name of the plot (meta) file to be displayed. This is the file created by OZIPM-4 with the suffix ".mta" as the extension. The plotting program will be executed after hitting the **ENTER** key.

6. If the **Plotter** option is chosen, the program will display a prompt reminding the user to configure the plotter if necessary. If the plotter needs to be reconfigured, then hit "**N**" and exit the program. Type "**PCONFIG**" to configure the plotter and repeat steps 1 to 4. At this point, answer "Y" to the reminder prompt. The next display will be a choice of one of the three Hewlett-Packard plotters available for plotting the isopleth diagram. Choose the appropriate plotter using the up or down arrow keys and hit the ENTER key. The plotting program will generate the hardcopy isopleth diagrams.

7. After all isopleth diagrams are generated, control will return to the primary option menu.

8. Repeat steps 1 through 7 for all desired plots.

9. After all plots are generated, hit the ESC key to access the six primary options, choose the **Quit** option to exit the program.

## VIEWING AN INPUT OR OUTPUT FILE

1. Change directory location to the subdirectory containing the OZIPM-4 input files using the DOS "**CD**" command.

2. Invoke the program by typing "**OZACCESS**". (Make sure the **PATH** statement is used.)

3. In the primary option menu, either hit the **L** key or with the left and right arrow keys move the cursor to the **Load/Save** option and hit the **ENTER** key.

4. Choose the **View** option to view an input or output file on the monitor. The system will ask for the name of the file to view. If the **ENTER** key is entered without entering a filename, a directory list is produced. Use the arrow keys to position the cursor to the desired file for viewing and hit the **ENTER** key. Use the page-up or page-down keys to move forward and backwards through the file. A

search feature is provided to search for specific information. For instance, the maximum 1-hour ozone can be found on an output file generated using the CALCulate option by hitting F3, typing "MAXIMUM", and hitting the F3 key a second time. The program will search for the next occurrence of the text string "MAXIMUM".

5. After viewing the file hit F10 to return to the primary option menu.

6. Hit the ESC key to access the six primary options, choose the Quit option to exit the program.

## EXITING THE PROGRAM

1. To leave the program, hit the ESC key to access the six primary options. Hit the Q key or with the left and right arrow keys position to the Quit option and hit the ENTER key. If any editing was performed during the session and has not been saved, the program will display a prompt asking the user if editing changes should be saved or abondoned before exiting the program.

# 4. DESCRIPTION OF THE OZIPM-4 PROGRAM

This chapter describes in greater detail the use of the six primary options available in the program. The screen menus displayed for each option are also presented in this chapter. Some general notes on operating the program are:

- Help messages are available for most OZIPM-4 options and parameters by hitting the **F1** key.
- Always hit the **SPACEBAR** to exit from a help message.
- The **ESC** key will return the OZIPM-4 to the primary option menu.
- Warm boot the system (using **CTRL+ALT+DEL** keys) should the system hang for any ryeason.

The six primary options are described in the following sections.

## EDIT OPTION

When the Edit option is accessed (either by hitting the E key or positioning to the Edit option with the left or right arrow keys) the program will display the 18 available input options (see Figure 4-1). The 18 options are described in detailed in "User's Manual for OZIPM-4 (Ozone Isopleth Plotting with Optional Mechanisms)" (EPA, 1989) and in Appendix A of this document. Choose the input option to edit by hitting the letter associated with the input option or using the up or down arrow keys to position to the desired input option and hitting the **ENTER** key.

Each of the 18 input options can be edited in a similar manner. Some general operations for each option are:

- Always hit the **ENTER** key after entering a value or the program will not retain the new value.
- After all modifications are made to an input option, hit the F10 key to save the modifications.
- An input option either defined during the current edit session or defined from a previous edit session can be cleared completely from the input file by hitting the **F9** key. The program will ask the user to verify that the option is to be cleared. Only use the F9 key to clear options which have been defined. Use the ESC key to abort an option which has not been defined.

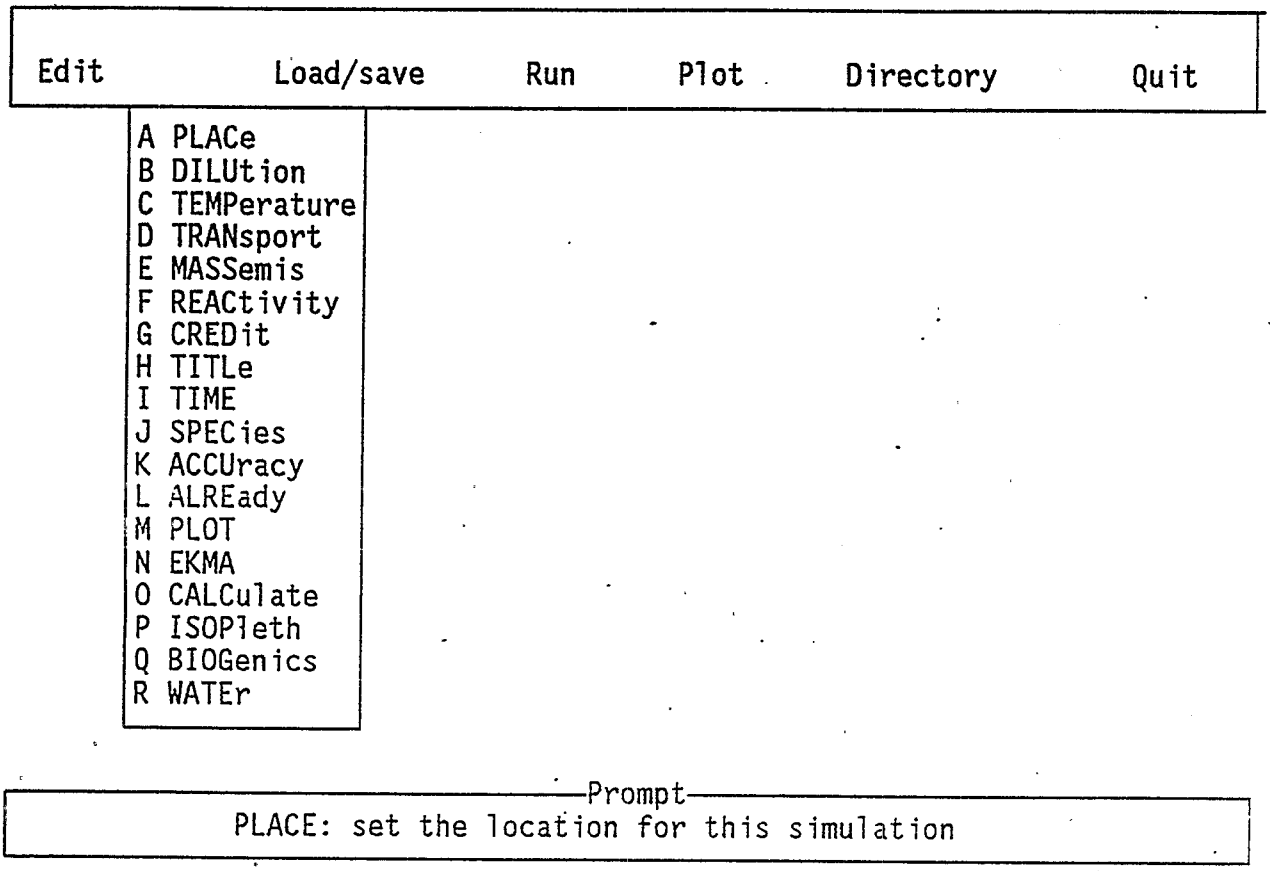



Figure 4-1. Example screen display of the 18 input options available in OZIPM-4.

- The **ESC** key will return to the primary option menu **without** storing any modifications.

- Use the **TAB** and arrow keys to move around the display screen.

- Data values which are not entered will be written to the input file with a value of zero. The OZIPM-4 main program will interpret zeroes as blanks for most parameters. Some input options do interpret zeroes as an actual number. For these input options a value must be entered explicitly even if default values are desired. Check the following subsections to determine where nonzero values must be entered. The data description line usually displays the default value for each input parameters.

- Input options which are not created or specified in the input file will be treated with default values as described in the EPA (1989) document.

- The OZIPM-4 system checks the minimum and maximum allowable values which can be entered in an input option. A value outside of the specified range will be flagged by the program and will not be accepted until the user enters a valid value. Similarly, if the user enters a nonnumeric value in a numeric data field, the program will notify the user that an invalid value has been entered and will not accept the value.

The display screens for each of the 18 input options contain a top banner describing the input option, a middle section to enter specific data values, a bottom banner section which contains a short description of the data to be entered, and a bottom line describing the key functions (see Figure 4-2 for an example of an input option display screen). The 18 input options are discussed in the following subsections.

### PLACe Option

The **PLACe** option can be accessed by hitting the **A** key or by using the up or down arrow keys to position to the **PLACe** option and hitting the **ENTER** key. The **PLACe** option screen will then be displayed (Figure 4-2). The **PLACe** input option contains seven input parameters (latitude, longitude, time zone, year, month, day, and the name of the location to be simulated). When the **PLACe** option is invoked, the user must enter all seven parameters even when default values are desired.

**Note:** The time zone can also be entered by hitting the **ENTER** key before entering a value. Choose the appropriate time zone using the left or right arrow keys.

PLACE Location and date for calculating light intensity.
---- If not used, PLACE defaults to Los Angeles on June 21, 1986.

Latitude:

Longitude:

Zone:

Year:

Month:

Day:

Name:

North latitude of location in decimal degrees (DF=34.058)

↑↓ :Locate Enter:Enter F1:help F10:Accept ESC:Reject F9:Clear

Figure 4-2. Example screen display of the PLACe option menu.

## DILUtion Option

The **DILU**tion option can be accessed by hitting the B key or by using the up or down arrow keys to position to the **DILU**tion option and hitting the **ENTER** key. The **DILU**tion option screen will be displayed as shown in Figure 4-3. The **DILU**tion option contains 5 input parameters (initial mixing height, final mixing height, starting time, ending time, and dilution rate before and after the mixing height change). If the **DILU**tion option is invoked, then the first four parameters must be entered even if default values are desired. Note that in city-specific calculations no dilution is assumed before and after the mixing height change. So, the dilution rate (before and after the mixing height change) parameter is generally set to zero. This parameter is in the program to provide compatibility with input files developed outside the program.

## TEMPerature Option

The **TEMP**erature option can be accessed by hitting the C key or by using the up or down arrow keys to position to the **TEMP**erature option and hitting the **ENTER** key. The **TEMP**erature option screen will be displayed as shown in Figure 4-4. The **TEMP**erature option contains 1 input parameter (the number of hours with varying hourly temperature values). Upon entering the number of hours which the temperature varies, the display screen will show the data field for entering the temperature values (Figure 4-5). There will be n+1 number of temperature data fields where n is the number of hours. Each temperature value represents the temperature at the beginning of the hour. Thus, the data field labelled "0:" will contain the temperature at start of the simulation.

## TRANsport Option

The **TRAN**sport option can be accessed by hitting the D key or using the up or down arrow keys to position to the **TRAN**sport option and hitting the **ENTER** key. The **TRAN**sport option screen will be displayed as shown in Figure 4-6. The **TRAN**sport option contains 6 main input parameters (surface $O_3$, aloft $O_3$, surface $NO_2$, aloft $NO_2$, surface NMOC, and aloft NMOC) and 18 data fields for the surface and aloft NMOC reactivities. If non-default NMOC reactivity values are desired, then enter the values into the appropriate data field. All reactivity data fields must be entered when one or more reactivity values are entered otherwise the program will interpret a blank data field as zero.

## MASSemiss Option

The **MASS**emiss option can be accessed by hitting the E key or by using the up or down arrow keys to position to the **MASS**emiss option and hitting the **ENTER** key. The **MASS**emiss option screen will be displayed as shown in Figure 4.7.

DILUTION Mixing height data to determine dilution.

Initial height:

Final height:

Starting time:

Ending time:

Dilution rate:

Initial mixing height in meters (DF=510)

↑↓ :Locate Enter:Enter F1:help F10:Accept ESC:Reject F9:Clear

Figure 4-3. Example screen display of the DILUtion option menu.

TEMPERATURE ---- Providing for varying temperatures during the simulation. If this option is not used, the temperature default to 303°K.

**Hours:**

Enter the number of hours of varying temperature (1-24)

↑↓ :Locate Enter:Enter F1:help F10:Accept ESC:Reject F9:Clear

Figure 4-4. Example screen display of the **TEMP**erature option menu.

TEMPERATURE ---- Provides for varying temperatures during the simulation. If this option is not used, the temperatures default to 303°K.

Hours: 11

| | | | | | |
|---|---|---|---|---|---|
| 0: | 1: | 2: | 3: | 4: | 5: |
| 6: | 7: | 8: | 9: | 10: | 11: |

Enter the temperature in degrees Kelvin

↑↓ :Locate Enter:Enter F1:help F10:Accept ESC:Reject F9:Clear

Figure 4-5. Example screen display of the TEMPerature option menu with the hourly temperature data fields.

TRANSPORT
----

Information on O3, NO2, and NMOC transported in the surface layer and in the air aloft that is entrained as the inversion rises. If TRAN is not used, concentrations default to 0.0

| | |
|---|---|
| Surface O3: | Aloft O3: |
| Surface NO2: | Aloft NO2: |
| Surface NMOC: | Aloft NMOC: |

Fill in the following ONLY if you want to change the default NMOC mix

| | | | | |
|---|---|---|---|---|
| Surface NMOC mix | ETH: | OLE: | ALD2: | FORM: |
| TOL: | XYL: | PAR: | ISOP: | NR: |
| Aloft NMOC mix | ETH: | OLE: | ALD2: | FORM: |
| TOL | XYL: | PAR: | ISOP: | NR: |

Transported O3 concentration in the surface layer (ppm)

↑↓ :Locate Enter:Enter F1:help F10:Accept ESC:Reject F9:Clear

Figure 4-6. Example screen display of the TRANsport option menu.

The **MASS**emiss option contains 4 main input parameters (number of hours of emissions, the 0600-0900 NMOC concentration, the 0600-0900 $NO_x$ concentration, and the initial mixing height) and up to 48 data fields for the VOC and $NO_x$ emissions. Blank data fields will be interpreted as zero emissions in the **MASS**emiss option. Upon entering the number of emission hours the data fields for the emission values will be displayed (see Figure 4-8).

## REACtivity Option

The **REAC**tivity option can be accessed by hitting the F key or by using the up or down arrow keys to position to the **REAC**tivity option and hitting the **ENTER** key. The **REAC**tivity option screen will be displayed as shown in Figure 4-9. The **REAC**tivity option contains 10 input parameters (the initial $NO_2/NO_x$ ratio, and the organic fractions for the 9 Carbon-Bond species). When the **REAC**tivity option is invoked, the user must enter a value for the initial $NO_2/NO_x$ ratio even if the default value is desired. All blanks in the organic reactivity data fields will be interpreted as zero if any nonzero organic fraction is entered.

## CREDit Option

The **CRED**it option can be accessed by hitting the G key or by using the up or down arrow keys to position to the **CRED**it option and hitting the **ENTER** key. The **CRED**it option screen will be displayed as shown in Figure 4-10. The **CRED**it option contains 7 main input parameters (a defeat option flag, the number of hours of CO emissions, the 0600-0900 CO concentration in the present year, the 0600-0900 aloft CO concentration in the present year, the aloft CO concentration in the future year, and the percent change in CO emissions from the present year to the future year) and up to 24 data fields for the hourly CO emissions. Blank data fields will be interpreted as zero emissions in the **CRED**it option.

Upon entering the number of emission hours the data fields for the emission values will be displayed (see Figure 4-11). Blanks entered in the emissions data fields will be interpreted as zero. The number of hourly CO emissions can be entered as either a positive or negative value depending on the units of the hourly emissions. If the user wishes to enter CO emissions as mass densities (units of $kg/km^2$), then the negative value of the number of hourly emissions should be entered. If the user desires to enter CO emissions expressed as the fraction of the initial 0600-0900 CO concentration, then a positive value of the number of hourly CO emissions should be entered.

The defeat option flag is an option provided in the mainframe versions of the OZIPM-4 program where multiple calculations (either with **EKMA**, **CALC**ulate, or **ISOP**leth options) can be performed and the user does not want to invoke the **CRED**it option for some of the calculations. In general, the defeat option flag will be set to zero.

MASSEMISS ---- Mass emission densities through which post-800 emission fraction are calculated

Hours: NMOC: NOX: Height:

Enter the number of hours of emissions

↑↓ :Locate Enter:Enter F1:help F10:Accept ESC:Reject F9:Clear

Figure 4-7. Example screen display of the MASSemiss option menu.

MASSEMISS ---- Mass emission densities through which post-800 emission fraction are calculated

```
Hours: 5                NMOC:          NOX:          Height:

1:          2:          3:          4:          5:



1:          2:          3:          4:          5:

Measured 0600-0900 NMOC emissions (ppmC)

↑↓ :Locate  Enter:Enter F1:help  F10:Accept  ESC:Reject  F9:Clear
```

Figure 4-8. Example screen display of the **MASS**emiss option menu with hourly emission fields.

REACTIVITY
----

Information on organic reactivity and the NO2/NOX ratio for the initial 6-9 AM mix and VOC and NOX emissions.

NO2/NOX

| | | | | |
|---|---|---|---|---|
| ETH: | OLE: | ALD2: | FORM: | TOL: |
| XYL: | PAR: | ISOP: | NR: | |

Enter the NO2/NOX fraction

↑↓ :Locate Enter:Enter F1:help F10:Accept ESC:Reject F9:Clear

Figure 4-9. Example screen display of the REACtivity option menu.

CREDIT
----

Allow for post-0800 CO emissions in EKMA calculations. Defaults are no post-0800 CO emissions, 1.2 ppm CO initial, and 0.5 ppm CO aloft.

Defeat: Hours: Height:

Present CO: Present aloft CO:

Future change: Future aloft CO:

Enter minus one (-1) to defeat this option in multiple runs (DF=0)

↑↓ :Locate Enter:Enter F1:help F10:Accept ESC:Reject F9:Clear

Figure 4-10. Example screen display of the CREDit option menu.

CREDIT
----

Allow for post-0800 CO emissions in EKMA calculations. Defaults are no post-0800 CO emissions, 1.2 ppm CO initial, and 0.5 ppm CO aloft.

```
Defeat:                 Hours:  5              Height:

Present CO:                                    Present aloft CO:

Future change:                                 Future aloft CO:


1:          2:          3:          4:          5:


        Initial mixing height.  Use only if HOURS is negative

↑↓ :Locate  Enter:Enter F1:help  F10:Accept  ESC:Reject  F9:Clear
```

Figure 4-11. Example screen display of the CREDit option menu with the hourly CO emissions data fields.

### TITLe Option

The TITLe option allows the user to enter a title for the specific simulation and can be accessed by hitting the **H** key or by using the up or down arrow keys to position to the **TITLe** option and hitting the **ENTER** key. The **TITLe** option screen will be displayed as shown in Figure 4-12. The title is entered in the area specified by the data field.

### TIME Option

The **TIME** option allows the user to specify a simulation time period other than the default time period of 0800 to 1800 LDT. The **TIME** option can be accessed by hitting the I key or by using the up or down arrow keys to position to the **TIME** option and hitting the **ENTER** key. The **TIME** option screen will be displayed as shown in Figure 4-13. The **TIME** option contains two data fields: the starting and ending times of the simulation. Both starting and ending times must be entered when this option is invoked. The values should be in military hours (e.g., 1300 LDT is 1 pm in the afternoon local daylight time).

### SPECies Option

The user can generate an isopleth diagram for up to five species found in the chemical kinetic mechanism through the use of the **SPECies** option. The **SPECies** option can be accessed by hitting the **J** key or by using the up or down arrow keys to position to the **SPECies** option and hitting the **ENTER** key. The **SPECies** option screen will be displayed as shown in Figure 4-14. The **SPECies** option contains 5 data fields for the five species of interest. Enter the name of the species of interest in each data field. The program will check the spelling of the names entered. If the name does not correspond to a species found in the chemical mechanism, the program will alert the user and provide a list of species names. If the user cannot recall the exact name of any species, then hitting the **ENTER** key displays a list of species names. The cursor will be located on the list of names. With the arrow keys move the cursor to the species of interest and hit the **ENTER** key. The species name will automatically be entered into the data field.

### ACCUracy Option

The **ACCUracy** option can be accessed by hitting the **K** key or by using the up or down arrow keys to position to the **ACCUracy** option and hitting the **ENTER** key. The **ACCUracy** option screen will be displayed as shown in Figure 4-15. The **ACCUracy** option contains 4 input parameters (error tolerance for the chemical integration scheme, two tension factors for the isolines on an isopleth diagram, and a stop flag to perform simulations up to the ozone peak). Any of the four input parameters may be left blank if desired. The OZIPM-4 main program will interpret blank data fields in this option as default values.

TITLE A title for the current simulation. If not used, TITLE defaults
---- to "Standard Ozone Isopleth Conditions.'

Title:

↑↓ :Locate Enter:Enter F1:help F10:Accept ESC:Reject F9:Clear

Figure 4-12. Example screen display of the TITLe option menu.

TIME  Starting and ending times for this simulation.
----

Starting:

Ending:

Starting time for simulation based on a 24-hour clock, e.g., 0800

↑↓ :Locate  Enter:Enter F1:help  F10:Accept  ESC:Reject  F9:Clear

Figure 4-13. Example screen display of the TIME option menu.

SPECIES ---- Names of 1-5 species for isopleth plots, or concentration profile plots if the CALCULATE option is used. 03 is the default for the SPECIES option.

Species 1:

Species 2:

Species 3:

Species 4:

Species 5:

Enter species abbreviation, e.g., 03, or enter blank field for list

↑↓ :Locate Enter:Enter F1:help F10:Accept ESC:Reject F9:Clear

Figure 4-14. Example screen display of the SPECies option menu.

## ALREady Option

OZIPM-4 isopleth diagram calculations from a previous computer run can be used to restart OZIPM-4 to complete the isopleth diagram calculation through the use of the **ALREady** option. The **ALREady** option can be accessed by hitting the **L** key or by using the up or down arrow keys to position to the **ALREady** option and hitting the **ENTER** key. The **ALREady** option screen will be displayed as shown in Figure 4-16. The only input parameter required in the **ALREady** option is the number (positive value only) of simulations performed previously.

## PLOT Option

The **PLOT** option is used to define the plot size of the isopleth diagram and the size of the labels on the diagram. The **PLOT** option can be accessed by hitting the **M** key or by using the up or down arrow keys to position to the **PLOT** option and hitting the ENTER key. The PLOT option screen will be displayed as shown in Figure 4-17. The **PLOT** option contains 5 input parameters (label location, grid type, length of the abscissa, length of the ordinate, size of the isoline labels, and size of the axis labels). The user can enter values other than defaults for any of the five data fields. Blank fields will be interpreted as default values by OZIPM-4.

## EKMA Option

The **EKMA** option is used to calculate VOC control requirements in OZIPM-4. The **EKMA** option can be accessed by hitting the **N** key or by using the up or down arrow keys to position to the **EKMA** option and hitting the **ENTER** key. The **EKMA** option screen will be displayed as shown in Figure 4-18. The **EKMA** option contains 11 main input parameters (base-year ozone, the NMOC/$NO_x$ ratio, the percent change in $NO_x$ emissions, a future year transport flag, an EKMA tabular report flag, a flag to perform an EKMA calculation at a specific NMOC level, 0600-0900 measured NMOC, 0600-0900 measured $NO_x$, predicted base-year NMOC location, predicted base-year $NO_x$ location, and the specific change in NMOC) and 6 data fields (which are needed only when the transport flag is declared) for the future-year precursor concentrations transported in the surface layer and entrained from aloft.

The input parameters, base-year ozone, the NMOC/$NO_x$ ratio, the percent change in $NO_x$ emissions, the 0600-0900 measured NMOC and $NO_x$ concentrations) must contain nonblank values in the **EKMA** option. All other data fields may contain a blank entry.

ACCURACY Change the accuracy of the isopleth diagram and stop simulation after any ozone maximum.

Tolerance:

Tension:

Tension:

Stop:

Enter error tolerance for integration routine (0.1-0.00001; DF=0.003

↑↓ :Locate Enter:Enter F1:help F10:Accept ESC:Reject F9:Clear

Figure 4-15. Example screen display of the ACCUracy option menu.

ALREADY Include results from previous simulations. This front-end assumes
---- that the simulation results will be input from another file.

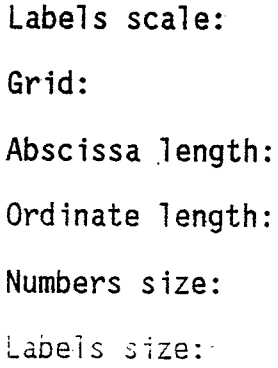
Number:

Number of previous simulations to be input

↑↓ :Locate Enter:Enter F1:help F10:Accept ESC:Reject F9:Clear

Figure 4-16. Example screen display of the ALREady option menu.

PLOT ---- Activates the drawing of the isopleth diagram on an off-line plotter.




Scaling factor for location of labels on isopleth (0.1-0.8, DF=0.6)

↑↓ :Locate Enter:Enter F1:help F10:Accept ESC:Reject F9:Clear

Figure 4-17. Example screen display of the **PLOT** option menu.

## CALCulate Option

The CALCulate option is used to perform a simulation at a single point on an isopleth diagram. The CALCulate option can be accessed by hitting the O key or by using the up or down arrow keys to position to the CALCulate option and hitting the ENTER key. The CALCulate option screen will be displayed as shown in Figure 4-19. The CALCulate option contains 5 input parameters (the initial NMOC, initial $NO_x$, a flag to provide detailed output of the simulation, the initial time to print instantaneous concentrations, and the interval to print subsequent instantaneous concentrations). The initial NMOC and $NO_x$ concentrations are the only required input data. The rest of the input data fields may contain blank (or zero) entries if the user desires to use the default values.

## ISOPleth Option

The ISOPleth option is used to generate isopleth diagrams. The ISOPleth option can be accessed by hitting the P key or by using the up or down arrow keys to position to the SPECies option and hitting the ENTER key. The SPECies option screen will be displayed as shown in Figure 4-20. The ISOPleth option contains 6 input parameters (the maximum 0600-0900 NMOC concentration, the maximum 0600-0900 $NO_x$ concentration, the number of isolines to plot, a flag to print time of peak value and solar noon, the number of species to plot, and an edit flag). Upon entering the number of isolines to plot, the screen will display the appropriate number of data fields to enter the isoline values (Figure 4-21). When more than one species to plot are specified (through the SPECies option), the edit flag is used to access the isoline data fields for the different species. For instance, if the user wishes to enter isoline values for the second species to plot, a value of 2 would be entered in the edit flag data field and the data fields will appear in the middle of the screen. To enter isoline values for another species, the user would enter the appropriate value in the edit data field. Note that the order of the species to plot must be in the same order as that set in the SPECies option.

## BIOGenics Option

The BIOGENICS option is used to input post-0800 emissions of up to five biogenic species. To access the BIOGenics option, hit the Q key or by using the up or down arrow keys to position to the BIOGenics option and hit the ENTER key. The BIOGenics option screen will be displayed (see Figure 4-22). The BIOGenics option contains three main inputs (the number of hours of biogenic emissions, the number of biogenic species, and the initial mixing height). Upon entering the number of hours of biogenic emissions, the data fields for the emission values will be displayed (Figure 4-23). The middle portion of the menu shows the input parameters for each of the biogenic species. Choose the species to edit or view by entering a number representing the order of the biogenic species (e.g., if terpenes is the first species,

```
EKMA   Perform a VOC emission requirement calculation.
----

    Ozone:          NMOC/NOX:          Change:          Transport:

                    Report:            Flag:

    Measured NMOC:          Calculated NMOC:          Changed NMOC:

    Measured NOX:           Calculated NOX:

           Enter the following only if the Transport item is nonzero

    Surface O3:             Surface NMOC:             Surface NOX:

    Aloft O3:               Aloft NMOC:               Aloft NOX:


    Enter base-case ozone concentration (ppm)

↑↓ :Locate    Enter:Enter    F1:help    F10:Accept    ESC:Reject    F9:Clear
```

Figure 4-18. Example screen display of the EKMA option menu.

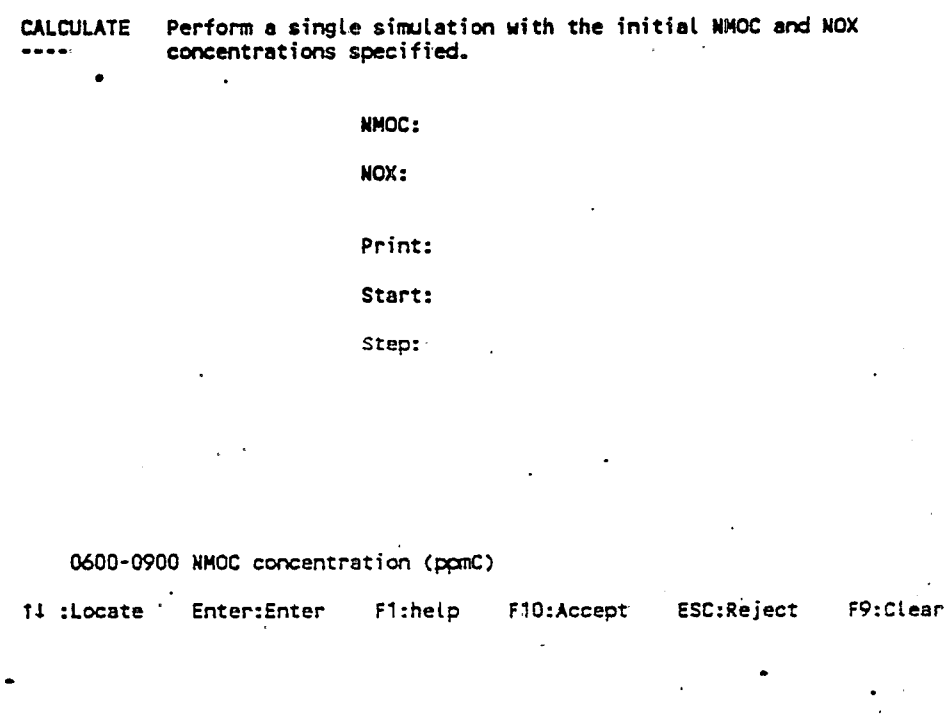



Figure 4-19. Example screen display of the CALCulate option menu.

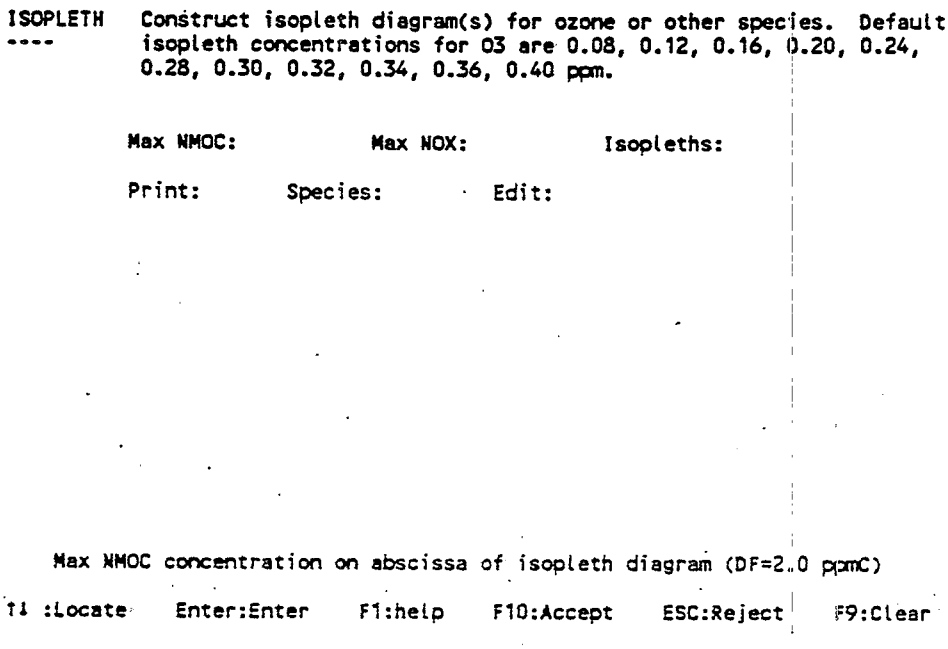



Figure 4-20. Example screen display of the ISOPleth option menu.

```
ISOPLETH   Construct isopleth diagram(s) for ozone or other species.  Default
----       isopleth concentrations for O3 are 0.08, 0.12, 0.16, 0.20, 0.24,
           0.28, 0.30, 0.32, 0.34, 0.36, 0.40 ppm.

           Max NMOC: 2.        Max NOX: .14       Isopleths: 5

           Print:       Species:         Edit: 1

   1:          2:          3:          4:          5:




      Enter one (1) to print solar noon and max 1-hour concentration

↑↓ :Locate    Enter:Enter    F1:help    F10:Accept    ESC:Reject    F9:Clear
```

Figure 4-21. Example screen display of the ISOPleth option menu with data fields for the isoline values.

then enter 1, etc). Enter the input values for the current biogenic species by using the **TAB** or arrow keys to move around the menu. Blanks in any of the fields will be interpreted as zeroes. Be sure to hit the **ENTER** key after typing a value so that the program will accept the value. After entering all values, hit the **F10** key so that the program can accept the option.

A list of commonly occurring biogenic species along with their molecular weights and bond fractions are listed in Table 4-1 as a quick reference.

### WATEr Option

The **WATEr** option is used to input hourly varying relative humidities in percent. The relative humidities are used along with the ambient temperatures to calculate the water vapor concentration. To access the **WATEr** option, hit the **R** key or by using the up or down arrow keys to position to the **WATEr** option and hit the **ENTER** key. The **WATEr** option screen will be displayed as shown in Figure 4-24. The WATEr option contains two main inputs (the number of hours with varying water concentrations and the atmospheric pressure). Upon entering the number of hours with varying water concentrations, the data fields for the relative humidity values will be displayed (Figure 4-25). Use the **TAB** or arrow keys to move around the menu and enter the input values. Remember to hit the **ENTER** key after each entry in order to retain the value. Blanks in any fields will be interpreted as zeroes. Be sure to hit the **F10** key after entering all values so that the program can accept the option.

### LOAD/SAVE OPTION

The Load/save option is used to load an OZIPM-4 input file for editing or execution, save input files for future use, and to clear the OZIPM-4 memory to start a fresh session. The display screen for the Load/save option is shown in Figure 4-26. The four operations in the Load/save option are discussed in the following subsections.

### Load option

To access the Load option either type the **L** key or use the up or down cursor key to position on the Load option and hit the **ENTER** key. Figure 4-27 shows an example of the screen display for the Load option. By default all OZIPM-4 input files will have a filename extension of "**.INP**". It is recommended that the user follow this convention to organize the various input and output files used in the program. To load an existing input file, type the name of the file (without the "**.INP**" extension) and hit the **ENTER** key. An alternative method of loading an input file is to hit the **ENTER** key before typing a name. This will produce a directory list of all files with names

```
BIOGENICS Allow for post-0800 biogenic emissions.  If the BIOG
 ----     option is not used, defaults are no post-0800 biogenic emissions,
          and no transported surface and aloft concentrations of biogenics.

          Hours:        Species:       Height:

     Number of species to view/edit: 1 Name:          Molwt:
     CB4 flag:              Present surface:          Aloft:
     Future change:         Future surface:           Aloft:

     Species Profile (fill in only if CB4 flag equals 1)
     ETH:        OLE:        ALD2:        FORM:
     TOL:        XYL:        PAR:          NR:

     Hourly emissions--

     Enter the number of emission hours

↑↓ :Locate  Enter:Enter F1:help  F10:Accept  ESC:Reject  F9:Clear
```

Figure 4-22. Example screen display of the BIOGenics option menu.

BIOGENICS Allow for post-0800 biogenic emissions. If the BIOG
---- option is not used, defaults are no post-0800 biogenic emissions, and no transported surface and aloft concentrations of biogenics.

Hours: 11 Species: Height:

Number of species to view/edit: 1 Name: Molwt:
CB4 flag: Present surface: Aloft:
Future change: Future surface: Aloft:

Species Profile (fill in only if CB4 flag equals 1)
ETH: OLE: ALD2: FORM:
TOL: XYL: PAR: NR:

Hourly emissions--

1: 2: 3: 4: 5: 6:
7: 8: 9: 10: 11:

Enter the number of biogenic species (DF=0)

↑↓ :Locate Enter:Enter F1:help F10:Accept ESC:Reject F9:Clear

Figure 4-23. Example screen display of the BIOGenics option menu with hourly emission fields.

Table 4-1

MOLECULAR WEIGHTS AND SPECIES BOND FRACTIONS
OF SOME COMMON BIOGENIC SPECIES

| Species | Molecular Weight. | ETH | OLE | ALD2 | FORM | TOL | XYL | PAR | NR |
|---|---|---|---|---|---|---|---|---|---|
| A-Pinene | 136.24 | -- | 0.5 | 1.5 | -- | -- | -- | 6.0 | -- |
| B-Pinene | 136.24 | -- | 1.0 | -- | -- | -- | -- | 8.0 | -- |
| 3-Carene | 136.23 | -- | 2.0 | -- | -- | -- | -- | 6.0 | -- |
| d-Limonene | 136.24 | -- | 1.0 | 2.0 | -- | -- | -- | 4.0 | -- |
| Isoprene | 68.13 | -- | 2.0 | -- | -- | -- | -- | 1.0 | -- |
| Terpenes | 136.24 | -- | 1.0 | -- | -- | -- | -- | 8.0 | -- |

ending with ".INP" (Figure 4-28). With the arrow keys, position to the desired input file and hit the **ENTER** key to load the selected input file.

### Save option

To access the Save option either type the **S** key or use the up or down arrow keys to position on the Save option and hit the **ENTER** key. Figure 4-29 shows an example of the screen display for the Save option. The display screen for the Save option is similar to the Load option discussed above. If the user wishes to overwrite the original file, then just hit the **ENTER** key. To save an input file with a different filename, type the name of file to write and hit the **ENTER** key. An alternative method of saving an input file is to hit the **ENTER** key before typing a name. This will produce a directory list of all files with names ending with ".INP" (Figure 4-30). With the arrow keys, position to the desired input file and hit the **ENTER** key to save into the selected input file.

### View option

The View option can be used to view an existing file (either an input or an output file). To access the View option either type the **V** key or use the up or down arrow keys to position on the View option and hit the **ENTER** key. Enter the name of the desired file to view. If the **ENTER** key is hit before typing a filename, a directory list will be produced showing the names of the files in the current directory. With the arrow keys, position to the desired file and hit the **ENTER** key to select the file. The first 24 lines of the file will be displayed on screen. The **Page-up** and **Page-down** keys can be used to move backwards and forwards through the file. The up and down arrow keys will move through the file line by line. The F3 key can be used to search for specific text strings. To search for a string, hit the F3 key followed for the search string. Hitting the F3 key again will begin the search. After viewing the file, hit the F10 key to return to the primary menu.

### Clear option

The program has the capability to edit multiple sets of input files during a single interactive session through the Load and Save options. After saving an edited input file, the user can clear the memory space to start a new edit session with the Clear option. After clearing the memory space, the user can create a new input file or load an existing input file. To access the Clear option either type the **C** key or use the up or down arrow keys to position on the Clear option and hit the **ENTER** key. The memory space will automatically clear. If any edit changes were performed in the current session and the changes have not been saved, the program will prompt the user to verify clearing the memory space.

WATER Allows for varying water concentrations during the simulation. If
---- this option is not used, the concentrations default to 20,000 ppm

Hours:

Pressure:

Enter the number of hours of varying relative humidity (1-24)

↑↓ :Locate Enter:Enter F1:help F10:Accept ESC:Reject F9:Clear

Figure 4-24. Example screen display of the WATEr option menu.

WATER Allows for varying water concentrations during the simulation. If
---- this option is not used, the concentrations default to 20,000 ppm

Hours: 10

Pressure:

| | | | | | |
|---|---|---|---|---|---|
| 0: | 1: | 2: | 3: | 4: | 5: |
| 6: | 7: | 8: | 9: | 10: | |

Enter the percent relative humidity for this hour

↑↓ :Locate Enter:Enter F1:help F10:Accept ESC:Reject F9:Clear

Figure 4-25. Example screen display of the WATEr option menu with hourly relative humidity fields.

## RUN OPTION

The RUN option has been disabled. ALL OZIPM-4 runs should be submitted using the batch procedure outlined in Chapter 5.

Typical CPU execution times varies among different PCs. For reference purposes, to execute a single calculation on an IBM PC/XT running at 8 MHz with a 8 MHZ math coprocessor takes about 110 secs. The same computer without a math coprocessor requires over 500 secs. A single calculation on an IBM AT computer running at 6 MHz with a math coprocessor requires about 90 secs. A single calculation on an IBM 386 AT running at 16 MHz with a 16 MHz math coprocessor takes about 26 secs. Typical EKMA calculations requires about 8 to 10 single calculations. Therefore, to perform an EKMA calculation on an IBM PC/XT with a math coprocessor would take about 15 to 20 mins. It takes about 4 to 5 hours to generate an isopleth diagram (which requires 121 single calculations) on an IBM PC/XT running on 8 MHz with a math coprocessor.

## PLOT OPTION

WARNING

The OZIPM-4 code does not contain a graphics package needed to write plotter output to a metafile. The user must supply a graphics package and compile/link it with OZIPM-4, in order to produce metafiles that can be plotted.

The Plot option allows the user to view isopleth diagrams generated from an OZIPM-4 run either on the display screen (if a graphics card is installed) or on an Hewlett-Packard (HP) pen plotter. A metafile generated from the OZIPM-4 program must be available to use the **PLOT** option. If a metafile has been deleted, it can be recreated using the **ALREady** input option available in the program assuming the results file has not been deleted. Load the input file and add the **ALREady** option to the input file using the Edit primary option. Don't forget to check the input and output filenames before executing the OZIPM-4 main program, especially the name of the file containing the previous results. After executing the main program, choose the Plot option by using the left or right arrow keys or hitting the **ESC** key and the **P** key. The Plot menu will be displayed as shown in Figure 4-31.

### Display option

To display the isopleth diagrams on the monitor screen, a graphics card must be installed. If one is installed, then hit the **D** key or use the up or down arrow keys to position on the Display option and hit the **ENTER** key. The program will ask for the name of the metafile to be plotted. Enter the name of the metafile leaving off the default extension "**.MTA**" if it is used. Upon hitting the **ENTER** key to accept the selected filename, the OZIPM-4 system will execute the plotting program "**OZPLOT**". Each isopleth diagram will be displayed on the monitor screen. After viewing the isopleth diagram, hit the **ENTER** key to view another diagram if more than one is generated or to return control to the program.

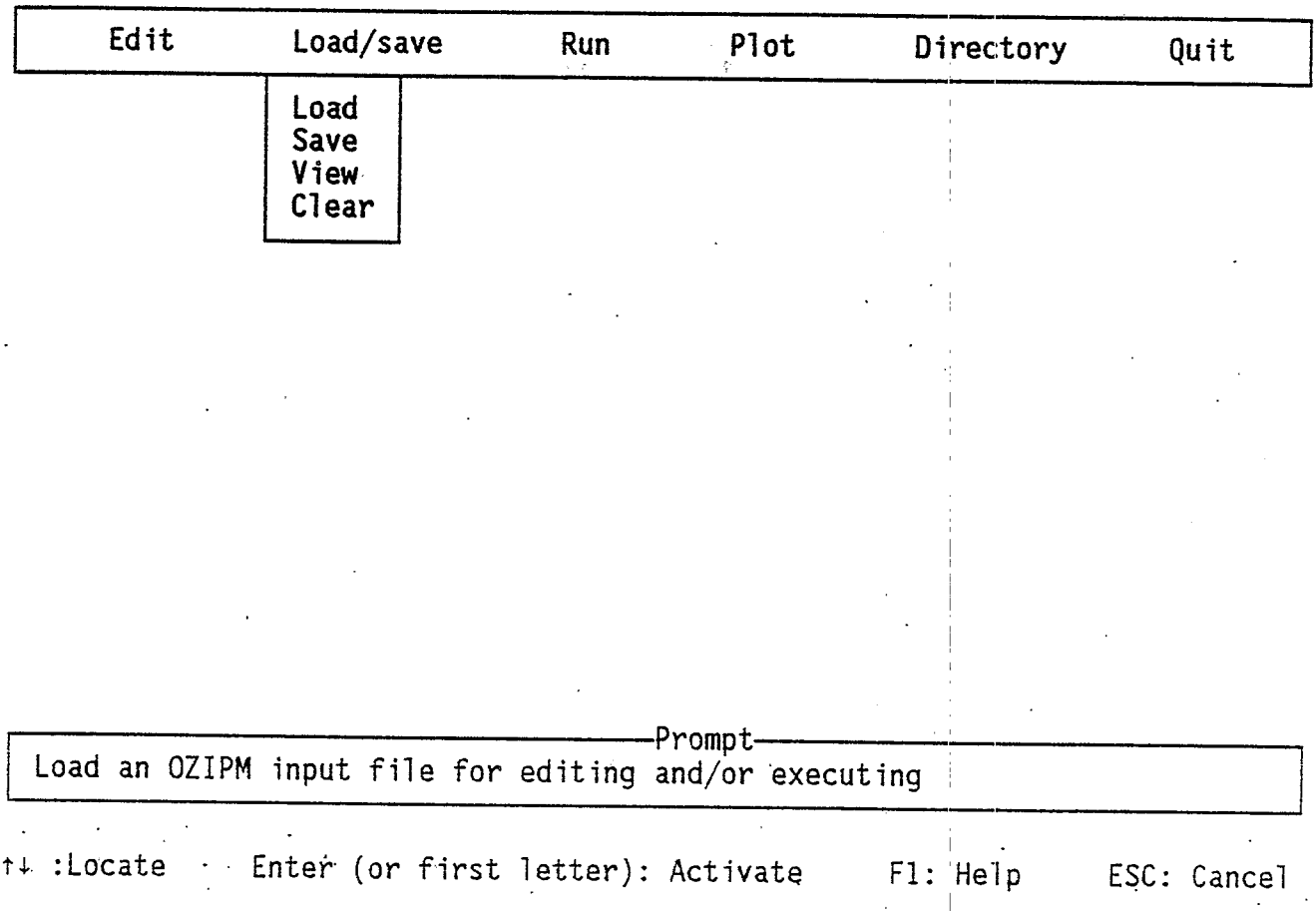



Figure 4-26. Example screen display of the Load/save option menu.

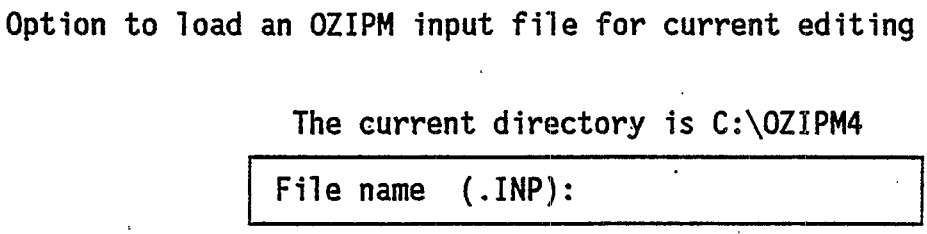



Figure 4-27. Example screen display of the Load option menu.

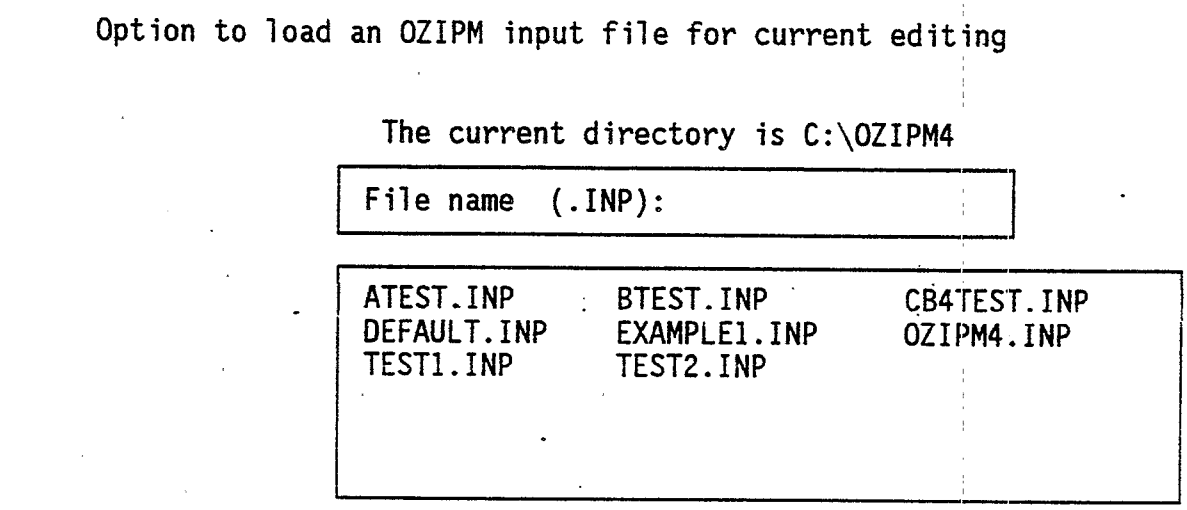



Figure 4-28. Example screen display of the Load option menu with a directory list of the input files.

Save an edited OZIPM input file for future editing

The working directory is C:\OZIPM4

File name (.INP):

Figure 4-29. Example screen display of the Save option menu.

Save an edited OZIPM input file for future editing

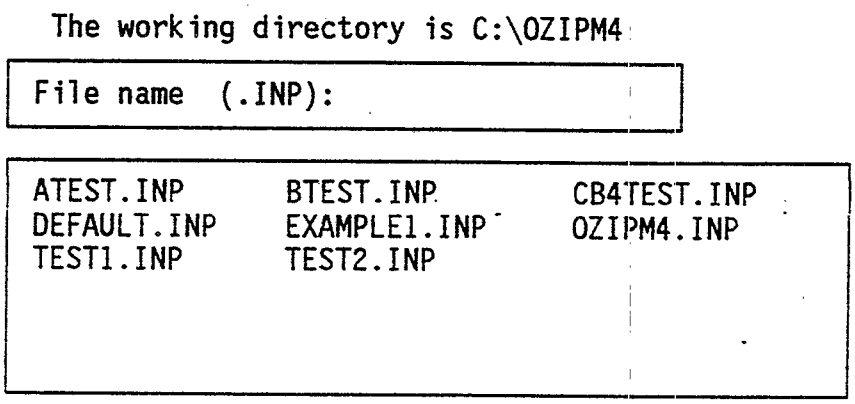



Figure 4-30. Example screen display of the Save option menu with a directory list of the input files.

## Plotter option

The Plotter option allows the user to plot isopleth diagrams on hard copy pen plotters. Pen plotters currently supported are the Hewlett-Packard 2-pen (model 7470A), 6-pen (model 7475A), and 8-pen (model 7550A) plotters. Before one can generate a hard copy plot, the system must be configured such that the plotter is attached to the printer port (usually LPT1). Hewlett-Packard pen plotters are generally configured to operate from the serial (or COM) port. So, the COM port must be redirected to LPT1. This can be accomplished using the DOS "MODE" command. To redirect output to LPT1 from a COM port, the following DOS commands must be entered:

**MODE LPT1:=COM@:** where @ is 1,2,3, or 4, and

**MODE COM@:baudrate,parity,databits,stopbits,P**

where baudrate, parity, databits, and stopbits, are set for the specific computer system. To facilitate entering the above commands, a batch file (called **PCONFIG.BAT**) is provided to automatically redirect the COM port. The settings used in the batch file must be changed for the specific system configuration. Lines 36 and 37 of the batch can be modified using any text editor such as "EDLIN". To execute the batch file, type "**PCONFIG**". After the hard copy plots are generated, reset the redirection by typing:

MODE LPT1:

To generate a hard copy plot, type the P key or use the up or down arrow key to position to the Plotter option and hit the **ENTER** key. The user will be warned to verify that the plotter has been appropriately configured before continuing. Type "**Y**" to continue or "**N**" to return to the primary option and leave the program to configure the plotter. Once the plotter has been configured, return to the program and answer "**Y**" to the warning message. A list of the pen plotters will be displayed on the screen. Choose the appropriate plotter using the up or down arrow keys and hit the **ENTER** key to accept the selection. Make sure the paper is properly loaded before hitting the **ENTER** key. The OZPLOT plotting program will be executed and the isopleth diagram will be generated on the pen plotter. After each isopleth diagram has been plotted, hit the ENTER key to either return control to the program or to begin plotting the next isopleth diagram.

If the plot is saved in a diskfile, then the file can be copied onto a floppy diskette along with the **PCONFIG.BAT** file. The floppy diskette is then taken to a computer system with an attached pen-plotter. Follow the instructions for executing **PCONFIG.BAT** as described above. To plot the file, type "**PRINT filename**". NOTE: This method can only do one plot. Multiple plots invoked with the SPECies options cannot be done using this method. To plot multiple species follow the procedures outlined in chapter 5 on using the OZPLOT program in stand-alone mode.

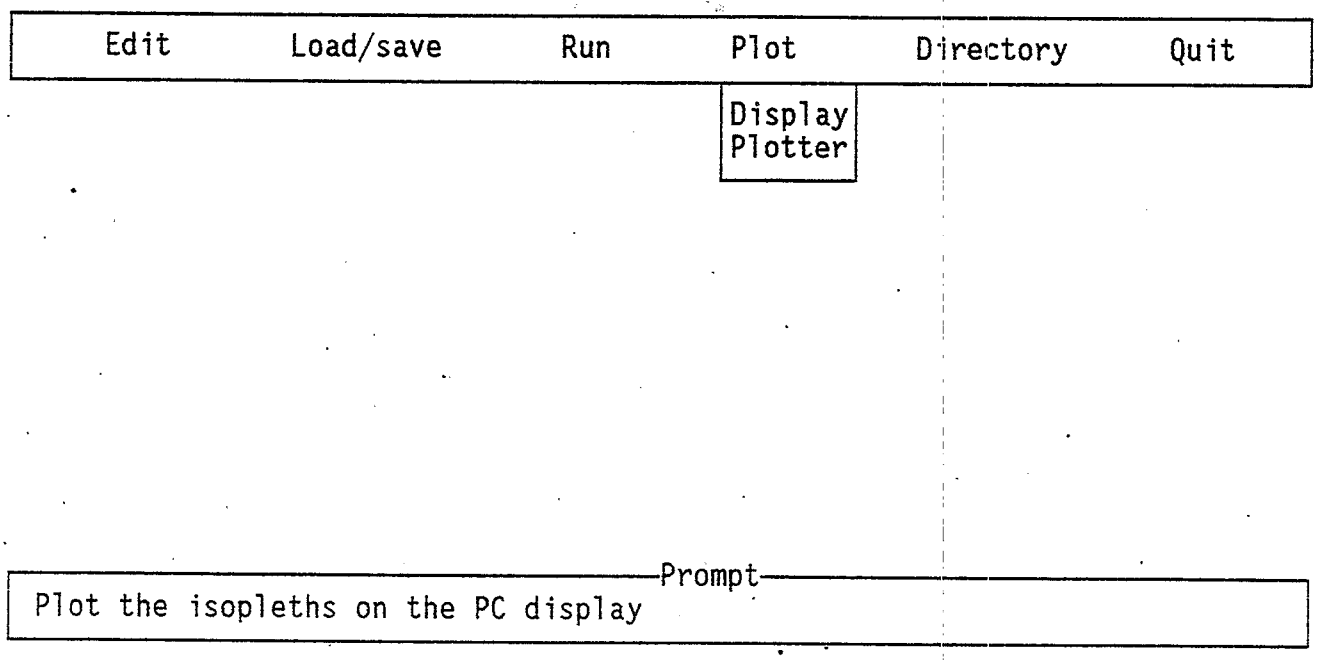



Figure 4-31. Example screen display of the Plot option menu.

## DIRECTORY OPTION

The Directory primary option sets the current directory as the working directory for the current session. This option can also be used to save the current directory as the default working directory so that future OZIPM-4 session will automatically set the current directory as the working directory. To access the Directory primary option, hit the **ESC** key followed by the **D** key or using the left or right arrow keys, position to the Directory option and hitting the **ENTER** key. The menu as shown in Figure 4-32 will be displayed.

To set the current directory as the working directory, choose the **W**orking option by hitting the **W** key or by using the up or down arrow key to position on the **W**orking option and hitting the **ENTER** key. The program will prompt for the name of the working directory. Enter the full pathname of the current directory including the drive specification (e.g. C:\MYDIR). This option allows the user to move to different subdirectories. The working directory is only retained during the current session.

To retain the current directory as the default working directory upon startup of the program, choose the **S**ave option by hitting the **S** key or by using the up or down arrow keys to position to the **S**ave option and hitting the **ENTER** key. The user will be prompted for the pathname of the current directory to be saved. Enter the full pathname including the drive specification. The pathname will be saved in a file called "WHIZ.SYS" created in the current directory. This option allows the user to create a "WHIZ.SYS" file in every subdirectory containing input and output files. Future startup of the program in any working directory will automatically set that directory as the default directory.

## QUIT OPTION

The **Q**uit primary option is used to exit the OZIPM-4 system. To exit the program, hit the ESC key followed by the **Q** key or use the left or right arrow key to position to the **Q**uit option. If there were no edit modifications performed during the current session, the system will return to the DOS environment. If edit modifications were made to the input file and the input file has not been saved, the program will prompt the user for verification that edit changes will not be saved. If the user answers "**Y**" a second prompt will be displayed to reconfirm the exit. If the user answers **N**, OZIPM-4 will return to the primary option menu so that the user can save the edited input file.

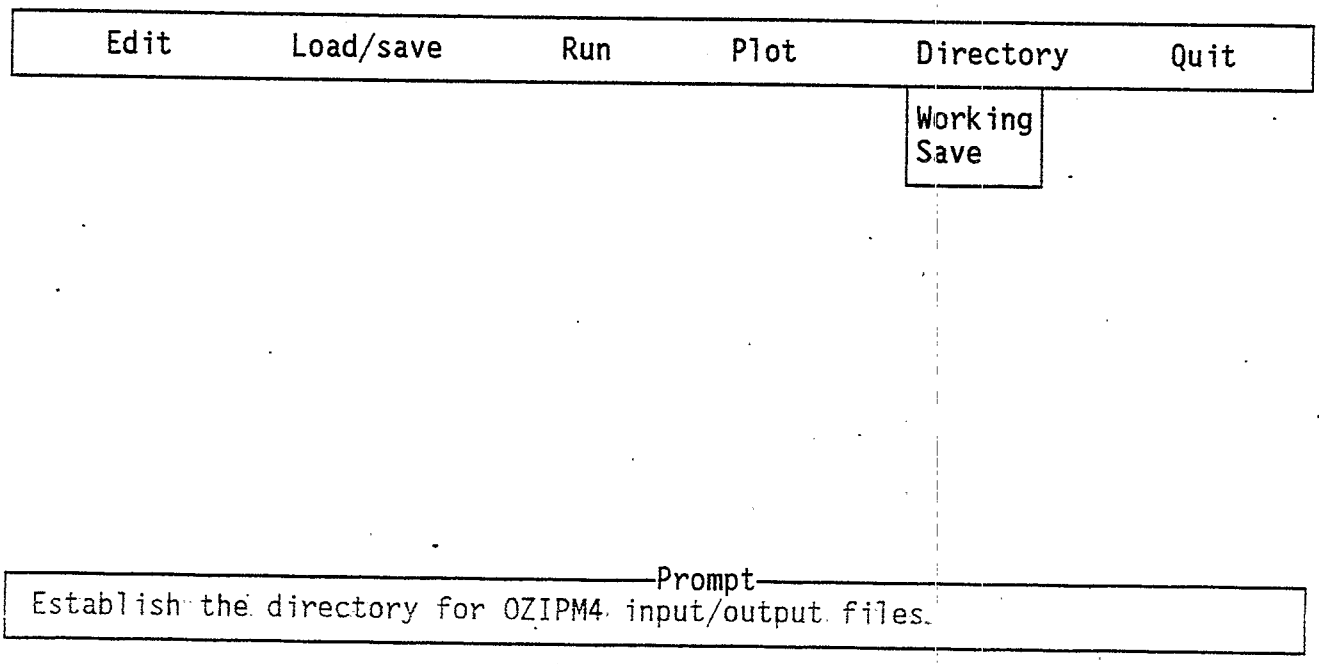



Figure 4-32. Example screen display of the Directory option menu.

# 5. RUNNING OZIPM-4 AND OZPLOT IN "STAND-ALONE" MODE

The previous chapters discussed how to prepare input files in the interactive mode. To run OZIPM-4 simulations, the user must use the procedures outlined here. The RUN option in the interactive program has been disabled. This chapter describes how to run the OZIPM-4 main program and the OZPLOT plotting program without accessing the interactive system.

## RUNNING OZIPM-4

The OZIPM-4 executable file "OZPC.EXE" can be executed independently by typing (in the current working directory):

OZPC *iofiles1* [BATCH]

The OZIPM-4 main program will be invoked with a file containing the names of the input and output files needed to execute the program. In the above command line, the file *iofiles1* contains the names of the input and output files. Note that *iofiles1* is only a generic name. The structure of the *iofiles1* is as follows:

line 1: pathname or filename of the input file

line 2: pathname or filename of the output file

line 3: pathname or filename of the file containing previous results file (needed only if the **ALR**Eady option is used).

line 4: pathname or filename of the file containing the current isopleth results (needed only if the **ISOP**leth option is used).

line 5: pathname or filename of the plot metafile (needed only if the **ISOP**leth option is used).

line 6: pathname or filename of the file containing the EKMA tabular report (needed only if the report flag of the **EKMA** option is set).

The first two lines must be entered, the rest are used only if the stated OZIPM-4 options are invoked. The beginning of each statement **must** contain a one letter identifier followed by a "=". The one letter identifiers are defined as follows:

I - for the Input file

O - for the Output file

P - for the Previous results file

R - for the file containing new Results

M - for the file containing the plots of the isopleth diagrams.

E - for the EKMA report file

The ***iofiles1*** file can be created using a standard text editor such as "EDLIN". An example of the ***iofiles1*** would be as follows:

```
i=D:\OZIPM4.INP\TEST1.INP
o=D:\OZIPM4.OUT\TEST1.OUT
p=C:\OZIPM4.RES\TEST1.AL1
r=C:\OZIPM4\TEST1.ALR
E=C:\OZIPM4\TEST1.EKM
m=C:\OZIPM4\TEST1.MTA
```

The above example shows the use of the one letter identifier followed by the pathname of the file. Note in this example that the input file is stored in a different directory than the output file and the results file. The use of an ***iofiles1*** allows the user to enter a very long pathname if needed.

The second parameter on the OZIPM-4 command line is an optional parameter which will switch off user prompts to end the OZIPM-4 program. One can set up a batch file to execute multiple OZIPM-4 runs without user intervention. By using a standard text editor such as "EDLIN", one can create a batch file RUN.BAT with the following lines:

```
OZPC iofiles1 BATCH
OZPC iofiles2 BATCH
OZPC iofiles3 BATCH
OZPC iofiles4 BATCH
OZPC iofiles5 BATCH
```

The batch file will execute the OZIPM-4 program five times each time with a different set of input and output files. To execute the batch file, type the batch file name. Such batch files can be setup and executed overnight to provide maximum use of the computer.

## RUNNING OZPLOT PLOTTING PROGRAM

The OZPLOT plotting program, **OZPLOT.EXE**, provided on the distribution disks can be executed independent of the interactive system by typing:

**OZPLOT *iofiles1* [plotter device]**

NOTE: Make sure that the plotter has been properly configured with **"PCONFIG.BAT"** before executing the plotting program.

The command line is similar to the OZIPM-4 command line discussed above except that the name (or pathname) of the metafile is entered. The second optional argument tells the **OZPLOT** program the model of the Hewlett-Packard pen plotter to be used:

**HP2** - Hewlett-Packard 2-pen (HP-7470A)

**HP6** - Hewlett-Packard 6-pen (HP-7475A)

**HP8** - Hewlett-Packard 8-pen (HP-7550A)

If a pen plotter is not available on the computer system, the files "OZPLOT.EXE", "PCONFIG.BAT", and the metafiles to be plotted, can be copied to a floppy diskette and taken to a computer system with a pen plotter.

## REFERENCES

EPA (1989), "User's Manual for OZIPM-4 (Ozone Isopleth Plotting with Optional Mechanisms/Version 4)", EPA-450/4-89-009a, Volume 1, U.S. Environmental Protection Agency, Research Triangle Park, North Carolina.

Hogo, H., and M. W. Gery (1988), "User's Guide for Executing OZIPM-4 with CBM-IV or Optional Mechanisms", Volume 1, SYSAPP-88/001, Systems Applications, Inc., San Rafael, California.

# APPENDIX A

## INPUT FORMAT FOR OZIPM-4 OPTIONS

INPUT FORMAT FOR OZIPM-4 OPTIONS

| Option | Line No. | Column | Contents |
|---|---|---|---|
| ACCURACY | Increase or reduce the mathematical accuracy of the isopleth diagram by using more or less accurate interpolation, etc. | | |
| | 1 | 1-4 | ACCU |
| | | 11-30 | Not read |
| | | 31-40 | Error tolerance in the numerical integration routine, from 0.1 to 0.00001; (DF = 0.003) |
| | | 41-50 | Tension factor for hyperbolic spline functions used in first stage of interpolation from 0.001 to 50.; (DF = 1) |
| | | 51-60 | Tension factor for hyperbolic spline functions used in plotting isopleth lines (high tensions lead to straight lines drawn between the points obtained from the first stage), from 0.001 to 50.; (DF = 1) |
| | | 61-70 | If any nonzero value is entered in this field, simulations will terminate after any ozone maximum; no entry produces results over the total simulation period |

| Option | Line No. | Column | Contents |
|---|---|---|---|
| ALREADY* | Include results from a previous run. | | |
| | 1 | 1-4 | ALRE |
| | | 11-20 | Number of previous simulations to be input<br><br>If the number is positive, then read the following lines. If the number is negative, then read previous simulation results from an external file |
| | 2 | 1-10 | NMOC concentration |
| | | 11-20 | $NO_x$ concentration |
| | | 21-30 | Maximum 1-hour average ozone concentration, ppm |
| | | 31-40<br>41-50<br>51-60<br>61-70 | Maximum 1-hour average concentrations (ppm) of any other species for which isopleths are to be constructed. These values are optional depending on the number of species declared on the SPECIES line. (Must be in the same order as listed on the SPECIES line.) |

*Can only be used with the ISOPLETH options.

| Option | Line No. | Column | Contents |
|---|---|---|---|
| BIOGENICS | Allow for post-0800 biogenic emissions. If the BIOG option is not used, defaults are no post-0800 biogenic emissions, and no transported surface concentrations and aloft concentrations of biogenics. | | |
| | 1 | 1-4 | BIOG |
| | | 11-20 | Number of emission hours. Must be equal to number of hours set in EMIS or MASS options. (Expressed as a negative number) |
| | | 21-30 | Enter the number of biogenic species (DF=0, max=5). |
| | | 31-40 | Initial mixing height. Used to convert mass units in $kg/km^2$ to ppm. Units must be in meters. |
| | The next set of lines are repeated for each biogenic species. | | |
| | 2+ | 1-4 | Species name. (Note: If Isoprene is used then the default name should be ISOP). |
| | | 11-20 | Flag to treat biogenic species as a specific molecular species or as Carbon Bond IV species (Enter a nonzero value in order to treat the biogenic species as CB-IV species). Note: Isoprene is the only biogenic species currently treated specifically in the CB-IV mechanism. |
| | | 21-30 | Present-day concentration transported in the surface layer (DF=0) |
| | | 31-40 | Present-day concentration transported aloft (DF = 0.0) |
| | | 41-50* | Percent change in biogenic emissions for the future year |

*Not used with CALC and ISOP options.

| Option | Line No. | Column | Contents |
|---|---|---|---|
| | | 51-60** | Future-year concentration transported in the surface layer (DF=0) |
| | | 61-70** | Future-year concentration transported aloft (DF = 0.0) |
| | | 71-80 | Not read |
| | 3+ | 1-10 | Species molecular weight (Units of gm/moles) |
| | 4+ (optional) | 1-10<br>11-20 | If a nonzero value is entered on columns of line 2, the species profiles by bond group of the biogenic species is entered here. |
| | | 11-20 | The species profiles should be in the following order: ETH, OLE, ALD2, FORM, TOL, XYL, PAR, and NR. |
| | | 61-70 | Continue on next line (if necessary). |
| | | 71-80 | Not read |
| | 5+ | 1-10 | Present-day hourly biogenic emissions ($kg/km^2$) |
| | | 11-20 | (continue on next line if necessary) |
| | | 61-70 | |

**Not used with CALC and ISOP option

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

| Option | Line No. | Column | Contents |
|---|---|---|---|
| CREDIT | Allow for post-8 a.m. CO emissions in EKMA calculations. Defaults are no post-8 a.m. CO emissions, 1.2 ppm CO for the 6-9 a.m. measurement and 0.5 ppm CO aloft. | | |
| | 1 | 1-4 | CRED |
| | | 11-20 | Enter a negative number to defeat use of this option in multiple runs. |
| | | 21-30 | Number of emission hours entered as a negative number. Must be equal to the number of hours set in MASS option. |
| | | 31-40 | Initial mixing height. |
| | 2 | 1-10 | Species names. CO is the only name allowed. |
| | | 11-20 | 6-9 a.m. present day CO concentration |
| | | 21-30 | Not read |
| | | 31-40 | Present day CO transported aloft (DF = 0.5) |
| | | 41-50 | Percent change in CO emissions and 6-9 a.m. concentration for the future year |
| | | 51-60 | Not read |
| | | 61-70 | Future year CO transported aloft |
| | 3 | 1-10 | Present hourly emissions of CO |
| | | 11-20... | in $kg/km^2$ |

| Option | Line No. | Column | Contents |
|---|---|---|---|
| DILUTION | Read site-specific information on initial and final mixing heights. Dilution is calculated using the characteristic curve. | | |
| | 1 | 1-4 | DILU |
| | | 11-20 | Initial mixing height, Z1, meters (DF = 510 m) |
| | | 21-30 | Final mixing height, Z2, in same units as initial mixing height (DF = 630 m) |
| | | 31-40 | Starting time of mixing height change (2400 hour) (DF = 0800) |
| | | 41-50 | Ending time of mixing height change (2400 hour) (DF = 1500) |
| | | 51-60 | Dilution rate in percent per hour before and after the mixing height change (DF = 0) |
| | | 61-80 | Not read |

| Option | Line No. | Column | Contents |
|---|---|---|---|
| EKMA | Used to perform a VOC emission requirement calculation. | | |
| | 1 | 1-4 | EKMA |
| | | 11-20 | Base-case ozone concentration, ppm |
| | | 21-30 | NMOC/$NO_x$ ratio (If the value is negative, the base-year NMOC and $NO_x$ levels have been determined in a previous simulation and are entered on line 3. Future-year calculations are performed based on the base-year NMOC and $NO_x$ levels.) |
| | | 31-40 | Percentage change in $NO_x$ emissions; positive number for increase, negative number for decrease (DF = 0) |
| | | 41-50 | Change in transport option indicator; if nonzero, input line 2 is required (DF = 0) |
| | | 51-60 | Option to generate report of change in ozone as a function of change in VOC emissions; if 1., generate tabular report; if 2., generate tabular report and write results on file. (DF = 0., i.e., no report or file generated) |
| | | 61-70 | Flag to do a calculation at a specified NMOC level. The NMOC level is expressed as a percent change from the base year level. The value is placed on line 2, Columns 61-70. Any nonzero value may be used as the flag. |

| Option | Line No. | Column | Contents |
|---|---|---|---|
| EKMA | The next line is included only if a nonzero entry is specified on line 1 for the transport option (41-50) and/or the flag option (61-70) | | |
| | 2 (optional) | 1-10 | Concentration of ozone transported in surface layer for post-control conditions, ppm; (DF = base-case level). A negative value activates the use of the future ozone transport estimate curves shown in Figure 3. (A value less than -100 activates the use of the dashed line shown in Figure 3.) |
| | | 11-20 | Concentration of ozone transported aloft for post-control conditions, ppm; (DF = base-case level). A negative value activates the use of the future ozone transport estimate curves shown in Figure 3. (A value less than -100 activates the use of the dashed line shown in Figure 3.) |
| | | 21-30 | Concentration of NMOC transported in the surface layer for postcontrol conditions, ppmC; (DF = base-case level). |
| | | 31-40 | Concentration of NMOC transported aloft for post-control conditions, ppmC; (DF = base-case level). |
| | | 41-50 | Concentration of $NO_x$ transported in surface layer for post-control conditions, ppm; (DF = base-case level) |
| | | 51-60 | Concentration of $NO_x$ transported aloft for post-control conditions, ppm; (DF = base-case level) |

| Option | Line No. | Column | Contents |
|---|---|---|---|
| | | | The following line must be included. |
| EKMA | 3 | 1-10 | Measured 6-9 a.m. NMOC (value used in emission density calculations) (DF = 0) |
| | | 11-20 | Measured 6-9 a.m. $NO_x$ (value used in emission density calculations) (DF = 0) |
| | | 21-30 | Calculated NMOC that yields base case $O_3$. Declared if a negative NMOC/$NO_x$ ratio is entered on line 1(DF = 0) |
| | | 31-40 | Calculated $NO_x$ that yields base case $O_3$. Declared if a negative NMOC/$NO_x$ ratio is entered on line 1 (DF = 0) |
| | | 41-50 | Change in NMOC level (percent) for specific calculation after the base-year ozone is estimated. (Used only if column 61-70 of line 1 is nonzero.) |

| Option | Line No. | Column | Contents |
|---|---|---|---|
| ISOPLETH | | | Construct isopleth diagrams for $O_3$ and other species according to the input parameters. Default isopleths for $O_3$ are 0.08, 0.12, 0.16, 0.20, 0.24, 0.28, 0.30, 0.32, 0.34, 0.36, and 0.40 ppm. |
| | 1 | 1-4 | ISOP |
| | | 11-20 | Maximum NMOC concentration on abscissa of isopleth diagram; (DF = 2.0 ppmC) |
| | | 21-30 | Maximum $NO_x$ concentration on ordinate of isopleth diagram; (DF = 0.28 ppm) |
| | | 31-40 | Number of ozone isopleths to be drawn, from 1. to 20.; (DF = 11) |
| | | 41-50 | Any nonzero value will activate the printing of solar noon and the time of the center of the maximum 1-hour average ozone concentration for each simulation |
| | | 51-60 | Not read |
| | | 61-70 | Number of species to plot. This number corresponds to the number of species entered on the PLOT option. |
| | 2 (optional) | 1-10 | Ozone concentration of 1st isopleth, ppm |
| | | 11-20 | Ozone concentration of 2nd isopleth, ppm |
| | | 21-30 | Ozone concentration of 3rd isopleth, ppm |
| | | 31-40 | Ozone concentration of 4th isopleth, ppm |
| | | 41-50 | Ozone concentration of 5th isopleth, ppm |
| | | 51-60 | Ozone concentration of 6th isopleth, ppm |
| | | 61-70 | Ozone concentration of 7th isopleth, ppm |

| Option | Line No. | Column | Contents |
|---|---|---|---|
| | 3 (optional) | 1-10 | Ozone concentration of 8th isopleth, ppm |
| | | . | |
| | | . | |
| | | . | |
| | | 61-70 | Ozone concentration of 14th isopleth, ppm |
| | 4 (optional) | 1-10 | Ozone concentration of 15th isopleth, ppm |
| | | . | |
| | | . | |
| | | . | |
| | | 51-60 | Ozone concentration of 20th isopleth, ppm |

| Option | Line No. | Column | Contents |
|---|---|---|---|
| MASSEMISS | Used to supply mass emission densities through which post-0800 emission fractions are computed. | | |
| | 1 | 1-4 | MASS |
| | | 11-20 | Number of hours of emissions (max = 24.)(expressed as a negative number) |
| | | 21-30 | Initial NMOC concentration (used to compute NMOC emission fractions, ppmC) |
| | | 31-40 | Initial $NO_x$ concentration (used to compute $NO_x$ emission fractions, ppm) |
| | | 41-50 | Mixing height at start of simulation, in meters |
| | The next line is repeated if more than 7 hours of emissions are specified. The number of entries must equal the number of hours specified on line 1. | | |
| | 2 | 1-10 | VOC emission density for hour 1, $kg/km^2$ |
| | | 11-20 | VOC emission density for hour 2, $kg/km^2$ |
| | | . | |
| | | . | |
| | | 61-70 | VOC emission density for hour 7, $kg/km^2$ |
| | The next line is repeated if more than 7 hours of emissions are specified. The number of entries must equal the number of hours specified on line 1. | | |
| | 3 | 1-10 | $NO_x$ emission density for hour 1, $kg/km^2$ |
| | | 11-20 | $NO_x$ emission density for hour 2, $kg/km^2$ |
| | | . | |
| | | . | |
| | | 61-70 | $NO_x$ emission density for hour 7, $kg/km^2$ |

| Option | Line No. | Column | Contents |
|---|---|---|---|
| PLACE | Input city-specific information on light intensity. Default values correspond to Los Angeles on June 21, 1986. | | |
| | 1 | 1-4 | PLAC |
| | | 11-20 | Latitude, in decimal degrees north of the equator (DF = 34.058) |
| | | 21-30 | Longitude, in decimal degrees west of Greenwich meridian (DF = 118.250) |
| | | 31-40 | The time zone, in hours from Greenwich mean time (DF = 7.0) |
| | | 41-50 | The year (DF = 1986) |
| | | 51-60 | The month of year (DF = 6) |
| | | 61-70 | The numerical day of month (DF = 21) |
| | 2 (optional) | 1-24 | The name of the place can be entered anywhere in columns 1-24. Include this line only if a new value is entered for the latitude or longitude on the previous line. |

| Option | Line No. | Column | Contents |
|---|---|---|---|
| PLOT | Activates the drawing of the isopleth diagram on an off-line plotter. | | |
| | 1 | 1-4 | PLOT |
| | | 11-20 | Scaling factor for the location of labels for each ozone isopleth. The value should be between 0.1 and 0.8.; (DF = 0.6) |
| | | 21-30 | If nonzero, a grid is overlaid onto the diagram. If the value is positive and nonzero, a grid is overlaid on the diagram using a different color pen (if available)<br><br>If the value is negative, a grid with line of different patterns (e.g., dot-dash) is overlaid on the plot. The absolute value of this number corresponds to different patterns and textures |
| | | 31-40 | Length (in inches) of the abscissa (NMOC scale) of the isopleth diagram; (DF = 8.5) |
| | | 41-50 | Length (in inches) of the ordinate ($NO_x$ scale) of the isopleth diagram; (DF = 5.95) |
| | | 51-60 | Size (in inches) of the numbers to be printed on the axes and of the characters in the title; (DF = 0.10) |
| | | 61-70 | The size (in inches) of the labels on the ozone isopleths and the division marks on the axis; (DF = 0.07) |

| Option | Line No. | Column | Contents |
|---|---|---|---|
| REACTIVITY* | Contains site-specific information on organic reactivity and $NO_2/NO_x$ ratio for the initial 6-9 AM mix and the VOC and $NO_x$ emissions. | | |
| | 1 | 1-4 | REACT |
| | | 5-10 | Not read |
| | | 11-20 | The number of primary organic species in the chemical mechanism (DF=9) |
| | | 21-30 | The $NO_2/NO_x$ fraction |
| | 2 | 1-10 | The reactivity for each of the organic species (up to 7 on a line) represented as the fractions of total NMOC. Continue on next line (if necessary) |
| | | 61-70 | |
| | | 71-80 | Not read |

*If the REACTIVITY option is not used, the default fractions are those shown in Table 5, Section 4.

| Option | Line No. | Column | Contents |
|---|---|---|---|
| SPECIES | This option allows the user to plot isopleths for any species found in the kinetic mechanism or to plot concentration-time profiles for species besides $O_3$ if the CALCULATE option is used. | | |
| | 1 | 1-4 | SPEC |
| | | 11-20 | Number of species to be plotted (DF = 1). Max = 5 |
| | | 21-80 | Not read |
| | | 1-4<br>11-14<br>21-24<br>31-34<br>41-44 | The alphanumeric symbol of the species of interest; left-justified (DF = 03 [ozone]) |
| | | 45-80 | Not read |

| Option | Line No. | Column | Contents |
|---|---|---|---|
| TEMPERATURE | | | A varying diurnal temperature profile may be used during the simulation with this option. Temperature values should be in units of degrees K. Values are read for the initial time and at the end of each hour. If there are n hours, there should be n+1 temperature values. |
| | 1 | 1-4 | TEMP (DF = 303 K) |
| | | 11-20 | Number of hours (n) of varying temperature (MAX = 24) |
| | | 21-30 | Temperature at time t = 0 |
| | | 31-40 | Temperature at time t = 1 hr |
| | | 41-50 | Temperature at time t = 2 hr |
| | | 51-60 | Temperature at time t = 3 hr |
| | | 61-70 | Temperature at time t = 4 hr |
| | | 71-80 | Not read |
| | | | If more than 4 hours of values, continue on next line |
| | 2+ (optional) | 1-10 | Continuation of temperature values |
| | | . . . | |
| | | 61-70 | |
| | | 71-80 | Not read |

| Option | Line No. | Column | Contents |
|---|---|---|---|
| TIME | Reset starting and ending times for simulations with this option. | | |
| | 1 | 1-4 | TIME |
| | | 5-10 | Not read |
| | | 11-20 | Starting time for simulations based on 24-hour clock (DF = 0800) |
| | | 21-30 | Ending time for simulations (DF = 1800). Note: Maximum difference is 24 hours |
| | | 31-80 | Not read |

| Option | Line No. | Column | Contents |
|---|---|---|---|
| TITLE | Input a new title. If this option is not activated, the default title is "Standard Ozone Isopleth Conditions." | | |
| | 1 | 1-4 | TITL |
| | 2 | 1-72 | The title can be placed anywhere in line between columns 1-72 |

| Option | Line No. | Column | Contents |
|---|---|---|---|
| TRANSPORT | Option for site-specific information on $O_3$, $NO_2$, NMOC transported in the surface layer and in the air aloft that is entrained as the mixing height rises. (If TRAN option is not used, concentration of transported species is 0.) | | |
| | 1 | 1-4 | TRAN |
| | | 11-20 | Transported ozone concentration in the surface layer (ppm) |
| | | 21-30 | Ozone entrained from aloft (ppm) |
| | | 31-40 | If nonzero and positive:* Transported NMOC in the surface layer (ppmC) |
| | | 41-50 | If nonzero and positive:* Total NMOC entrained from aloft (ppmC) |
| | | 51-60 | Transported $NO_x$ in the surface layer (ppm) |
| | | 61-70 | $NO_x$ entrained from aloft (ppm) |
| | | 71-80 | Not read |
| | 2 (optional) | 1-10 | If a nonzero negative value is entered in columns 31-40 of the TRAN line, the total NMOC transported in the surface layer is entered here (ppmC). |
| | | 11-20 . . . . | The fraction of the total NMOC for each of the organic species transported in the surface layer (should be in the following order: ETH, OLE, ALD2, FORM, TOL, TYL, PAR, ISOP, and NR. |
| | | 61-70 | Continue on next line (if necessary) |
| | | 71-80 | Not read |

*The default carbon fractions for NMOC transport in the surface layer and for NMOC aloft are given in Table 5, Section 4.

| Option | Line No. | Column | Contents |
|---|---|---|---|
| TRANSPORT | | | |
| | 3 (optional) | 1-10 | If a nonzero negative value is entered in columns 41-50 of the total NMOC entrained from aloft is entered here (ppmC) |
| | | 11-20 | The fraction of the total NMOC entrained for each of the organic species entrained from aloft. Continue on next line (if necessary) |
| | | . | |
| | | . | |
| | | . | |
| | | . | |
| | | 61-70 | |
| | | 71-80 | Not read |

| Option | Line No. | Column | Contents |
|---|---|---|---|
| WATER | | | Allows for varying water concentration profile. This option must follow the TEMPerature option. Information is entered regarding the number of hours with varying water concentrations, the hourly relative humidity, and the atmospheric pressure. The relative humidity values are read for the initial time and at the end of each hour. If there are n hours, there should be n+1 relative humidity values. If the WATE option is not used, the default water concentration is 20000 ppm. |
| | 1 | 1-4 | WATE (DF = 20000 ppm) |
| | | 11-20 | Number of hours of varying water concentrations. (MAX = 24) |
| | | 21-30 | Enter the atmospheric pressure; units of inches of Hg. (DF=29.92 inches of Hg which is equal to 1 atm) |
| | 2 | 1-10 | Relative humidity (in percent) at time t = 0 |
| | | 11-20 | Relative humidity at time t = 1 hr |
| | | 21-30 | Relative humidity at time t = 2 hr |
| | | 31-40 | Relative humidity at time t = 3 hr |
| | | 41-50 | Relative humidity at time t = 4 hr |
| | | 51-60 | Relative humidity at time t = 5 hr |
| | | 61-70 | Relative humidity at time t = 6 hr |
| | | 71-80 | Not read |
| | 3+ (optional) | 1-10 | Continuation of relative humidity values |
| | | . . . | |
| | | 61-70 | |
| | | 71-80 | Not read |

| Option | Line No. | Column | Contents |
|---|---|---|---|
| bbbb | A blank line must follow all input lines to terminate the program. | | |
| | 1 | 1-4 | Blanks |

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

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**16. ABSTRACT**

OZIPM-4 is a model which allows the user to estimate the volatile organic compound (VOC) control requirement for a city in order to achieve the national ambient air quality standard for ozone.

This document describes a PC-based system which assists the user in creating input files.

**17. KEY WORDS AND DOCUMENT ANALYSIS**

| a. DESCRIPTORS | b. IDENTIFIERS/OPEN ENDED TERMS | c. COSATI Field/Group |
|---|---|---|
| ozone<br>VOC control strategies<br>photochemical modeling | | |

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