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USEPA / Office of Toxic Substances

Graphical Exposure Modeling System

G E M S USER'S GUIDE

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DISCLAIMER

This edition of the user's guide is a preliminary document and is presented only as a DRAFT. It has not been released formally by the Office of Toxic Substances, Office of Pesticides and Toxic Substances, U.S. Environmental Protection Agency, and should not, at this stage of development, be construed to represent EPA policy. It is being circulated for comments on technical merit and policy implications.

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HOW TO USE THIS MANUAL

This is a NEW User's Guide for the Graphical Exposure Modeling System (GEMS). New enhancements to GEMS through the spring of 1988 are reflected in this document, which is intended to replace all previous versions.

Chapter One gives you a broad introduction to GEMS and how it works. You'll learn how to communicate with the program, and what to expect for your efforts. You will want to read this section since it contains previously un-presented information. After reading this section you should be ready to use the system. If you are not experienced in GEMS use, you may want to read the additional chapter which describes the GEMS procedures you want to use.

Because of our desire to provide fresh information to you as quickly as possible, we have decided to release the new User's Guide in stages. The introduction is being issued first, to provide you with a logical understanding of overall GEMS capabilities. Additional chapters referenced in Chapter 1 (the Introduction) are in various stages of production, and will be released upon individual completion.

A number of useful tables will be provided at the end of the completed volume, including information which is refered to in a number of places in the text. These tables provide information which is useful to a GEMS user but which did not fit in at any particular place in the user's guide.

The glossary at the end of the volume provides definitions for terms used in the text. This User's Guide includes a topical index to help you quickly find just the information you seek.

Many people have contributed greatly to the compilation of your user's guide. We would like to thank all of them for their efforts, especially the following people, (listed alphabetically) without whose individual efforts the project would not have been completed. Andy Battin, Jon Chen, Nancy Chiu, Terri Grasso, Loren Hall, Pat Harrigan, Dr. Russ Kinnerson, James Pillotte, Scott Rheingrover, Kellie Scialabba, John Thomas, Cathy Turner, and Stuart Wollman.

If you have comments on the manual, please drop us a line and share them with us. You can use the User Response Form at the end of the Guide or drop us a line directly. Its your feedback that will direct the publication of the next GEMS User's Guide.

Herb Hunt
Dalroy Ward
GSC, May 1988

Foreward

The Graphical Exposure Modeling System (GEMS) was first developed in 1981. The first version of GEMS consisted of only a few modeling tools with limited application, and of potential use to only a few scientists. Today, GEMS has evolved into a system that combines the power of over 40 different modeling and statistical analysis tools into one easy-to-use system. GEMS is used by over 250 scientists working at EPA headquarters and its regional offices, other Federal agencies, and State and local environmental and human health departments.

Several proprietary systems have been incorporated into GEMS including the powerful analysis and graphic display tool, Statistical Analysis System (SAS). These separate systems each has a user's guide available for those users who are not familiar with their individual operation. In addition, each of the environmental models in GEMS has its own user's guide. In this document, we have provided only brief overviews of the function of each of these separate systems, along with a quick reference to commands utilized within each. The reference section of this guide lists the model and system specific user's guides.

This publication has evolved from several previous writings by many different authors. We hope to provide on these pages a clear and concise guide to GEMS use for the user who already has a basic understanding of the functioning of the various component systems. *Editorial comments are not only welcomed, but encouraged.*

Every attempt has been made to insure that the contents of this users guide are correct and presented in the most useful manner. However, GEMS is an ever evolving system, and the possibility exists that even while we were writing these pages, the system may have outgrown the paper. We apologize, and hope that the next update will reach you soon. If you find documentation bugs, take a moment to report them to us by using the GEMS trouble reporting procedures outlined in Section 8.1. Thanks!

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Chapter 1 - Introduction

The amount of data on which policy decisions are based has created an ever increasing burden for planners. There needs to be a way to evaluate a large volume of information quickly and accurately. To answer this need, the Office of Toxic Substances (OTS) has developed the Graphical Exposure Modeling System (GEMS). GEMS is an interactive information management tool designed to allow the quick and meaningful analysis of environmental problems. Figure 1-1 illustrates the functional relationship of the various GEMS components.

1.1 Who Uses GEMS

GEMS was originally designed for use by EPA scientists and modelers who needed a tool to provide comprehensive policy planning support to EPA administrators. It has subsequently evolved into a tool for use by a wider range of environmental professionals, including those at the state level, as well as other federal agencies such as the Department of Energy. Plans are now in the works to increase the scope of GEMS use by making it available to local communities and several international agencies. The environmental scientist at virtually every level from federal to local community will eventually be able to use this tool to provide policy and planning support for a broad range of environmental issues.

1.2 How GEMS Works

Like most scientists elsewhere, the EPA turned to the computer to help solve their number crunching tasks. GEMS was developed to provide interactive analysis of information in a

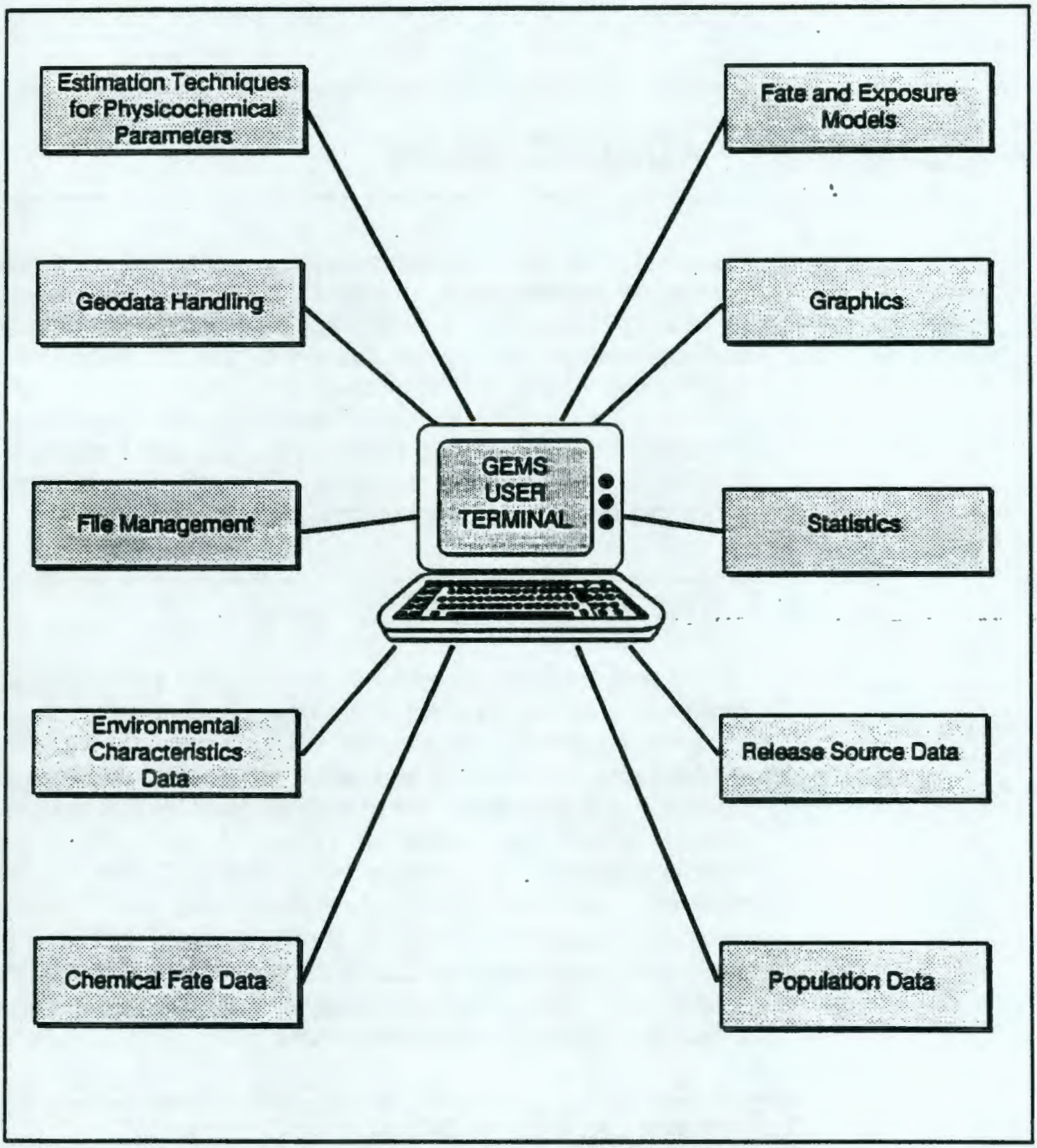

FIGURE 1-1. GEMS Components

broad range of databases of interest to scientists and policy makers. Data such as census information on population distributions are used in studies with other data such as chemical fate or modeling data. Often many databases are utilized in producing GEMS outputs.

GEMS is an operating environment that ties together several previously discrete analysis tools into a coordinated system that allows for multiple types of analysis. These discrete systems are handled under a common environment that makes a user's data available to multiple individual modules of GEMS. Data produced by certain GEMS models, for example, could then be utilized to provide graphic analysis.

GEMS allows the user to:

- Estimate chemical properties.
- Assess the fate of chemicals in receiving environments.
- Model resulting chemical concentrations.
- Determine the number of people potentially exposed.
- Estimate the resultant human exposure and risk.

While some modeling knowledge is required to operate the models, the use of GEMS as the host environment for accessing these models is extremely simple and requires only minimal computer skill.

The modular design of GEMS supports the implementation of additional features on an ad hoc basis. Modules already implemented include:

- Molecular Structure Entry
- Physicochemical Property Estimation
- Fate of Atmospheric Pollutants
- Air Models
- Soil Models
- Water Models
- State/County Map
- Geographical Data Manipulation and Mapping
- Census Data Retrieval

HELP is always available to the user at the touch of a key, and even an AUTOHELP facility is available to assist new users,

which provides help messages every step of the way. More experienced users may elect not to use the menu navigation system by simply issuing direct commands to GEMS to access specific functions. Menus are used to set up models and provide information input to GEMS. There is also a "prompt mode" available for users who feel more comfortable in an interactive dialog rather than menu selection. This range of user options provides broad support to users of any skill level.

1.3 GEMS on the EPA VAX Cluster

GEMS resides on the VAX Cluster of computers maintained by EPA at Research Triangle Park (RTP), North Carolina. The VAX Cluster currently consists of two VAX 8600's and one VAX 11/785. You must have an account on this system to access GEMS. If you do not currently have an account contact:

Ms. Cathy Turner at (202) 382-3929 / FTS 382-3929

She will send you information on opening an account. When you receive your account confirmation from the National Computer Center (NCC) at RTP be sure to keep it in a safe place. When you log onto the system, you will need to know the Username you were assigned, the initial Password for your Username and the Project to which your work will be charged.

1.3.1 Getting to the Port Selector

With a valid account on the RTP system you may use your modem and terminal or PC to log onto the system. The actual connection to the VAX Cluster is accomplished by using one of the following access methods:

1. Washington, DC Direct Access
2. Regional Dial Access
3. DECnet Access
4. TYMNET Access

You will need to investigate which of these alternatives is best suited for your needs. Some incur additional charges, while some are toll-free. These methods are discussed in the following sections. If you are in metro Washington, D.C., or in

the area of one of the regional access numbers, TYMNET access is not available.

Yet another access method is available for international users. More about international access is discussed in Section 1.3.1.4.

1.3.1.1 Washington DC - Direct Access

From the metropolitan Washington DC area, you access the Cluster by dialing the local access number for the communications line to RTP, 488-3671. This number will allow you to access the port selector at RTP. TYMNET nodes in the metropolitan DC area can not access the RTP computer, you must use one of the direct access numbers. 488-3671 supports both 1200 and 2400 baud,or 488-1515 for 1200 baud only. For calls from DC, your communication parameters should be 7 data bits, even parity. For information on what happens after you dial this access number, go to Section 1.3.2 for instructions on use of the port selector.

1.3.1.2 Regional Dial Access

To use the Regional Data Switch, dial the appropriate number listed in Table 1-1 below.

TABLE 1-1. Regional Dial Access Numbers for 300 and 1200 Baud Operation as of 3/1/88

REGION	OFFICE LOCATION	TEL. NUMBER	FTS
I	Boston, MA	(617) 565-3774	8 835-3774
II	New York, NY	(212) 264-1554	8 264-1554
III	Philadelphia, PA	(215) 597-0103	8 597-0103
IV	Atlanta, GA	(404) 347-7285	8 257-7285
V	Chicago, IL	(312) 353-2468	8 353-2468
Lab	Cincinnati, OH	(513) 569-7821	8 684-7821
VI	Dallas, TX	(214) 655-6409	8 255-6409
VII	Kansas City, KS	(913) 371-8118	8 757-8118
VIII	Denver, CO	(303) 293-1400	8 564-1400
IX	San Francisco, CA	(415) 495-0168	8 454-0168
Lab	Las Vegas, NV	(702) 798-3101	8 545-3101
X	Seattle, WA	(206) 442-4423	8 399-4423

These numbers should be used if you are working in an EPA regional office or either of the two EPA labs, or if you these numbers are local calls to you. When calling some of these regional data switches, you may be prompted for a device type. For example, the Region II Network users must first select [illegible] for ASCII 1200 baud. Generally, if you have an IBM PC or a VT100 emulator, respond to terminal-type prompts with [illegible] An alternative is to simply hold down the control key and press the [illegible] key five times. You will get a message welcoming you to the system and asking for a system choice. These choices will include PDP, NCC, and TCP.

To access the VAX Cluster, the home of the GEMS system, select [illegible] This will provide you with access to the NCC IBM through the protocol converter. Regions V and VI will be prompted with **"Commtex Data Exchange. Enter terminal's device type:"**. Type [illegible] for help and respond to the following prompts according to the terminal type you are using. The next message you will see will ask you to select the mainframe you want to use, select [illegible] After this point, the process will be identical to the procedures described in Section 1.3.2, The RTP Port Selector. For more detailed information on what to do next, go to this section.

1.3.1.3 DECnet ACCESS

If you have a local VAX which is on the EPA DECnet network, you can access the VAX Cluster across the network. To do so, log into your local VAX and then use the VAX/VMS SET HOST command to connect to the Cluster.

SET HOST VAXTM1 for access via DECnet

or

SET HOST/X29 VAXTM1 for access over the X.25 network

Your system must have DEC PSI available, and your system manager must have set up the address file in order to use the X.25 link. Check with your system manager to determine if DEC PSI is available and set up on your system.

If your network link is at 9600 baud or less you should use the X.25 network for access to the Cluster. At such low speeds, the DECnet overhead can make editing a tedious process at best. By using this method, you bypass the port selector and connect directly to the Cluster.

1.3.1.4 TYMNET

TYMNET is available if you are outside of the cities with regional offices listed in Table 1-1 and without access to toll-free numbers. To use TYMNET, you will need to call NCC at (919) 541-4506 (FTS 629-4506) to find the number for your area. When you call NCC to get the phone number, make sure you ask for the number that supports the speed at which you plan to communicate (1200 or 2400 baud). When you are using TYMNET, your terminal should be set to 8 data bits, no parity. When you dial the TYMNET number, TYMNET will respond with:

- **Enter your terminal id:** (at 300 baud)
- **$xx%!@xxxx$&x%x%#** (at 1200 baud)
  (The garbage may be a couple of lines.)
- You will see nothing immediately following carrier detection at 2400 baud.

If you are calling at 1200 baud, don't worry about the garbage, that's normal. In all cases enter an *A* in response. You don't need to wait until the text is finished before typing "A". At 2400 baud, you will see nothing until you enter "A".

You will then see:

Please Log In:

Respond with:

EPA1 for 1200 baud

or

EPA2400 for 2400 baud operation

If you are using a 2400 baud line, you will need to know the TYMNET password. To learn the TYMNET password for 2400 baud operation, you should contact NCC at (919) 541-4506.

Once you have successfully gotten to this point, the TYMNET network will advise you of a successful connection with a message like:

NODE xxxx HOST 1038 EPA IS ONLINE

Congratulations, you are now connected to the port selector at RTP. Continue with the procedure discussed in Section 1.3.2 below.

If you are having trouble logging into the system, and believe you are doing everything right, there may be a problem with the computer itself. The National Computer Center maintains a status phone to let users know if there are problems with the system. You can call (FTS) 629-2969, or (919) 541-2969 to check on the current system status.

TYMNET International Access

To obtain information for accessing the NCC computer from overseas, first dial your local TYMNET node. At the **Please Log in** prompt, type *INFORMATION* to enter the TYMNET Information Service. At the Main Menu select the entry for International Access.

TYMNET provides access to and from over 70 foreign countries, and you can obtain a listing by selecting #1 from the second menu. For detailed information on a specific country that is on the list, select option #2. You will be prompted to enter the name of the country, and then will be given information including a contact in that country (name, address, telephone number, and telex) and technical information including access, speeds and protocols supported, and prices. Inbound and outbound rates are listed in Menu Item #4; customer support information is provided in option #7.

TYMNET Customer Support and Trouble-Shooting services are available to help in placing an international call. The toll-free number is (800) 336-0149. When trying to locate NCC's international address you may be asked to contact a communications consultant in external network services at (703) 356-6993.

1.3.2 The RTP Port Selector

Once you have connected to the port selector, you are almost there. Enter one or two carriage returns to bring up the port selector menu. (If you enter too many returns, you will be disconnected). The menu will look like this:

```
Welcome to the Environmental Protection Agency National Computer
                        Center

Please enter one of the following
                    IBMPSI for IBM
                    UNI for SPERRY
                    TCP for 3270 Emulation
                    FMO for FMO PDP
                    VAX for VAX
                    PRIME for PRIME
                    EMAIL for EMAIL via X25
Enter Selection:
```

FIGURE 1-2. Initial Messages

At this prompt, enter VAX. Now you are finally at the VAX Cluster and ready to log into the computer. Once you tell the port selector to connect you to the VAX, you will see:

Connected.

Now enter a few carriage returns (one or two) until you get the computer's attention. It will then respond with:

Username:

Enter the username which was assigned to you by the RTP accounts personnel. You will then see:

Password:

Enter the password for your username. If this is your first time logging in, then enter the password which was given to you on your account authorization information from RTP. Otherwise enter your current password. If this is your first time logging on, remember to change your password when you finish logging in.

After entering your password, if you see **User authorization failure**, then you have entered either your username or password incorrectly. The system will re-prompt you for your username and password. If you enter everything as entered on the account authorization information you received from RTP, then give User Support a call (800) 334-2400, or (FTS) 629-7862 for assistance in solving the access problem.

```
Welcome to the US EPA VAX Cluster - Timesharing VAX 8600
*****************************************************************
VAX USER SUPPORT: (FTS)629-7862 or 919-541-7862 or 800-334-2405
*****************************************************************
VAX 8600 Operations Status Phone: (FTS)629-2969 or 919-541-2969
For the Weekly Operations Schedule Type:  OPERATIONS_SCHEDULE
*****************************************************************

Last interactive login on ...
Last non-interactive login on ...
*****************************************************************
                    CURRENT NEWS ALERTS
- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -

************TYPE "NEWS ALERT#" TO VIEW AN ALERT*************
```

FIGURE 1-3. VAX Cluster Messages

Project:

At this point you enter the project which has been assigned to you, it will be listed under "account" on your account authorization sheet. You cannot finish the login procedure without this information. If you cannot remember your project then type LOGOUT to log off of the system and find the account authorization information that you received from RTP

to confirm that your account had been set up. This will have the project information.

Once you have completed the process of logging into the system you will see the VAX/VMS prompt, the dollar sign ($). This indicates that the system is ready and waiting for input from you. Under some circumstances you may have a system prompt of the node ID in the network (i.e.: CASTOR> or VAXTM1>) rather than the "$." If your account is setup in this manner, then substitute your prompt for the "$" we use in this manual for illustration.

VAX/VMS uses the Digital Command Language (DCL) as the interface between you and the VAX. One of the most useful of the DCL commands is the "HELP" command. This will access the VAX/VMS on-line help function. You can simply type *HELP* or type *HELP option*.

For example you can enter *HELP COPY* for help on the copy command. You can get help on any DCL command in this manner. To give you a hand, if this is your first time on a VAX, we present several useful concepts below.

If this is your first time logging into your account, you should IMMEDIATELY change your password to something you won't forget. The VAX requires this change for security reasons. If you forget to change your password, your username will be locked against use once you log off after your initial session. Then you will have to call USER SUPPORT to have your Username unlocked. When changing your password try to choose something which only you can guess. Avoid using words that others might guess such as your spouse's or child's name, your middle name, or other words that are easily associated with you. Remember you are responsible for guarding the security of your password. Memorize the password and do not keep it written down next to your terminal or in your office. To help insure the security of your password, the system will not display your password as you enter it. Looking over your shoulder will not allow others to see your entry.

To change your password, enter:

```
$ SET PASSWORD
```

You will be prompted for your old password, new password, and verification: once you have entered your currently valid password, you will be asked to enter the new password that you want to use in the future. To verify your entry of the new password, you will be asked to enter it a second time. BE SURE TO REMEMBER YOUR PASSWORD. IF YOU FORGET IT, YOU WILL LOSE ACCESS TO YOUR ACCOUNT.

When you log in to the system you will be in your main directory. At this point you can edit files, create sub-directories, or run a program, for example: GEMS. Remember, however, that if this is your first time logging on, you must set up the GEMS environment before you can run GEMS. Be sure to learn about creating sub-directories as they are very useful for organizing your files. If you put everything you do into your main directory, it will get very cluttered and it will be difficult to find the files you are interested in. In the next two paragraphs we'll introduce a few DCL commands to you and give a short description of how file names work on the VAX. If you are new to VAX computers, please be sure to read both of these sections.

File names under VAX/VMS have two components, the file name and the file type in the format:

filename.filetype

The file name can have from one to 39 characters chosen from the letters A through Z, the numbers 0 through 9, and the underscore (_) and dollar sign ($). The file type can be from 0 to 39 characters from the same set of characters. The file name and the file type are separated by a period (.). Some examples of legal file names are:

LOGIN.COM	DATA.
GENERAL.DAT	GAMS_ISC01.CONC

The system recognizes a number of default file types for special purposes. Use of these file types should be limited to the types of files they are meant for:

FILE TYPE	USE
COM	DCL Command procedure (example: LOGIN.COM)
DIR	Directory or subdirectory
EXE	Executable file
OBJ	Object file created by a compiler or assembler
FOR	Source file for FORTRAN compiler
MAI	VAX/VMS Mail file

In addition to a file name and type, every file has a version number assigned to it when it is created or revised. When you initially create a file it has a version number of 1. As you modify the file the version number is increased by one each time. The system will maintain all versions of a file. You should use the PURGE command to delete all versions but the highest numbered (most current) one.

A wildcard character is a symbol that you can use with many DCL commands to apply the command to several files at once, rather than specifying each file individually, or to select a sub-set of the available files in a directory. The wildcard characters are the asterisk (*) and the percent sign (%). The asterisk matches any number of characters in a file name or file type:

```
DIRECTORY *.DAT
```

DIRECTORY *.DAT would give you a list of all files in your directory with the file type of DAT. The percent sign matches only a single character in the position at which it is specified:

```
DIRECTORY CHAPT%.TXT
```

DIRECTORY CHAPT%.TXT would list out files such as CHAPT1.TXT, CHAPT2.TXT, but would not list CHAPT.TXT or CHAPTIX.DAT.

1.3.3 Setting Up GEMS

Once you have successfully logged into the VAX Cluster computers you must setup your LOGIN.COM file in order to gain access to GEMS. If you do not yet have a LOGIN.COM file, you can simply copy over a sample file which is provided to help you set up your account to use GEMS. To copy this file, enter:

```
$ COPY USER32$DISK:[GEX.LOGIN]LOGIN.COM *
```

If your LOGIN.COM file already exists, you must edit this file and add the following line.

```
$@USER32$DISK:[GEX]GEMSUSER.COM
```

In order to gain access to GEMS, you will have to re-execute your LOGIN.COM. To do this simply enter:

```
$@LOGIN
```

Your LOGIN.COM is executed automatically each time that you log into the system so it will not be necessary for you to execute this file yourself with each future login.

1.3.4 Running GEMS

After following the procedures in Section 1.3.3, your LOGIN.COM sets up the GEMS execution structure for you. All you will need to do to run GEMS is enter:

```
$ GEMS
```

See Section 1.4, Using GEMS, for additional information on using the system.

1.3.5 Things to Know

The first time you run GEMS, a number of files and directories will be created in your account. The most important of these is the sub-directory GEMSLIB. This directory will be created by GEMS under your primary directory. If your primary directory was [GEMSUSER] then you would have the new directory [GEMSUSER.GEMSLIB]. This directory is very important. It contains your GEMS User Dataset Library. You should never delete the files in this directory or the directory itself except from within GEMS. If you delete files within this directory, you lose access to that dataset and run the risk of damaging your User Dataset Library. If it is damaged, you will lose access to the rest of your data.

If you run the Estimation Procedure routines, you will have a number of files ending in the extension .SFS created in your main directory. These files are important to the execution of these programs and are used to store the structures which you are entering. If you delete these files, you will lose access to the structures which you have previously entered. If you no longer need access to previously entered structures, you can delete these files to conserve disk space.

Files will also be created, in your directories, as you run some of the models accessible through GEMS or when you use the EXPORT feature under GEMS File Management. Files existing outside of the GEMS file management structure must be managed by you. You may save or delete these files as you deem appropriate.

Remember, if you have not accessed a file for 45 days, it will automatically be archived to conserve disk space, and will be available only after recalling it from archive. To learn how to retrieve a file from archive type *HELP TAPE RESTORE* or consult the NCC VAX Users Guide.

Changing file protections can be very helpful in preventing the accidental erasure of your files. To change file protection, use the VAX/VMS SET PROT command:

SET PROT=(S:REWD,O:REWD,G:REWD,W:REWD)

FILENAME.EXT

You can change the protection for various categories of users:

S(ystem)	System level Usernames
O(wner)	Yourself
G(roup)	Usernames under the same project as yours
W(orld)	All other Usernames

Remember that you must remove a protection from all categories after yours. For instance, if you have removed "Delete permission from O(wner)" but you have left it in for "W(orld)," you will still be allowed to delete the file.

The protection codes are:

E to be allowed to execute a file. Mainly applies to .COM and .EXE files. Allows a user to execute the file without being able to read or write the file.

R for read permission. Users in the applicable category will be allowed to read the file. This level of protection also allows a user to make a copy of the file.

W for write permission. Users will be allowed to write new information to the file. Be very careful in allowing this level of protection.

D A user will be allowed to delete the file. Omit this protection to prevent yourself or others from being able to inadvertently delete this file.

1.4 Using GEMS

If you have successfully completed Section 1.3 of this manual, you should now have logged on to the computer system and have access to GEMS. Before you actually run and use GEMS, there are some concepts you should keep in mind.

1.4.1 GEMS Menus

GEMS comes with two basic types of menus, navigational menus and parameter editing menus. Knowing the differences between the two will be helpful in understanding how the system works and how to use the system most efficiently.

1.4.1.1 Navigational Menus

Navigational Menus help you navigate your way through GEMS. They present you with a list of options from which to select. When you select one, you will proceed to either another navigational menu or a parameter editing menu. To get to many GEMS functions, you may have to go through several navigational menus.

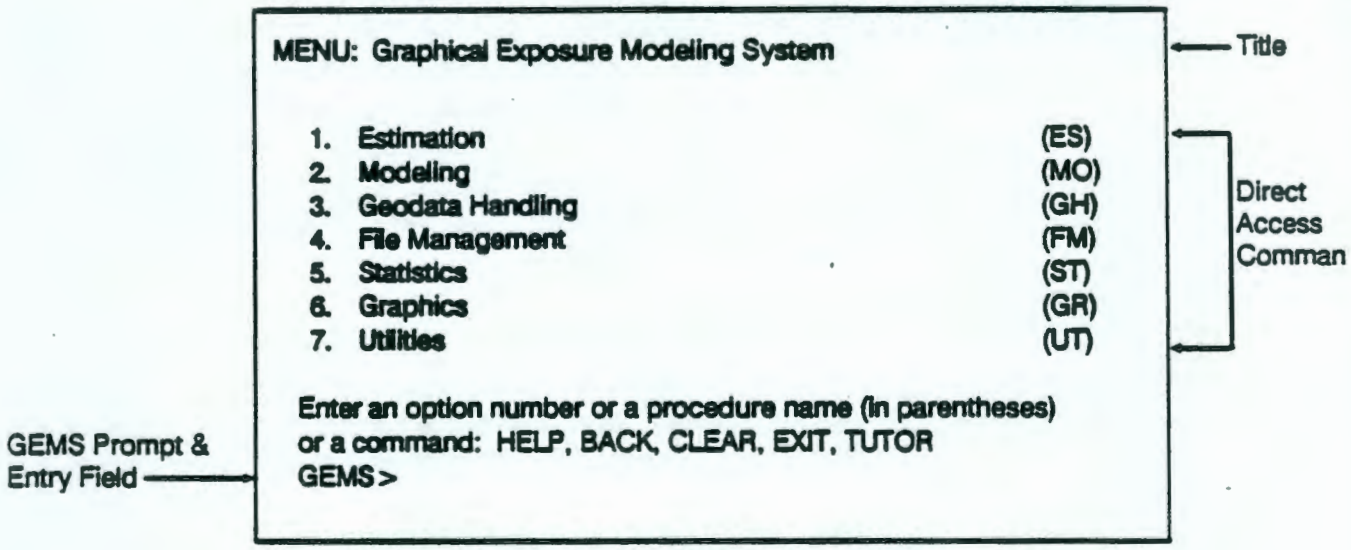

FIGURE 1-4. Typical Navigational Menu

Title:	This is the title of the menu. If you have problems at a menu, writing down the procedure you were using (the title of the menu) can greatly assist the support staff in solving any problem.
Reference number:	Each parameter on the menu will have an associated reference number. Enter this number to select the operation or procedure.
Description:	The name of the operation that is associated with the number preceding it is presented.
DAC:	The Direct Access Command for the procedure or operation. (See below for a discussion of DAC's).
Entry Field:	This is the area of the screen where you will enter your function selection.

To select an option from the menu, you need only type the reference number associated with that item.

Once you are familiar with GEMS, you can issue a Direct Access Command (DAC) for the functions that you want to use. The Direct Access Command lets you name a destination without relying on the system navigational menus for guidance. This can save you time and keystrokes when you know exactly what you want to do and the proper command to do it. Remember, however, that DAC's are available only from navigational menus.

At navigational menus, you can type *HELP* to bring up a help screen that explains your current menu. You can also type *HELP n* where n is the reference number, and you will get specific help about that selection.

The DAC feature is very powerful and useful, but you should take care in its use. The problem with relying on the Direct Access Commands too heavily is that you miss many of the other useful features which are available through GEMS. After navigating through the menu screens, you will reach the

procedure you desire. Once there, you will use the Parameter Editing Menus.

1.4.1.2 Parameter Editing Menus

Parameter Editing Menus are the menus which are used to enter values into GEMS for specific parameters needed by a GEMS procedure in its execution. Several conventions exist in editing menus which you should be aware of. A field which contains an asterisk (*) will have a default value applied if you do not change it. Many menus used in setting up input for the models used in GEMS have default values already in place in the parameter fields. These values should only be used if you have verified that they make sense for your application. While an attempt has been made to select values which will apply in many situations, it cannot be assumed that the default value will apply in any specific situation. Finally remember that DACs will not work at a parameter editing menu.

Title →

MENU: Monthly Climate Data for Year 1

Ref.	Parmname	Parameter Description	Parameter Value	Index
1.	TA	Air Temperature (deg C)	15.08	(1)
2.	NN	Cloud Cover (frac.)	0.77	(1)
3.	S	Relative Humidity (frac.)	0.84	(1)
4.	A	Short Wave Albedo (frac.)	0.19	(1)
5.	REP	Evapotranspiration (cm/day)	0.00	(1)
6.	MPM	Rain Depth (cm/month)	13.86	(1)
7.	MTR	Mean Storm Duration (days)	0.24	(1)
8.	MN	Number of Storm Events (#/mnth)	11.00	(1)

Reference Numbers

Enter one or more combinations of: reference or parameter name and value(s)[ref1 value1, ref2 value2, ...] or a command: HELP, NEXT, BACK, END, CLEAR, EXIT

GEMS Prompt & Entry Field →

GEMS>

FIGURE 1-5. Typical Parameter Editing Menu

Title: This is the title of the menu. If you have problems in GEMS, writing down the procedure you were in and the title of the menu you were at can greatly help in finding and solving the problem.

Reference Number:	Each parameter on the menu will have a reference number associated with it. This is the number which you will use to specify which parameter you want to assign a new value to.
Parameter Name:	The name of the parameter. Every attempt has been made to associate a meaningful name with the parameters.
Description:	A short description of the parameter.
Value:	This field displays the current value of the parameter. Many parameters will be initially displayed with no value. You must specify a value for all items on the menu which do not have default values.
Index:	This lets you know if a parameter is a single value or an array parameter. If this field is blank, it is a single value. If the parameter is an array parameter (i.e., it can take on more than one value), this field will initially have a "(1)" displayed there. This indicates that the value of the first index is being displayed on the menu.
Entry Field:	This is the area of the screen where you will enter your information to fill the editing screen.

Now that you know a bit about the menu, here's how you modify parameter values in the menu.

To modify a parameter you type its reference number followed by a space and then the new value: *1 NEW VALUE* If you are using a DEC video terminal or Tektronix 41xx series terminal, the new value for the parameter will be displayed on the menu, after a CR, to indicate that the value has been changed. If you are entering values for an array parameter then you should enter just the reference number. You will then

be prompted for the values for each element of the array. You end the process by entering just a carriage return for a value. You will then be returned to the same menu and the value of the last element of the array will be displayed and the number of elements in the array will be indicated by the index field.

You can use the SHOW command to examine the value of a specific element of the array. Use is simple, just type the command *SHOW PAR-NAME(INDEX)* where you replace PAR-NAME with the name of the parameter, and INDEX with the number of the element you want to see. The value and index fields will be updated with the information you requested.

By typing *HELP* you can bring up a general help screen about the menu, or by typing *HELP n* , where 'n' is the reference number, you can bring up help for a specific parameter on the menu.

When entering data you may also put more than one reference number on a line. Separate the entries using commas (*1 new value,2 another new value,3 the third new value*) to modify the values for Items 1, 2 and 3.

Once you have finished entering values into this menu, you type *NEXT* to proceed to the next menu. If the menu you were on is the last in the sequence, then the NEXT command will proceed to run the program.

Should you decide that you want to end the procedure you are in prior to finishing your work, you can type *END* to end the current procedure and return to the previous navigational menu or *CLEAR* to end the current procedure and return to the main GEMS menu.

1.4.2 Entering GEMS

If you have set up your LOGIN.COM file as explained in Section 1.3.2 then you will be able to simply enter the command *GEMS* to run GEMS. If you have not yet setup your LOGIN.COM file, turn to Section 1.3.2 and do so before proceeding.

When you enter GEMS, it will print out the GEMS NEWS file to let you know about any new procedures or updates which have been made to GEMS recently. Once you have seen the GEMS NEWS, it's time to select your terminal type:

```
MENU: Terminal Type Specifications

   1. VT100-compatible terminal          2. Tektronix 4010 terminal
   3. VT100 with TEK41040 emulator       4. Tektronix 4014 terminal
   5. 80 column ASCII terminal           6. Tektronix 4105 terminal
   7. 132 column ASCII terminal          8. Tektronix 4106 terminal
   9. LA120 DECwriter terminal          10. Tektronix 4107 terminal

Please identify your terminal type by number
?
```

FIGURE 1-6. Terminal Selection Menu

Enter the number which corresponds to the terminal with which you logged onto the computer. This lets GEMS set up conversational parameters for such functions as full-screen display. This is important! Many GEMS features will only display on a particular terminal type (i.e., while you may run one of the mapping options on any terminal, a TEKTRONIX or compatible terminal is required to display the map). GEMS will still let you request these functions but will simply store the map or graphic which is created in your library for later viewing on the proper terminal. Once you have entered your terminal type GEMS gives you the official Welcome:

```
                GRAPHICAL EXPOSURE MODELING SYSTEM

                        Version 8.1

                      Developed by
                GENERAL SCIENCES CORPORATION

                          For
            U.S. ENVIRONMENTAL PROTECTION AGENCY
        OFFICE OF PESTICIDES AND TOXIC SUBSTANCES
```

FIGURE 1-7. GEMS Welcome Screen

After a few seconds the main GEMS menu will appear.

```
MENU: Graphical Exposure Modeling System

  1. Estimation                    (ES)
  2. Modeling                      (MO)
  3. Geodata Handling              (GH)
  4. File Management               (FM)
  5. Statistics                    (ST)
  6. Graphics                      (GR)

Enter an option number or a procedure name (in parentheses)
or a command: HELP, HELP option, BACK, CELAR, EXIT, TUTOR
GEMS >
```

FIGURE 1-8. GEMS Main Menu

You are now ready to begin work. From this menu you can either navigate through the available choices to the function that you want to use or use the menu DAC to jump there directly (as discussed above). The DAC is displayed at the far right of the selection screen. For instance, to advance to the Environmental Models section of GEMS you could either enter 2 from the main menu or enter MO.

Each of the items on the main menu is the subject of a chapter in this manual. Because of the complexities of Chemical Property Estimation and Modeling, separate User's Manuals have been written for these functions. In Chapters 2 and 3, we will provide you with a broad overview of these operations and refer you to the appropriate detailed user's guide. In Chapters 4 through 8, we present a much more detailed discussion of GEMS procedures used in support of the modeling and estimation operations. For now, here's a short overview of each function.

Chemical Property Estimation

The Estimation option provides you with a variety of procedures which can be used to estimate a number of properties on a wide range of chemicals. These procedures fall into two classifications: Structure Entry (SFILES and

SMILES programs) and Property Estimation (CLOGP, CHEMEST, NEWCHEM, AUTOCHEM, and FAP programs). More about Chemical Property Estimation can be found in Chapter 2.

Environmental Modeling

The GEMS Modeling functions provide access to a variety of computer models which simulate the effects of chemicals released to air, water, and soil. The models are grouped by media into the categories of AIR, WATER, SOIL, and MULTI-MEDIA. The AIR models deal with the fate of contaminants released into the atmosphere. The WATER models deal with the fate of a contaminant in surface water bodies, and the SOIL models address transport and fate of a contaminant in soil and ground water systems. The MULTI-MEDIA models deal with the transport and fate of a contaminant as it moves through the atmosphere, soil and surface water. All of these models produce estimated concentrations of the contaminant under study. Many of these models create GEMS datasets which may be used in subsequent analyses. More about Modeling can be found in Chapter 3.

Geographic Data Operations

Geographic Data Handling allows access to mapping routines and to specialized data retrieval operations which access data by location (latitude/longitude) or geographic codes (such as state name or State FIPS code, county name or County FIPS code, etc.). Please remember that the mapping operations are viewable only on Tektronix or compatible terminals at present. More about Geodata handling operations can be found in Chapter 4.

GEMS File Management Operation

File Management allows for the creation and manipulation of GEMS datasets, some of which can be used as the input for other GEMS procedures. This capability also allows you to import data from outside of GEMS for use with GEMS

procedures. More about the File Management Operation can be found in Chapter 5.

Statistics

The Statistics option provides the user with a variety of statistical analysis capabilities and functions. This capability has been implemented using routines from the International Mathematical and Statistical Library (IMSL) and from the Statistical Analysis System (SAS). More about Statistics can be found in Chapter 6.

Graphics

Selection of the Graphics option allows you to display data from the datasets in the system and/or your own dataset library. Many of the models installed in GEMS create GEMS datasets containing the results of the model's execution, which are usable by the GEMS graphics progams. This allows you to graphically represent information and modeling results to assist in analysis. Many of the graphics available through this operation have been implemented utilizing SAS Graphics capabilities. Most GEMS graphics require the use of a Tektronix compatible terminal, or a PC running Tektronix emulation software for viewing the graphs. More about Graphics can be found in Chapter 7.

Utilities

The Utilities operation allows access to a number of useful capabilities. Particularly important under this operation is the Problem Reporting utility, allowing GEMS users to communicate with the GEMS system staff. This feature can be used to send problem reports, complements, and development suggestions and requests to the staff. A number of VAX/VMS utilities are also available under this GEMS Operation. More about Utilities can be found in Chapter 8.

1.4.3 GEMS Datasets

One of the most important concepts that must be mastered for a full understanding of GEMS is that of the GEMS Dataset. There are several types of GEMS Datasets. GEMS User

Datasets are datasets which have been created by and are only accessable to a GEMS user. These are the datasets in your GEMS User Dataset Library. These Datasets are either temporary or permanent. Temporary Datasets are those which have been created during a GEMS session and which have not yet been saved. Permanent Datasets are those which have been saved and remain available from session to session. When GEMS procedures and models create new datasets, they are created as temporary. This is to help you conserve disk space. Temporary datasets are automatically deleted at the end of a GEMS session. If you do not need continuing access to a dataset, you should simply allow this deletion to take place in order to leave as much space available on the disk as possilble. Whenever you exit from GEMS, you will be given a list of new datasets which were created during the current session. You will then be given an opportunity to save the new datasets, rescuing them from automatic and certain deletion.

The other type of dataset is the SYSTEM INSTALLED Dataset. These datasets are owned and maintained by the system and are available to all GEMS users. These datasets remain available from session to session and cannot be deleted or modified by GEMS users. Datasets of this category contain data which has been found to be useful in performing environmental modeling by GEMS users. Many of these datasets are accessed automatically by various GEMS functions, or you can use them with various GEMS functions to create subsets which are useful for your own applications. For information relating to specific SYSTEM INSTALLED datasets please see Chapter 9.

Both User and SYSTEM INSTALLED datasets may be displayed by using the DATASET procedure under the OUTPUT function of the FILE MANAGEMENT operation. The DATASET procedure is documented in Chapter 5 (File Management) and you should review this section in order to gain a full understanding of the procedure.

An important concept which will help you understand the GEMS datasets is that of the data "group". Data groups are used to store information so that variables such as latitude and

longitude which may have many records associated with them can be placed into one group and then the repeating records placed into another group with a link variable between them. This saves a great deal of disk space. If you do not realize which group a variable is in you can get quite confused when attempting to use a GEMS dataset. (see Chapter 9 - Datasets)

The LIST DATASET command allows you to see all of your available datasets. Subcommands allow you to list selected datasets:

Enter a subcommand: TEMP, UON, UOFF, UALL, SON, SOFF, SALL, ALL, HELP, Return to end.
?

TEMP	All temporary datasets
UON	All on-line user datasets
UOFF	All off-line user datasets
UALL	All user datasets
SON	All System on-line datasets
SOFF	All system off-line datasets
SALL	All system datasets
ALL	All datasets
HELP	Brings Help

After you have identified a dataset of interest, the LIST VARIABLES command will allow you to list the variables in that dataset. If you are in a GEMS procedure that has specified a dataset, you will be shown the variables of that dataset. If you have not previously specified a dataset, GEMS will ask you to name one. The LIST DATASET command also has available several subcommands to allow you to specify which variables you would like to list.

Enter a subcommand: INT, REAL, CHAR, ALL, HELP, Return to end
?

INT	All integer variables

REAL	All real variables
CHAR	All character variables
ALL	All variables
HELP	Brings Help

The variables will be displayed by group.

The command DATASET will allow you to change the dataset for which you are listing the variables. Note: you can not do a LIST DATASET command from within LIST VARIABLES, or a LIST VARIABLES from within LIST DATASETS

Often throughout this user's guide we will refer to your User Dataset Library. When we use this term we are referring to the data files and your MAP, GRAPH, REPORT, and TABLE datasets as well.

MAPS are created by the various GEMS mapping procedures, generally found in the GeoMap procedures under the Geodata Handling operation. These datasets can only be displayed. No further manipulation can be performed on these data. Datasets may be reviewed by using the MAP procedure under the OUTPUT function of the FILE MANAGEMENT operation.

GRAPHS are created by the GEMS graphics procedures found under the GRAPHICS operation on the main menu, as well as a number of specialized graphics procedures which are available for use with several of the models. These datasets can only be displayed. Further manipulation of the file is not allowed. These datasets may be reviewed by using the GRAPH procedure under the OUTPUT function of the FILE MANAGEMENT operation.

REPORT datasets store model output files. These files are placed within a structure which will allow you to better manage them. These datasets are usually text files which may be typed through use of the REPORT procedure under the OUTPUT function of the FILE MANAGEMENT operation. No further manipulation can be done to these datasets.

TABLES are generated by several GEMS procedures, for example, STATISTICS - Contingency tables. These datasets

may be viewed by using the TABLE procedure under the OUTPUT function of the FILE MANAGEMENT operation.

The LIST MAPS, GRAPHS,... commands all act identically to the LIST DATASET command except for the absence of system maps, graphs, etc.

The LIST MAPS, et al. command offers you several useful subcommands:

Enter a subcommand: TEMP, ON, OFF, ALL, HELP, Return to end.
?

TEMP	All temporary maps, etc.
ON	All on-line maps, etc.
OFF	All off-line maps, etc.
ALL	All maps, etc.
HELP	Brings Help

1.4.4 Exiting GEMS

Now that you have mastered getting into GEMS, and have learned a little of the fun you can have with the system, it's time to learn how to leave GEMS.

If you are at any GEMS menu, you can simply type EXIT to leave the system. GEMS will then ask you to confirm your intention to leave the system:

Enter YES to confirm the EXIT command; type NO to restart GEMS...
?

If you haven't entered the EXIT command by mistake, confirm with YES and GEMS will check to see if you have created any new datasets while you were on the system. If you have, GEMS will ask if you want to SAVE them:

Temporary data created in the current session...

Datasets: ONE TWO THREE
Graphs: G1 G2
Maps: MAP1 MAP2

Press return to delete them, or enter "ALL" to save them, or enter only names of those temporary data to be saved.
?

Once you have taken care of these housekeeping chores, GEMS will return you to VMS, and you will see the VMS prompt.

$

Remember, if you are using GEMS for the first time, you must change your password before you log-off the VAX or you will not be allowed to log-on again!

Once at the VMS prompt, you can continue to use the system or log out. To log out, type **LOGOUT**.

1.4.5 TGEMS

A special version of GEMS is used to make new procedures available for testing. This version of GEMS is called TGEMS. If you have set up the GEMS environment in your LOGIN.COM file, you can access this version by typing **TGEMS**. TGEMS is provided in order to make new procedures available to you as soon as possible during development. While procedures are not installed into TGEMS until they have been tested, these procedures are not always fully operational. Care should be taken when using any procedure in TGEMS. If you have a problem using TGEMS procedures, you should report it using the normal GEMS problems report method. The TGEMS menus may be different than those in GEMS, which are documented in this manual. This is because of new or updated procedures in TGEMS. The User's Guide is only updated when a procedure becomes operational and is installed into GEMS.

1.4.6 Reporting Problems

If a problem occurs while you are running GEMS or TGEMS, please let us know. It's easy, just use the PR procedure under the utilities menu, or send MAIL to the username GEX. It will help us understand your problem is you will remember to provide us with as much of the following information as possible.

- Date and Time the problem occured.
- Menu title of the menu on which you had problem.
- What happened. (Describe the problem as fully as possible.
- Error Messages (if any) that you received.

Remember, the more you can tell us about what happened, the better we can help. After you submit the problem report, we'll get back to you with an answer as soon as possible.

1.5 Commands Summary

GEMS has its own set of navigation and control commands segregated into four basic functional groups. The commands discussed here are universally operable in GEMS. Additional commands may be functional in isolated sections of the system, and will be discussed as part of the discussion of those sections of GEMS. Note that the commands work as single word commands except where otherwise noted.

Help Commands obtain information about the system:

HELP	AUTOHELP	NOAUTOHELP
LIST	TUTOR	REVIEW
QUEUE	SHOW	

Navigation Commands allow you to move through the system:

BACK	END	CLEAR
EXIT	NEXT	GO

Operational Mode Commands support selection methods for data input:

MENU PROMPT

Parameter Commands are used to change your operating parameters:

RESET STORE RESTORE

These commands, listed alphabetically, include the following; unless specified, the command and the syntax are identical, that is to say, you enter the command exactly as it is written.

COMMAND	FUNCTION
AUTOHELP	Turns automatic help facility on, see "NOAUTOHELP" for a clue on how to turn it off.
BACK	Used to return to the previous prompt or menu screen.
CLEAR	Used to return to Main GEMS menu and restart the procedure selection operation.
EXIT	Used to leave GEMS. When EXITing, you must confirm your intention to leave the system. As you EXIT, GEMS will ask you if you want to SAVE any temporary GEMS datasets you have created during the current session. If you do not specifically save them, they will be deleted.
HELP	Used to call-up screens of system-help information. This help function is context sensitive. Entry of the HELP command affords you an opportunity to ask for specific help. If you enter *HELP*, you will be given general help for your current screen. If you enter *HELP n* (where n is an option number on your current menu), you will be provided with help specific to that option.
LIST	LIST DATASETS lists the available user and system-installed GEMS datasets. LIST GRAPHS, LIST TABLES, LIST

	REPORTS, and LIST MAPS all list the available graphs, tables, reports, or maps in your user GEMS library. LIST VARIABLES lists the variables in the GEMS dataset you specify. LIST COMMANDS is used to list available commands. NOTE: There are two versions of this command, with the suffix "S" as in LIST MAPS, you will see a full list, without the "S", as in LIST MAP the list will be in abbreviated form.
MENU	Selects the Menu-Mode of system operation. This is the default mode, the alternate is PROMPT. The MENU command can also be used to refresh the screen if you are in menu mode.
NEXT	Calls the next parameter specification menu. Not applicable to navigational menus.
NO AUTOHELP	Turns off the AUTOHELP function.
PROMPT	Used to invoke the User Prompt mode of operation. Alternate mode is MENU.
QUEUE	Displays the current jobs in the system batch queue.
RESET	Resets parameter values to the default values on the original parameter editing menu.
RESTORE	RESTORE file-name, used to recall specification parameters saved with the STORE command.
REVIEW	Re-displays the current menu or previously entered parameter values in parameter editing menus.
SHOW	SHOW reference/parameter name displays current parameter values.
STORE	Used to store responses to parameter editing menus for later recall.
USERCMD	Displays available facility-defined commands.

Consult the sections of this manual which describe individual procedures for commands that are a part of individual programs, and are not detailed above.

1.6 Communication with PCs

As GEMS has grown, the number of GEMS users has also grown. This growth brought with it several problems, not the least of which was the prospect that the number of users would exceed the number which could be accommodated with the available processing power. The prospect loomed on the horizon that increasing numbers of GEMS users would result in a serious degradation in system response speed. An alternative was to utilize the increasing base of available PC processing power to absorb some of the new user demands.

1.6.1 PCGEMS

In order to meet the growing demands of EPA modelers for access to GEMS features, the Personal Computer (PC) version of the Graphical Exposure Modeling System (PCGEMS) has been adapted from the VAX version. PCGEMS has many of the same features as GEMS but is accessible at a local level on a desk top computer. PCGEMS features work both independently and in concert with their more powerful counterparts on the mainframe. PCGEMS was created to meet two primary needs. First, PCGEMS reduces reliance on the VAX based GEMS by making GEMS capabilities independently available on a PC, and second, added capabilities allow a user to do preliminary work at the PC, send this information to GEMS on the VAX, and use the VAX based GEMS to perform the more demanding model runs.

PCGEMS is designed to reduce the reliance on the VAX based GEMS by providing the following independent capabilities:

1. Estimating the properties of chemicals such as octanol/water coefficient and boiling point, providing general chemical information of a chemical as well as

information necessary to feed into the environmental models; it also estimates the fate of atmospheric pollutants in water and air.

2. Allowing use of environmental models which simulate the effects of chemicals released to the air, water and soil or groundwater. Plans are underway to include features to assess the risk to the ecology presented by chemicals and give estimates of the danger these chemicals may present to the environment.

In addition to these stand-alone features, PCGEMS was designed to work in concert with the GEMS on the EPA VAX Cluster at RTP. While PCGEMS has many useful features, it is not intended to accomplish all of the functions of its more powerful VAX namesake. However, PCGEMS has the capability to allow GEMS users to use PCs as work stations in preparation for using GEMS. The easy-to-use upload/download features of PCGEMS provide a painless way to transfer data to and from GEMS on the VAX. In PCGEMS, you create datasets, build input files, and then transfer the information to GEMS on the VAX to access the more powerful GEMS capabilities. This PC-based pre-processing of data allows you to:

1. Work on a PC at times when the VAX is unavailable.
2. Reduce computer charges by shifting work to the PC.
3. Make use of powerful PC software packages in file preparation.
4. Keep local copies of vital data or programs.

The sections that follow provide more information on the communications capabilities built into PCGEMS to support this method of using GEMS. Refer to the PCGEMS User,s Guide for more details on PCGEMS

1.6.2 Communications methods to GEMS on the Cluster

There are a number of programs available to manage the transfer of files between the PC and the VAX. Kermit and CrossTalk are both tools in the standard EPA software

distribution. PCPLOT is another useful terminal emulation package that makes a PC look like a Tektronix 4010 to the VAX. PCPLOT is typical of a number of similar products that allow you to use the graphics capabilities of GEMS operations on your personal computer.

Before you attempt to transfer a GEMS dataset to your PC, you must first use the G2VAX procedure to export the dataset from GEMS to a VAX file. You can not transfer a GEMS dataset directly from the VAX to your PC.

For each of the file transfer methodologies discussed below, a modem and the requisite software is assumed.

1.6.2.1 Communications with Kermit

Load Kermit by typing the command *KERMIT* then you will see the Kermit system prompt:

KERMIT-MS

If you do not have an initialization file for Kermit, then enter:

SET BAUD 1200 sets the communications speed to 1200 baud

SET PA EVEN sets the parity to even if calling on the Washington Direct Line.

SET PA NONE sets the parity to none if calling on the TYMNET network.

Now type:

CONNECT

Your PC will now act as a terminal emulator; that is to say your PC now looks like a regular computer terminal to the VAX. You can now login to the VAX in the normal manner by entering *ATDT (phone number)* for a Hayes compatible modem. If you do not have a Hayes compatible modem, see your

modem's user's guide for instructions on how to dial. Follow the instructions in Section 1.3 for logging in to the system.

To download a VAX file to the PC:

1. At the VMS prompt $, enter the command *KERMIT* to enter the Kermit file transfer program.

2. Enter *SEND (filename)* on the VAX. You may use wild cards to send multiple files with the same command (i.e., SEND *.FOR).

3. Enter ^] (^ = Control) and while holding down the control key enter C. This returns you to the MS-DOS KERMIT prompt. Type *REC* (to receive). KERMIT will then display an information screen to tell you what file it is currently receiving and how large it is. You may have to enter a CR (carriage return) to start the transfer.

4. When KERMIT has finished the transfer, just type C an d you will be reconnected to the VAX.

To upload a PC file to the VAX:

1. Type *KERMIT* on the VAX, to enter the Kermit file transfer system. NOTE: If you are transferring a binary file (*.EXE), type *SET FILE TYPE BINARY* on the VAX.

2. Enter *REC* on the VAX. This will put the VAX into the receive mode.

3. Enter ^] (^ = control) and enter C. This brings you back to MS-DOS KERMIT, from this command level, type *SEND (filename)*. Wildcards are permitted, for example, SEND *.TXT. Kermit will display an information screen to tell you which file is being transferred, and the transfer progress. You may have to enter a CR to start the transfer.

4. When Kermit has finished the transfer, you can enter a C to be reconnected to the VAX.

1.6.2.2 Communications with CrossTalk

Load CrossTalk by typing the command *CrossTalk*. NOTE: A quick look at the status of CrossTalk is available by pressing the HOME key. The ESC key is used prior to entering any command.

If the CrossTalk software has already been set up for the VAX, enter the number corresponding to the appropriate command file. If none has been established:

Press the *HOME* key to see the status screen.
Press *ESC* to receive the COMMAND line.

Type the command prefix followed by the associated data to

SPeed	2400	DUplex	Full
DAta	7	EMulate	VT-100 or VT-52
POrt	(1)*	MOde	Call
PArity	Even	CWait	Delay 5
STop	1	LWait	Delay 20

(* - Assumes modem on port 1)

set the following parameters:

Log on to the VAX:

Type *GO* at the Command prompt to dial the currently loaded phone number. If a new telephone number is to be selected, type *NU* followed by the number, then type *GO*.

To download a VAX file to the PC:

1. Press the *ESC* key to go to command mode.

2. Type CAPTURE , followed by the drive designation for the drive where you want to write the incoming file, followed by the name you want to give to the file. (i.e., CAPTURE A:file.ext).

3. Type the information on the VAX (i.e., TYPE file.ext)
The file will then be transmitted from the VAX to the PC onto the specified drive and with the name you assigned.

4. Press the ESC key to go to command mode, and type CAPTURE OFF to save the file to disk.

To upload a file from the PC to the VAX:

1. First make certain that you are in the VAX line editor, EDIT, or in any system mode which will accept input data.

2. Press ESC to go into the command mode, and enter the command SEND, followed by the drive designation and file name of the file you wish to send to the VAX. (i.e.,SEND A:file.ext)

3. Exit from EDIT by pressing the ^Z (^ = control key) to save the file on the VAX.

To exit from XTALK, press the *ESC* key and enter QUIT.

1.6.2.3 Communications with PCPLOT

PCPLOT is just one of the many commonly used programs for Tektronix 4010 terminal emulation. We illustrate it's use here only because GEMS users have successfully used it.

To upload or download files to the VAX using the PCPLOT program is simple with PCPLOT. Enter PCPLOT with the DOS level command PCPLOT. PCPLOT will first display a terminal type.

Make sure the terminal type is set it to either "1" or "2". If not, press ^T before proceeding. NOTE: A complete list of PCPLOT commands is available by pressing ^H.

Logon to the VAX by calling the appropriate telephone number with the ATDT (phone number) command.

To download a VAX file to the PC:

1. Depress the ALT key and press the F key at the same time to name the destination file. This key combination will be refered to as ALT/F for the rest of this section. Include drive and full file specification in the name.

2. To copy the VAX file, enter ALT/I to accept the host file. All terminal output will then be copied to the file you named.

3. To close the file, enter ALT/Q after the file has been downloaded.

To upload a PC file to the VAX:

1. You must be in the line editor, EDIT, in insert mode, or any other system mode which can accept input data.

2. Enter ALT/O to open the file on the PC.

3. Enter ALT/U to start uploading.

4. Enter ALT/R to close the file when uploading has been completed.

5. Exit from EDIT on the VAX to save the file.

When finished uploading or downloading using PCPLOT, enter ALT/X to exit to DOS command level.

- END CHAPTER ONE -

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GEMS User's Response Form

We appreciate your feedback on this User's Guide. If you could take a few moments to share your comments, it will help us in the continuing effort to provide you with professional user documentation. Please share your evaluation of this document's:

Content

Organization

Readability

Style & Format

Specific Problems, or Comments:

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PleaseMail to:
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GSC-TR8645

GRAPHICAL EXPOSURE MODELING SYSTEM

(GEMS)

USER'S GUIDE

VOLUME 2. MODELING

Prepared for:

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APPENDIX A: Air Models

APPENDIX B: Surface Water Model

APPENDIX C: Soil and Groundwater Models

APPENDIX D: Multimedia Models

DISCLAIMER

This document is a preliminary draft. It has not been released formally by the Office of Toxic Substances, Office of Pesticides and Toxic Substances, U.S. Environmental Protection Agency, and should not at this stage be construed to represent Agency policy. It is being circulated for comments on its technical merit and policy implications.

A number of copyrighted or trademarked computer software programs have been mentioned in this user's guide. Mention of these software programs does not reflect endorsement by EPA or GSC.

1. INTRODUCTION

The Graphical Exposure Modeling System (GEMS) is an interactive computer system developed by General Sciences Corporation under the auspices of the modeling section in the Exposure Evaluation Division (EED), Office of Toxic Substances (OTS) of Environmental Protection Agency (EPA). GEMS provides a simple user-interface for environmental modeling, physiochemical property estimation, statistical analyses, and graphic display. GEMS is installed on the OTS VAX 11/780 computer in Research Triangle Park, North Carolina, and is accessible to Washington, D.C. through dial-up lines.

Volume 1 of the GEMS User's Guide, the Core Manual, provides details about accessing GEMS system interaction, terminal session control, terminal-type descriptions, menu and prompt operation modes, control commands, and on-line system messages. Please consult Volume 1 for this information. This document assumes that the user is familiar with GEMS and thus, only details the Modeling Operation.

The purpose of Volume 2, Modeling, is to comprehensively guide the user through this GEMS Operation. It is written so that no specialized knowledge of computer programming is necessary.

The Modeling Operation provides a variety of computer models that can simulate, predict and analyze the effects of chemicals released in the air, water and soil. The models are grouped into the categories of AIR, WATER, SOIL and MULTI-MEDIA. The AIR models deal with contaminants released in the atmosphere. The WATER models deal with the fate of a contaminant in surface water bodies. The SOIL models deal with transport and fate of a contaminant in subsurface soil-water systems. The MULTIMEDIA models deal with the transport and fate of a contaminant in the atmosphere, soil, and surface water.

One of the most significant and unique aspects of GEMS is its capability to support interactively the operation of a variety of fate and exposure models. GEMS design allows for two levels of model implementation, involving either partial or full integration of a model.

Complete model integration fulfills the requirements:

(1) Direct access to the model from GEMS and return to GEMS when the model operations are completed;

(2) Prompting the user for essential model input parameters from GEMS, instead of directly within the model, thereby providing a consistent format for the user interface and constant access to standard control commands.

(3) Conversion of the output data/graphics/tables from each model into a standard format, which can be saved and retrieved through GEMS;

Of these three requirements, the first one is mandatory for inclusion in GEMS, while fulfillment of the other two depends upon the individual model and its input/output. At present, SESOIL, AT123D, SWIP, and INPUFF are fully integrated. The three criteria for model integration described above also serve as a stepwise procedure for model integration. Table 1-1 illustrates the current implementation status of the models available in GEMS.

All models currently implemented in GEMS have some kind of user prompting for essential input data, although in many cases this prompting occurs within the models rather than within GEMS. While user prompting within the models simplifies access to the model, the format and versatility of the prompting is quite varied. User prompting within GEMS, such as that found in the AT123D and SWIP implementation, has the advantages of providing a consistent format for user interaction and allowing the use of common GEMS control commands during the prompting sequence.

All models implemented in GEMS store some input and/or output files in the user's VAX directory. When GEMS is invoked from a subdirectory, these input and output files are automatically located in that subdirectory. Users are encouraged to set up a subdirectory structure to handle each major model or model run.

The space requirements for setting up and running various models vary greatly. Users should consult the model user's guide or model documentation for any information regarding space requirements.

TABLE 1-1. Implementation Status of Models Available in GEMS

ENVIRONMENTAL MEDIA MODELED	MODEL NAME	MODEL OUTPUT TO GEMS FILE MANAGEMENT	GEMS CONTROLLED PROMPTING	PROMPTING WITHIN MODEL
Air	GAMS*	No*	Yes	No
Air	INPUFF	Yes	Yes	No
Air	PTMAX	No	No	Yes
Air	PTDIS	No	No	Yes
Air	BOXMOD	No	No	Yes
Surface Water	EXAMS II**	No	Yes**	Yes
Soil	SESOIL	Yes	Yes	No
Soil	PRZM	No	No	Yes
Groundwater	AT123D	Yes	Yes	No
Groundwater	SWIP	Yes	Yes	No
Multimedia	ENPART	No	Yes	No
Multimedia	TOX-SCREEN	Yes	Yes	No
Multimedia	UTM-TOX	No	No	No

* GAMS stands for GEMS Atmospheric Modeling Subsystem and consists of the Industrial Source Complex Long-Term (ISCLT) model and the TOXBOX urban area source model. These models are able to access data on the distribution of surrounding populations to calculate exposures as well as environmental concentrations. Linking model outputs to GEMS is expected to be completed in FY87.

** A front-end is being implemented in GEMS for this model.

2. MODEL SUMMARIES

Brief summaries of the models within the Modeling Operation are given in the following subsections. These summaries are given to provide the user with an overall view of the models. More detailed information on any specific model may be obtained from the model documentation referenced for each model.

The GSC user's guides for models with GEMS controlled prompting are provided in the following appendices:

- o Appendix A - User's Guides for GEMS Atmospheric Modeling Subsystem (GAMS) and INPUFF
- o Appendix B - User's Guide for EXAMS II
- o Appendix C - User's Guides for SESOIL, AT123D, and SWIP
- o Appendix D - User's Guides for ENPART and TOX-SCREEN

The user's guide for EXAMS II will be released when the model is completely implemented in GEMS. For the PRZM and UTM-TOX models, GSC has installed them in GEMS without implementing model output to GEMS nor providing controlled prompting. Refer to Sections 2-8 and 2-13 for information related to these two models. The PTDIS, PTMAX and BOXMOD air models also lack controlled prompting, and the model outputs have not been implemented to GEMS. Refer to Sections 2-3, 2-4, and 2-5 for information related to these three models.

2.1 Air Models

2.1.1 GEMS Atmospheric Modeling Subsystem (GAMS)

Overview

The OTS Graphical Exposure Modeling System (GEMS) Atmospheric Modeling Subsystem (GAMS) allows multiple atmospheric models to be used for multiple release sources to examine overlapping exposures. The Industrial Source Complex Long-Term (ISCLT) model and the TOXBOX area source model are implemented in GAMS to estimate annual average atmospheric concentrations. GAMS integrates the atmospheric concentrations estimates of the two models with a population distribution data base to estimate exposure and risk.

Description

GAMS can currently treat up to twenty source categories with up to fifty emission type entries within each category for an unlimited number of source locations for ISCLT modeling. TOXBOX is implemented in GAMS to estimate annual average concentrations for all U.S. urban populations. Land areas used for the urban populations were obtained from a 1980 Bureau of the Census publication (Census 1983). The urban population comprises all persons living in the 366 urbanized areas (UAs) and in the 3827 places of 2,500 or more inhabitants outside urbanized areas. (The total 1980 U.S. urban population modeled by TOXBOX is 167,050,922 persons.)

The concentration estimates generated by the models are stored at the 1980 Census block group and enumeration district (BG/ED) geographic level. The population data base, which includes latitude/longitude coordinates of all BG/ED's, was obtained from Donnelly Marketing Information Services. By assigning concentration estimates at this detailed population distribution level, GAMS accounts for increments of concentration from any number of sources that may impact an individual BG/ED. This tracking avoids multiple counting of populations when sources are close enough to one another that surrounding BG/ED are impacted by more than one source.

Exposure and risk calculations are performed by GAMS for each BG/ED population by source category and emission type from the ISCLT results, by source category from the TOXBOX results, and across all source categories from the overlapping results from both models. Excess risk over background is currently estimated within GAMS by using a unit risk value. The risk is calculated as the product of the estimated concentration and the unit risk value. The unit risk value must be in the units of inverse microgram per cubic metre. Brief descriptions of ISCLT and TOXBOX are given.

ISCLT

The ISCLT model was developed by Bowers et al. (1980) for the Source Receptor Analysis Branch, Office of Air Quality Planning and Standards, U.S. Environmental Protection Agency. ISCLT combines and enhances various dispersion model algorithms into a computer program that can be used to assess the air quality impact of emissios from the wide variety of sources associated with an industrial source complex. The GEMS version of ISCLT is from EPA's UNAMAP (user's network for Applied Modeling of Air Pollution).

The ISCLT model is a sector-averaged model that extends and combines basic features of the Air Quality Display Model (AQDM) and the Climatological Dispersion Model (CDM). The long-term model uses statistical wind summaries to calculate annual ground-level concentration or deposition values.

For plumes comprised of particulates with appreciable gravitational settling velocities, ISCLT accounts for the effects on ambient particulate concentrations of gravitational settling and dry deposition. Alternately, ISCLT can be used to calculate dry deposition.

ISCLT accepts the following source types: stack, area and volume. The volume source option is also used to simulate line sources. The steady-state Gaussian plume equation for a continuous source is used to calculate ground-level concentrations for stack and volume sources. The area source equation in ISCLT is based on the equation for a continuous and finite crosswind line source. Procedures suggested by Huber and Synder (1976) and Huber (1977) are used to evaluate the effects of the aerodynamic wakes and eddies formed by buildings and other structures on plume dispersion.

A wind-profile exponent law is used to adjust the observed mean wind speed from the measurement height to the emission height for the plume risk and concentration calculations. The Pasquill-Gifford curves (Turner 1970) are used to calculate lateral and vertical plume spread. ISCLT has the option of a rural mode or one of two urban modes. Time dependent exponential decay of the pollutant can also be included in the model.

TOXBOX

TOXBOX was developed by the General Sciences Corporation for the Office of Toxic Substances, EPA. The model is an atmospheric area source model based on the work of Hanna (1972, 1977, 1980). The model is applicable to regions containing many diffuse emission sources within their boundaries, such as an urban area source. TOXBOX is a steady-state box model, which assumes no upwind background concentrations. Dry deposition, precipitation scavenging, and chemical removal processes are accounted for in the continuity

equation for material entering and leaving the box above the modeled regions.

The model computes a weighted average concentration based on stability frequency of occurrence. The stability frequencies and their corresponding average winds speeds are computed from running five year annual average STability ARray (STAR) data compilations.

INPUT

GAMS contains a wide range of options and the atmospheric models, particularly ISCLT, require a substantial amount of input data. The data requirements are therefore summarized in Figure 2-1. The dashed arrows indicate optional transfers between prompt groups where the direction of transfer is based on your response to the prompts. Solid arrows represent no option transfer between prompt groups.

Because of the sophistication level of GAMS, a GAMS INterface, GAMSIN, prompts you for the information required to set up and perform the desired modeling scenario.

OUTPUT

If you request to save the ISCLT and/or TOXBOX model output, the file names will consist of the run name followed by "ISC", followed by the three digit site number for each of the ISCLT model output files; and the run name followed by "TOXBOX" for the TOXBOX model output file. The file type of ISCLT and TOXBOX, the model output files from the performance of GAMS, is ".OUT".

The ISCLT and TOXBOX model-wide and the multi-model exposure and risk summary tables are written to a single output file. The file name consists of the study name and the file type is ".postout".

All of the above files are written to the user's VAX subdirectory. Because of the potentially large space requirements of a GAMS run, users should have a minimum of a 20,000 block quota allocated to them.

References

Bowers, J.F., et al. 1980. Industrial Source Complex (ISC) Dispersion Model User's Guide (Volume I), PB80-133044. Research Triangle Park, N.C: U.S. Environmental Protection Agency, Office of Air Quality Planning and Standards.

Census. 1983. 1980 Census of Population. Vol. 1: Characteristics of Population. Number of Inhabitants. PC80-1-A1.

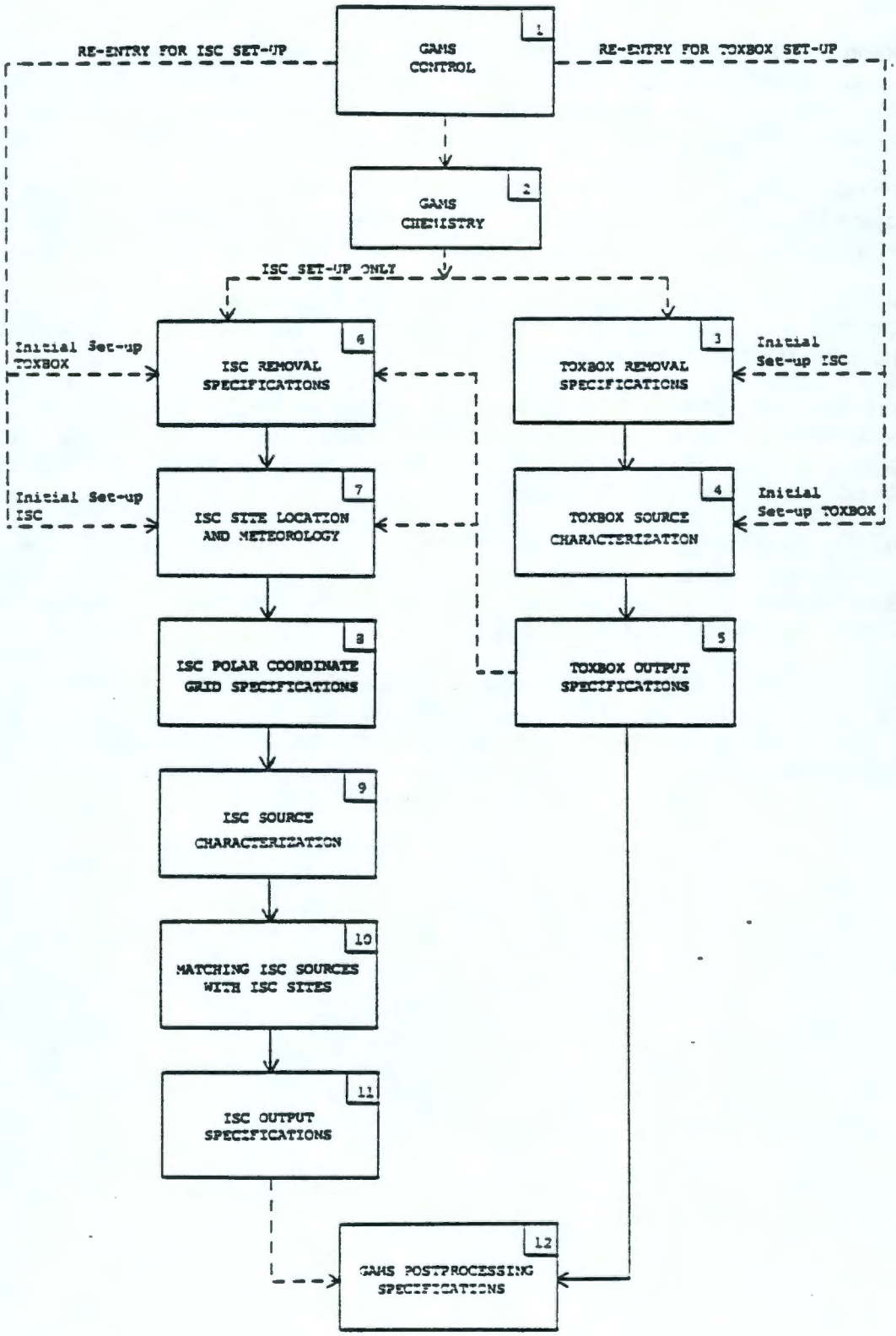

FIGURE 2-1. Sequence of GAMSIN logical prompt groups.

Hanna, S.R. 1972. Dry deposition and precipitation scavenging in the ATDL computer model from multiple point area sources. Oak Ridge, TN: Air Resources Atmospheric Turbulence and Diffusion Laboratory. ATDL Contribution File No. 71.

Hanna, S.R. 1977. A stability correction term for a simple urban dispersion model. Oak Ridge, TN: Air Resources Atmospheric Turbulence and Diffusion Laboratory. ATDL Contribution File No. 77/15.

Hanna, S.R. 1980. Atmospheric removal processes for toxic chemicals. Draft. Oak Ridge, TN: ATDL progress report to ORNL under EPA Multimedia Modeling Project.

Huber, A.H. 1977. Incorporating building/terrain wake effects on stack effluents. Preprint Volume for the Joint Conference on Applications of Air Pollution Meteorology. Boston, Massachusetts: American Meteorological Society.

Huber, A.H. , and Synder, W.H. 1976. Building wake effects on short stack effluents. Preprint Volume for the Third Symposium on Atmospheric Diffusion and Air Quality. Boston, Massachusetts: American Meteorological Society.

Turner, D.B., 1970. Workbook of Atmospheric Dispersion Estimates. PHS Publication No. 999-AP-26. Cincinnati, Ohio: U.S. Department of Health, Education and Welfare, National Air Pollution Control Administration.

2.1.2 INPUFF

Overview

INPUFF (Peterson et al. 1984) is an atmospheric model capable of addressing the accidental release of a substance over several minutes or of modeling the more typical continuous plume from a stack. INPUFF is capable of simulating moving point sources as well as stationary sources.

Description

INPUFF is a Gaussian plume, INtegrated PUFF model with a wide range of applications. The implied modeling scale is from tens of meters to tens of kilometers. Computations in INPUFF can be made for a single point source at up to 25 receptor locations. Up to 144 separate meteorological periods of the same length may be used to characterize the meteorology during the event.

INPUFF utilizes three distinct dispersion algorithms. For short travel time dispersion, the user has the option of using either the Pasquill-Gifford (P-G) scheme (Turner 1970) or the on-site scheme (Irwin 1983). The third dispersion algorithm is used for long travel times in which the growth of the puff is assumed proportional to the square root of travel time.

INPUT

INPUFFIN is a sequence of menus and/or prompts that is used to set up your INPUFF modeling scenario and create the INPUFF input file. Figure 2-2 depicts the sequence of menus, and prompt group in the case of Supplemental Climatological Data, within INPUFFIN. INPUFFRUN is a single menu with three parameters that is used to set up an execution of the INPUFF model.

OUTPUT

The INPUFF model output is written to a GEMS REPORT. The REPORT can be displayed at your terminal by using the Output Option in the File Management Operation of GENS.

The output begins with printing the title of the run, which can be up to 60 characters in length. The next printed information is a list of options, followed by a list of the input parameters. Next are the source data followed by a printout of meteorological conditions used in the execution of the model for the current simulation period. These are followed by five pieces of information regarding how INPUFF simulates the release, including: simulation period, simulation time, puff release rate, minimum source-receptor distance, and dispersion type.

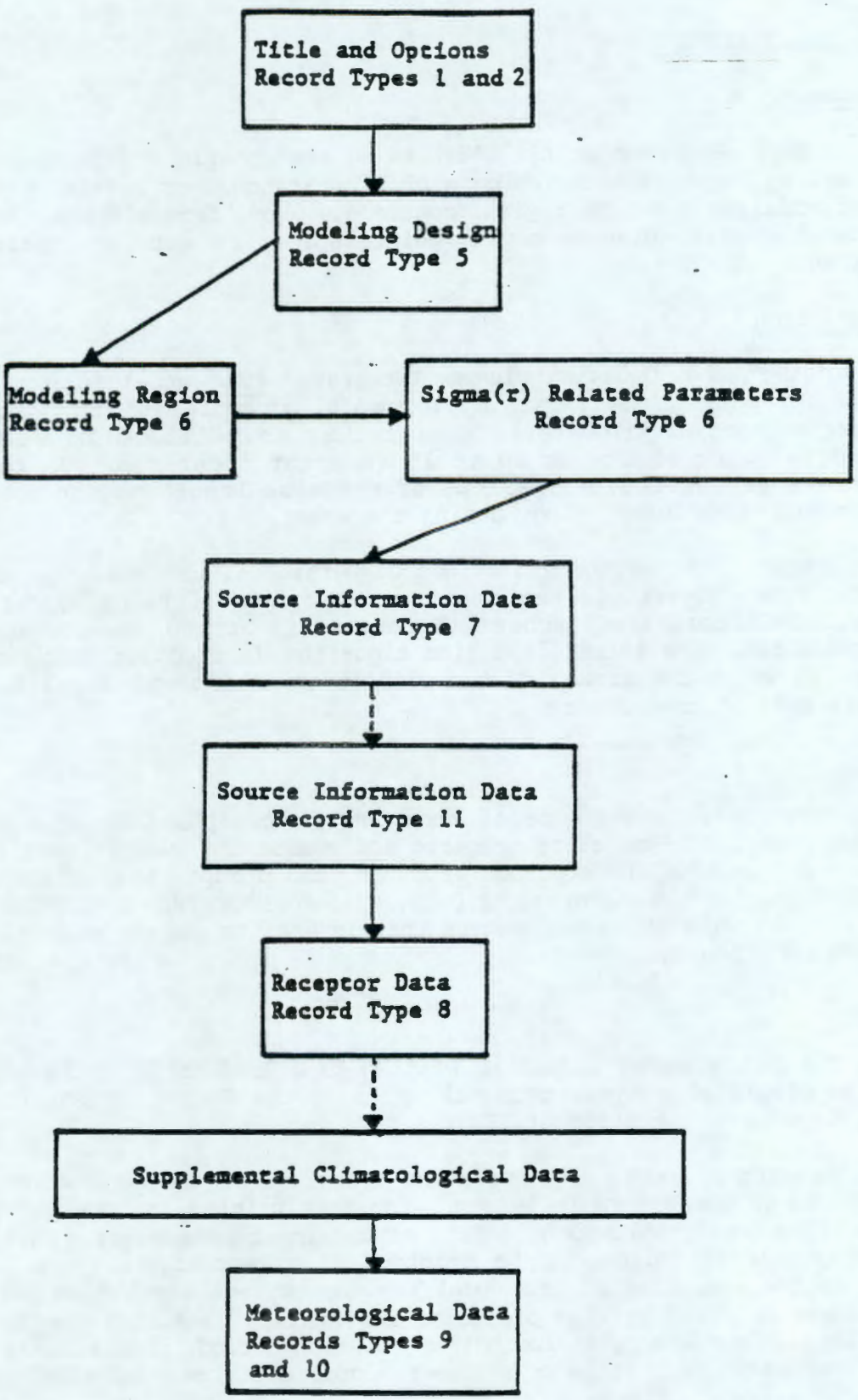

FIGURE 2-2. INPUFFIN Sequence

The next two output sections are optional. If IPIC = 1, then intermediate concentrations are written every INC seconds. The time period for which the averages are appropriate is printed in the first line of the intermediate concentration output. If IPCC = 1, then information on each puff is printed each ITIME, in addition to average concentrations at each receptor. Finally, a table of average concentrations is output, giving averages for each receptor for all meteorological periods.

References

Irwin, J.S. 1983. Estimating Plume Dispersion - A Comparison of Several Sigma Schemes. J. Climate Applied Meteorol. 22: 92-114.

Peterson, W.B., Catalano, J.A., Chico, T., and Yuen, T.S. (1984). INPUFF - A SINGLE SOURCE GAUSSIAN PUFF DISPERSION ALGORITHM User's Guide. Research Triangle Park, NC: U.S. Environmental Protection Agency, Environmental Sciences Research Laboratory. Contract No. EPA 68-02-3750.

Turner, D.B. 1970. Workbook of Atmospheric Dispersion Estimates. Office of Air Programs Publication No. AP-26 (NTIS PB 191 482). Research Triangle Park, NC: U.S. Environmental Protection Agency.

2.1.3 PTMAX

Overview

PTMAX (Turner and Busse 1973) is a short-term atmospheric model applicable to point sources. The model, which was obtained from EPA's UNAMAP (User's Network for Applied Modeling of Air Pollution), performs an analysis of the maximum hourly concentrations from a single point source as a function of atmospheric stability and wind speed.

The maximum ground-level hourly concentration estimated by PTMAX may be used to screen various emission scenarios. The distance of maximum concentration may be used to assign receptor locations for input to other models.

Description

PTMAX is a steady-state Gaussian plume point source model. It assumes that the source is continuous, that none of the material emitted is removed from the plume as it moves downwind, and that there is complete reflection at the ground. The final plume height used for each computation is determined using Briggs' plume rise methods.

Input

Input to the program consists of ambient air temperature and characteristics of the source, such as emission rate, physical stack height, and stack gas temperature. Either the stack gas volume flow or both the stack gas velocity and inside diameter at the top of the stack are required.

Output

Outputs of the program consist of effective height of emission, maximum ground-level concentration, and distance of maximum concentration from the release point for each condition of stability and wind speed. This output is written directly to the user's terminal and to a data file, FORØ77.DAT, under the user's computer account directory. At the end of a PTMAX run, the output file may be renamed, printed, and reviewed. Once the user returns to GEMS operation level from the PTMAX program, a saved output file is not directly accessible from GEMS.

Reference

Turner D.B., and Busse A.D. 1973. User's guides to the interactive version of three point source dispersion programs: PTMAX, PTDIS, and PTMTP. Preliminary draft. Research Triangle Park, NC: U.S. Environmental Protection Agency, Meteorological Laboratory.

2.1.4 PTDIS

Overview

PTDIS (Turner and Busse 1973) is a short-term atmospheric model applicable to point sources. The model, which was obtained from EPA's UNAMAP (User's Network for Applied Modeling of Air Pollution), estimates hourly concentrations directly downwind of a single point source at distances specified by the user.

The estimated hourly concentrations from the PTDIS model may be used to screen various emission scenarios. PTDIS is most applicable when the user requires concentration estimates at specific travel distances from a point source.

Description

PTDIS is a steady-state Gaussian plume point source model. It assumes that the source is continuous, that none of the material emitted is removed from the plume as it moves downwind, and that there is complete reflection at the ground. The effect of limiting upward vertical dispersion by defining a mixing height is possible, and gradual plume rise to the point of final rise is considered, using Briggs' plume rise methods.

Input

Input to the program consists of distances at which calculations are to be made, ambient air temperature, atmospheric stability class, wind speed, mixing height, and emission rate. The user is given the option of specifying effective height of emission or having it calculated. To have the plume rise calculated, characteristics of the source, such as physical stack height and stack gas temperature, are required. Either the stack gas volume flow or both the stack gas velocity and inside diameter at the top of the stack are required.

Output

Primary output of the program consists of a table with height of emission and ground-level hourly concentration given for each downwind distance specified. This output is written directly to the user's terminal and to a data file, FORØ55.DAT, under the user's computer account directory. At the end of a PTDIS run, the output file may be renamed, printed, and reviewed. Once the user returns to GEMS operation level from the PTDIS program, a saved output file is not directly accessible from GEMS.

Reference

Turner, D.B., and Busse, A.D. 1973. User's guides to the interactive version of three point source dispersion programs: PTMAX, PTDIS, and PTMTP. Preliminary draft. Research Triangle Park, NC: U. S. Environmental Protection Agency, Meteorological Laboratory.

2.1.5 BOXMOD

Overview

BOXMOD was developed by the General Sciences Corporation for the Office of Toxic Substances, EPA. The model is an interactive simple atmospheric area source model based on the work of Hanna (1972, 1977, 1980). BOXMOD is appropriate for use when screening chemicals for potential health or environmental problems. The model is applicable primarily to regions containing many diffuse emission sources within their boundaries, such as an urban area source. BOXMOD may be used for averaging periods of less than a day, but estimated concentrations are more nearly accurate using an averaging period greater than a few days up to annual averages.

BOXMOD is used to calculate the atmospheric concentration for a single area where the location and width of the area are input by the user. The TOXBOX model within GAMS calculates the atmospheric concentration for 366 UAs and 3738 places across the country. With BOXMOD, the user has the option of a solution to the box model assuming either a uniform or Gaussian concentration distribution in the vertical and has the option of selecting STAR and auxiliary climatological data or supplying their own climatological data. With TOXBOX, the STAR and auxiliary data are automatically used and a Gaussian solution is used for the model.

Description

BOXMOD is a steady-state box model, which assumes no upwind background concentration. Dry deposition, precipitation scavenging, and chemical removal processes are accounted for in the continuity equation for material entering and leaving the box above the modeled region. The user has the option of selecting a solution to the box model, based on the assumption of uniform or Gaussian concentration distribution in the vertical. If Gaussian is selected, you have the option to use STAR summary and auxiliary data.

The model calculates a single pollutant concentration applicable to the entire region based on a uniform area emission rate. The box is assumed square with a north-south, east-west geographic orientation.

Input

Input to the program consists of the latitude and longitude for the center of the area, and the width and emission rate of the area; either the STAR station index number or wind speed , stability type, and precipitation rate and frequency under the Gaussian options, or windspeed, mixing depth, and precipitation rate and frequency under the uniform option; particle radius and density, or molecular weight if a gas, for estimating the dry deposition speed; and the time constant applicable to the chemical removal process.

Output

Outputs of the program consist of a reiteration of all input values, as well as the estimated values for the scavenging coefficient, deposition speed and pollutant atmospheric concentration. This output is written directly to the user's terminal and to a data file, FORØ33.DAT, under the user's computer account directory. At the end of a BOXMOD run, the output file may be renamed, printed, and reviewed. Once the user returns to GEMS operation level from the BOXMOD program, a saved output file is not directly accessible from GEMS.

Reference

Hanna, S.R. 1972. Dry deposition and precipitation scavenging in the ATDL computer model for dispersion from multiple point and area sources. Oak Ridge, TN: Air Resources Atmospheric Turbulence and Diffusion Laboratory. ATDL Contribution File No. 71.

Hanna, S.R. 1977. A stability correction term for a simple urban dispersion model. Oak Ridge, TN: Air Resources Atmospheric Turbulence and Diffusion Laboratory. ATDL Contribution File No. 77/15.

Hanna, S.R. 1980. Atmospheric removal processes for toxic chemicals. Draft. Oak Ridge, TN: ATDL progress report to ORNL under EPA Multimedia Modeling Project.

2.2 Surface Water Model

2.2.1 Exposure Analysis Modeling System II (EXAMS II)

The Exposure Analysis Modeling System (EXAMS) was developed by EPA's Environmental Research Laboratory in Athens, Georgia (1981), for rapid evaluation of the behavior of synthetic organic chemicals in aquatic ecosystems. Based on both the physical/chemical properties of a compound and on the relevant environmental characteristics of the ecosystem, EXAMS simulates the ultimate distribution and concentration of the compound resulting from a specified pattern of release into the ecosystem.

A new EXAMS version, EXAMS II, was developed recently to enhance the modeling capabilities and options of EXAMS. With EXAMS II, the user is able to elect either the original long-term, steady-state analysis mode or the new spike analysis model which performs simulation based on user-specified initial conditions and time factors. At the completion of a simulation run, EXAMS II provides new options for plotting and/or listing of a variety of parameter combinations (e.g., Time vs. Concentration, Compartment 1 vs. Compartment 2, etc.). EXAMS II can also make multiple runs on the basis of an extended, continuous time frame upon request.

An environmental data base has also been developed for EXAMS II to contain monthly average water quantity/quality data and general characteristics for thirty (30) major river systems (9 for streams and 21 for lakes/reservoirs). This data base has been interfaced with EXAMS II under GEMS so that the user can select data from the data base via a series of questions and responses. The selected data may then be read in and stored by the user as an EXAMS "environment." Subsequent retrieval of an environment using EXAMS' command "RECALL" can then be made to provide input data for model execution.

Description

EXAMS II is a deterministic model based on a set of process equations, which account for the interactions between the chemistry of a compound and the environmental forces that shape the compound behavior in the ecosystem. The loading, transport, and transformations of a compound are balanced in the model in accordance with a mass conservation law. The ecosystem is represented by a set of N-compartments; each depicting a unique, constant, uniform entity of the ecosystem.

Input

Three major data input files are required by EXAMS II: the environmental data file, the chemical data file, and the loading data file. The environmental data file contains information describing the environment in terms of climactic, biological, hydrologic, and sedimentary characteristics. Each of the variables required by the data file has a direct bearing on the compound behavior. Monthly values may be used for environmental parameters or they may be constrained to single time-invariant values within a given compartment of the ecosystem. As such, those variables are termed "canonical" descriptions of the environment and are regarded as representing average or typical values of the environment. The chemical data file contains information related to the various chemical characteristics of the compound of interest. Examples of those data requirements include compound solubility, molecular weight, partition coefficients, hydrolysis rate constants, and biodegradation rate. The loading data file provides information concerning the compound loading input to the ecosystem, as well as to the system background loadings in stream flow, rainfall, interflow, nonpoint source flow, and drift.

EXAMS II has an interactive interface, which allows a user to have direct access to the input data files for data storing, updating, and retrieval via simple commands. A generalized flowchart for EXAMS II data entry is shown in Figure 2-3.

Output

EXAMS II output is comprised of up to 20 different types of tables which include summaries of the input data used in the analysis; a time trace of the average concentrations during the simulation period; distributions among aqueous chemical species at various times; locations of the minimum and maximum concentrations at various times; the fate of the compound in the form of the percent of loading, half-life, and mass flux expressed for each of the transport and transformation processes considered; a post load decay kinetics analysis, and the ultimate chemical concentrations and distribution in the ecosystem and the time required for the system self-purification after cessation of the chemical loading. A more detailed discussion of the output tables is presented in the original EXAMS User's Manual and System Documentation (EPA 1981), and in the updated Training Guide and Reference Manual for EXAMS II (EPA 1984).

The complete model output is written to a data file, REPORT.DATA, in the user's computer account directory. At the end of an EXAMS II run, this data file may be renamed, printed, and reviewed.

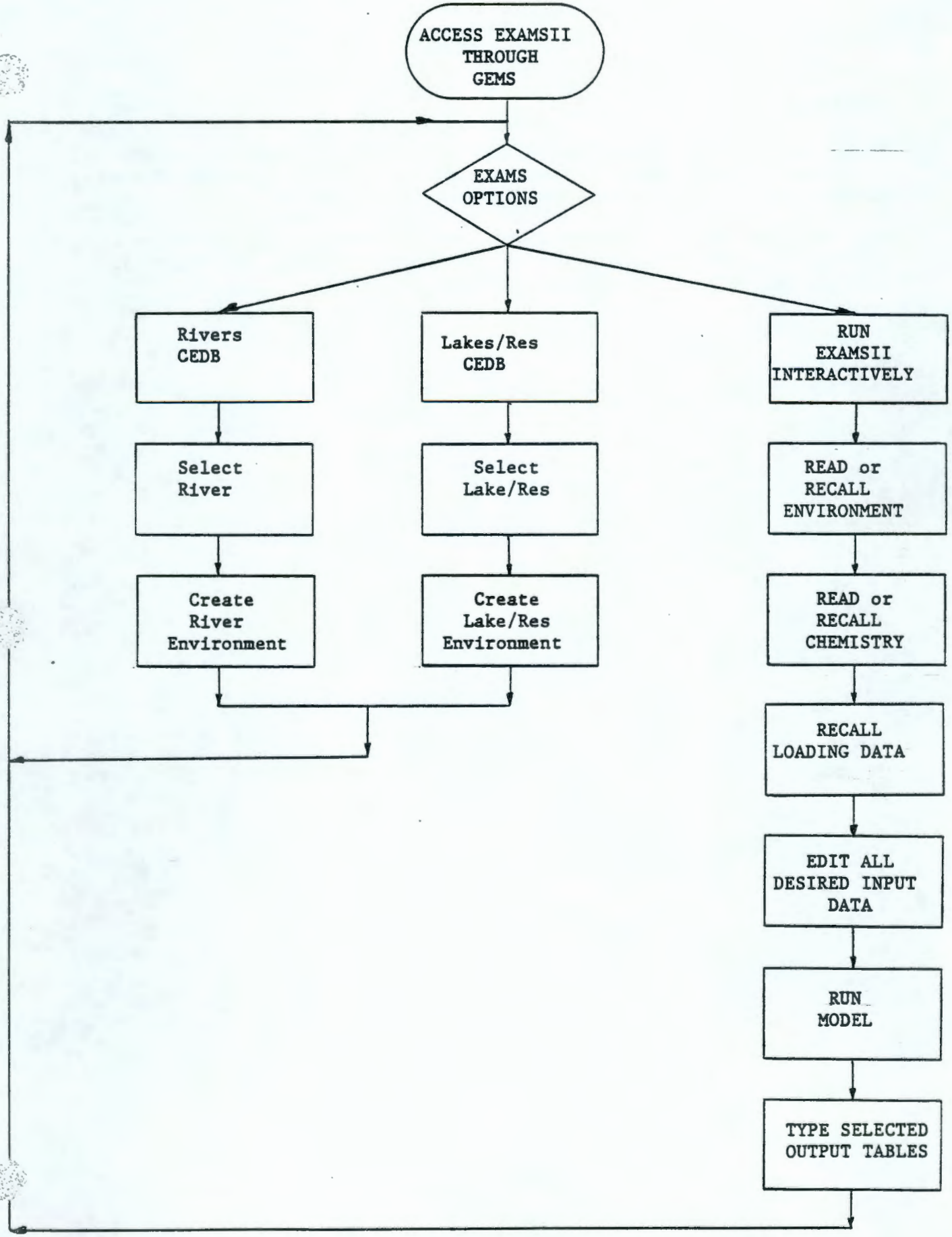

FIGURE 2-3. Flow chart showing EXAMS Execution.

Reference

U. S. Environmental Protection Agency (EPA). 1981. Exposure Analysis Modeling System (EXAMS): User Manual and System Documentation. Athens, GA: U. S. Environmental Research Laboratory.

U.S. Environmental Protection Agency (EPA). 1984. Exposure Analysis Modeling System: Training Guide and Reference Manual for EXAMS II. Athens, GA: U.S. Environmental Research Laboratory.

2.3 Soil and Groundwater Models

2.3.1 SESOIL

Overview

SESOIL is a seasonal soil compartment model developed by Bonazountas and Wagner (1984) for the Office of Pesticides and Toxic Substances, EPA. The model is designed for long-term environmental pollutant fate simulations that can describe water transport (quality/quantity), sediment transport (quality/quantity), and pollutant transport/transformation.

General Sciences Corporation (GSC) implemented SESOIL in GEMS and developed input and output data management systems to support its operation. The input data management system, SESIN, uses interactive prompts to assist the user in the preparation of SESOIL input data files. The output data management system, SESOILFM, allows the user to store the SESOIL output data in GEMS, making it possible to utilize the file manipulation capabilities of GEMS for data analysis and graphic interpretation.

The SESOIL model is useful for a wide range of applications, including the screening and detailed review of new chemicals. For example, it can be used to compare a large number of chemicals for their resulting effects when released into nonsite-specific environments; it can be used to provide necessary evaluative information in a site screening management plan; or it can be treated as a detailed site-specific pollutant transport modeling tool.

Description

The SESOIL model simulates a user-specified soil column which extends from the ground surface to the saturated zone. The soil column is divided into a number of compartments, each compartment representing a homogeneous soil layer. Simulation of the transport/transformation processes within each compartment and between compartments are based upon three cycles: 1) water cycle, which takes account of the hydrologic balance; 2) the sediment cycle, which accounts for resuspension (due to wind) and sediment washload (due to rainfall); and 3) the pollutant cycle which accounts for the transport and transformation processes directly affecting the fate of the pollutant.

SESOIL has options allowing the user to select from a number of levels of modeling application; each level associated with certain temporal and spatial resolution characteristics, and each having different specific input requirements. The most commonly utilized level for OTS applications is Level 3 which performs calculations on a monthly basis and uses a 3-layer soil column. Recent model enhancements allow spatial resolution of up to 4 soil layers.

Input

Requirements for the input data include a climatologic, soil, and chemical specific data; pollutant application data file(s), containing information concerning the size of the study area, depth to groundwater, ratio relationships among soil layers, and pollutant input from various sources; and data file containing model execution information.

To facilitate the preparation of these input data files, GSC developed SESIN, a SESOIL input data file management system, which provides step-by-step guidance to assist the user in performing the formulation, editing, and naming of SESOIL input data files (GSC 1984). A flowchart showing the steps required to enter data using SESIN is shown in Figure 2-4.

Output

SESIN output results include hydrologic balance calculations and the distribution of the chemical in the soil column. Specifically, the following are included:

- Resulting hydrologic relationships among precipitation, surface runoff, infiltration, evapotranspiration, soil moisture, and groundwater runoff;
- Temporal and spatial pollutant concentration distributions in soil-air, soil-moisture;
- Temporal and spatial pollutant concentration distributions on soil particles; and
- Leachate (pollutant mass) migration from the unsaturated soil zone to groundwater.

GSC developed SESOILFM, a SESOIL output data file management system, which allows the user to create a GEMS data set of more than 60 SESOIL output variables (GSC 1984). The user can utilize GEMS file management capabilities for output data manipulation, analysis, and interpretation. One example of the use of GEMS capabilities is the display of information (e.g., concentration vs. time) in graphics, such as scattergrams, bar charts, and histograms.

After each SESOIL run, the complete model output is written to a data file, SESOUT.DAT, in the user's computer account directory. The user can review, rename, or request a hardcopy print of this output dataset.

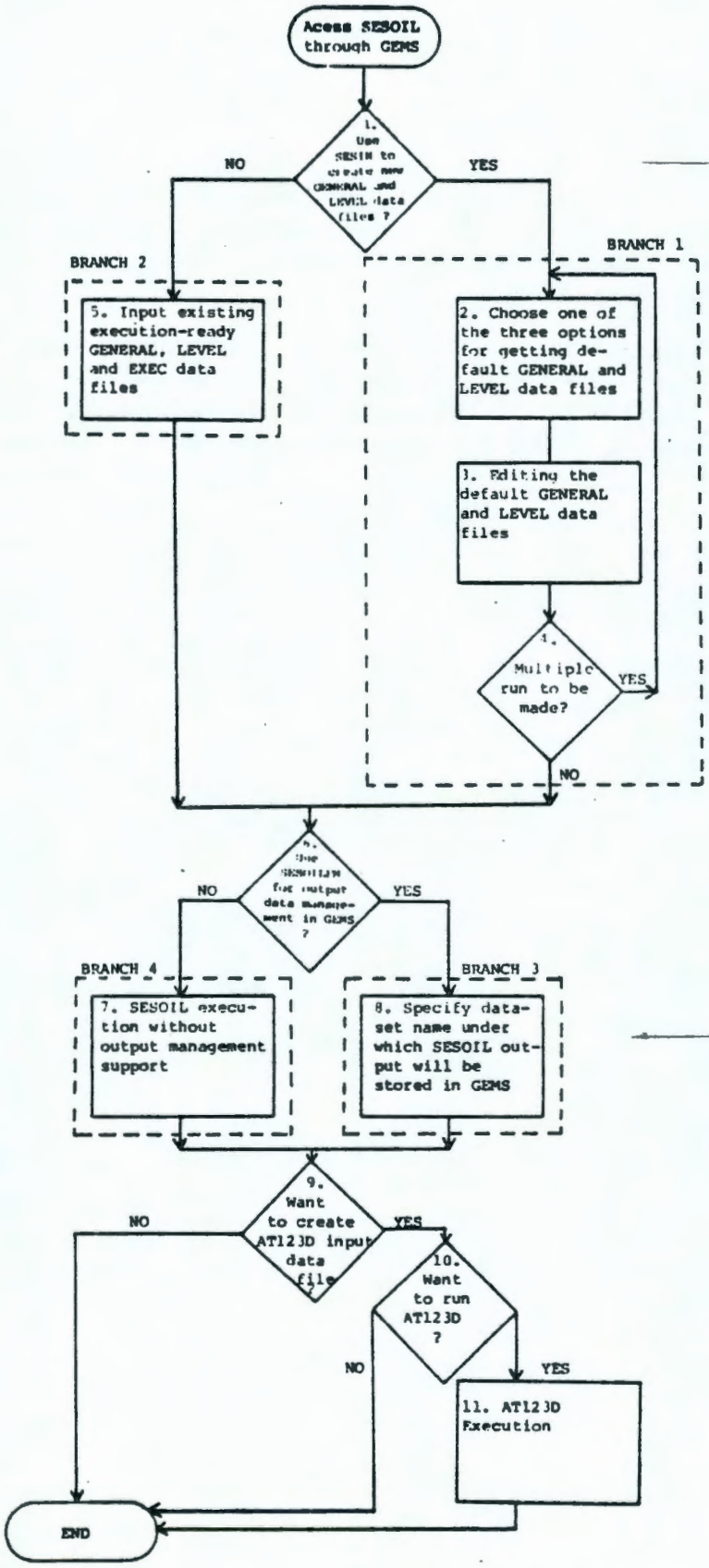

FIGURE 2-4 FLOWCHART FOR SESOIL EXECUTION WITH DATA MANAGEMENT SYSTEM SUPPORT

References

Bonazountas, M., and Wagner, J. 1984. SESOIL: A seasonal soil compartment model. Cambridge, MA: Arthur D. Little, Inc. Prepared for U. S. Environmental Protection Agency, Office of Toxic Substances. Contract No. 68-01-6271.

General Sciences Corporation (GSC). 1984. User's guide to SESOIL execution using the data management supporting systems, SESIN and SESOILFM. Landover, MD. Prepared for U. S. Environmental Protection Agency, Office of Toxic Susbstances. Contract No. 68-01-6618.

2.3.2 PRZM

Overview

The Pesticide Root Zone Model (PRZM) is a dynamic model which simulates the vertical movement of pesticides in the unsaturated soil, within and below the plant root zone, and extending to the water table, using generally available input data that are reasonable in spatial and temporal requirements. The model consists of hydrology and chemical transport components that simulate runoff, erosion, plant uptake, leaching, decay, foliar washoff and volatilization (implicitly) of a pesticide. It was developed by the Environmental Research Laboratory of the Environmental Protection Agency in Athens, Georgia (Carsel et al. 1984).

Description

PRZM is a dynamic, compartmental model for use in simulating chemical movement in the unsaturated soil systems within and below the plant root zone. Time-varying transport, including advection, and dispersion, are represented in the program. PRZM has two major components: hydrology and chemical transport. The hydrology component for calculating runoff and erosion is based on the Soil Conservation Service curve number technique and the universal soil loss equation. Evapotranspiration is estimated from pan evaporation data or by an empirical formula if input pan data are unavailable. Evaportranspiration is divided among evaporation from crop interception, evaporation from soil, and transpiration from the crop. Water movement is simulated by the use of generalized soil terms including field capacity, wilting point, and saturation. Drainage from loose, porous and tighter compact soils is simulated. To produce soil water and solid phase concentrations, the chemical transport component calculates pesticide uptake by plants, surface runoff, erosion, decay, vertical movement, foliar loss, dispersion, and retardation. A finite difference numerical solution, using a backwards difference implicit scheme, is employed.

Input

To complete a simulation using a dynamic hydrologic model such as PRZM, three efforts are required: (1) the input stream for the model must be developed, (2) the climatic data must be placed on a file in the required model format, and (3) time-series output has to be analyzed. ANPRZM reduces the time to accomplish Item 1 of the three efforts required of a simulation with PRZM.

ANPRZM is a FORTRAN program designed to provide interactive capability for PRZM to create, check, and update input streams of data. ANPRZM was developed to reduce the time and effort required in setting up hydrologic models for calibration/verification/production analyses. ANPRZM also was designed to be helpful to the inexperienced user and yet be efficient for the experienced user. PRZM input

consists of watershed pesticide characteristics such as field capacity, wilting point, curve number, crop type, partition coefficient, and decay rate.

For the category of input, ANPRZM provides easy creation of the files by prompting the user for parameters, checking the parameters for agreement to acceptable ranges, and providing default values. The user may decide to change an option within PRZM, which can affect other input required. ANPRZM will provide checks for such situations, thus saving time from submitting jobs that fail due to missing data. A detailed flow diagram of the PRZM structure is provided in Figure 2-5.

Output

There are four output files which include daily, monthly and yearly hydrological summaries; the pesticide mass balance; the pesticide concentrations over space and time; and time series output of selected parameters.

Reference

Carsel, R.F., Smith, C.N., Mulkey, L.A., Dean, J.D., and Jowse, P. 1984. User's manual for the pesticide root zone model (PRZM). Athens, GA: U.S. Environmental Protection Agency, Environmental Research Laboratory.

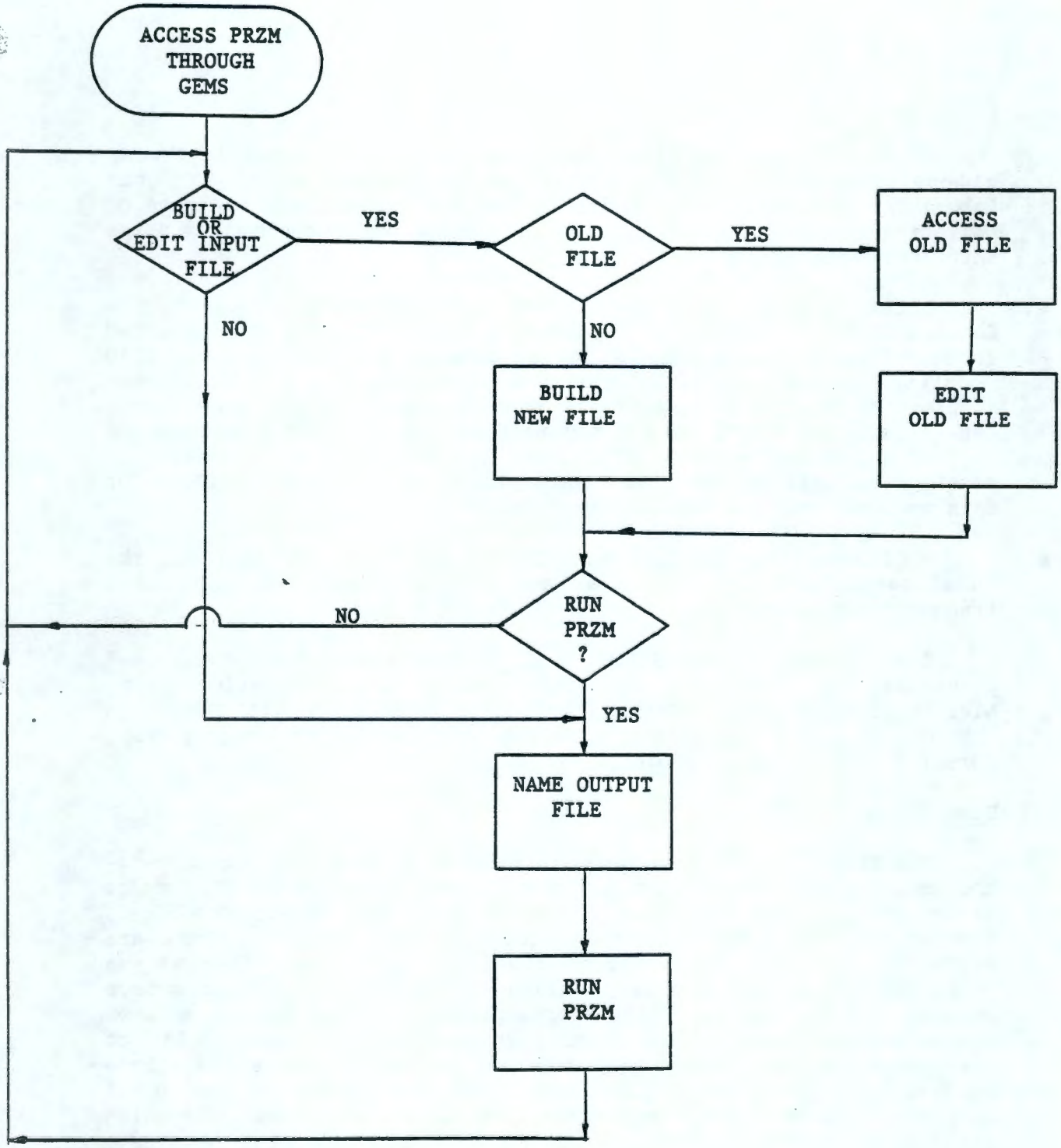

FIGURE 2-5. Flowchart of ANPRZM Execution.

2.3.3 AT123D

Overview

AT123D is an analytical transient one-, two-, and/or three-dimensional computer model developed by the Oak Ridge National Laboratory (Yeh 1981). The model is designed to estimate the rate of pollutant transport/transformation in a groundwater system (i.e., the saturated zone).

Under contract with the Office of Toxic Substances, EPA, the General Sciences Corporation implemented AT123D in GEMS and developed input and output data management systems in support of the AT123D modeling operation. The input data management system (AT123DIN) uses interactive prompts to assist the user in preparing the model input data file. The output data management system (AT123DOUT) allows the user to store the selected AT123D output results in GEMS, making it possible to utilize the file manipulation capabilities of GEMS for data analysis and graphical interpretation.

AT123D has been coupled with SESOIL, a model designed for the unsaturated zone, to serve as a complete subsurface pollutant transport modeling tool.

The combination of SESOIL and AT123D models have been used previously for estimating the likely pollutant concentrations (e.g., Nitrilotriacetic Acid (NTA) and Polychlorinated Biphenyls (PCBs)) in the groundwater downgradient from potential polluting sources (e.g., domestic septic tanks, landfill sites).

Description

The AT123D model is designed to provide an efficient and easy-to-use tool for the groundwater pollutant transport analysis. The model is capable of handling three different pollutant types: chemical, radioactive, and heat. The model contains many options. There are eight types of pollution source configuration to be selected: a point source, a line source parallel to the x-axis, a line source parallel to the y-axis, a line source parallel to the z-axis, an area source perpendicular to the x-axis, an area source perpendicular to the y-axis, an area source perpendicular to the z-axis, and a volume source. The patterns of source releases acceptable to the model include: instantaneous, continuous, and finite duration. Selection can also be made to define the aquifer dimension in terms of finite depth and finite width, finite depth and infinite width, infinite depth and finite width, or infinite depth and infinite width. The mechanisms of transport considered by the model include advection, hydrodynamic dispersion, adsorption, and decay/degeneration.

Inputs

AT123D requires one input data file containing the following information:

- o job title
- o model execution specifications
- o aquifer size and loading source size configurations
- o soil and waste properties
- o location coordinates where the solutions are desired

To facilitate the preparation of this input data file, GSC developed an input data management system, AT123DIN (GSC 1983). This system provides step-by-step prompts to assist the user in performing the formulation, editing, and naming of the AT123D input data file. A flow chart showing the steps required in creating an input dat file using AT123DIN is shown in Figure 2-6.

Output

Output results of AT123D include:

- o a summary of all input hydrologic, chemical, physical, soil, and execution specification parameters considered in the model simulation,
- o tabular presentation of the estimated pollutant concentration distribution in the groundwater at different time intervals and at different locations pre-specified by the user along the X, Y, and Z directions.

GSC developed an output data management system, AT123DOUT, to allow the user to create, for each AT123D simulation run, a GEMS dataset containing all of the AT123D output parameters (GSC 1985). The user can utilize GEMS file management capabilities to manipulate, analyze, and interpret those output parameters in the dataset. One example of the use of GEMS capabilities is the display of information (e.g., concentration vs. time) in graphics, such as scattergrams, barcharts, or histograms.

After each AT123D run, the complete model output is written to a data file, AT123DOUT.DAT, in the user's computer account directory. The user can review, rename, or request a hardcopy print of this output data file.

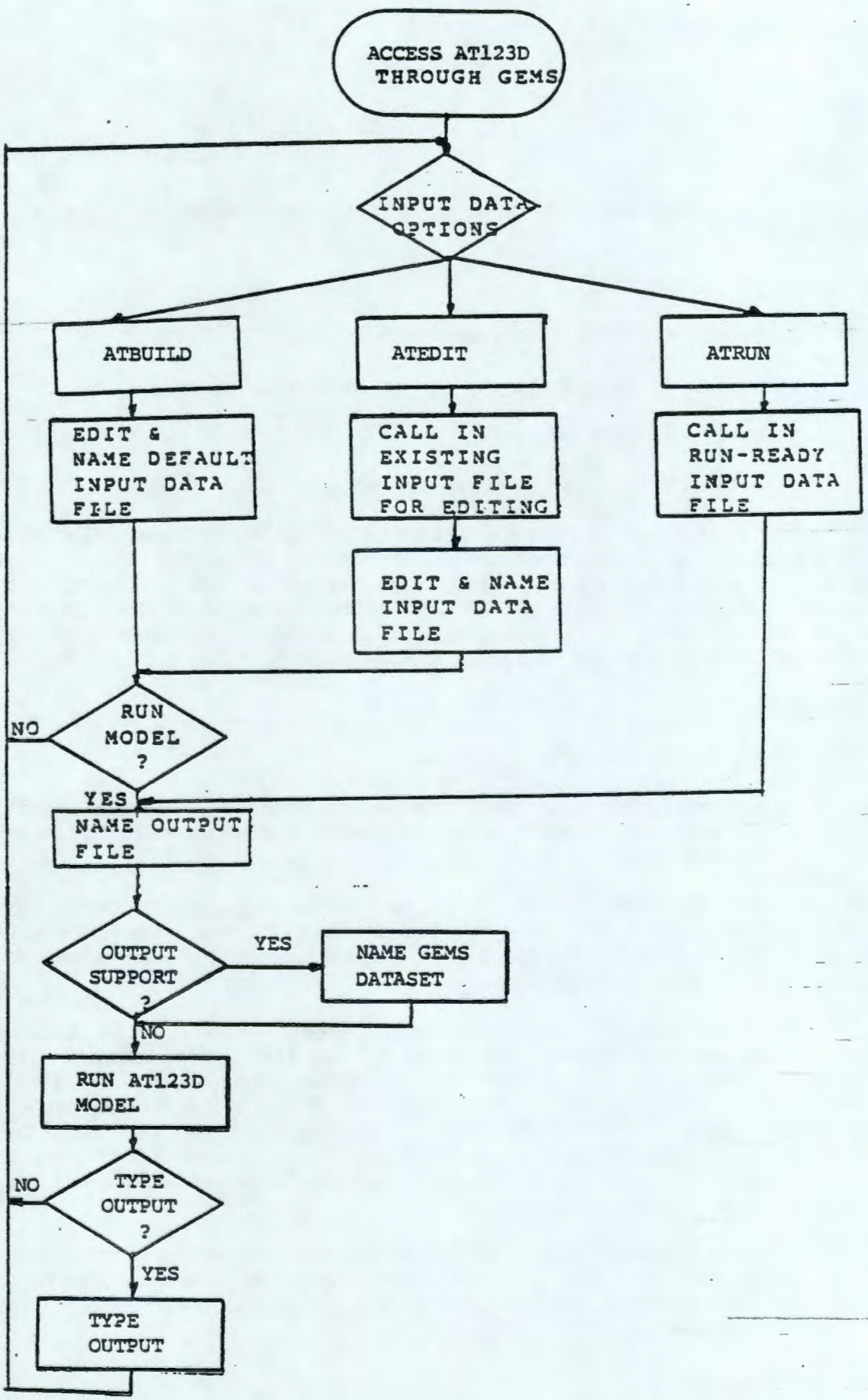

FIGURE 2-6. Flowchart of AT123D Execution with Data Management System Support

References

Yeh, G.T. 1981. AT123D: analytical transient one-, two-, and three-dimensional simulation of waste transport in the aquifer system. Oak Ridge, TN: Oak Ridge National Laboratory. ORNL5602.

General Sciences Corporation (GSC). 1985. User's guide to AT123D execution using the data management supporting systems AT123DIN and AT123DOUT. Landover, MD. Prepared for U. S. Environmental Protection Agency, Office of Toxic Substances. Contract No. 68-01-3970.

2.3.4 SWIP

Overview

SWIP is a three-dimensional numerical computer model for simulating pollutant (chemical and thermal) transport/transformation in a groundwater system (i.e., the saturated zone), with or without wells. It was originally developed by Intercomp, Inc. for the U.S. Geological Survey to investigate problems associated with the disposal of wastes into deep wells (Intercomp 1976). The model was subsequently modified for more general applications to include free water surface, vertical recharge, equilibrium-controlled linear adsorption and a first-order irreversible rate reaction (Intera 1979).

General Sciences Corporation (GSC) has implemented a data management supporting system for the input data support of the SWIP modeling operation. The SWIP Data Management Supporting System uses interactive prompts and parameter menus to the user in the preparation of the SWIP model input data file. Through the use of the Data Management Supporting System, a user can access various commands to perform efficient data entry, manipulation, and editing.

Description

The SWIP model incorporates the finite-difference approximation, and has options for several matrix solution techniques. It treats steady or transient flow in heterogeneous and/or isotropic media. In addition, it has options for treating flow in one-, two-, or three-dimensional cartesian or cylindrical coordinates. The model also incorporates a wellbore model for calculation of pressures, heat loss, and flow rates in the wells.

Input

The SWIP input data consists of a single file which is divided into the following 5 data groups:

- Program controls
- Fluid and aquifer properties
- Initial aquifer conditions
- Recurrent data, and
- Well plotting data

The program controls data consist mainly of control parameters, which control the major options in the model such as selection of solution of equations, wellbore calculations, output listings, and dimensioning of arrays. The fluid and aquifer properties consist mostly of aquifer and fluid properties, and grid system description data. The initial aquifer conditions describe the initial concentrations, temperatures, and fluid velocity in the aquifer. The recurrent data is read before each time step (or period) when you which to change the well conditions, internal time step calculations,

solution technique, aquifer recharge conditions, or output controls for the simulation period. The recurrent data is repeated in a loop as many times as is specified. The well-plotting data is needed for plotting pressures, temperatures, and concentrations in the wells; and is also repeated in a loop for each well specified.

A generalized flowchart showing the steps required for inputting SWIP model data using the data management system support is shown in Figure 2-7.

Output

The output results of the SWIP model include pressures, temperatures, and concentrations in the specified aquifer grid block centers at each specified time step. In addition, total quantities of water, heat, and contaminant mass pumped by each well for each specified time step are given. Contour maps of pressure, temperature and/or concentration at any specified time steps can be obtained, and plots of any or all of these three quantities in each well versus time, may also be obtained. It should be mentioned that the contour maps and well plots are outputted in character mode, and are therefore not of high quality resolution. The SWIP output is written to a file in the user's current directory. The file name is specified by the user as the response to a prompt.

References

General Sciences Corporation (GSC). 1985. User's guide to SWIP model execution using data management supporting system. Landover, MD. Prepared for U.S. Environmental Protection Agency, Office of Toxic Substances. Contract No. 68-02-3970.

Intera, Inc. 1979. Revision of the Documentation for a Model for Calculating the Effects of Liquid Waste Disposal in Deep Saline Aquifers. U.S. Geological Survey, Water-Resources Investigations 79-96, July 1979.

Intercomp, Inc. 1976. A Model for Calculating the Effects of Liquid Waste Disposal in Deep Saline Aquifer, Part I and II. U.S. Geological Survey, Water-Resources Investigations 76-61, June, 1976.

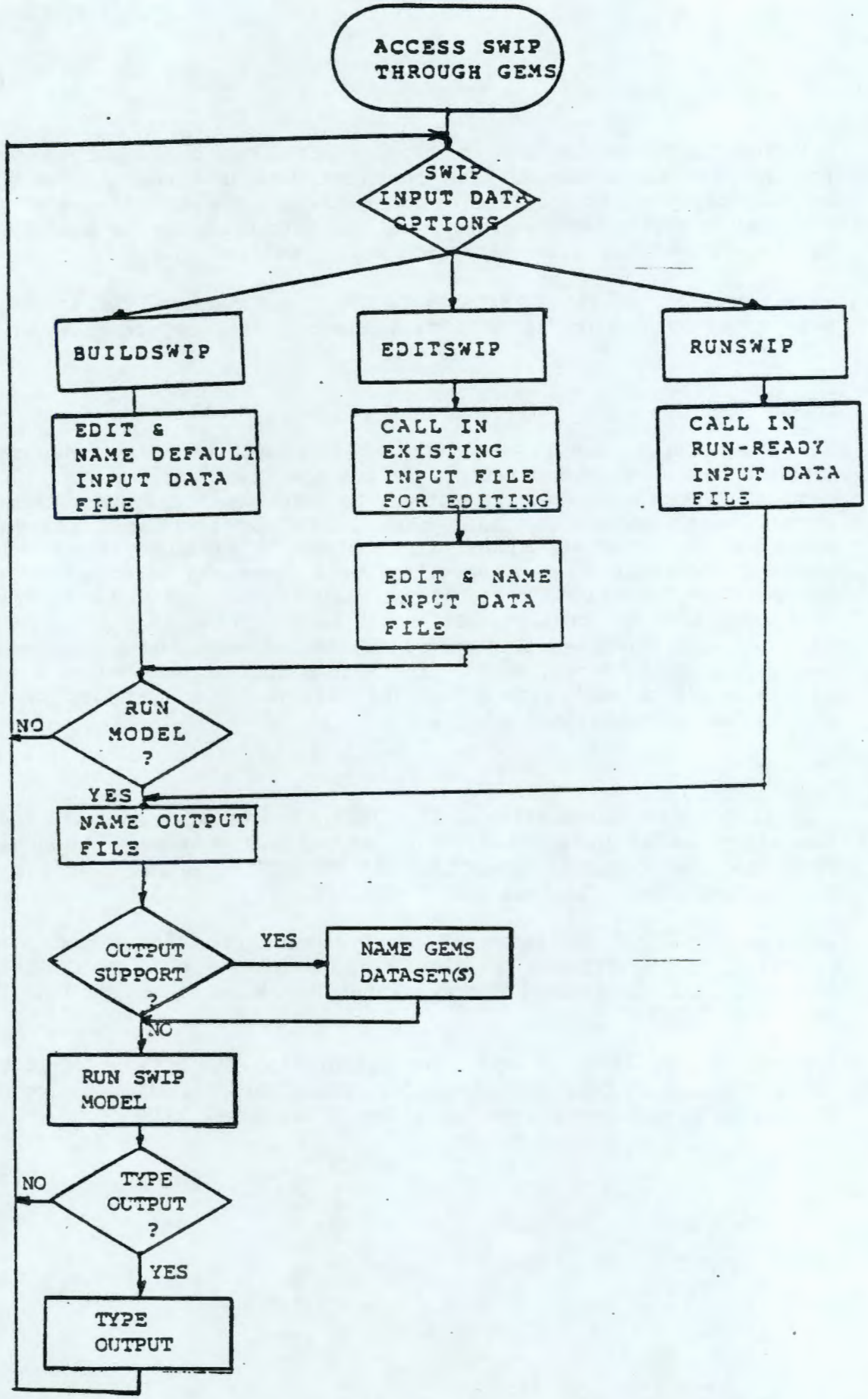

FIGURE 2-7. Flowchart for SWIP Execution with Data Management System Support.

2.4 Multimedia Models

2.4.1 Environmental Partitioning Model (ENPART)

Overview

ENPART is an environmental partitioning model developed by the General Sciences Corporation and the Exposure Evaluation Division's Modeling Section, Office of Toxic Substances, EPA. The model is designed to perform a first-level screening analysis from a minimum set of chemical-specific input data. The purpose of this analysis is the identification of the most important environmental exposure pathways, the estimation of the substances' environmental persistence, and their bioconcentration potential.

Description

The model is adapted from the fugacity approach to equilibrium partitioning as described by McKay (1979). In this approach, the equilibrium concentration ratios between environmental compartments are calculated from simple physical/chemical data, such as molecular weight, solubility, and vapor pressure. In ENPART, this approach was modified by the addition of environmental parameters, such as compartment size, intercompartment transport, and degradation, to yield a second level of concentration and mass partitioning (dynamic partitioning). The environment ENPART models consists of three compartments: air, water and soil. The water compartment is subdivided into four components: water, suspended sediment, biota, and bottom sediment. For the last three components, only equilibrium processes are considered. In equilibrium partitioning, only equilibrium processes defining the time-independent "steady state" environmental conditions are allowed to determine the estimated final distribution of the chemical. In dynamic partitioning, the chemical distribution is controlled by compartment-related transformation rates and intercompartment chemical transport.

Input

Data input to the model is via several interactive user prompts, the sequences of which vary with the information available to the user. Many of the ENPART input parameters can be estimated within the model or are assigned default values. A complete description of ENPART input is presented in the model documentation (Wood et al. 1982; Pilotte et al. 1985).

Output

Output of ENPART consists of intercompartment concentration and mass ratios, concentration and mass partitioning factors, and a ranking analysis for both equilibrium and dynamic partitioning. In addition, dynamic partitioning provides an estimate of the chemical persistence.

ENPART is designed as an interactive model and, therefore, the output is provided to the user's terminal during a model run. In addition, a summary of the modeling results is written to a file during each model run. This summary file, SUMOUT.TRM, is available for renaming, reviewing, or printing at the terminal at the end of the model run, but it is not available for use with GEMS file management and graphics capabilities.

References

Mackay, D. 1979. Finding fugacity feasible. Env. Sci. & Tech., 13, 1218.

Wood W., Nold A., Lefler J., and Pilotte J. 1982. Environmental partitioning model. Landover, MD: General Sciences Corporation. Prepared for U. S. Environmental Protection Agency, Office of Toxic Susbstances. Contract No. 68-01-6618.

Pilotte, J. and Kinkel, W. 1985. User's guide to environmental partitioning model. Landover, MD: General Sciences Corporation. Prepared for U.S. Environmental Protection Agency, Office of Toxic Substances. Contract No. 68-01-3970.

2.4.2 TOX-SCREEN

Overview

TOX-SCREEN was developed by Hetrick and McDowell-Boyer (1982, 1983) for the Office of Pesticides and Toxic Substances, U.S. EPA. It was designed as a multimedia screening-level model which assesses the potential fate of toxic chemicals released to the air, surface water, or soil. Four types of surface water bodies are considered: lakes, rivers, estuaries, and oceans. The model is simple in nature and is intended to be used as a screening device to identify chemicals that are unlikely to pose problems even under conservative assumptions.

General Sciences Corporation implemented TOX-SCREEN in GEMS and developed an input data management system TOXIN, to support its operation. TOXIN uses interactive prompts to assist the user in the preparation of TOX-SCREEN input data files for the air, water, and soil phases.

There is no output data management system available for the TOX-SCREEN operation at this time.

Description

The multimedia nature of TOX-SCREEN requires that physical/chemical processes which drive transport of chemicals across air-water, air-soil, and soil-water interfaces be simulated. Such media interactions are handled explicitly in the model, in most cases with the use of deposition velocities, transfer rate coefficients, and mass loading parameters. Monthly pollutant concentrations in air, surface water, and soil reflect both direct input to any or all of the media from a specified source(s) and subsequent interaction via processes such as volatilization, atmospheric deposition, and surface runoff. The user must select the types of water bodies (i.e., river, lake, estuary, or ocean), if any, to be considered in any given simulation, as well as specify whether the pollutant is directly released to air or water and/or directly applied to soil.

For the atmospheric dispersion simulation, a modified Gaussian plume equation was adapted for use in estimating downwind concentrations of a particular chemical emitted from a point source. A simple urban diffusion model was adopted for use in estimating ground-level pollutant concentrations over area sources.

For the aquatic dispersion, an equation similar to that used in the EXAMS model was used to estimate the monthly pollutant mass in rivers and lakes. A one-dimensional steady-state model was used for simulating dispersion of pollutants in estuaries and a steady-state Gaussian-type linear diffusion model was used in oceans.

TOX-SCREEN employs the SESOIL model to estimate pollutant concentrations in the soil media following introduction via direct application and/or interaction with other media.

Input

The input data files required by TOX-SCREEN include the following:

1. SESOIL EXEC data file

2. SESOIL GENERAL data file

3. SESOIL LEVEL3 data file

4. Model Flags data file

5. Air Parameters data file

6. Water Parameters data file

7. Bioaccumulation Parameters data file

To facilitate the preparation of these input data files, GSC developed TOXIN, a TOX-SCREEN input data management system, which provides step-by-step guidance to assist the user in performing the formulation, editing, and naming of TOX-SCREEN input data files. Figure 2-8 depicts the sequence of menus within TOXIN that pertain to the model flags, Air, Water, and Bioaccumulation data files. The SESOIL data files are handled by the SESIN interactive data entry menus.

Output

TOX-SCREEN provides estimates of the fate of pollutants once released into the air, water, and/or soil environments. Depending on the nature of outputs generated, the following major types of output files can be expected:

1. Results generated by SESOIL

2. Summary of TOX-SCREEN input data

3. Results generated if the water body is a lake

4. Results generated if the water body is a river

5. Results generated if the water body is an estuary

6. Results generated if the water body is an ocean

7. Results generated from the food chain bioaccumulation calculations

References

McDowell-Boyer, L.M., and Hetrick, D.M. 1982. A multimedia screening-level model for assessing the potential fate of chemicals released to the environment. Oak Ridge, TN: Oak Ridge National Laboratory. ORNL/TM-8334.

McDowell-Boyer, L.M., and Hetrick, D.M. 1983. User's manual for TOX-SCREEN: A multimedia screening-level program for assessing the potential fate of chemicals released to the environment. Oak Ridge, TN: Oak Ridge National Laboratory. ORNL/TM-8570.

2.4.3 UTM-TOX

Overview

The Unified Transport Model for Toxic Materials (UTM-TOX) was developed at the Oak Ridge National Laboratory (1983) for the U.S. Environmental Protection Agency. It is a multimedia model designed for predicting the dispersion of pollutants through air, soil, and water. The model calculates the atmospheric dispersion of up to 20 chemicals from a maximum of 10-point, 10-line, and 10-area sources; deposition of one chemical at a time in both wet and dry form on foilage or the surface of the earth followed via the transport through runoff and erosion; percolation through the soil to a stream channel; and transport in the stream channel to the outfall of a watershed.

During each of these phases of transport, many chemical processes can be represented in the model, including exchange with the soil, solubilization, degradation, volatization, photolysis, and hydrolysis. Each of these processes is represented in the model in a useful and direct manner by the incorporation of three previous models, ATM,, WHTM, and SEDMNT, which treat atmospheric, hydrologic, and soil transport of pollutants, respectively. Thus, with UTM-TOX, the user can track a contaminant through the ecosystem, tabulate budgets for the partitioning of the contaminant, calculate the concentration of the contaminant in many compartments of the ecosystem, and reliably assess the impact of the contaminant.

Description

ATM calculates the dispersion of airborne pollutants. It is a Gaussian plume model that determines the spreading of material emitted from a point source, a line source, or an area source from calculations of the sigma values, vertical and horizontal widths of the plume. These sigma values are determined empirically and are representative of plumes of less than 50 km in length.

When the program is used in an annual or monthly mode, 16 sectors are used to describe the direction from which the wind blows. The concentration of the pollutant is assumed to be uniformly azimuthally distributed over the whole sector because of the meandering of the plume.

WHTM calculates the transport of pollutants through portions of the watershed. In the hydrologic cycle, the continuous processes of transpiration and evaporation driven by precipitation lead to interflow beneath the surface of soil, recharge and discharge of an aquifer, and establishment of flow in the stream channel. These processes are quite complex within themselves, and the model provides a parametric summary of these that is completely deterministic and very useful for purposes of simulating runoff and transport. The modeled cycle also includes uptake by vegetation, erosion, solubilization of absorbed material from the litter, transport from

the litter, and infiltration into an unsaturated region of the soil where the root zone occurs.

SEDMNT models the aquatic transport of pollutants by sediment. This mode of transport is important because of sorbtion-desorbtion of a chemical on sediment can determine its fate. SEDMNT considers each reach of a stream channel to have a suspended-load layer that travels with the stream; a bed layer that is deposited at the bottom of the channel and is subject to resuspension; and a resident-bed layer that is more permanent. The fluxes among these various layers are calculated with (1) Stokes's Law fall velocities, (2) the shear stresses within each layer, (3) the particle sizes of the sediment, and (4) the load-carrying capability of the stream channel. The thicknesses of the different layers can change during the course of a simulation in response to the sediment deposit and/or resuspension in the progress of stream flow transport.

Input

The input data required by UTM-TOX include monthly wind roses, hourly precipitation, solar radiation, daily maximum and minimum temperatures, soil characteristics, topographic information, surface water characteristics, sediment characteristics, and the physiochemical properties and transformation rates associated with the chemical.

All input data are read by UTM-TOX through ten (10) input data files. As discussed in the UTM-TOX user's manual, each input file contains a group of input parameters to be coded according to a pre-specified format. Presently, there is no interactive front-end data management system available to assist the user in preparing these ten (10) input data files; the user has to manually set up these ten input data files in order to execute UTM-TOX. UTM-TOX is operational in GEMS, and the user is prompted for the 10 input data files (GSC 1984). The model is then run in batch mode. A previous study is available which is intended as an aid to the user in estimation of many of the input parameters required by UTM-TOX (GSC 1985).

Output

The output consists of plots and tables summarizing the average monthly and annual chemical concentrations in wind sectors, in saturated and unsaturated soil layers, in runoff, and out of each reach. Additionally, listing of input data is also presented to facilitate cross referencing.

UTM-TOX produces three output data files: UTMTOX1.OUT, UTMTOX2.OUT, and UTMTOX3.OUT. These output files will be stored in the user's computer account directory after completion of each UTM-TOX run. Presently, there is no interactive back-end data management system available for UTM-TOX to allow the user to store output into

GEMS for subsequent output graphical display, analysis, and interpretation using GEMS utility services.

Reference

Oak Ridge National Laboratory. 1983. A user's manual for UTM-TOX, the unified transport model. Oak Ridge, TN. ORNL/TM-8182.

General Sciences Corporation (GSC). 1984. Implementation of the UTM-TOX Model. Landover, MD. Prepared for U.S. Environmental Protection Agency, Office of Pesticides and Toxic Substances. Contract No. 68-01-6618.

General Sciences Corporation (GSC). 1985. Characterization of data base requirements for implementation of UTM-TOX under GEMS: parameter senstivity study. Landover, MD. Prepared for U.S. Environmental Protection Agency, Office of Pesticides and Toxic Substances. Contract No. 68-02-3970.

OBTAINING A NON-EPA ACCOUNT TO ACCESS THE GRAPHICAL EXPOSURE MODELING SYSTEM
December 1988

This bulletin is directed to those outside of EPA, both government agencies and industry, who are interested in using the Graphical Exposure Modeling System (GEMS). GEMS resides on the VAX Cluster located at the National Computer Center in Research Triangle Park, North Carolina. The paragraphs below describe the steps required to open an account on the VAX Cluster. There is a modest charge to use the VAX Cluster. Check the billing section of this bulletin for more information. If you have any questions about opening an account, please contact Cathy Turner at (202) 382-3929.

STEP #1: APPLICATION FOR ACCOUNT

You may apply for an account on the Cluster at any time. The process of opening an account for non-EPA GEMS users takes between 2 to 4 weeks. In the paragraphs below you will find instructions on how to go about opening your account. As a non-EPA GEMS user, you must obtain an account to use GEMS through the National Technical Information Service (NTIS). Call Cathy Metzler, our NTIS representative at (703) 487-4807. Give her your name and address and request that she send you an online license and billing agreement for the NCC VAX Cluster to use GEMS. You should complete only one licensing and billing agreement for use by yourself and any contractors working for you who also use GEMS. However, be sure to provide a list of those who will be using GEMS, so that individual user-ids can be created for each. Cathy can answer any questions you may have about this phase of the process.

On the Online License Agreement, there is a space for you to fill in the name of the database or system to which you desire access. You should enter "Graphical Exposure Modeling System (GEMS)" here. NTIS requires that you complete both copies of this form and return it to them. The charges for GEMS use for Fiscal Year 1988 are included with the licensing and billing agreement and are repeated in the billing section of this bulletin for your information. How this adds up for some typical GEMS applications is also included in the billing section. These charges will be the same for EPA users.

Once you have completed the forms, return them to Cathy Metzler at the address given on the cover sheet of the forms. I recommend that you keep a copy of the completed forms and check with Cathy in one week to verify that she has received the originals. Call her if you have any questions regarding filling out the forms. About two weeks after you send in the Licensing and Billing Agreement, you will receive the TSSMS Account Authorization Notice. (TSSMS stands for the Time Sharing Services Management System.) This notice will inform you of your user-identification and the account you are authorized to use on the VAX Cluster.

Please read this notice carefully for its explanation your user-id, password, and account, also referred to as project. Attached to the notice is a postcard that **must** be returned to the TSSMS Office by the date indicated, verifying that you have reset your password. Failure to respond by the due date will result in your user-id being removed from the VAX Cluster. The password resetting procedure is described in the section that follows.

STEP #2: LOGGING ON TO THE CLUSTER

You must log on to the VAX Cluster as soon as possible after receiving your TSSMS Account Authorization Notice and before the due date stamped both on the attached postcard and at the bottom of the notice. Before logging in, you must configure your terminal or your communications software to transmit and receive ASCII data in full duplex mode, using even parity and 7-bit data word length. Communication rates may be 300, 1200, or 2400 baud (bits per second). You will access the VAX Cluster through the NCC Port Selector. Those of you located in D.C. can access the port selector using 488-1515 for 300 and 1200 baud communica-tions, or 488-3671 for 1200 and 2400 baud lines. Those of you outside the D.C. area may use the TYMNET telephone network. Contact the Telecommunications Group at NCC, (919) 541-4506, to find out how you can access the port selector using TYMNET. The port selector screen looks like this:

```
WELCOME TO THE ENVIRONMENTAL PROTECTION AGENCY

                HEADQUARTERS DATA SWITCH


TO ACCESS:                          TYPE:

IBM (TTY)                           NCC, IBMPSI
IBM 3270 Emulation                  NCC, TCP
EPA/DIALCOM ELECTRONIC MAIL         EMAIL
PRIME                               system name
VAX                                 NCC, system name
MODEM POOL                          MODEM, 999-9999
OTHER SERVICES                      HELP

Enter selection:
```

You should respond with the words NCC, VAXA. You will then receive a username prompt, enter your user-id at this prompt. Next, you will be prompted for your password. Enter your password as indicated in your TSSMS Account Authorization Notice. Finally, you will be prompted for the project you are authorized to use; this is also listed in the TSSMS Notice as your account.

Once you have correctly responded to all these prompts, you will receive a series of system news banners and then the dollar sign prompt ($) will appear. The first thing you must do is reset your password. Remember that passwords must have at least 6 characters. Note that the VAX Cluster will automatically log

you off if your account is inactive for more than 20 minutes. You will no longer be able to leave your terminal unattended in the middle of a GEMS session. However, due to the charges that will accrue due to connect time alone, it will be unlikely that you will want to do this.

STEP #3: PASSWORD RESETTING

The procedure to reset your password is identical to that used on the OTS VAX. The procedure is repeated here for your information. Don't forget to mail in that postcard once you've got your password reset. Once you've reset your password, please remember that on the VAX Cluster, as on the OTS VAX, passwords must be reset every 90 days. Keep an eye open for the password expiration message. If you let it expire, you will have to contact the TSSMS office at (919)-541-3629.

1) At the $ prompt, type the words SET PASSWORD.

2) The system will prompt you for the old password, meaning the password set for you by TSSMS; what you type in will be masked - you won't be able to see it.

3) The system will prompt you for a new password, which must be at least six letters long. Your entry here will also be masked. Please note: your new password must be different from the old one.

4) The system will prompt you for verification, which requires you to enter your new password again. This functions as a spelling check, to verify that you entered the intended new password. Again, your entry here will be masked.

STEP #4: USING GEMS

GEMS is already up and running on the VAX Cluster. You can access GEMS by simply typing GEMS at the $ prompt. It is not necessary to have any of the files from your previous account to use the system on the VAX Cluster. Please use the Problem Report function in the GEMS Utilities menu if you have any problems. We will be contacting you one month after sending you this bulletin, to check on your progress. We will also ask you for your user-id, as we will be creating a mailing list for use in sending VAX-Mail messages. Please give us a call if you haven't heard from us within that period of time.

BILLING

User billing for NTIS accounts will start up as soon as an account is opened. You can get more detailed information about the charge-back system from NTIS. Currently, the VAX Cluster consists of two processors, an 8650 (VAXA) and an 8600 (VAXB). By the end of January, the 8600 processor will be upgraded to an 8650. The CPU rate for using the 8650 processor is $238.00 per CPU hour. The rate for the 8600 is $169.00 per CPU hour. (These rates were based on the CPU performance ratios of the 2 processors, and will result in about the same CPU charge per application.) There will also be a connect charge of $9.00 per connect hour. Please notice that CPU usage will be in the region of seconds, and therefore charges for CPU use will be small; however, the charges for connect hours will be a significant contribution to your costs. Also, please note that disk block storage (storing the files in your account) is $0.075 per 1,000 blocks per day. Cost for lines printed at the Computer Center in North Carolina (using the VAX PRINT command) is $1.50 per 1,000 lines. These charges will be the same for our EPA accounts.

We are providing you with some information on the average costs entailed in running various GEMS applications in the table below, for your use in estimating costs for your usage of GEMS for your ADP (automated data processing) budget. The estimates are based on running the programs by experienced users. Note that costs do not include retrieving and reviewing model output or storage of model output. (Less CPU time is involved in these processes than in those included in the table.)

GEMS Capability	CPU time (seconds)	Connect time* (minutes)	Cost* dollars
Retrieve CENSUS data for a single site	6	10	1.90
Use CENBAT to retrieve CENSUS data for 10 sites	9	12	2.40
Run AUTOCHEM for 1 chemical, all properties	6	5	1.20
Run ENPART, both steady state and dynamic processes	9	10	2.10
Run GAMS for 1 chemical 1 or 2 sites, up to 5 stacks	6	15	2.70
Run EXAMS with all input already entered	12	7	1.90
Extract CEDB environment information for a river	14	6	1.90
Run SESOIL with minor modification of input datasets	8	22	3.90
Run AT123D	15	16	3.40

* Includes time from login to logoff, running in 1200 baud. CPU times for 2400 baud will be the same, connect times will be somewhat shorter.

USER SUPPORT

In order to use GEMS effectively, you may be interested in obtaining user support. GEMS manuals and training are available through General Sciences Corp. This company has been the Agency's contractor in the development and refinement of GEMS for the past seven years, and has extensive experience in the use and applications of the system. You may also find it helpful to engage their services for as-needed user support for questions you encounter in using the system or help on special applications you are developing. Contact Mr. Jon Chen at (301)-953-2700 for information on obtaining manuals and training, and on setting up a user support contract. The address is General Sciences Corp., 6100 Chevy Chase Drive, Suite 200, Laurel, MD, 20707.

FILES AND TAPE STORAGE

On the VAX Cluster, files that haven't been opened for 45 days will be automatically archived to tape. Each user should figure on having and using one tape to store their inactive files. We will explain more about personal tapes in a future mailing. Tape storage charges are expected to be about $10.00 per month, with the rate for tapes you send to the Computer Center for your own use set at around $15.00 per month. The tape management system on the VAX Cluster is TAPESYS, and the procedurs you may need are described in the NCC VAX User's Guide. Soon after receiving your new account, the computer center will send you a Profile Sheet. You can request a copy of the VAX User's Guide on this sheet. The computer center is also currently working to develop an on-line version of this document for easier reference.

GEMS MANUAL

A new GEMS manual is in the works, integrating all previously available information on GEMS capabilities and including detailed explanations of the procedures as they apply to the VAX Cluster. The manual will consist of several chapters, each focusing on a separate GEMS function: the introductory chapter (which includes the information described above) and chapters on chemical property estimation, modeling, graphics and geodata handling, dataset manipulation, and statistics. Chapters 1 (the core manual), 2 (property estimation), and 8 (GEMS Utilities) have been completed. Contact Cathy Turner to obtain a copy of these chapters. Ask to have your name placed on our mailing list, and we will send you subsequent chapters as they are completed.

PCGEMS: BETA-TEST VERSION

We are pleased to announce that the beta-test version of PCGEMS is ready for distribution. There have been a number of changes to the software, including added capabilities and a major reorganization to make the PCGEMS software modular. This allows you to use the various PCGEMS capabilities and datasets without having to store the entire program in one sub-directory on their computer's hard disk. The modules and datasets may be accessed directly from the floppy diskettes or Bernoulli cartridges on which they are stored.

PCGEMS CAPABILITIES

A list of the modules and datasets available on PCGEMS is attached. Note that you must have the Core System Module in order to run PCGEMS. All other capabilities are available but optional. Please note that at this time, CLOGP3 (in the Property Estimation module) is available only to those working in Federal and State government offices; due to an agreement EPA made with the developer, we are unable to provide this software to government contractors and other private companies.

Although we are presently unable to distribute the dataset of measured and estimated properties for the Superfund Title III Section 313 List of Chemicals, we expect it to be available very soon. The dataset will be formatted such that property values can be imported directly into PCGEMS models to facilitate your analyses. The PCGEMS Mapping module will also be available soon and will include the State/County mapping capability. We will announce the availability of the Title III properties dataset, the Mapping module and the supporting state and county boundaries, FIPS codes and Reachtrace files as soon as they are available.

DISTRIBUTION

Our contractor, General Sciences Corporation (GSC) will handle the distribution of the beta-test version of PCGEMS. We are providing you with an order form on which you may specify which PCGEMS modules you wish to obtain. The order form lists the modules and datasets available in this version of PCGEMS, and the fee for each. Please note that these charges are based solely on the costs to GSC incurred by purchasing the disks or cartridges, copying the software, and mailing PCGEMS and the User's Manual to you.

On the order form you will see a series of dollar amounts to the right of each PCGEMS module and dataset. Each amount corresponds to the kind of disk or cartridge on which you would like to receive your copy of PCGEMS. PCGEMS is available to you on a variety of media. These include floppy diskettes: double density (360 KB) or high density (1.2 MB), or $3^1/_2$ inch (720 KB) diskettes; and on either 10 MB and 20 MB Bernoulli cartridges.

FILLING OUT THE FORM

To fill out the order form, first identify the PCGEMS modules and datasets you will need, and the media on which you would like to receive your copy. Use the first column if you are requesting floppy diskettes. At the top, indicate which type of diskette you use. Then move down the column and indicate which module you want by writing in the quantity desired in the space to the right of the cost for that module. All copies of PCGEMS require the Core System Module. This core system includes the PCGEMS system disks, the Data Management disks, and the Utilities disks.

Supporting datasets are identified for the appropriate model or function. Note that two databases have been sub-divided by EPA Region and may be obtained either complete or by one or more regions. They are the Population and ReachScan datasets. Be sure to specify the regions you desire on the order form. The cost listed is per region; you will have to multiply that cost by the number of regions you are requesting. When ordering a single EPA Region, you may want to consider including the regions surrounding your own to avoid problems with releases that originate from or extend beyon the regional boundaries. A list of EPA Regions and the states included in each Region is attached.

If you wish to receive your copy of PCGEMS on Bernoulli cartridges, use the second column (10 megabyte capacity) or the third column (20 megabyte capacity). Note that only the entire PCGEMS system, and only the complete datasets are available with Bernoulli cartridges. Indicate the total cost of each module or dataset in the right hand column of blanks, and indicate the grand total at the bottom. Costs for postage and handling are already included.

For assistance, please contact Cathy Turner at (202) 382-3929.

MODULES AVAILABLE IN BETA-TEST PCGEMS

MODULE or DATASET	CONTAINS
Core System Module	Configuration File, Data Management, and Utilities Functions
Property Estimation	PCLOGP, PCCHEM, PCFAP, and PCHYDRO. Note: PCLOGP only available to Federal and State users
Air Models	ISCLT and PTPLU models
Surface Water Models	EXAMS II and ReachScan models
Soil and Groundwater Models	SESOIL and AT123D models
Multimedia Model	ENPART model
Graphics	Wind Rose
CAS/SMILES File for PCLOGP and PCCHEM	Cross-reference file for locating SMILES notation by CAS number
Population Data for ISCLT	BG/ED data from the 1980 Census by EPA Region
STAR Data for ISCLT and Wind Rose	Atmospheric conditions for weather stations around U.S.
River/Facility Data for ReachScan	Flow data and locations of dischargers and drinking water facilities
Climate Data for SESOIL	Precipitation and evapo-transpiration statistics
Zipcode File for Wind Rose	Cross-reference file for latitude/longitude of zipcodes

E.P.A. Regions

Population Data used by the ISCLT model is available by EPA Region. River/Facility Data used by the ReachScan model, is also available by EPA Region. The map and the list below are provided to allow you to determine the EPA Region for your area(s) of interest.

Regions	Regions	Regions
4 — Alabama	1 — Maine	3 — Pennsylvania
10 — Alaska	3 — Maryland	1 — Rhode Island
9 — Arizona	1 — Massachusetts	4 — South Carolina
6 — Arkansas	5 — Michigan	8 — South Dakota
9 — California	5 — Minnesota	4 — Tennessee
8 — Colorado	4 — Mississippi	6 — Texas
1 — Connecticut	7 — Missouri	8 — Utah
3 — Delaware	8 — Montana	1 — Vermont
3 — D.C.	7 — Nebraska	3 — Virginia
4 — Florida	9 — Nevada	10 — Washington
4 — Georgia	1 — New Hampshire	3 — West Virginia
9 — Hawaii	2 — New Jersey	5 — Wisconsin
10 — Idaho	6 — New Mexico	8 — Wyoming
5 — Illinois	2 — New York	9 — American Samoa
5 — Indiana	4 — North Carolina	9 — Guam
7 — Iowa	8 — North Dakota	2 — Puerto Rico
7 — Kansas	5 — Ohio	2 — Virgin Islands
4 — Kentucky	6 — Oklahoma	
6 — Louisiana	10 — Oregon	