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API'S DECISION SUPPORT SYSTEM FOR EXPOSURE AND RISK ASSESSMENT (DSS)

VERSION 2.0

HEALTH AND ENVIRONMENTAL SCIENCES DEPARTMENT
PUBLICATION NUMBER 4685
MARCH 1999

API's Decision Support System for Exposure and Risk Assessment (DSS)

Version 2.0

Health and Environmental Sciences Department

API PUBLICATION NUMBER 4685

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MARCH 1999

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STEP
Strategies for Today's Environmental Partnership

American Petroleum Institute Environmental, Health, and Safety Mission and Guiding Principles

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The members of the American Petroleum Institute are dedicated to continuous efforts to improve the compatibility of our operations with the environment while economically developing energy resources and supplying high quality products and services to consumers. We recognize our responsibility to work with the public, the government, and others to develop and to use natural resources in an environmentally sound manner while protecting the health and safety of our employees and the public. To meet these responsibilities, API members pledge to manage our businesses according to the following principles using sound science to prioritize risks and to implement cost-effective management practices:

PRINCIPLES

- To recognize and to respond to community concerns about our raw materials, products and operations.
- To operate our plants and facilities, and to handle our raw materials and products in a manner that protects the environment, and the safety and health of our employees and the public.
- To make safety, health and environmental considerations a priority in our planning, and our development of new products and processes.
- To advise promptly, appropriate officials, employees, customers and the public of information on significant industry-related safety, health and environmental hazards, and to recommend protective measures.
- To counsel customers, transporters and others in the safe use, transportation and disposal of our raw materials, products and waste materials.
- To economically develop and produce natural resources and to conserve those resources by using energy efficiently.
- To extend knowledge by conducting or supporting research on the safety, health and environmental effects of our raw materials, products, processes and waste materials.
- To commit to reduce overall emission and waste generation.
- To work with others to resolve problems created by handling and disposal of hazardous substances from our operations.
- To participate with government and others in creating responsible laws, regulations and standards to safeguard the community, workplace and environment.
- To promote these principles and practices by sharing experiences and offering assistance to others who produce, handle, use, transport or dispose of similar raw materials, petroleum products and wastes.

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ACKNOWLEDGMENTS

THE FOLLOWING PEOPLE ARE RECOGNIZED FOR THEIR CONTRIBUTIONS OF TIME AND EXPERTISE DURING THIS STUDY AND IN THE PREPARATION OF THIS REPORT:

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Development of version 1.0 of API's Exposure and Risk Assessment Decision Support System (API DSS) was a joint effort between DuPont Environmental Remediation Services (DERS), Woodward-Clyde Consultants (WCC) and BBT Design and Optimization (BBT). The overall project manager was Lynn Spence.

Key Woodward-Clyde individuals included Atul Salhotra, Viru Raparthi, Jeff Rousch, Phil Mineart, Marco Lobascio and Rob Schanz.

Bill and Bev Thompson, of BBT (Nassau, New York), assisted with the development of the graphical user interface.

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API DSS
QUICK START SHEET

Before calling Technical Support, please review the following document to see if your question is addressed.

Hardware and Software Requirements

The API DSS requires the following configuration:

- An Intel® 486 (with math coprocessor) or any 100%-compatible machine
- Windows® 3.1®, NT, 95®, or 98®
- At least 8 megabytes of RAM
- At least 8 megabytes of free space on the hard-disk drive
- Microsoft EXCEL® version 5.0 for Windows®

Installation Procedure

The following steps will install the DSS on your computer; a new Windows® program group as well as a "API DSS 2.0" icon will be installed into your Windows® desktop. An uninstall option is available under the API DSS program group. The uninstall option will delete the DSS files and directory along with the API DSS icon and group.

For Windows® 3.1:

Step 1 Insert Distribution Disk #1 in drive A or B.
Step 2 Select "File" from the Program Manager menu and "Run" from the pull-down menu. Enter the following command in the dialog box:

```
a:\install.exe
```

Select OK on the Run dialog box.
Step 3 Follow the instructions in the installation package.

For Windows® 95, 98, and Windows® NT:

Step 1 Insert Distribution Disk #1 in drive A or B.
Step 2 Select the "Start" button and then "Run..." from the pop-up menu. Enter the following command in the "Open" dialog box:

```
a:\install.exe
```

Select OK.
Step 3 Follow the instructions in the installation package.

Previous page is blank.

Running the DSS

<u>Starting DSS under Windows® 3.1:</u>

Double-click on the "API DSS 2.0" icon in the API DSS group.

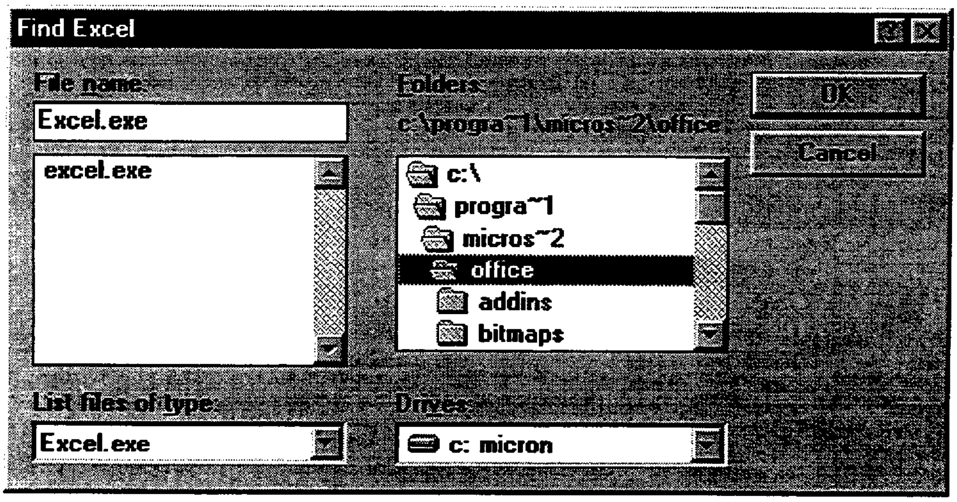
<u>Starting DSS under Windows® 95, 98, and Windows® NT:</u>

Double-click on the "API DSS 2.0" icon from the Windows desktop or select "Programs", "API DSS", and "API DSS 2.0" from the Start menu.

Starting the DSS is the only time you need to double-click. Double-clicks are not required from within the DSS software and will be misinterpreted. **All clicking within the DSS must be single clicks.**

<u>Locating EXCEL for the DSS</u>

When the DSS is opened for the first time, the user will be asked to "browse" (using a file menu) to the location where EXCEL® is loaded on their system. Using the file menu shown, the user should change the directory until the file "EXCEL.exe" is shown in the "File name:" box.



Find Excel

File name: Excel.exe

excel.exe

Folders: c:\progra~1\micros~2\office

c:\
progra~1
micros~2
office
addins
bitmaps

List files of type: Excel.exe

Drives: c: micron

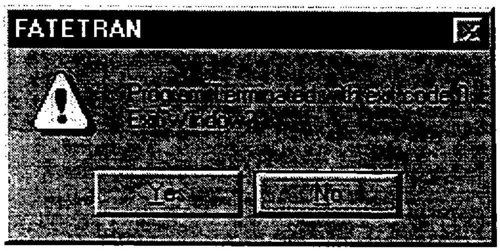
Remember, EXCEL® may be located on a network drive. Once the location of EXCEL® has been identified this window will not appear again. If you are unable to locate EXCEL® for the time being, select "Cancel"; you can still use the DSS however you will be unable to bring up the FORTRAN results in EXCEL® automatically. When the DSS is opened the next time it will ask again for the location of EXCEL® (it will do this until the location has been established).

NOTE: If you are unable to locate EXCEL® but can still open EXCEL® from your Windows® desktop, you may run the EXCEL® macros externally from the DSS to view the FORTRAN results.

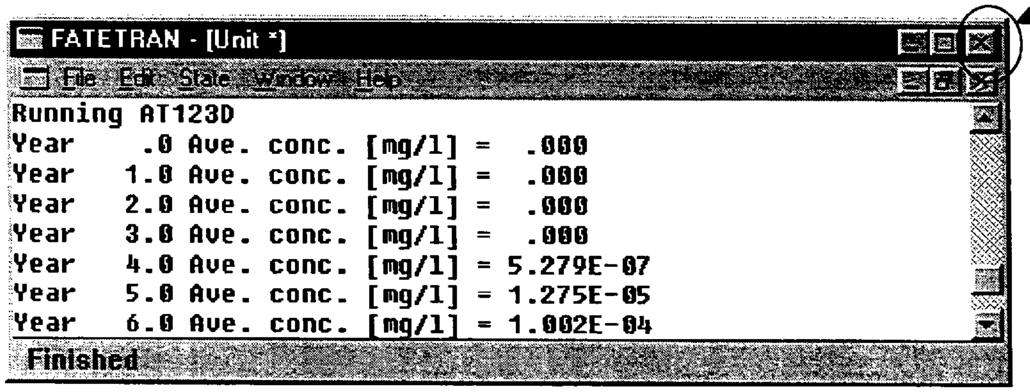
- If you have just run the fate and transport models, open EXCEL® (from your Windows® desktop not the DSS) and open the file called "APIDSSTP.xls".
- If you have just run the chemical intake model, open open EXCEL® (from your Windows® desktop not the DSS) and open the file called "APIDSSRK.xls".

Running the FORTRAN codes:

Upon successful execution of any of the DSS's FORTRAN models, Windows will display the message, 'Program Terminated with exit code 0. Exit Window?'



You will be prompted to click on 'Yes' or 'No'. **This is not an error message!** If you click on 'Yes' the FORTRAN runtime window will be closed and you will be returned to the DSS. If you select 'No' you can browse back up through the FORTRAN output (AT123D displays groundwater concentration with time); when you are through, close the FORTRAN runtime window (by selecting "File", "Exit", or double-click on the window control box) and you will be back in the DSS.



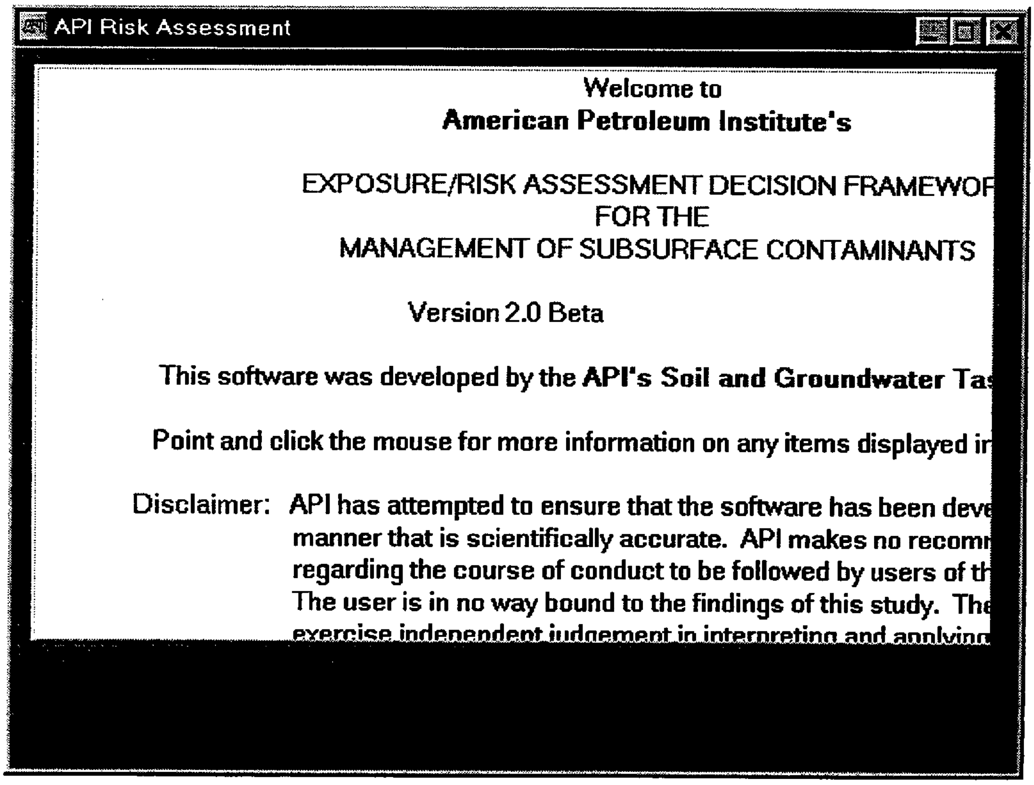
```
Running AT123D
Year     .0 Ave. conc. [mg/l] =  .000
Year    1.0 Ave. conc. [mg/l] =  .000
Year    2.0 Ave. conc. [mg/l] =  .000
Year    3.0 Ave. conc. [mg/l] =  .000
Year    4.0 Ave. conc. [mg/l] = 5.279E-07
Year    5.0 Ave. conc. [mg/l] = 1.275E-05
Year    6.0 Ave. conc. [mg/l] = 1.002E-04
```

Window control box—for closing window

Saved Files from DSS Version 1.x

Saved files from previous DSS versions are not compatible with version 2.0. Too many additional features were added (especially in the SESOIL inputs) to keep the compatibility option. The easiest way to get the old data into the new version is to print out the "Data Requirements" summary from the previous version and then retype in the data.

If the Initial Screen Looks Like This:



Welcome to
American Petroleum Institute's

EXPOSURE/RISK ASSESSMENT DECISION FRAMEWO
FOR THE
MANAGEMENT OF SUBSURFACE CONTAMINANTS

Version 2.0 Beta

This software was developed by the **API's Soil and Groundwater Ta**

Point and click the mouse for more information on any items displayed i

Disclaimer: API has attempted to ensure that the software has been dev
manner that is scientifically accurate. API makes no recom
regarding the course of conduct to be followed by users of t
The user is in no way bound to the findings of this study. Th
exercise independent judgement in interpreting and applying

You need to set the "Font" option in your Windows' display panel to "Small Fonts". The API DSS must be run with the small fonts option. To do this, select "Settings" from the Windows Start Menu and then select "Control Panel". Then select "Display". Under the "Settings" tab make sure that "Small fonts" are selected under the "Font Size" option (not "Large Fonts"). Click on the OK button.

EXECUTIVE SUMMARY

The American Petroleum Institute's (API) Exposure and Risk Assessment Decision Support System (DSS) has been developed to assist environmental professionals in estimating human exposure and risk from contaminated sites. The DSS is a valuable, user-friendly tool that can be used to (i) estimate site-specific risks, (ii) identify the need for site remediation, (iii) develop and negotiate site-specific cleanup levels with regulatory agencies, and (iv) efficiently and effectively evaluate the effect of parameter uncertainty and variability on estimated risk.

The API DSS Version 2.0 consists of four modules. The Development of Risk Scenario module allows the user to develop a conceptual model for estimating the risk. The Receptor Point Concentration module allows explicit entry of receptor point concentrations or estimates the concentrations by contaminant fate and transport modeling. The fate and transport models included in the DSS are: SESOIL, VADSAT, and Jury unsaturated zone models; AT123D and VADSAT saturated zone models; and Farmer's, Jury's, VADSAT and Thibodeaux's air emission models linked with a box or Gaussian dispersion model. The Chemical Intake and Risk Calculation module uses estimated or user-entered receptor point concentrations to estimate chemical intake by a human receptor for several different exposure routes. Further, this module uses the estimated dose and chemical-specific toxicity (slope factor or potency value for carcinogens and the reference dose for non-carcinogens) to estimate carcinogenic risk and noncarcinogenic hazard index. Finally, the Risk Presentation module allows the user to view the results of the analysis in tabular and graphical formats. The DSS includes databases accessed by the various modules and contains chemical-specific fate and transport properties, toxicity properties and default uptake parameters for 86 chemicals. Report-ready tables and graphs depicting the exposure and risk results can be printed.

The Chemical Intake and Risk Calculation module of the DSS can be implemented in either deterministic or Monte Carlo simulation modes. The latter is used to quantify the uncertainty in the exposure and risk results due to uncertainty in the input parameters.

The DSS runs under the Microsoft Windows® 95, 98, 3.1, or NT environments. It is user friendly and includes online help. The software accesses FORTRAN codes to perform computations and relies on EXCEL® spreadsheet software (version 5.0 or higher) to present results in report-ready tabular and graphical formats.

System Limitations

DSS limitations include:

- The maximum number of chemicals for a DSS session is limited to twenty.
- The DSS can only consider one receptor at a time. This limitation was imposed to simplify system output and its interpretation. If a user wants to analyze the risk posed to two different receptors, he or she may run the DSS twice. Default parameter values from the first analysis can be saved and then retrieved for the second analysis.
- The DSS includes six routes of exposure as discussed in Section 6.0. Other exposure routes such as the ingestion of produce grown in contaminated soil or the inhalation of indoor air in confined spaces (such as basements), are not addressed. Depending on the site-specific conditions, these routes of exposure may be significant.

Other assumptions and limitations include:

- The EPA Uptake Biokinetic model for lead is not included in the software. If lead is added to the DSS database, it will be treated in the same manner as other chemicals requiring a slope factor or reference dose.
- Risks are additive; chronic effects are additive.
- Risks are carcinogenic only. Teratogenicity, mutagenicity, etc., are not considered.
- Chronic toxicities are not specified by toxic effect or affected organ.
- Fate and transport models may assume steady-state and compositional equilibrium between phases at all times.

- Risk is to a maximally exposed individual. Population risks are not addressed.
- Subchronic risks are not addressed by the DSS. The database does not contain toxicity values for subchronic exposures (less than two years).
- Risks/chronic effects to children can be calculated by assuming that a child is a "small adult." It is assumed that potency factors, RfDs, apply to children as well as adults.

Differences Between Version 2.0 and 1.0

The following additions and/or changes to the software have been made in version 2.0:

- The VADSAT model was added.
- The new SESOIL code (1996) was incorporated and the interface was updated to allow the user full access to all of the SESOIL options (except the erosion module).
- Monte Carlo capabilities were removed for the fate and transport models.
- The new AT123D version developed by H.S.I. GeoTrans (for the EPA) was incorporated. (This version of AT123D corrected a problem with the pulse source option in the original AT123D code.)
- The AT123D coordinate system was changed to make it more intuitive to use.
- The user may now enter time step size for AT123D. Using smaller time steps will help reduce the number of cases where oscillations in the solution occurred.
- A new capability was added to import concentration-time series data generated by models external to the DSS.
- A user interface was added to allow users to append or modify the toxicological and physical/chemical property databases directly from the DSS.

1.0

OVERVIEW OF THE DECISION SUPPORT SYSTEM

1.1 INTRODUCTION

This section presents an overview of the American Petroleum Institute's (API) Exposure and Risk Assessment Decision Support System (DSS) Version 2.0. The DSS is a valuable user-friendly tool that can estimate risks at sites contaminated by petroleum hydrocarbons and other contaminants. While the DSS is a convenient tool for preparing a relatively complex level of risk assessment, it should be run by personnel knowledgeable in risk assessments.

The exposure/risk assessment process is a multidisciplinary process requiring expertise in data collection and site characterization, contaminant fate and transport modeling, toxicology, environmental chemistry, and data analysis. Both federal and state guidance encourage the use of site-specific risk assessments as well as the evaluation of uncertainty in estimated risk (e.g., EPA Risk Assessment Guidance for Superfund and the Texas Risk Reduction Rules). It is important to develop a computerized framework to provide a consistent and cost-effective approach for determining risk and cleanup levels at sites with subsurface contamination. The development of the DSS is a first step in ensuring a consistent approach.

1.2 DESCRIPTION OF THE RISK ASSESSMENT PROCESS

As described by the National Academy of Sciences (1983), the risk assessment process consists of four steps: (1) hazard identification, (2) exposure assessment, (3) dose-response assessment, and (4) risk characterization. These steps are illustrated in Figure 1-1 and briefly described below. Details are available in EPA (1989a).

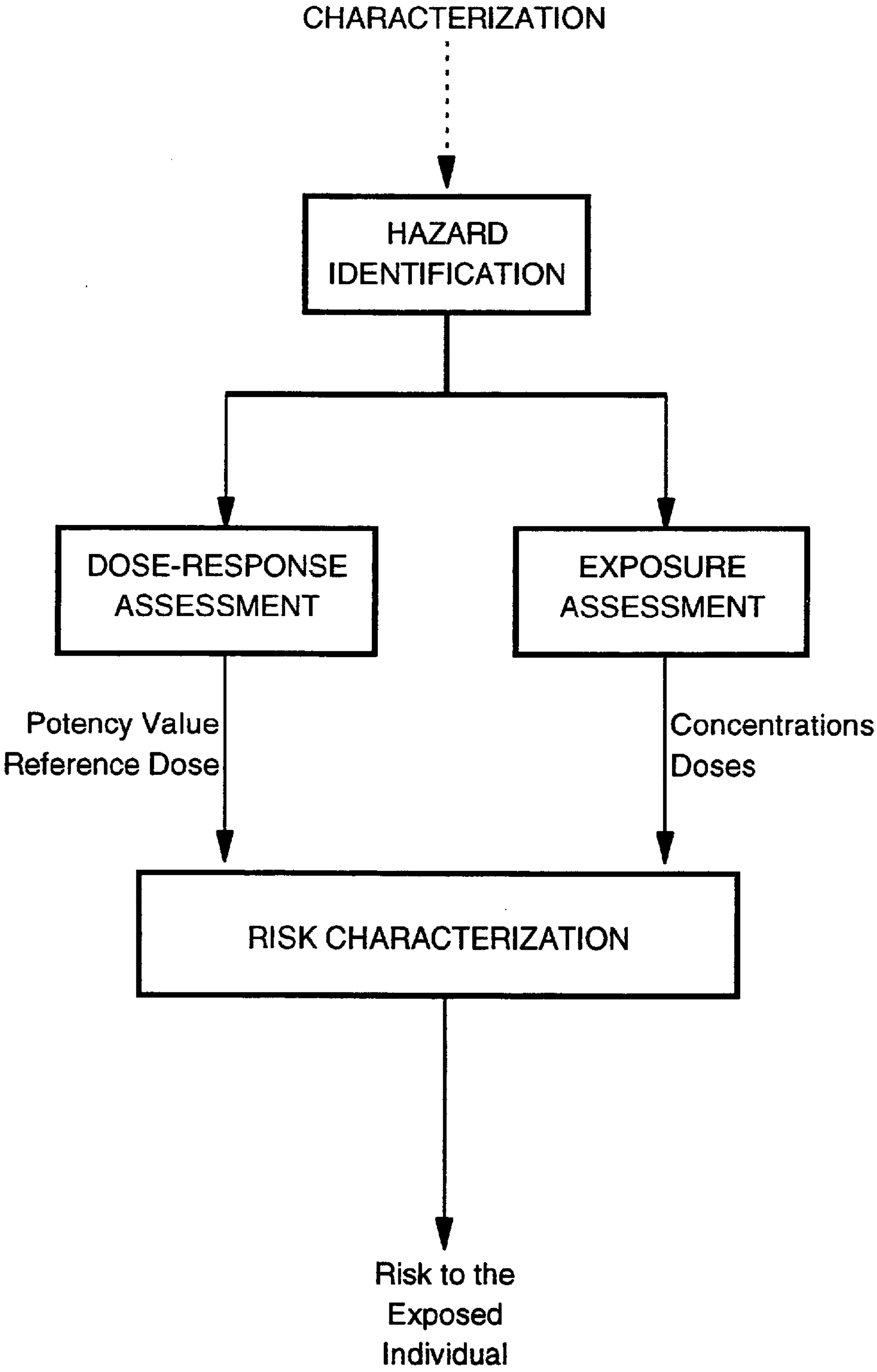


Figure 1-1. Schematic of the Risk Assessment Process.

In the hazard identification step, the chemicals of concern and the hazard (carcinogenic or other adverse health effects) associated with exposure to these chemicals are determined. This step necessitates collection of site-specific information to characterize the site in terms of source-, media-, chemical-, and receptor-specific characteristics. Potential receptors of concern and exposure routes are also identified in this step.

The objective of the exposure assessment step is to estimate intake by the receptor(s) identified in the previous step. This is a two-step process. First, the concentrations in the contact media (soil, air, groundwater), termed "receptor point concentrations" are estimated, and then the intake (or dose) is calculated for the receptor. Receptor point concentrations are actual or projected concentrations in site media to which a receptor (human) may potentially be exposed for particular pathways. For example, a receptor point concentration for groundwater could be the contaminant concentration projected to occur at a hypothetical or actual well location some distance from a source. Estimation of the receptor point concentrations is a key component of the exposure assessment step. This estimation often involves the use of contaminant fate and transport models and historical site data to simulate the movement of the chemicals of concern from the source to the receptor point. Contaminant fate and transport modeling should be calibrated with site-specific data. Once receptor point concentrations have been estimated, contaminant intake by the receptors is estimated.

Toxic effects of the chemical are identified and quantified in the dose- response assessment step. For carcinogenic chemicals, toxicity is quantified by estimating the chemical-specific potency value (also called slope factor). For non-carcinogenic chemicals, toxicity is quantified as the chronic reference dose, an estimate of the threshold daily level of exposure to the human population, including sensitive subpopulations, that may cause a deleterious health effect.

Finally, the risk characterization step combines the results of exposure and dose-response assessments to evaluate site-specific risk to the exposed populations. Each of these steps is described in detail in the subsequent sections of this manual.

The risk assessment process described above is very general in its application. Most state and federal regulations and associated guidance documents require risk assessments be conducted according to this process. However, there are many differences in the actual details of any given risk assessment. For example, risk may be based on arithmetic or geometric mean concentrations in the contact media. Similarly, there are a number of ways in which chemical concentrations reported as below the analytical detection limit may be treated. Additional variations exist in the estimation of the frequency and magnitude of contact media uptake. Details of these variations are not discussed in this manual. The manual and software generally follow the guidance presented in EPA (1989a).

1.3 OVERVIEW OF THE DECISION SUPPORT SYSTEM

This DSS consists of four modules coupled together into an integrated, user-friendly exposure/risk assessment framework. These modules are Development of Risk Scenario, Receptor Point Concentrations, Chemical Intake and Risk Calculation, and Risk Presentation.

The Development of Risk Scenario module allows the user to develop a conceptual model of the site for the purposes of risk assessment. In this conceptual model, the user identifies chemicals of concern, relevant uptake routes, and the specific models to estimate receptor point concentrations. Prior to running this module, an adequate site assessment should have been conducted, which helps ensure that the location is sufficiently well understood so that appropriate data are used in the DSS. This step corresponds to the last part of a “Hazard Identification” step shown in Figure 1-1.

The Receptor Point Concentrations module includes models to simulate contaminant fate and transport from source to receptor, thereby estimating receptor point concentrations. These models include atmospheric emission and dispersion models, and unsaturated and saturated zone contaminant transport models. It is important that the models used be calibrated with field data to help prevent inaccurate estimates. Alternatively, the user may enter directly into this module site-specific measured receptor point concentrations or those estimated by models external to the DSS. The Receptor Point Concentrations module corresponds to the first part of the "Exposure Assessment" step shown in Figure 1-1.

The Chemical Intake and Risk Calculation module uses the computed or user-entered receptor point concentrations or user-entered concentrations to estimate chemical intake by the human receptor for several different exposure routes. These routes include ingestion of contaminated water and soil, inhalation of air containing volatile contaminants, and dermal contact with contaminated soil and water. This module also estimates the carcinogenic risk and non-carcinogenic effect (hazard index) due to these exposures. The Chemical Intake and Risk Calculation module corresponds to the second part of the "Exposure Assessment" step shown in Figure 1-1. Usually, toxicity parameters are obtained from EPA databases or other sources of published values. These toxicity parameters are specified in this module. Obtaining (or deriving) the toxicity parameters for the chemicals of concern corresponds to the "Dose-Response Assessment" step shown in Figure 1-1.

Finally, the Risk Presentation module uses EXCEL® to present the estimated chemical intake, carcinogenic risk, and hazard index. Several graphical and tabular options for presentation of results are available to the user. The results shown in the Risk Presentation module correspond to the "Risk Characterization" step shown in Figure 1-1.

An important aspect of this DSS is not only its ability to estimate the risk but also to evaluate the uncertainty in the risk estimates due to uncertainty in, and variability of, the input parameters. This uncertainty is quantified by using the Monte Carlo simulation technique. Monte Carlo simulation generates a probability distribution of the risk. From this distribution, the range as well as the most likely value (i.e., the 50th percentile) and the upper bound (i.e., the 95th percentile) can be estimated.

1.4 REPORT ORGANIZATION

This report includes the technical details and other information necessary to understand API DSS Version 2.0. Section 2.0 describes the overall structure of the decision framework and the hardware and software requirements of the system.

Section 3.0 includes instructions for using the DSS. Section 4.0 describes the details of the Development of Risk Scenario module and the development of a conceptual model of the site for the purposes of the risk assessment. Section 5.0 presents instructions on how to use the Receptor Point Concentration module. (The appendices of this manual contain detailed descriptions of the fate and transport models.) Section 6.0 describes the Chemical Intake and Risk Calculation module and includes the mathematical relationships used to estimate the intake, risk, and hazard index for each exposure route. Section 7.0 describes the Risk Presentation module and the available output formats. Sections 8.0 and 9.0 describe the DSS Monte Carlo uncertainty analysis procedures and the contents of the DSS databases, respectively.

This report also includes several appendices that provide the details of each fate and transport model included in the DSS, limited guidance for estimating values of selected input parameters, the probability distributions that can be used to describe the uncertainty and variability in the input variables, and the cumulative probability distributions based on data presented in the Exposure Factors Handbook (USEPA, 1989b).

2.0
STRUCTURE OF THE DECISION SUPPORT SYSTEM

In the following sections the various components of the DSS, as well as overall system requirements, software architecture, and flow of information will be described.

2.1 SYSTEM REQUIREMENTS

The DSS is a Windows®-based software and will run under Windows® 3.1 or Windows® 95 and 98 with the following minimum hardware and software requirements.

2.1.1 Minimum Hardware Requirements

The API DSS requires the following configuration:

- An Intel® 486 or any 100%-compatible machine running at 25MHz or faster
- At least 8 megabytes of RAM
- Math coprocessor
- At least 8 megabytes of free space on the hard-disk drive

2.1.2 Software Requirements

The API DSS requires the following software:

- Microsoft Windows® 3.1, 95, 98, or NT
- Microsoft EXCEL® 5.0 (or higher version) for Windows®

2.2 DSS ORGANIZATION

The DSS consists of four modules as shown in Figure 2-1. These are the (i) Development of Risk Scenario, (ii) Receptor Point Concentrations, (iii) Chemical

Intake and Risk Calculation, and (iv) Risk Presentation modules. Each of these modules accesses databases and runs different computational codes as needed. The options available in, and data generated by, each module are shown in Figure 2-1. The structures of the databases are described in Sections 6 and 9. FORTRAN computational codes are run in both the Receptor Point Concentrations and the Chemical Intake and Risk Calculation modules as discussed in Section 2.3. DSS results are presented using EXCEL® macros. These macros are discussed in Section 2.4.

2.3 FORTRAN CODES

FORTRAN codes are used in the DSS for estimating receptor point concentrations and for calculating dose and risk. Fate and transport codes used to estimate receptor point concentrations are run in a deterministic mode. The risk calculation code may be run either deterministically or in a Monte Carlo mode. The risk calculation code is linked to a Monte Carlo software code so that uncertainty analyses can be performed easily. Details of the Monte Carlo code are discussed in Section 8.0.

The DSS collects all the information necessary to run each FORTRAN code, generates an input file on the hard drive, then runs the code. A new window appears and the FORTRAN code runs in this window, so the user can track the progress of the simulation. Successful completion of the FORTRAN run results in a message on the screen "Error Code = 0", see Figure 2-2. The user is also prompted to close the window and return to the DSS (select "Yes"). If the user wants to scroll through the screen output generated by the code, he or she can leave the window open (select "No") and look at the output. Before returning to the DSS, the user must close the FORTRAN window (select "File" from the menu bar, then "Exit", see also Section 3.3.6).

1. DEVELOPMENT OF RISK SCENARIO MODULE

Purpose: To **define** the risk scenario being evaluated.

User Identifies:

Chemicals of concern
Exposure routes
Method(s) of estimating Receptor Point Concentrations

Module Output:

Once the above information is specified a summary of data required to perform analysis based on selected options can be generated from the main screen.

2. RECEPTOR POINT CONCENTRATIONS MODULE

Purpose: To ***enter*** or ***estimate*** receptor point concentrations.

User Input: Receptor point concentrations and/or data for the fate and transport models.

The following transport models are available to estimate receptor point concentrations in the contact media:

Contact Media	Model		
Groundwater:	SESOIL linked with AT123D		
	VADSAT		
	Jury linked with AT123D		
	AT123D		
Air:	Emissions	Dispersion	Particulate
	Jury	Box	Cowherd
	Thibodeaux-Hwang	Gaussian	
	Farmers		
	VADSAT		

Module Output:

EXCEL® tables and charts.
FORTRAN output files summarizing all inputs and results.

Figure 2-1. Overview of the DSS.

3. CHEMICAL INTAKE AND RISK CALCULATION MODULE

Purpose: To **calculate** chemical dose and risk.

User inputs:

Exposure data
Toxicity data

Output:

EXCEL® charts and tables containing the risk assessment results.
FORTRAN output file (INTAKE.OUT) summarizing all inputs and results.

4. RISK PRESENTATION MODULE

(can also be accessed from the Chemical Intake and Risk Calculation module)

Purpose: To **present** results from the risk assessment.

No user input.

This module uses the EXCEL® spreadsheet to present report ready tables and charts of dose, risk and hazard index.

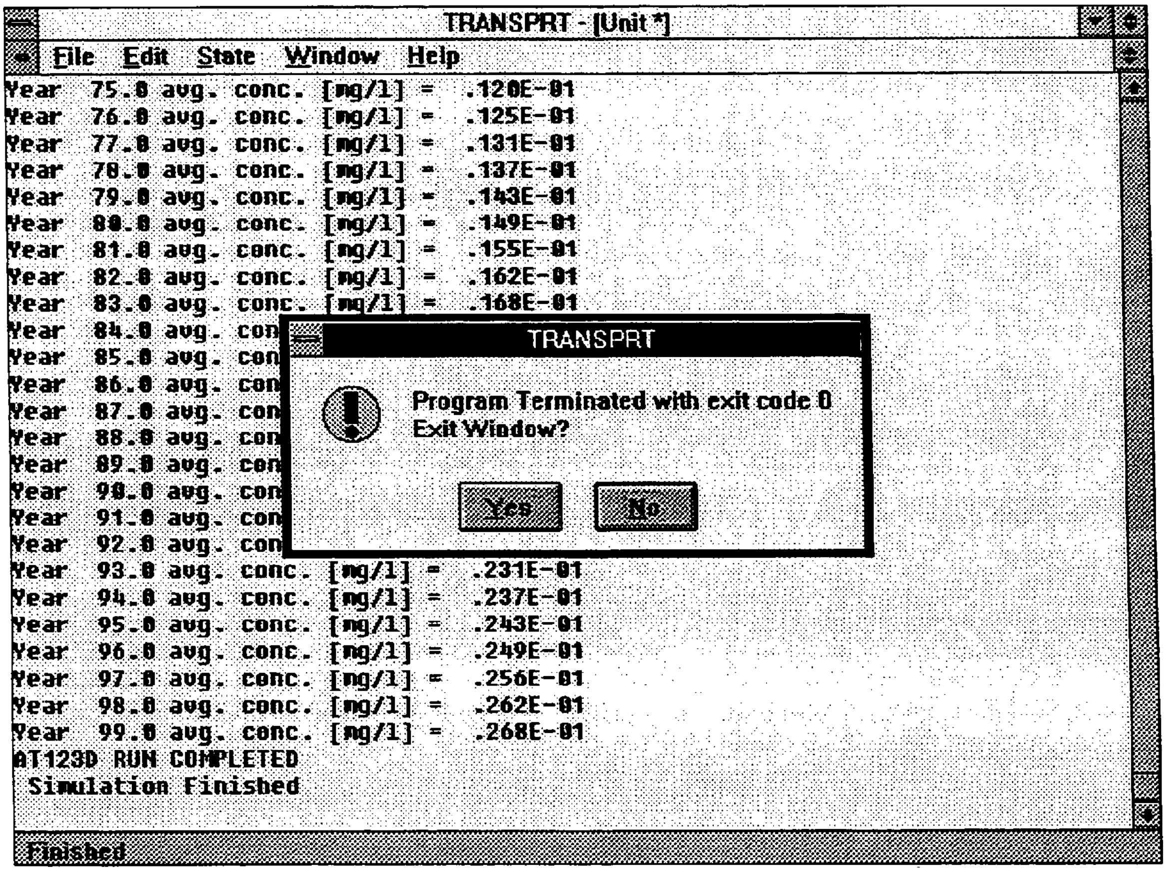
Module Output:

User can print or save the charts and tables and load them into other word processing programs.

Figure 2-1. Overview of the DSS (concluded).

2.4 EXCEL® MACROS FOR PRESENTATION OF RESULTS

The EXCEL® spreadsheet is used by the DSS to present results of the analysis. EXCEL® macros are used to provide the specialized functions for the DSS. These macros bring up a new menu item within EXCEL® allowing the user to select various tables and charts of results for both receptor point concentrations (accessed in the Fate and Transport module) and risk and hazard indices (the Risk Presentation module).



```
Year  75.0 avg. conc. [mg/l] =  .120E-01
Year  76.0 avg. conc. [mg/l] =  .125E-01
Year  77.0 avg. conc. [mg/l] =  .131E-01
Year  78.0 avg. conc. [mg/l] =  .137E-01
Year  79.0 avg. conc. [mg/l] =  .143E-01
Year  80.0 avg. conc. [mg/l] =  .149E-01
Year  81.0 avg. conc. [mg/l] =  .155E-01
Year  82.0 avg. conc. [mg/l] =  .162E-01
Year  83.0 avg. conc. [mg/l] =  .168E-01
Year  84.0 avg. con
Year  85.0 avg. con
Year  86.0 avg. con
Year  87.0 avg. con
Year  88.0 avg. con
Year  89.0 avg. con
Year  90.0 avg. con
Year  91.0 avg. con
Year  92.0 avg. con
Year  93.0 avg. conc. [mg/l] =  .231E-01
Year  94.0 avg. conc. [mg/l] =  .237E-01
Year  95.0 avg. conc. [mg/l] =  .243E-01
Year  96.0 avg. conc. [mg/l] =  .249E-01
Year  97.0 avg. conc. [mg/l] =  .256E-01
Year  98.0 avg. conc. [mg/l] =  .262E-01
Year  99.0 avg. conc. [mg/l] =  .268E-01
AT123D RUN COMPLETED
 Simulation Finished
```

```
Program Terminated with exit code 0
Exit Window?
```

Figure 2-2. FORTRAN Code Completion.

The EXCEL® spreadsheet is accessed directly by the DSS; the user does not have to exit the DSS to run EXCEL®. After a FORTRAN run has been completed successfully, the EXCEL® button on the DSS screen becomes available. When selected with the mouse, the EXCEL® spreadsheet comes up automatically.

Once in EXCEL® there is a new menu option called "DSS" on the menu bar at the top of the EXCEL® window. When chosen, the "DSS" menu option brings up more menus from which the user can choose specific tables and graphs.

The EXCEL® macros create plots and tables of model output as shown in Section 7.0; however, users are free to modify the plots (using the standard EXCEL® commands) if they prefer a different font or type of plot. Also, the user can modify the format of the tables if desired (again, using standard EXCEL® commands). The tables and charts can be printed directly from EXCEL® just as from any other EXCEL® spreadsheet.

3.0
INSTRUCTIONS FOR USING THE DECISION SUPPORT SYSTEM

The DSS is designed to be user friendly with online help. This section will describe the installation procedures, as well as describe some of the system limitations.

3.1 INSTALLATION PROCEDURE

For Windows® 3.1:

Step 1 Insert Distribution Disk #1 in drive A or B.

Step 2 Select "File" from the Program Manager menu and "Run" from the pull-down menu. Enter the following command in the dialog box:

```
a:\install.exe
```

Select OK on the Run dialog box.

Step 3 Follow the instructions in the installation package.

For Windows® 95, 98, and Windows® NT:

Step 1 Insert Distribution Disk #1 in drive A or B.

Step 2 Select the "Start" button and then "Run..." from the pop-up menu. Enter the following command in the "Open" dialog box:

```
a:\install.exe
```

Select OK.

Step 3 Follow the instructions in the installation package.

3.2 STARTING A SESSION

To start the DSS, double-click on the API DSS icon in your Windows® desktop. The main menu of the DSS is shown in Figure 3-1. This screen has five buttons in the center. The top four correspond to the four modules of the API DSS. Only the first button is enabled, indicating that this step must be performed first. When the first step has been performed the other buttons will become available as appropriate.

At the bottom of the screen are four buttons: Quit, Load a Session, Help, and Save a Session. The Help button, when chosen with the mouse, brings up the help system for the DSS. The help system provides help for the current screen; the user is free to view the help index and display help for any listed topic. When Quit is chosen, the user will be prompted to save the session before exiting. When the "Load a Session" button is chosen, the user will be prompted to load a previously saved file. The "Save a Session" button allows the user to save data entered in the current session without having to leave the DSS.

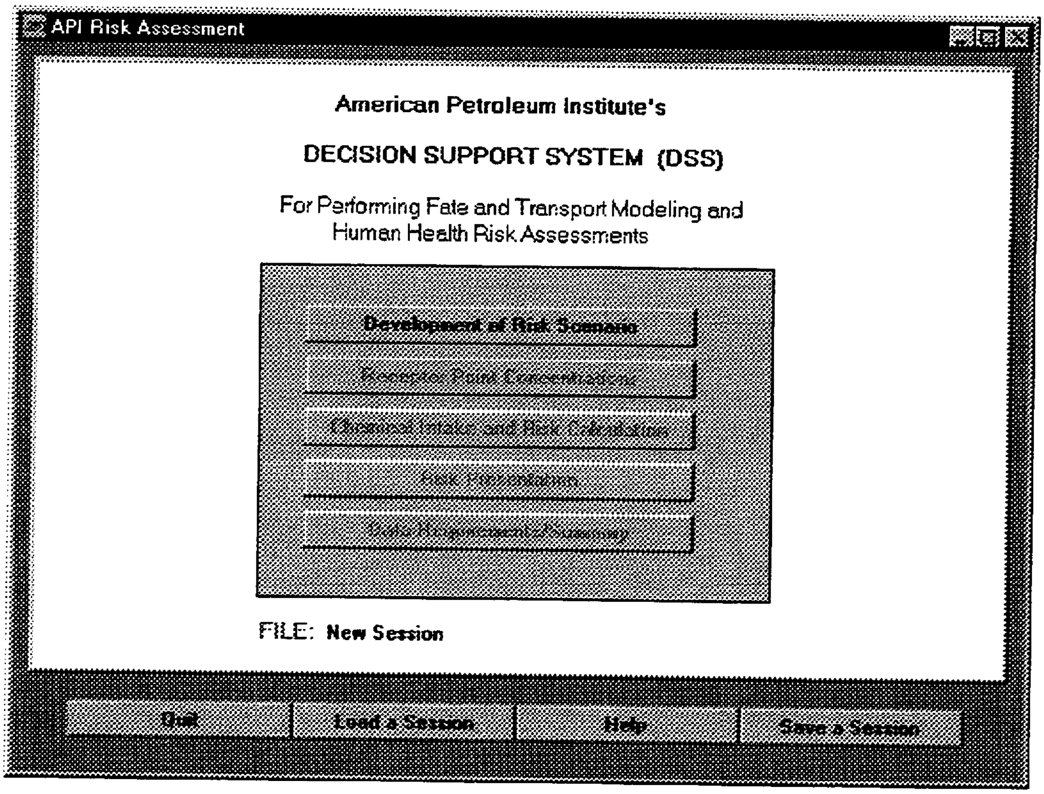


Figure 3-1. The Main Menu.

3.3 HOW TO USE API DSS

This section describes the screen formats observed when using the DSS and the types of information available from the different modules. It is recommended that the user run the DSS while reading this section.

3.3.1 Choose Options With a Single-Click

The only time the user should double-click the mouse is to start the DSS from the Windows® desktop or to close a window. Once in the DSS, the user chooses options such as buttons or hypertext by single-clicking with the mouse button.

3.3.2 Hypertext

Hypertext is special text (highlighted in green) which can be selected as a topic by clicking with the mouse. Selecting hypertext usually displays additional information on the word or phrase that was highlighted. Hypertext in the DSS is highlighted in green. The mouse cursor changes to a hand when it is over Hypertext.

3.3.3 Screen Layout in the DSS

The basic format of the DSS screens consists of a maximized window with a title bar and a control menu (the box at the left side of the title bar, refer to Figure 3-1). The title bar shows the application name "API Risk Assessment." The control menu allows the window to be minimized or moved. The control menu allows the user to switch to other Windows® programs if desired. Another way to minimize the window is to click on the down arrow on the right side of the title bar.

3.3.4 Buttons, Drop-Down Lists, and Edit Boxes

Within the modules, the user should click on the button corresponding to the desired step. After entering all the appropriate information for that step, the user is returned to the module window and the box next to the selected button will be checked.

Occasionally, some of the buttons will be disabled (shaded) indicating that other information is needed before that step can be performed. For example, in the AT123D initial input screen the aquifer data cannot be entered until the AT123D model control parameters are chosen. Once these control parameters have been entered the aquifer data buttons will become available.

Edit boxes are used wherever the user may want to change the default values (e.g., model parameters, title boxes). These boxes may be edited by clicking on the edit box with the mouse and typing a new value.

A drop-down list (i.e., a box with a down arrow on the right) is used to select a value from a list of options. When the down arrow is selected, a list will appear and the user can select any item on the list. When an item from the list is selected, the drop-down list will close and the new default will appear in the box. This type of drop-down list is used to choose among the various distribution types in the Monte Carlo mode.

3.3.5 HELP System

The DSS has on-line help that is available from every screen. This feature can be activated by choosing the HELP button (located at the bottom of the screen) with the mouse. This displays the Help Window that has (i) topic specific information and (ii) a menu bar at the top with six buttons (Contents, Search, Back, Copy, Print and Quit) that perform the following functions:

Contents:	Displays the list of contents (modules and databases) of the DSS.
Search:	Displays a list of all the HELP topics (in alphabetical order) included in the DSS. The user may choose any topic to view information on that topic.
Back:	Displays the previous topic.
Copy:	Copies the contents of the HELP window into the Windows® Clipboard. The text can then be transferred to a word processing file.

Print:	Sends the HELP text directly to the printer
Quit:	Closes the window and returns the user to the DSS.

Note, some of the text displayed in the HELP window is highlighted in green. This is HYPERTEXT and can be selected by the user (by clicking) to view additional information on the topic.

3.3.6 Running FORTRAN Codes

The computational elements of the DSS are written in FORTRAN and include (i) the models in the Receptor Point Concentrations Module and, (ii) the algorithms to compute dose, carcinogenic risk and the hazard index in the Chemical Intake and Risk Calculation Module. The FORTRAN codes are executed by selecting the "Run" button. This button is not available until all the data required to run the FORTRAN codes have been entered. Quantitative data can be entered in either floating point, integer, or exponential form. The number of significant digits is left to the user's discretion. The interface performs limited range checking but users are cautioned to enter the appropriate value and not rely solely on the interface to check the appropriateness of a data value.

The DSS runs each FORTRAN code in a window that displays the code's output as it is generated. The sole objective of the screen output is to monitor the progress of the computations (e.g., the number of Monte Carlo runs completed). At the completion of the run a message is displayed on the screen which shows (i) an error code of either 1 or 0 and (ii) a query prompting the user to exit the FORTRAN window (Figure 2-2). An error code of 0 indicates successful completion of the FORTRAN code. An error code of 1 indicates an unsuccessful completion - probably due to an error in the data entered. **In either case (an error code of 0 or 1) the user must exit the FORTRAN window before proceeding further.**

An "MSLANGLOAD" (Microsoft Language Loader) error may occur if too many Windows® applications are open or the computer does not have enough memory (RAM). If an MSLANGLOAD error occurs, the user should make sure that all other Windows® applications are closed (e.g., EXCEL®, DOS Shell, File Manager).

After the run has been successfully completed and the FORTRAN window has been closed, the DSS allows the user to select one of two options: (i) "View Charts and Tables in EXCEL," or (ii) "View FORTRAN Results." EXCEL® outputs are discussed in Section 3.3.7 below. For SESOIL, AT123D, and Jury's model, these FORTRAN output files are similar to the output files a user would obtain by running these models outside the DSS. The FORTRAN output files may be printed from the interface.

3.3.7 Using EXCEL® with DSS

After running the FORTRAN code, the user can review the results in EXCEL® provided the directory containing EXCEL® has been added to the DOS path specified in the AUTOEXEC.BAT file (see Section 3.1). When running EXCEL® the user can view tables and charts showing the results of the analysis by choosing the "DSS" option that has been added to the standard EXCEL® menu bar. These charts and tables can be printed or saved by using the "print" or "save" option respectively under the "file" menu. The tables contain the name of the analysis entered by the user before running the FORTRAN codes.

To exit EXCEL®, use the "Return to DSS" option under the DSS menu item.

3.4 MONTE CARLO AND DETERMINISTIC MODES

The user can choose to run the risk calculation FORTRAN code in either a deterministic mode or a Monte Carlo mode. The default option is the deterministic mode, as indicated by the solid bullet in the first screen of the Chemical Intake and Risk Calculation module and each fate and transport model's main screen. To choose Monte Carlo mode, the user may click on the words "Monte Carlo." A new edit box will appear so the user can enter the number of Monte Carlo runs desired. The maximum number of runs is 10,000.

Under the Monte Carlo option, the format of the user input screens is altered. Whereas the deterministic input screens have only one edit box for each parameter, the Monte Carlo input screens allow the user to choose a distribution from a drop-down list and then enter the statistical parameters needed to describe the distribution for each parameter. Available statistical distributions are: constant, normal, log-normal, exponential, uniform, and triangular. The statistical parameters that describe the distribution are mean, mode (for triangular distributions), standard deviation, minimum, and maximum. Additional details are included in Section 8.0 and Appendix K.

3.5 PRINTING

There are several places in the DSS where the user can print information, assuming that Windows® has been configured to print. (If Windows® has not been configured to print, the user should follow the instructions in the Windows® manual and set up the appropriate printer.) The main screen of the API DSS has an option to print a summary of the data requirements for a given analysis. This summary is available from a button on the main module screen.

The tables and charts presented in EXCEL® can also be printed. These are designed to be report-ready; the user can easily print them directly from EXCEL®. Users experienced with EXCEL® may wish to reformat the tables and charts. Again, the charts can be saved as text files and brought into a word processing program.

The FORTRAN output files can also be printed. These output files ("*.out") are neither formatted nor report-ready; they are merely designed to provide summary statistics to the experienced user. After running any FORTRAN code, the user has the option to view a summary of the FORTRAN output. These files can be opened with a word processor (such as Microsoft Word®, or Write®) and reformatted.

3.5.1 Performing a Screen Dump to the Windows® Clipboard

The following steps describe how to perform a screen dump from the screen to the Windows® Clipboard.

Make sure the information you want to copy is on the screen. Press PRINT SCREEN. The contents of the screen are copied onto the Clipboard. If the above procedure does not copy the screen onto the Clipboard, you may not have an enhanced keyboard. Try pressing ALT+PRINT SCREEN or SHIFT+PRINT SCREEN to copy the screen.

Choose the Clipboard Viewer icon in the Windows Main group to view the contents of the Clipboard. Switch to the destination application, i.e., the application from which you want to print (such as MS Word®, EXCEL® or Paintbrush®). Place the insertion point where you want the information from the Clipboard to appear. From the application's Control menu, choose Edit. From the Edit menu, choose Paste. The screen can now be printed from the application.

3.6 QUITTING AND SAVING USER PREFERENCES

Whenever a user quits a session in the DSS the user is prompted to save choices and results. Similarly, the data can also be saved without exiting the DSS by choosing the "Save a Session" button on the main screen. The information is saved in a user-specified file as compiled code (not editable). When a new session is started, the user has the option to load any of the previously saved files. Information from this file will appear as defaults for the current analysis.

3.7 LOADING A SAVED FILE

After a session has been saved (Section 3.6) it can be reloaded at a later time. This is accomplished by choosing the "Load a Session" button from the main menu (Figure 3-1). Clicking on the "Load a Session" button brings up a file selection window showing the files with the extension *.sav. If the saved file has a different extension the user can find the file by entering "*.*" in the "File Name:" edit box. If the saved file is in another directory or drive the user can change directories by choosing the appropriate directory from the boxes in the window.

The saved file contains all the data entered in the session and the FORTRAN code results if a successful run was made. To transfer the saved file to another directory (or computer) just copy the saved file to the new directory (or computer).

3.8 SYSTEM LIMITATIONS

DSS limitations include:

- The maximum number of chemicals for a DSS session is limited to twenty.
- The DSS can only consider one receptor at a time. This limitation was imposed to simplify system output and its interpretation. If a user wants to analyze the risk posed to two different receptors, he or she may run the DSS twice. Default parameter values from the first analysis can be saved and then retrieved for the second analysis.
- The DSS includes six routes of exposure as discussed in Section 6.0. Other exposure routes such as the ingestion of produce grown in contaminated soil or the inhalation of indoor air in confined spaces (such as basements), are not addressed. Depending on the site-specific conditions, these routes of exposure may be significant.

Other assumptions and limitations include:

- The EPA Uptake Biokinetic model for lead is not included in the software. If lead is added to the DSS database, it will be treated in the same manner as other chemicals requiring a slope factor or reference dose.
- Risks are additive; chronic effects are additive.
- Risks are carcinogenic only. Teratogenicity, mutagenicity, etc., are not considered.
- Chronic toxicities are not specified by toxic effect or affected organ.
- Fate and transport models may assume steady-state and compositional equilibrium between phases at all times.

- Risk is to a maximally exposed individual. Population risks are not addressed.

- Subchronic risks are not addressed by the DSS. The database does not contain toxicity values for subchronic exposures (less than two years).

- Risks/chronic effects to children can be calculated by assuming that a child is a "small adult." It is assumed that potency factors, RfDs, apply to children as well as adults.

4.0
DEVELOPMENT OF RISK SCENARIO MODULE

4.1 OVERVIEW OF THE MODULE

An important first step in conducting a risk assessment is to develop a conceptual model of the site. Key elements of the conceptual model include identification of the contaminated media, the chemicals of concern, the types and locations of receptors, the relevant routes of exposure, and the manner in which the receptor point concentrations for each chemical are to be estimated. The Development of Risk Scenario module allows the user to define a conceptual model for the site-specific risk assessment by specifying three types of information. These are categorized as:

i) chemicals of concern,
ii) routes of concern, and
iii) method for estimating receptor point concentrations.

Figure 4-1 shows the "Development of Risk Scenario" input screen. The first button is where the chemicals of concern are chosen. The second button is where the routes of exposure and the method for estimating receptor point concentrations are identified.

4.2 CHEMICALS OF CONCERN

Figure 4-2 shows the Chemicals of Concern screen. Chemicals of concern are selected from this list by clicking on the chemical(s) with the mouse and then choosing “Add→.” A selected chemical may be deselected by clicking on it and selecting “←Remove.” Version 2.0 of the DSS allows the user to select up to 20 chemicals of concern from a total of 48 chemicals included in the database. Use the up and down arrows to scroll through the chemicals listed in the database. New chemicals may be added to the DSS by choosing “Add Chemical to Database.”

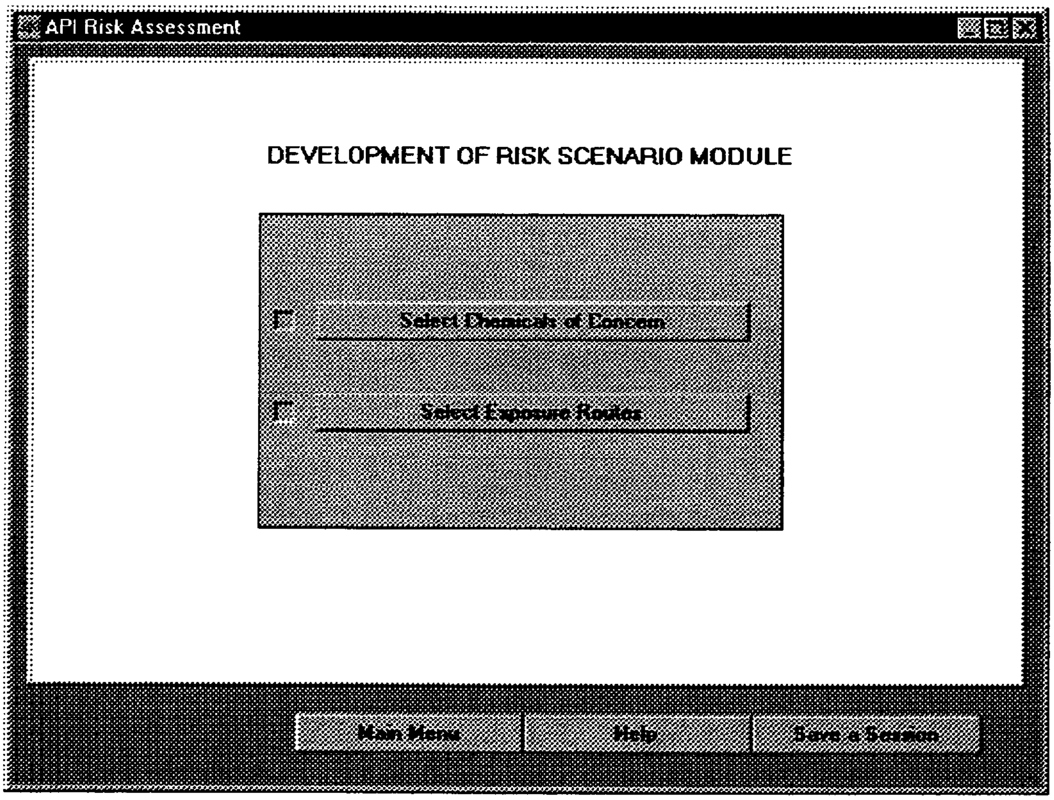


Figure 4-1. Development of Risk Scenario Screen.

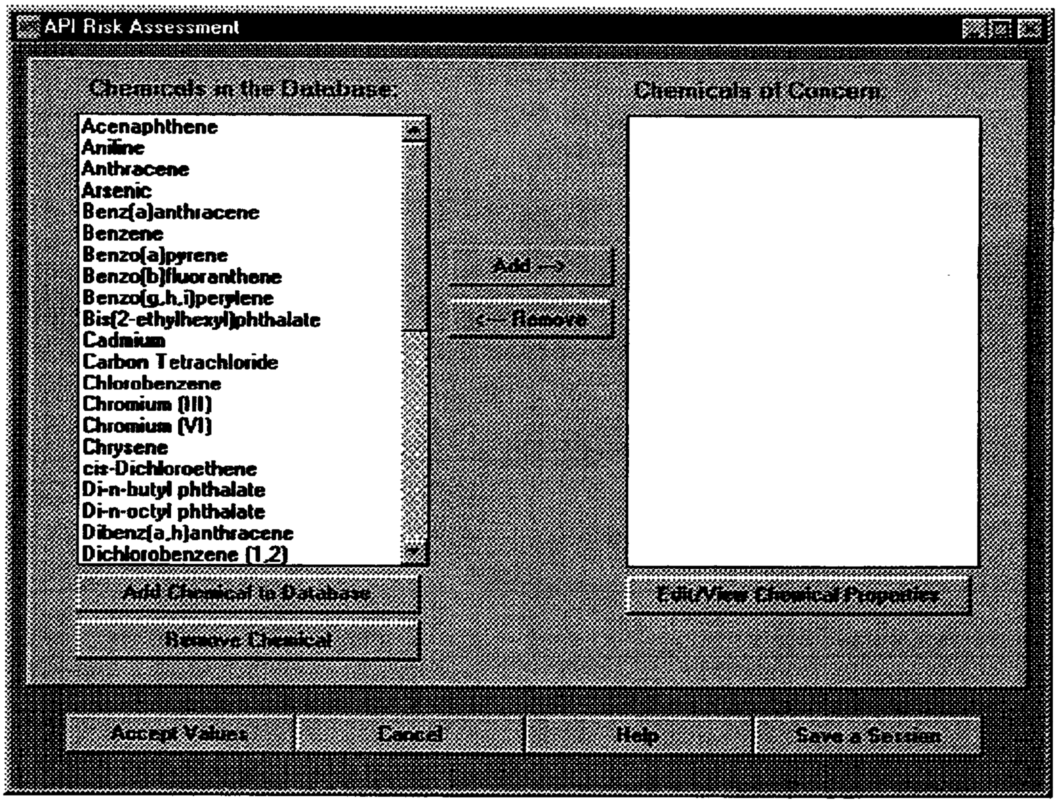


Figure 4-2. Selecting Chemicals of Concern.

The process for selecting chemicals of concern is described in the EPA Risk Assessment Guidance for Superfund manual (RAGS, EPA 1989a). Section 5.8 of the RAGS guidance lists the criteria for identifying chemicals of potential concern using site-specific information. Briefly, the initial chemical list should include chemicals that were:

1) positively detected in at least one sample;
2) detected at levels significantly elevated above levels of the same chemicals detected in associated blank samples;
3) detected at levels significantly elevated above naturally occurring background levels;
4) only tentatively identified but may be associated with the site historically; or
5) transformation (daughter) products of chemicals demonstrated to be present.

This initial list can be slimmed down using toxicity/concentration screens, etc. See the RAGS guidance for more information.

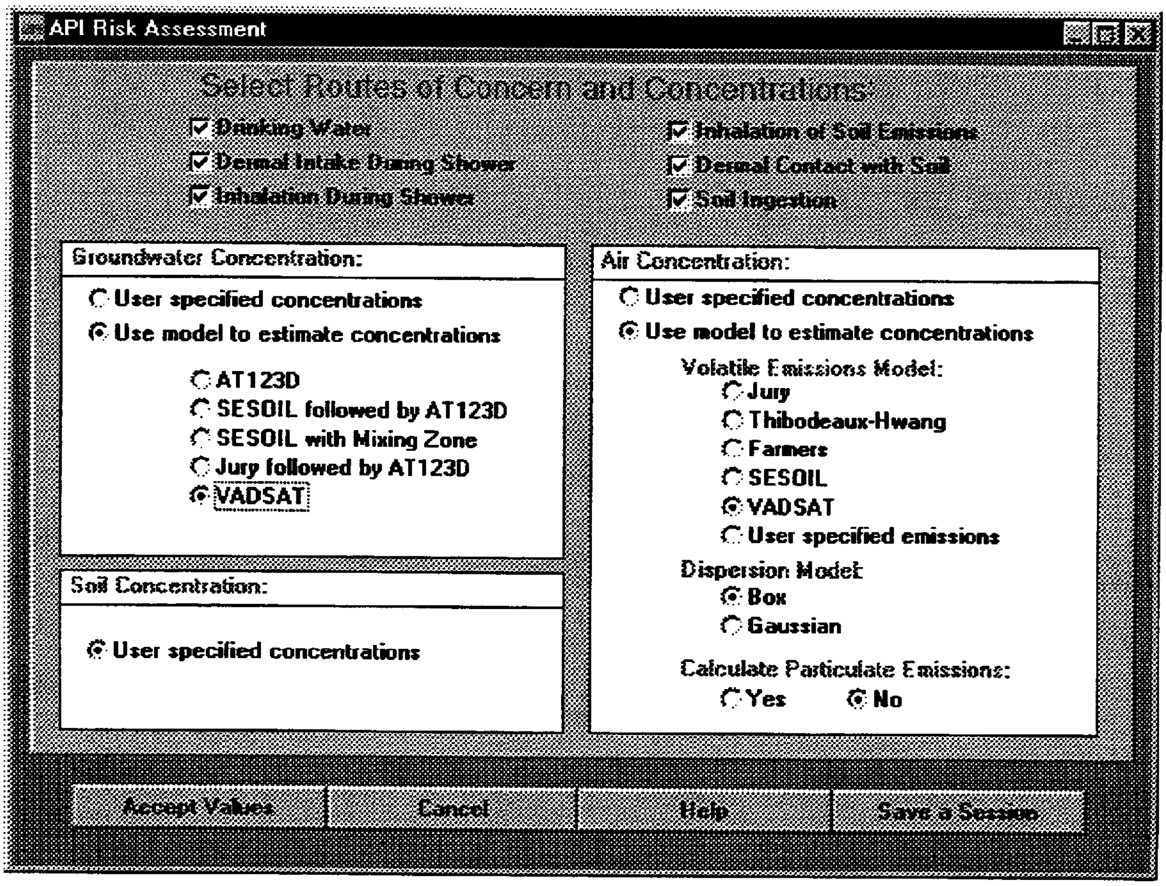
4.2.1 Edit/View Chemical Properties

By selecting this button, the user may view or change the values for the chemical properties for each chemical in the API DSS database. Please note, if the values are changed in this location they will be permanently changed in the database. If the values were changed mistakenly, the user either can change them back (using the values presented in the manual, Table 9-1) or reload the API DSS from the installation disks. This process will just overwrite the files used to run the program and will not overwrite any saved session files.

4.3 ROUTES OF CONCERN

From the Development of Risk Scenario screen, the user must also choose the exposure routes of concern. There are six routes available in the DSS:

1) Ingestion of Drinking Water
2) Dermal Absorption while Bathing
3) Inhalation while Showering
4) Inhalation of Soil Emissions
5) Dermal Contact with Soil
6) Ingestion of Soil



Select Routes of Concern and Concentrations:

☑ Drinking Water
☑ Dermal Intake During Shower
☑ Inhalation During Shower
☑ Inhalation of Soil Emissions
☑ Dermal Contact with Soil
☑ Soil Ingestion

Groundwater Concentration:
○ User specified concentrations
● Use model to estimate concentrations
  ○ AT123D
  ○ SESOIL followed by AT123D
  ○ SESOIL with Mixing Zone
  ○ Jury followed by AT123D
  ● VADSAT

Soil Concentration:
● User specified concentrations

Air Concentration:
○ User specified concentrations
● Use model to estimate concentrations
  Volatile Emissions Model:
  ○ Jury
  ○ Thibodeaux-Hwang
  ○ Farmers
  ○ SESOIL
  ● VADSAT
  ○ User specified emissions
  Dispersion Model:
  ● Box
  ○ Gaussian
  Calculate Particulate Emissions:
  ○ Yes ● No

Figure 4-3. Selecting Routes of Concern.

These routes are displayed on the top of the "Select Routes of Concern" screen (Figure 4-3). The user should select exposure routes based on the receptor type and expected location of the receptor. For example, if risks to an on-site resident are being estimated, then all the above routes may be of concern. On the other hand, if an on-site worker is being considered, the shower routes may be eliminated leaving inhalation of soil emissions, dermal contact with soil, soil ingestion, and ingestion of groundwater as routes of concern. Of course, if showers are available to the workers at the site (and the showers use groundwater) then the shower routes should be considered for a worker scenario.

Table 4-1 lists suggested exposure routes for different combinations of receptor type and the contaminated media. As an example, if soil is contaminated at a given site and the receptor is an off-site resident, ingestion of contaminated soil and dermal absorption of chemicals due to contact with soil are not considered viable routes of concern. However, chemicals may leach from the soil into groundwater so the groundwater routes are potential routes of concern. Similarly, chemicals may volatilize from the soil into the air, making inhalation of soil emissions a pathway of concern.

When a route of concern is selected from the interface, the associated media concentration box (below the Routes of Concern) becomes available. For example, when the user selects "Drinking Water" as a route of concern, the "Groundwater Concentration" group becomes available indicating that the user needs to specify the methodology for estimating receptor point concentrations. This process is explained in the following section.

4.4 RECEPTOR POINT CONCENTRATION ESTIMATION METHODOLOGY

Receptor point concentrations in the contact media are necessary variables for computing chemical intake. Depending on the routes of concern identified, receptor point concentrations may be required for air, groundwater, and soil. For example, if the only exposure routes to be analyzed are ingestion of soil and dermal absorption of chemicals due to contact with soil, the only receptor point concentrations required are the concentrations in soil.

In general, receptor point concentrations for each medium can be estimated by: (i) analysis of site-specific data, or (ii) application of fate and transport models. In the "Select Routes of Concern" screen (Figure 4-3), the user identifies the method to be used to estimate concentrations for each medium of concern (groundwater, soil, and/or air).

TABLE 4-1. Suggested Routes of Exposure for Selected Receptor Type and Contaminated Medium.

		Possible Routes of Exposure					
Receptor Type and Location	Contaminated Media	1	2	3	4	5	6
On-site Resident	Soil	•	•	•	•	•	•
	Groundwater	•	•	•	—	—	—
	Air	—	—	—	•	—	—
Off-site Resident	Soil	•	•	•	•	—	—
	Groundwater	•	•	•	—	—	—
	Air	—	—	—	•	—	—
On-site Worker	Soil	—	—	—	•	•	•
	Groundwater	•	—	—	—	—	—
	Air	—	—	—	•	—	—
Off-site Worker	Soil	—	—	—	•	—	—
	Groundwater	•	—	—	—	—	—
	Air	—	—	—	•	—	—
Visitor	Soil	—	—	—	•	•	•
	Groundwater	—	—	—	—	—	—
	Air	—	—	—	•	—	—

1. Ingestion of water
2. Dermal absorption while showering
3. Inhalation while showering
4. Inhalation of emissions from soil
5. Dermal contact with soil
6. Ingestion of soil

If the first option is selected (using site-specific data), the receptor point concentrations are entered by the user in the Receptor Point Concentrations module. If the second option is selected (using fate and transport models), the user must specify which model(s) will be used. The fate and transport models included in the DSS are described in Section 5.0 and Appendices A through H, and O. The available choices are shown in Figure 5-1. Receptor point concentrations may be user-entered for some media and calculated for others.

In some cases the fate and transport models are linked together. For instance, SESOIL (a vadose zone model) may be used to calculate contaminant mass loading to groundwater and volatile emission rates. Both of these outputs are used as inputs to other models. The loading to groundwater is used as an input to the saturated zone model, AT123D, and the volatile emission rates are used as input to an air dispersion model (either box or Gaussian) if the air pathway is being considered.

4.5 DATA REQUIREMENTS SUMMARY

The data required to estimate the risk at a site depend on the conceptual model developed. Thus, the necessary data depend on the type and location of the receptor, the contaminated media, the method of estimating receptor point concentrations, and the relevant routes of exposure. Based on the decisions made by the user, as discussed above, the DSS summarizes all the data that will be necessary to estimate the risk. This information is available from the "Data Requirements/Summary" button on the main API DSS screen (Figure 3-1).

An example of this summary is included in Table 4-2. Specific values for these parameters can be estimated based on a combination of site-specific field investigations, a literature search, professional judgment, or default values included in the DSS databases discussed in Section 9.0. It is recommended that while conducting a site assessment or risk assessment the user print this list and select values for each parameter before proceeding on to the site assessment or to the next module. Appendix J also includes a list of the input variables and guidance on estimating their values.

If the "Data Requirements/Summary" button is chosen after information has been entered in the DSS, the output will summarize the values entered.

Table 4-2. Printout of the Data Requirements/Summary Option.

```
API DSS Data Requirements            Example              10/25/97  10:08

DEVELOPMENT OF RISK SCENARIO
-------------------------------------------------
The following chemicals were selected:
          Benzene
          Ethylbenzene

The following exposure routes were selected:
          Drinking Water
          Inhalation During Shower

RECEPTOR POINT CONCENTRATIONS
-------------------------------------------------

User-Specified Receptor Point Concentration Distributions

Groundwater Concentrations [mg/L]
  Benzene                                                0.0
  Ethylbenzene                                           0.0


INTAKE PARAMETERS
-------------------------------------------------

 Analysis Type:          __

Body Weight and Lifetime
  Average Weight (kg)                                    __
  Lifetime (yrs)                                         __

Drinking Water
  Exposure Frequency [days/yr]                           __
  Exposure Duration [years]                              __
  Ingestion Rate [liters/day]                            __

Drinking Water Chemical Specific Parameters
  Benzene
    Bioavailability [fraction]                           1
  Ethylbenzene
    Bioavailability [fraction]                           1
```

Table 4-2. Printout of the Data Requirements/Summary Option (Concluded).

Inhalation During Shower	
Exposure Frequency [days/yr]	_
Exposure Duration [years]	_
Inhalation Rate [m^3/hr]	_
Time in Shower [hours/day]	_
Fraction Volatilized [-]	_
Shower Flow Rate [l/min]	_
Volume of Bathroom [m^3]	_
Temperature of the Water [C]	_
Droplet Diameter [cm]	_
Droplet Drop Time [s]	_
Liquid Mass Trans. Coeff. [cm/hr]	_
Gas Mass Trans. Coeff. [cm/hr]	_
Inhalation During Shower Chemical Specific Parameters	
Benzene	
Henry's Constant [(mg/L)/(mg/L)	2.49E-01
Bioavailability [fraction]	1
Ethylbenzene	
Henry's Constant [(mg/L)/(mg/L)	2.87E-01
Bioavailability [fraction]	1
Oral Toxicity Parameters	
Benzene	
Slope Factor [1/(mg/kg-day)]	0.029
Reference Dose [mg/kg-day]	ND
Ethylbenzene	
Slope Factor [1/(mg/kg-day)]	NA
Reference Dose [mg/kg-day]	0.1
Inhalation Toxicity Parameters	
Benzene	
Slope Factor [1/(mg/kg-day)]	0.029
Reference Dose [mg/kg-day]	ND
Ethylbenzene	
Slope Factor [1/(mg/kg-day)]	NA
Reference Dose [mg/kg-day]	2.86E-01

5.0

RECEPTOR POINT CONCENTRATION MODULE

A required step in the risk assessment process is to estimate the receptor point concentrations in the various contact media. Contact media are air, water, and soil that come in contact with or otherwise enter the human body. Receptor point concentrations are used to estimate the dose or intake (via the Chemical Intake and Risk Calculation module) and can be estimated by: (i) application of fate and transport model(s), (ii) analysis of site-specific data, or (iii) a combination of the two.

The API DSS can be used to estimate the chemical intake and risk from the six routes of exposure shown in Table 5-1. Specifically, the API DSS requires the following four receptor point concentrations:

- concentration in groundwater
- concentration in surface soil
- concentration in ambient air
- concentration in shower air (estimated from concentration in groundwater)

Table 5-1. Receptor Point Concentrations Required for Different Routes of Exposure.

ROUTE OF EXPOSURE	CONCENTRATION
Ingestion of contaminated groundwater	Concentration in groundwater
Inhalation while showering	Concentration in shower air
Dermal contact while bathing	Concentration in shower water
Ingestion of contaminated soil	Concentration in soil
Dermal contact with contaminated soil	Concentration in soil
Inhalation of outdoor air	Concentration in air

The Receptor Point Concentrations module allows the user to either directly specify concentrations (except for shower air concentrations) or to use fate and transport models to estimate these concentrations. The shower concentrations are estimated in the Chemical Intake and Risk Calculation Module. Table 5-2 lists the models included in the API DSS and the pathways associated with them. Figure 5-1 shows how the models are linked together.

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Table 5-2. Fate and Transport Models in the DSS by Model Type.

Model Type	Model Name	Processes Simulated	Receptor Point Concentrations Calculated
Vadose Zone	VADSAT	Leaching to groundwater Groundwater transport Volatile emissions	Groundwater
Vadose Zone	SESOIL	Leaching to groundwater Mixing in groundwater Volatile emissions	Groundwater (directly beneath source)
Vadose Zone	Jury	Leaching to groundwater Volatile emissions	None
Volatile Emissions Only	Farmers	Volatile emissions	None
Volatile Emissions Only	Thibodeaux-Hwang	Volatile emissions	None
Particulate (Dust) Emissions	Cowherd	Particulate emissions	None
Saturated Zone	VADSAT	Groundwater transport	Groundwater
Saturated Zone	AT123D	Groundwater transport	Groundwater
Air	Box	Mixing in a "box"	Air
Air	Gaussian	Transport downwind	Air

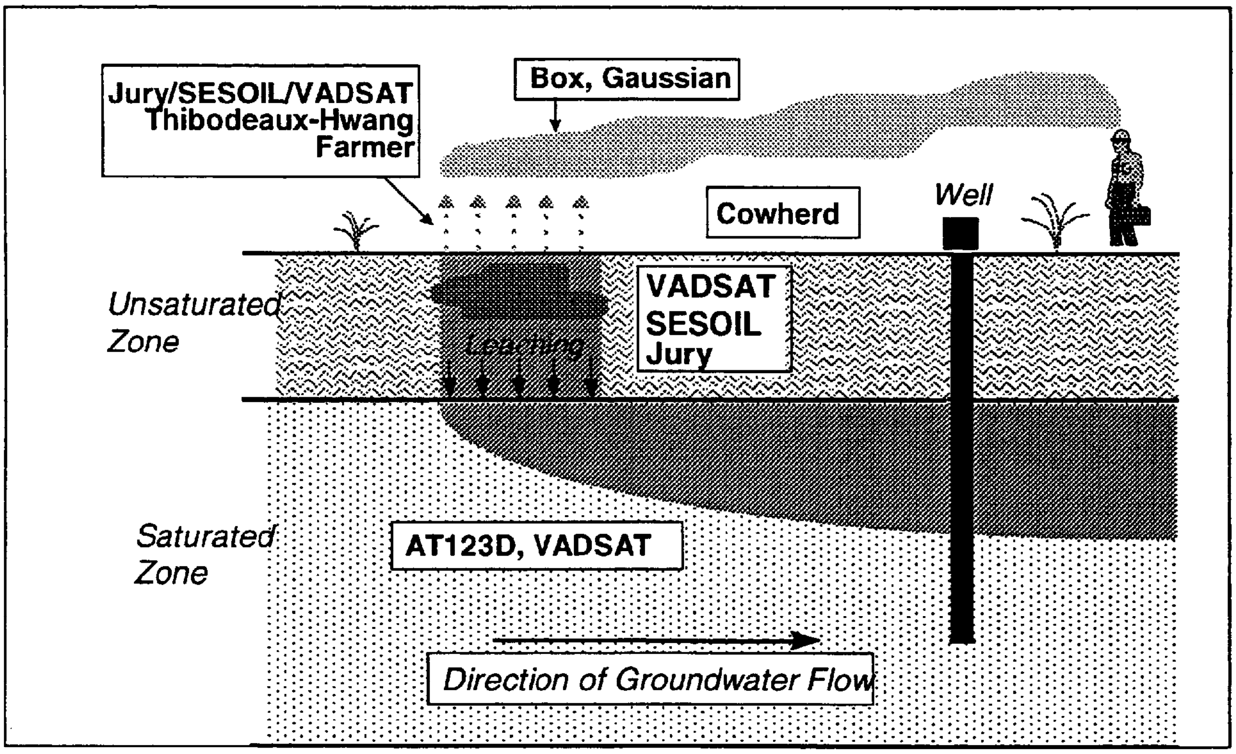
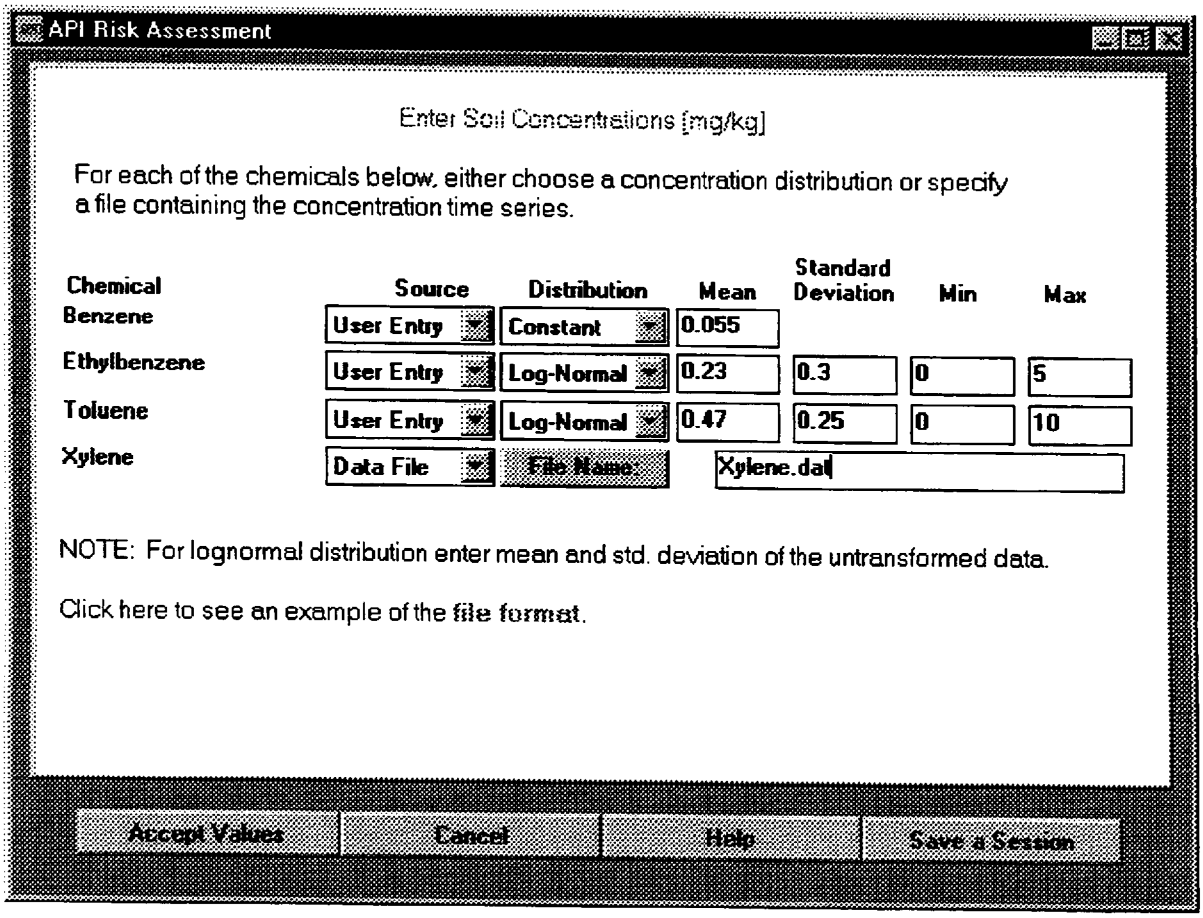


Figure 5-1. Schematic of the Models Included in the DSS.

5.1 ENTERING RECEPTOR POINT CONCENTRATIONS

If "User-Specified Concentrations" is selected in the Development of Risk Scenario module, the user will be prompted to enter concentrations in this module. Figure 5-2 shows a hypothetical input screen for soil concentrations for four chemicals. Please note, these are receptor concentrations (not necessarily source concentrations)—they will not be linked to any fate and transport model.



Enter Soil Concentrations [mg/kg]

For each of the chemicals below, either choose a concentration distribution or specify a file containing the concentration time series.

Chemical	Source	Distribution	Mean	Standard Deviation	Min	Max
Benzene	User Entry	Constant	0.055			
Ethylbenzene	User Entry	Log-Normal	0.23	0.3	0	5
Toluene	User Entry	Log-Normal	0.47	0.25	0	10
Xylene	Data File	File Name:	Xylene.dat			

NOTE: For lognormal distribution enter mean and std. deviation of the untransformed data.

Click here to see an example of the file format.

Figure 5-2. Entering Receptor Point Concentrations.

The screen contains two drop-down lists, one labeled **Source**, and the other **Distribution**. The source option allows the user to specify whether the concentration data are read from an external file or entered directly on this screen (the default). The external data file option allows the use of external time-series concentration data (not generated by one of the models in the DSS). The green hypertext, "file format," provides guidance on the file format required. **Note: If an external data file is entered, the Monte Carlo distributions can not be used for the same media—the selections shown in Figure 5-2 are just for illustration.**

If the external data file option is used, the time vs. concentration data should be contained in a separate file for each chemical. The length of the time series in each file should be equal if they are to be viewed using EXCEL®.

The **Distribution** drop-down list allows the user to specify a distribution for the concentration data. If a deterministic analysis is being performed, the constant option should be selected (the default). If a different distribution is selected, additional data will be required to specify the distribution (standard deviation, minimum, and maximums). For more information see Section 8, Monte Carlo Analysis.

5.2 OPTIONS TO ESTIMATE RECEPTOR POINT CONCENTRATIONS

Table 5-3 summarizes the fate and transport models included in the DSS. The following sections are organized by media for which the model estimates the concentrations.

5.2.1 Estimation of Groundwater Concentration

Groundwater concentrations can be estimated by a number of different fate and transport models in the DSS:

- VADSAT (vadose zone and saturated zone model)
- SESOIL linked with AT123D
- Jury linked with AT123D
- AT123D (for groundwater sources)
- SESOIL to mixing zone in groundwater (Summers)

All of these models use site-specific information to estimate concentrations in groundwater. Comprehensive descriptions of these models are presented in the Appendices of this manual.

VADSAT is a new model added to version 2.0 of the DSS. This model offers several advantages over SESOIL and Jury. It was developed specifically to handle mixtures such as total petroleum hydrocarbons (TPH). This is an important consideration if the contaminants of concern are part of a mixture because they will solubilize and transport differently than if they were the only contaminant present in the soil. For

Table 5-3. Summary of Fate and Transport Models in the DSS.

MODEL	Type of Model	Solution Technique	Conserves mass?	Can be used in the presence of free product?	Estimates media concentrations?	Processes Simulated	Source Inputs
SESOIL	Unsaturated Zone Model one-dimensional, dissolved solute transport and volatile emissions.	Lumped Semi-Numerical	Yes	Yes, make sure to calculate effective solubility	Groundwater (in mixing zone)	Leaching to groundwater, volatile emissions	Mass for each soil layer (kg)
Jury's Model	Unsaturated Zone Model one-dimensional, dissolved solute transport and volatile emissions.	Analytical	Yes	No	None, estimates volatile emissions and loading to groundwater	Leaching to groundwater, volatile emissions	Concentration (mg/kg) in contaminated zone
VADSAT	Unsaturated Zone Model coupled with its own Saturated Zone Model. Dissolved transport only, volatile emissions.	Analytical	Yes	Yes, automatically calculates effective solubility	Groundwater, volatile emissions	Leaching to groundwater, vol. emissions, adv./disp. in sat zone	Concentration (mg/kg) in contaminated zone
AT123D	Saturated Zone Model one-dimensional flow, estimates dispersion in three dimensions.	Semi-Analytical Uses a time step.	Yes	No, it does not check to see if concentrations exceed solubility	Groundwater	Advection and dispersion in the saturated zone	Mass loading (kg or kg/year), may be linked with SESOIL or Jury's Model
Farmer Model	Emission Model Only	Analytical	No (infinite source)	Yes	None, estimates volatile emission rate only	Volatilization	Concentration (mg/kg)
Thibodeaux-Hwang Model	Emission Model Only	Analytical	No (has a limited source but does not account for chemicals leaching or degrading)	Yes	None, estimates volatile emission rate only	Volatilization	Concentration (mg/kg)
Box Model	Air Dispersion Only Onsite receptor	Analytical	Yes	Not Applicable	Air	Estimates air concentrations given an emission rate	Volatile emission rate (kg/year), must be linked with a volatilization model
Gaussian Dispersion Model	Air Dispersion Only Offsite receptors	Analytical	Yes	Not Applicable	Air	Estimates air concentrations given an emission rate	Volatile emission rate (kg/year), must be linked with a volatilization model

example, benzene will leach out of a gasoline mixture at 1-3% of its pure phase solubility. This means that the concentrations will be lower in the soil and the source will last longer than for the case of pure benzene. VADSAT is a coupled VADose zone and SATurated zone model and may only be run in this linked mode.

AT123D is a saturated zone (only) model. Therefore, AT123D may be used for cases where the source is in the groundwater aquifer or it may be linked with the SESOIL or Jury vadose zone models for contamination originating in the vadose zone. AT123D can only simulate the transport of dissolved phase contaminants and cannot account for the presence of mixtures (it does not check effective solubility).

The SESOIL and Jury vadose zone models are quite different from each other and have been included in the DSS because they offer features not found in the other codes. SESOIL estimates the hydrology (all the other models require the user to enter the infiltration rate) and SESOIL can also handle multiple layers. Jury, on the other hand, assumes a uniform vadose zone but has a more sophisticated method for estimating volatile emissions. Jury does not address residual concentrations (concentrations high enough that the contaminant forms a fourth phase, non-aqueous phase liquid [NAPL]).

5.2.2 Estimation of Ambient Air Concentration

Ambient air concentrations are required to estimate intake due to inhalation of outdoor air. In the API DSS, these concentrations can either be specified by the user based on site-specific concentration measurements or estimated using the box or the Gaussian dispersion models. Typically, the box model is used to estimate ambient air concentrations when receptors are located on or near the contaminated site. The Gaussian model is used for receptors located further away from the source. Comprehensive descriptions of both these models are presented in Appendices G and H, respectively.

A key input for both of these models is the contaminant emission rate, which is the sum of the volatile and particulate emission rates. In the API DSS, this total emission rate can either be specified by the user or the emission rates can be estimated using emission models. Specifically, the API DSS includes the VADSAT, SESOIL, Farmer, Jury, and Thibodeaux-Hwang models for estimation of air emission rates. A comprehensive description of each of these models and the underlying assumptions are included in the Appendices.

The Farmer and Thibodeaux-Hwang models should be considered crude screening level models. They were included in the DSS to provide a quick "first look" to see if air emissions need to be considered. Briefly, the Farmer model assumes an infinite source of contaminant mass in the soil. The Thibodeaux-Hwang model assumes a finite source and estimates the average emission rate over a user-specified time period. This model does not account for any downward leaching of contaminants or other losses.

The Jury, SESOIL, and VADSAT models can also be used to estimate the emission rate. If other than a rough estimate of air emission is needed, it is recommended that these models be used to estimate volatile emissions rather than Farmer's or Thibodeaux-Hwang because the vadose zone models conserve mass and account for losses due to leaching and degradation.

The Farmer's and Thibodeaux-Hwang models estimate volatile emissions only. Particulate emissions are estimated using the Cowherd model. This is an empirical model based on wind tunnel experiments on mining soils. A comprehensive discussion of this model is presented in detail in Appendix F. The particulate emission rates and the volatile emission rates are added to yield the total emission rate used as an input to the box or Gaussian model.

5.2.3 Estimation of Concentration in the Shower Air

Air concentrations in the shower-stall are necessary to estimate the intake due to inhalation during showering. The shower air concentration is estimated by first estimating the contaminant mass that volatilizes from the water used for showering. This estimation is based on either the Foster and Chrostowski model described in Appendix I or by specifying a fraction of the total contaminant that volatilizes from shower water.

The concentration in the shower air is estimated by dividing the volatile mass by the volume of air in the shower. This concentration is then used to estimate the intake due to inhalation of the shower air.

5.3 ESTIMATION OF TIME-AVERAGED RECEPTOR POINT CONCENTRATION

The above sections present a discussion of the use of specific models to estimate receptor point concentrations. In the event that the models and their inputs are steady state, the receptor point concentrations do not vary in time and the estimated concentration is used directly to estimate the intake as discussed in Section 6.0. Examples include the direct application of the Farmer, Thibodeaux-Hwang, or Cowherd emission models coupled with a box or Gaussian model.

If the models or the inputs vary in time, the model output consists of a receptor point concentration that varies with time. For example, application of AT123D could result in a time varying concentration in the receptor well. However, in order to estimate exposure (dose), an average concentration over the exposure duration is needed for carcinogens. These average concentrations used to estimate the dose (refer to Section 7.0) are calculated internally by the API DSS in accordance with the following procedure. For non-carcinogens, the maximum concentration is used for calculation of hazard index.

The time-varying concentration values are analyzed to estimate the maximum running average concentrations taken over 5-year increments for up to 75 years (maximum likely human exposure duration). This results in 15 values, i.e., the maximum 5-year running average concentration, the maximum 10-year running average concentration, etc. Note, the maximum 5-year average concentration does not necessarily correspond to the average concentration for the first five years simulated. Rather, it corresponds to the five years surrounding the point in time when the maximum concentration occurred. Figure 5-3 shows an example.

In case the model is run for less than 75 years, the concentration is assumed constant for all averaging periods larger than the simulation time. For example, if the model is run for 37 years, the maximum 40-, 45-,....., and 75-year running average concentrations would be the same as the 35-year maximum running average concentration. These 15 concentrations are used to estimate the specific value used for estimating the dose. If the exposure duration is not a multiple of five, the next lowest averaging year is used for the concentration value. For example, if the exposure period is 37 years, the model calculates running average concentrations up to a 35-year averaging period.

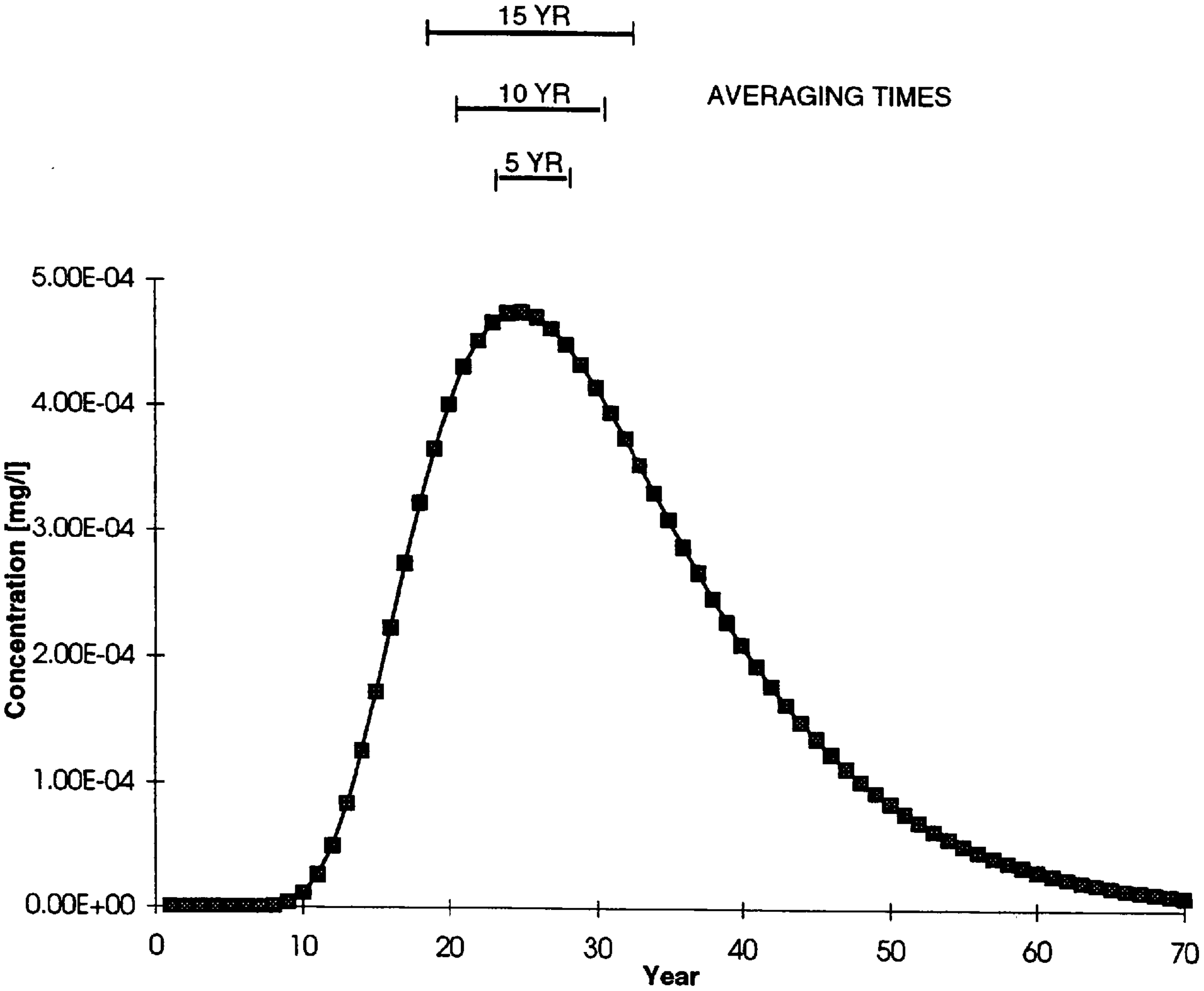


Figure 5-3. Schematic Showing the Estimation of Maximum Average Concentrations for Different Averaging Periods.

6.0
CHEMICAL INTAKE AND RISK CALCULATION MODULE

6.1 OVERVIEW OF THE MODULE

This module estimates the chemical intake and computes the human health risk due to this intake. Chemical intake is computed using equations (presented subsequently in this section) that include variables for exposure concentration, frequency, duration of exposure, body weight, and contact rates. The latter reflect the rates at which contaminated media (soil, water, air) come in contact with the receptor. The estimated intake is then used to quantify the risk for each exposure route, as discussed in Section 6.3.

The procedures used to compute intake are consistent with those described in EPA's Risk Assessment Guidance for Superfund (EPA, 1989a). Specifically this module can be used to estimate chemical intake for the following routes:

- Ingestion of contaminated water
- Inhalation while showering
- Dermal contact with contaminated groundwater
- Ingestion of contaminated soil
- Dermal contact with contaminated soil
- Inhalation of air containing chemical vapors or particulates.

These are typically the most important routes of exposure at petroleum contaminated sites. Other exposure routes, such as inhalation of contaminated indoor air or ingestion of produce grown in contaminated soil, may be important in certain situations but are currently not included in this module.

As shown in Table 6-1, two sets of default data are included in the DSS. These are the (1) EPA-recommended reasonable maximum exposure assumptions, and (2) average most-likely intake parameter values derived from EPA's Exposure Factors Handbook (EPA, 1989b) and Risk Assessment Guidance for Superfund Manual

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Table 6-1. Intake Parameters Database*.

(Page 1 of 2)

Parameter	Units	Default Maximum Exposure Value	Default Most-Likely Value
Common to all Routes			
Body Weight	[kg]	70 (Adult) 15 (Child)	70 (Adult) 15 (Child)
Lifetime	[years]	70	70
Ingestion of Drinking Water			
Exposure Duration	[years]	30	9
Exposure Frequency	[days/year]	365	350
Ingestion Rate	[liters/day]	2	1.4
Bioavailability	[mg/mg]	Chemical-Specific	Chemical-Specific
Inhalation During Shower			
Exposure Duration	[years]	30	9
Exposure Frequency	[days/year]	365	350
Exposure Time	[hours/day]	0.333	0.12
Inhalation Rate	[m^3/hour]	0.89	0.63
Bioavailability	[mg/mg]	Chemical-Specific	Chemical-Specific
Dermal Exposure in Shower			
Exposure Duration	[years]	30	9
Exposure Frequency	[days/year]	365	350
Exposure Time	[hours/day]	0.333	0.12
Total Skin Surface Area	[cm^2]	18150	18150
Permeability Coefficient	[cm/hour]	Chemical-Specific	Chemical-Specific

Table 6-1. Intake Parameters Database*.
(Page 2 of 2)

Parameter	Units	Default Maximum Exposure Value	Default Most-Likely Value
Inhalation of Volatile Soil Emissions			
Exposure Duration	[years]	30	9
Exposure Frequency	[days/year]	365	350**
Time Outdoors	[hours/day]	8	4
Inhalation Rate	[m^3/hour]	1.25	0.833
Bioavailability	[mg/mg]	Chemical-Specific	Chemical-Specific
Dermal Contact with Soil			
Exposure Duration	[years]	30	9
Exposure Frequency	[days/year]	365	350
Skin Surface Area (arms and hands)	[cm^2]	3120	3120
Adherence Factor	[mg/cm^2]	1.45	0.6
Absorption Coefficient	[mg/mg]	Chemical-Specific	Chemical-Specific
Ingestion of Soil			
Exposure Duration	[years]	30	9
Soil Contact Frequency	[days/year]	365	350
Soil Ingestion Rate	[mg/day]	200 (Child) 100 (Adult)	50 (Child) 10 (Adult)
Fraction Soil Contaminated	[mg/mg]	1	Site-Specific
Bioavailability	[mg/mg]	Chemical-Specific	Chemical-Specific

Note: the module allows the user to enter site-specific values for analysis. It is strongly recommended that site-specific values be used when available.

* U.S. EPA (1989a)

** U.S. EPA (1989b)

(EPA, 1989a). In the deterministic mode, these two data sets will be presented side-by-side on the screen. One of these data sets may be selected for analysis, or the user may enter his/her own data.

The equations in the DSS calculate an administered dose. The administered dose or intake is defined as the mass of a substance that comes in contact with an exchange boundary within an organism (e.g., gastrointestinal tract, skin, lungs) per unit body weight of that organism per unit time. Absorbed dose, on the other hand, is the mass of the substance that, after contact, penetrates the exchange boundaries, enters the metabolic system and causes the adverse health effect. This is sometimes referred to as the bioavailable dose. EPA (1989a) states that most toxicity values are based on administered doses and therefore the intakes calculated should be administered intakes. Occasionally toxicity values may be based on absorbed dose and then the administered dose should be adjusted to reflect the amount of chemical absorbed. The bioavailability terms in the DSS are used to make this adjustment. Unless a review of the toxicity data suggests otherwise, the bioavailability values should be left at their default value of 1.

For ingestion and inhalation exposure routes, the daily intake rate is equivalent to an administered dose. For dermal exposure routes, by which the chemical is absorbed directly into the bloodstream, the daily intake rate calculated by the DSS is equivalent to an absorbed dose. Even though the dermal doses usually represent absorbed doses, it is standard practice to use the oral toxicity value to calculate risk from the dermal pathways. This is how the risk from dermal exposures is calculated in DSS.

The equations used to estimate the intake for each of the routes of exposure included in the DSS are presented below.

6.2 DESCRIPTION OF EACH INTAKE ROUTE

The Chemical Intake and Risk Calculation module first estimates the intake of chemical that occurs during an exposure event. This intake rate, expressed in milligrams per day of chemical taken into the body per unit body weight (mg/kg-d), is then averaged over time for use in characterizing risk.

6.2.1 Ingestion of Drinking Water

Daily intake from ingestion of contaminated water is computed from the rate of water ingestion and the contaminant concentration in the drinking water source:

$$DI = b_i \, IR \, C_w / BW \tag{6-1}$$

where

DI = daily absorbed dose from water ingestion (mg/kg-d)
IR = water ingestion rate (l/d)
C_w = contaminant concentration in drinking water (mg/l)
BW = body weight (kg)
b_i = chemical-specific bioavailability for ingestion (mg/mg)

In the above equation, IR is the rate of ingestion from the contaminated water source only, and is not necessarily equal to the total daily fluid intake. For a contaminated water supply, IR would be the ingestion rate of tap water and drinks made from tap water. This intake estimate is conservative because it ignores the dilution of contaminated groundwater by pumping.

6.2.2 Inhalation While Showering

While showering, volatile compounds in domestic water are volatilized into the air within the shower stall, the bathroom, and the remainder of the household. Recent studies have shown that risks from inhalation while showering can be comparable to or greater than risks from drinking contaminated water (McKone, 1987). Daily inhalation intake during showering is computed as a function of the concentration of volatile chemicals in the shower air, the inhalation rate, and the duration of the shower:

$$DI = b_{sh} \, C_{sh} \, IH \, ET / BW \tag{6-2}$$

where

DI = daily absorbed dose from inhalation while showering (mg/kg-d)
C_{sh} = concentration of chemicals in shower air (mg/m^3)
IH = inhalation rate during showering (m^3/hr)
ET = shower duration (hr/day)

BW = body weight (kg)
b_{sh} = chemical-specific bioavailability for inhalation (mg/mg)

The concentration C_{sh} is estimated using the shower volatilization model described in Appendix I. The transport of chemical vapors from shower stall to other parts of the house and the subsequent inhalation of indoor air are not considered in the model presented in Appendix B or included in the DSS.

6.2.3 Dermal Absorption While Showering

During showers and baths humans may absorb dissolved contaminants across the skin into the bloodstream. The dose to humans by this route is computed as an absorbed dose rather than as an administered dose (or intake). The daily dose will depend upon the absorption characteristics of the chemical, the surface area of skin in contact with the water, and the duration of the bath or shower:

$$D_{abs} = 10^{-3}\, C_w\, SA\, PC\, ET / BW \qquad (6\text{-}3)$$

where

D_{abs} = dermal absorbed dose (mg/kg-d)
C_w = concentration of chemicals in water (mg/l)
SA = exposed skin surface area (cm^2)
PC = chemical-specific skin permeability constant (cm/hr)
ET = bath or shower duration (hr/day)
BW = body weight (kg)
10^{-3} = conversion factor from (l/cm^3)

The chemical-specific skin permeability constant is equal to the chemical diffusivity through the skin, cm^2/hr, divided by the skin thickness, cm. This method assumes that diffusion across the stratum corneum (skin layer) can be described by Fick's Law, and that the concentration in the bloodstream is small relative to the concentration in water. The permeability constant quantifies the diffusion properties of the skin and the chemical; values of PC are tabulated in the user's manual for the Pollutant Hazard Assessment System (U.S. Army, 1991) as well as EPA's Interim Report on dermal exposure assessment (1992). Section 9.2.7 presents the values contained in the DSS database as well as a method for estimating values.

6.2.4 Ingestion of Soil

Adults working outdoors may ingest soil orally through incidental contact of the mouth with hands and clothing. Soil ingestion by children is often the primary route of exposure from contaminated surface soils (Paustenbach, 1989a,b). Daily intake of contaminants in soil through this route is estimated as follows:

$$DI = 10^{-6}\, b_s\, C_s\, IR\, FI\, /\, BW \qquad (6\text{-}4)$$

where

DI = daily absorbed dose from soil ingestion (mg/kg-d)
C_s = concentration of chemicals in contaminated soil (mg/kg)
IR = ingestion rate of soil (mg/d)
FI = fraction of total ingested soil that is contaminated (mg/mg)
BW = body weight (kg)
10^{-6} = conversion factor from (kg/mg)
b_s = chemical-specific bioavailability for soil ingestion (mg/mg)

The total amount of soil ingested by adults and children is highly uncertain. The U.S. EPA recommends ingestion rates of 100 mg/d for adults and 200 mg/d for children. Calabrese et al. (1989) discuss methodologies for measuring soil ingestion rates. Paustenbach (1989a, b) presents data suggesting that actual rates may be as low as 10 mg/d for adults and 50 mg/d for children. The ingestion rate is sometimes expressed as the product of the total soil ingested and the fraction of the total soil that is contaminated, as above.

6.2.5 Dermal Contact with Soil

Soil contaminants may be absorbed across the skin into the bloodstream. Absorption will depend upon the amount of soil in contact with the skin, the concentration of chemicals in soil, the skin surface area exposed, and the potential for the chemical to be absorbed across skin. The steady-state dose absorbed is computed as follows:

$$D_{abs} = 10^{-6}\, C_s\, SA\, AF\, ABS\, /\, BW \qquad (6\text{-}5)$$

where

D_{abs} = dermal absorbed dose (mg/kg-d)
C_s = concentration of chemicals in soil (mg/kg)
SA = skin surface area exposed to soil per day (cm^2/d)
AF = soil-to-skin adherence factor (mg/cm^2)
ABS = fraction of chemical that is absorbed (mg/mg)
BW = body weight (kg)
10^{-6} = conversion factor from (kg/mg)

The absorption factor accounts for both contaminant desorption from soil and absorption across the skin, and is rarely known for a specific chemical. Paustenbach (1989a, b) indicates that petroleum contaminants in soils will absorb at a rate of 2 to 10 percent. Ryan et al. (1986) derive absorption factors for general classes of chemicals; they found that volatile organic compounds have absorption factors of 10 to 25 percent, while inorganics have absorption factors of 0.1 to 1 percent.

6.2.6 Inhalation of Soil Emissions

As discussed in Section 5.1.3, volatile and particulate emissions from the contaminated site mix with the on-site ambient air and are transported off site by advection and dispersion. On-site and off-site receptors may therefore be exposed to chemicals by inhalation. Inhalation intake is computed as follows:

$$DI = b_a\, C_a\, IH\, ET\, /\, BW \qquad (6\text{-}6)$$

where

DI = daily absorbed dose from inhalation of soil emissions (mg/kg-d)
C_a = concentration of chemical in ambient air (mg/m^3)
IH = inhalation rate (m^3/hr)
ET = exposure time (hr/day)
BW = body weight (kg)
b_a = chemical-specific bioavailability for inhalation (mg/mg)

The concentration of the chemical in the ambient air is the sum of vapor and particulate chemical concentrations. The inhalation rate for this exposure route should account for the type of activity occurring during the exposure time (e.g., outdoor work, light to moderate activity, resting). For residential exposure, the exposure time will typically equal the time spent at home, and an average daily inhalation rate may be representative of inhalation during multiple sets of activities (e.g., resting, light housework).

6.2.7 Estimation of Chronic and Lifetime Daily Intakes

The chronic daily intake (CDI) is used in the assessment of non-carcinogenic effects from chronic exposure, and is computed by averaging daily intake over the exposure period:

$$CDI = DI\ EF\ ED / (365\ AT) \qquad (6\text{-}7)$$

where

CDI = chronic daily absorbed dose (mg/kg-d)
DI = daily intake estimated using the equations presented above (mg/kg-d)
EF = exposure frequency (days per year)
ED = exposure duration (years)
AT = averaging time (years)

When evaluating non-carcinogenic effects the averaging time (AT) is equal to the exposure duration (ED).

The lifetime average daily dose (or intake) (LADD or LADI) is used to assess carcinogenic risk, and is estimated by averaging the daily intake over a human lifetime:

$$LADD = DI\ EF\ ED / (365\ AT) \qquad (6\text{-}8)$$

where

LADD = lifetime average daily absorbed dose (mg/kg-d)
AT = averaging time (years)

When evaluating carcinogenic effects the averaging time is equal to the length of a human lifetime (years). The exposure frequency (EF in Equations 6-7 and 6-8) corresponds to the number of daily exposure events that occur within a year and is specific to each site. For instance, in assessing dermal exposure to soils, the exposure frequency equals the number of days per year that the receptor comes in direct contact with soils (sometime during the day) at the site. The exposure duration is the number of years that the receptor is exposed, e.g., the number of years that the receptor lives or works in the vicinity of the site.

6.3 CALCULATION OF RISK

Risk calculation is the final step in the risk assessment process, and serves as the bridge between risk assessment and risk management. In this step, information on the toxicity of chemicals is combined with intake estimates discussed above to compute the potential risk to human receptors. If the computed risks exceed acceptable levels, results of this analysis should be carefully analyzed to identify alternative risk management options, or the need for more detailed modeling and/or monitoring to better estimate risk. EPA generally allows 10^{-6} to 10^{-4} excess risk.

The approach used here to quantify risk is consistent with EPA's guidelines for hazardous waste sites (EPA, 1989a). Similar procedures have been adopted in regulatory guidance for many states, including California (California Department of Health Services, 1990), Massachusetts (Massachusetts Department of Environmental Quality, 1989), and Florida (Florida Department of Environmental Regulation, 1989). The state of New Jersey essentially uses this approach to derive soil cleanup criteria for petroleum products, based on average exposure assumptions for soil ingestion (Stokman and Dime, 1986).

For each receptor, total risk and risk due to each chemical and each pathway of concern are evaluated. Separate calculation methodologies are provided for evaluating carcinogenic risk and non-carcinogenic effects; these are discussed in detail below.

6.3.1 Risk Calculation for Carcinogenic Effects

For carcinogens, risk is quantified as the incremental probability of an individual developing cancer over a lifetime. This risk, referred to as the individual excess lifetime cancer risk (IELCR), is the excess risk incurred by individuals exposed to the chemicals by the pathways and routes identified in the exposure assessment. This risk is quantified as the product of the slope factor (also referred to as the potency factor) and the lifetime average daily dose (LADD):

$$IELCR_{ij} = SF_{ij}\ LADD_{ij} \qquad (6\text{-}9)$$

where

$IELCR_{ij}$ = the individual excess lifetime cancer risk for chemical i, exposure route j (dimensionless)

SF_{ij} = the slope factor for chemical i, exposure route j $(mg/kg\text{-}d)^{-1}$

$LADD_{ij}$ = the lifetime average daily dose for chemical i, exposure route j (mg/kg-d)

This approach to estimating risk is based on the linear low-dose cancer risk model described by the EPA (1989a), and is valid for risks below 0.01. The model assumes that exposure to any amount of a carcinogen will increase the risk of cancer.

To assess total risk to receptors exposed to multiple chemicals and exposure routes, risks are assumed to be additive:

$$IELCR_{t} = \Sigma\ IELCR_{ij} \qquad (6\text{-}10)$$

where

$IELCR_{t}$ = the total individual excess lifetime cancer risk (dimensionless)

This method for estimating total risk assumes there are no synergistic or antagonistic interactions between chemicals.

6.3.2 Calculation of Hazard Index for Non-carcinogenic Effects

Non-carcinogenic effects are evaluated by assuming that there is a threshold level of exposure (i.e., the RfD) below which it is unlikely that sensitive populations will experience adverse health effects. Non-carcinogenic effects are characterized by comparing the chronic daily intake for each chemical and exposure route to the chemical- and route-specific RfD. This risk is quantified as the ratio of the chronic daily intake to the RfD:

$$HQ_{ij} = CDI_{ij} / RfD_{ij} \qquad (6\text{-}11)$$

where

HQ_{ij} = the hazard quotient for chemical i, exposure route j (dimensionless)

CDI_{ij} = the chronic daily intake for chemical i, exposure route j (mg/kg-d)

RfD_{ij} = the reference dose for chemical i, exposure route j (mg/kg-d)

The hazard quotient is an index of the potential for non-carcinogenic effects, and is not a probabilistic risk. If the value exceeds unity, there is the potential for adverse non-carcinogenic health effects, and some risk management may be necessary.

For receptors exposed to multiple chemicals and exposure routes, the potential for non-carcinogenic effects is quantified by the hazard index (HI), equal to the sum of the hazard quotients for each chemical and exposure route:

$$HI = \Sigma HQ_{ij} \qquad (6\text{-}12)$$

The hazard quotient is the ratio of a single substance exposure level over a specified time period to a reference dose for that substance. The hazard index is the sum of more than one hazard quotient for multiple substances and/or multiple exposure pathways.

This method of assessing overall hazard assumes that the effects from all chemicals are additive and neglects any synergistic or antagonistic effects among multiple chemicals. If the overall hazard index is greater than unity, a more detailed evaluation of the potential for adverse health effects should be conducted. In such an analysis, the risk assessor should evaluate the toxicity and endpoint (the specific adverse health effect) for each chemical in detail. Hazard indices can then be computed for each specific health effect. The DSS does not perform this effect-specific hazard evaluation.

6.4 SUMMARY OF DATA REQUIREMENTS

The data requirements summary for the Chemical Intake and Risk Calculation module is shown for each exposure route in Table 6-2. Values marked with an asterisk can either be calculated in the Fate and Transport module or be entered by the user in this module. These data can be entered as constant values or as a probability distribution by specifying the parameters of the distribution. The distributions are used for the Monte Carlo uncertainty analysis procedure described in Section 8.0. Default values and statistics for some of the input variables are available in the Exposure Factors Handbook (EPA, 1989b)

6.5 MODULE OUTPUT

Using the data discussed in Section 6.4 and the algorithms discussed in Sections 6.2 and 6.3, this module runs a FORTRAN program to estimate intake and risk. Specific output for each exposure route includes daily intake (see Equations 6-1 through 6-6), chronic daily intake (see Equation 6-7), lifetime average daily dose (see Equation 6-8), carcinogenic risk (see Equation 6-9), and hazard index (see Equation 6-11). The module also estimates cumulative values for these results by route and by chemical. Output is stored in 14 ASCII files shown in Table 6-3 which are used as input files to the Risk Presentation module discussed in Section 7.0.

A short summary of the FORTRAN output can be viewed and printed by choosing the "View FORTRAN Results" button. The Risk Presentation module is also available from the Chemical Intake Module by choosing the "View Charts and Tables in EXCEL" button. This is the same as choosing the "Risk Presentation" button from the main screen.

Table 6-2. Data Requirements Summary for the Chemical Intake Module.
(Page 1 of 2)

All Routes
    Body Weight [kg]
    Lifetime [years]

Drinking Water
    Exposure Frequency [days/yr]
    Exposure Duration [years]
    Ingestion Rate [liters/day]
  For each chemical of concern in groundwater:
    *Concentration [mg/l]
    Oral Reference Dose [mg/kg-d]
    Oral Slope Factor $[mg/kg\text{-}d]^{-1}$
    Bioavailability [mg/mg]

Inhalation During Shower
    Exposure Frequency [days/yr]
    Exposure Duration [years]
    Inhalation Rate $[m^3/hr]$
    Time in Shower [hours/day]
  For each chemical of concern in groundwater:
    *Concentration [mg/l]
    Inhalation Reference Dose [mg/kg-d]
    Inhalation Slope Factor $[mg/kg\text{-}d]^{-1}$
    Bioavailability [mg/mg]

Dermal Exposure in Shower
    Exposure Frequency [days/yr]
    Exposure Duration [years]
    Total Skin Surface Area $[cm^2]$
    Time in Shower [hours/day]
  For each chemical of concern in groundwater:
    *Concentration [mg/l]
    Dermal Permeability Coefficients [cm/hr]
    Oral Reference Dose [mg/kg-d]
    Oral Slope Factor $[mg/kg\text{-}d]^{-1}$

Table 6-2. Data Requirements Summary for the Chemical Intake Module.
(Page 2 of 2)

Inhalation of Volatile Soil Emissions
- Exposure Frequency [days/yr]
- Exposure Duration [years]
- Inhalation Rate [m^3/hr]
- Time Outdoors [hours/day]
- For each chemical of concern in air:
  - *Concentration [mg/m^3]
  - Inhalation Reference Dose [mg/kg-d]
  - Inhalation Slope Factor [mg/kg-d]$^{-1}$
  - Bioavailability [mg/mg]

Dermal Contact with Soil
- Exposure Frequency [days/yr]
- Exposure Duration [years]
- Skin Surface Area [cm^2]
- Adherence Factor [mg/cm^2]
- For each chemical of concern in soil:
  - *Concentration [mg/kg]
  - Dermal Absorption Factors [fraction]
  - Oral Reference Dose [mg/kg-d]
  - Oral Slope Factor [mg/kg-d]$^{-1}$

Ingestion of Soil
- Exposure Frequency [days/yr]
- Exposure Duration [years]
- Ingestion Rate [mg/day]
- Fraction Soil Contaminated [cc/cc]
- For each chemical of concern in soil:
  - *Concentration [mg/kg]
  - Oral Reference Dose [mg/kg-d]
  - Oral Slope Factor [mg/kg-d]$^{-1}$
  - Bioavailability [mg/mg]

---

* These concentrations can be entered by the user or they can be calculated using fate and transport models.

Table 6-3. Output Files from the Chemical Intake Module.

File Name	Contents
Dose1.dat	Daily Intakes, Chronic Daily Intakes and Lifetime Average Daily Intake for each chemical in the Drinking Water route.
Dose2.dat	Daily Intakes, Chronic Daily Intakes and Lifetime Average Daily Intake for each chemical in the Inhalation During Shower route.
Dose3.dat	Daily Intakes, Chronic Daily Intakes and Lifetime Average Daily Intake for each chemical in the Dermal Exposure During Shower route.
Dose4.dat	Daily Intakes, Chronic Daily Intakes and Lifetime Average Daily Intake for each chemical in the Inhalation of Soil Emissions and Particulates route.
Dose5.dat	Daily Intakes, Chronic Daily Intakes and Lifetime Average Daily Intake for each chemical in the Dermal Exposure to Soil route.
Dose6.dat	Daily Intakes, Chronic Daily Intakes and Lifetime Average Daily Intake for each chemical in the Ingestion of Soil route.
Risk1.dat	Excess Lifetime Cancer Risk and Hazard Quotient for each chemical in the Drinking Water route.
Risk2.dat	Excess Lifetime Cancer Risk and Hazard Quotient for each chemical in the Inhalation During Shower route.
Risk3.dat	Excess Lifetime Cancer Risk and Hazard Quotient for each chemical in the Dermal Exposure During Shower route.
Risk4.dat	Excess Lifetime Cancer Risk and Hazard Quotient for each chemical in the Inhalation of Soil Emissions and Particulates route.
Risk5.dat	Excess Lifetime Cancer Risk and Hazard Quotient for each chemical in the Dermal Exposure to Soil route.
Risk6.dat	Excess Lifetime Cancer Risk and Hazard Quotient for each chemical in the Soil Ingestion route.
Dosetot.dat	Daily Intakes, Chronic Daily Intakes and Lifetime Average Daily Intake for all of the chemicals summed across all of the routes analyzed.
Risktot.dat	Excess Lifetime Cancer Risk and Hazard Quotient for all of the chemicals summed across all of the routes analyzed.

7.0

RISK PRESENTATION MODULE

The last module in the DSS allows the user to view the results in several different formats depending on whether a deterministic or a Monte Carlo analysis of chemical intake and risk calculation was performed. Specific options are presented below. These risk results are calculated by the FORTRAN code in the Chemical Intake and Risk Calculation module. The Risk Presentation module uses EXCEL® macros to read the FORTRAN output files and present results. When this button is chosen (it can also be accessed from the Chemical Intake and Risk Calculation module) the EXCEL® spreadsheet is loaded automatically.

7.1 DETERMINISTIC ANALYSIS

Figure 7-1 shows how to access the results of the risk assessment. There are three table options and six chart options. Figures 7-2(a), 7-2(b), and 7-2(c) are examples of tables that are generated by selecting bar chart numbers 1, 2 and 3 indicated in Figure 7-2(a). Similarly, Figures 7-3(a) through 7-3(f) show the format for charts that can be generated. The risk/dose values on these tables and charts do not correspond to a specific example. These figures are included to illustrate the table formats only.

7.2 MONTE CARLO ANALYSIS

Figure 7-4 lists the available options for presenting the results in tables and charts. The user has the option to select any percentile for which the results are desired. Figure 7-5(a) shows the format of Table 1 and includes carcinogenic risk and hazard index for each chemical and route of exposure for the user-selected percentile. Figure 7-5(b) presents summary dose results for the selected percentiles. Figures 7-5(c) through 7-5(e) present key statistics for risk, hazard index, and dose. These include the minimum, maximum, median, and the user-selected percentiles as well as the 95th percentile value.

The chart options are analogous to those for the deterministic case. Specific values are picked from Table 1 (Figure 7-5a), i.e., the values plotted will be for the percentile selected in Table 1. In addition to these charts, the DSS allows the user to plot CDFs of risk and hazard index by route and by chemical as well as total risk and hazard index. The CDF menu is shown at the bottom of Figure 7-4. The box on the left shows the chemical or routes analyzed for which CDFs can be selected. Figure 7-6 is an example output of CDF obtained by selecting Option 2.

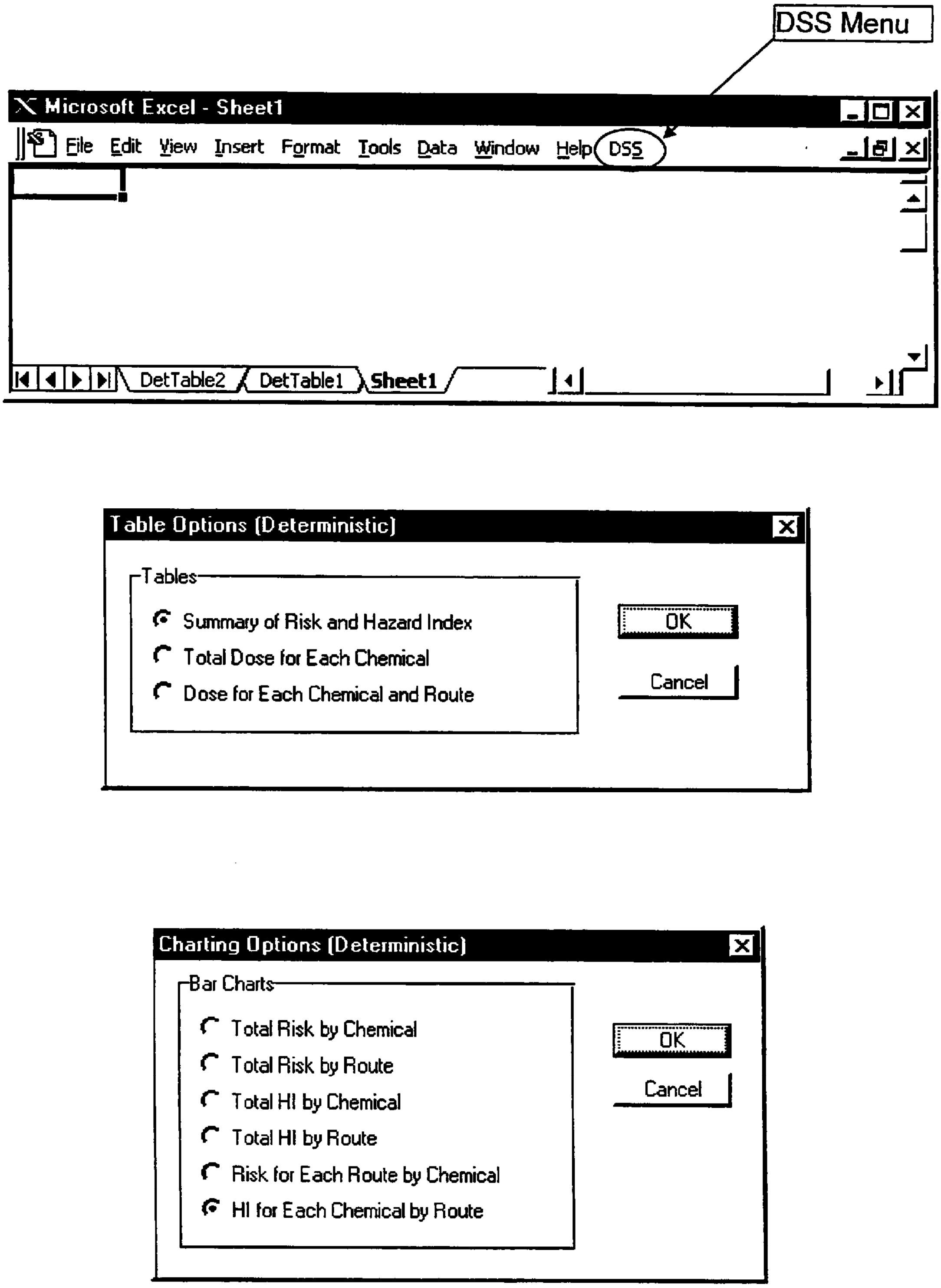


Table Options (Deterministic)

Tables

- ● Summary of Risk and Hazard Index
- ○ Total Dose for Each Chemical
- ○ Dose for Each Chemical and Route

Charting Options (Deterministic)

Bar Charts

- ○ Total Risk by Chemical
- ○ Total Risk by Route
- ○ Total HI by Chemical
- ○ Total HI by Route
- ○ Risk for Each Route by Chemical
- ● HI for Each Chemical by Route

Figure 7-1. The DSS Menu in EXCEL®: Table and Chart Options.

Example Problem from Appendix M

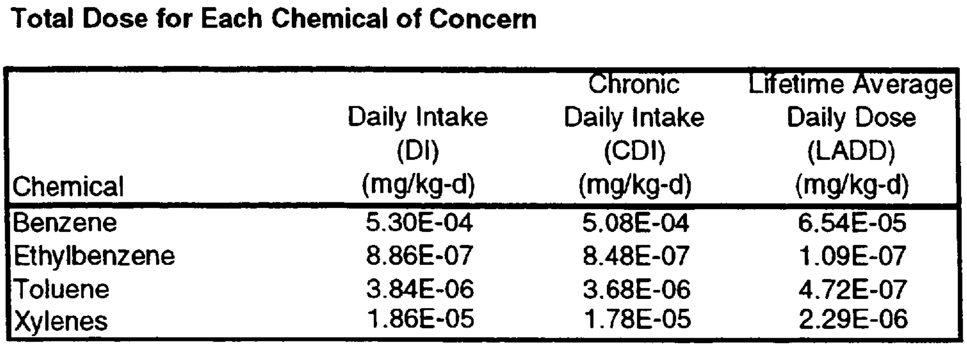
Carcinogenic Risk by Chemical for Each Route of Concern

Chemical	Drinking Water	Dermal Uptake During Shower	Inhalation During Shower	Inhalation of Soil Emissions	Total
Benzene	1.14E-06	3.73E-08	7.02E-07	1.84E-08	1.90E-06
Ethylbenzene	ND	ND	ND	ND	0.00E+00
Toluene	ND	ND	ND	ND	0.00E+00
Xylenes	ND	ND	ND	ND	0.00E+00
Total	1.14E-06	3.73E-08	7.02E-07	1.84E-08	1.90E-06

Hazard Index by Chemical for Each Route of Concern

Chemical	Drinking Water	Dermal Uptake During Shower	Inhalation During Shower	Inhalation of Soil Emissions	Total
Benzene	1.80E-01	5.88E-03	1.11E-01	2.91E-03	3.00E-01
Ethylbenzene	2.81E-06	3.24E-07	5.39E-07	1.31E-06	4.98E-06
Toluene	7.15E-06	5.02E-07	7.33E-06	1.15E-05	2.65E-05
Xylenes	4.93E-06	6.16E-07	2.74E-05	6.13E-06	3.91E-05
Total	1.80E-01	5.88E-03	1.11E-01	2.93E-03	3.00E-01

Figure 7-2(a). Example of Table Obtained by Selecting Deterministic Table 1.



Total Dose for Each Chemical of Concern

Chemical	Daily Intake (DI) (mg/kg-d)	Chronic Daily Intake (CDI) (mg/kg-d)	Lifetime Average Daily Dose (LADD) (mg/kg-d)
Benzene	5.30E-04	5.08E-04	6.54E-05
Ethylbenzene	8.86E-07	8.48E-07	1.09E-07
Toluene	3.84E-06	3.68E-06	4.72E-07
Xylenes	1.86E-05	1.78E-05	2.29E-06

Figure 7-2(b). Example of Table Obtained by Selecting Deterministic Table 2.

Dose by Chemical for Each Route of Concern (mg/kg-day)

Drinking Water

	Intake	Value
Benzene	DI	3.18E-04
	CDI	3.05E-04
	LADD	3.93E-05
Ethylbenzene	DI	2.93E-07
	CDI	2.81E-07
	LADD	3.61E-08
Toluene	DI	1.49E-06
	CDI	1.43E-06
	LADD	1.84E-07
Xylenes	DI	1.03E-05
	CDI	9.87E-06
	LADD	1.27E-06

Dermal Uptake During Shower

	Intake	Value
Benzene	DI	1.04E-05
	CDI	1.00E-05
	LADD	1.29E-06
Ethylbenzene	DI	3.38E-08
	CDI	3.24E-08
	LADD	4.17E-09
Toluene	DI	1.05E-07
	CDI	1.00E-07
	LADD	1.29E-08
Xylenes	DI	1.28E-06
	CDI	1.23E-06
	LADD	1.58E-07

Inhalation During Shower

	Intake	Value
Benzene	DI	1.96E-04
	CDI	1.88E-04
	LADD	2.42E-05
Ethylbenzene	DI	1.63E-07
	CDI	1.56E-07
	LADD	2.01E-08
Toluene	DI	8.71E-07
	CDI	8.35E-07
	LADD	1.07E-07
Xylenes	DI	5.72E-06
	CDI	5.48E-06
	LADD	7.05E-07

Inhalation of Soil Emissions

	Intake	Value
Benzene	DI	5.16E-06
	CDI	4.94E-06
	LADD	6.36E-07
Ethylbenzene	DI	3.96E-07
	CDI	3.79E-07
	LADD	4.88E-08
Toluene	DI	1.37E-06
	CDI	1.31E-06
	LADD	1.68E-07
Xylenes	DI	1.28E-06
	CDI	1.23E-06
	LADD	1.58E-07

Figure 7-2(c). Example of Table Obtained by Selecting Deterministic Table 3.

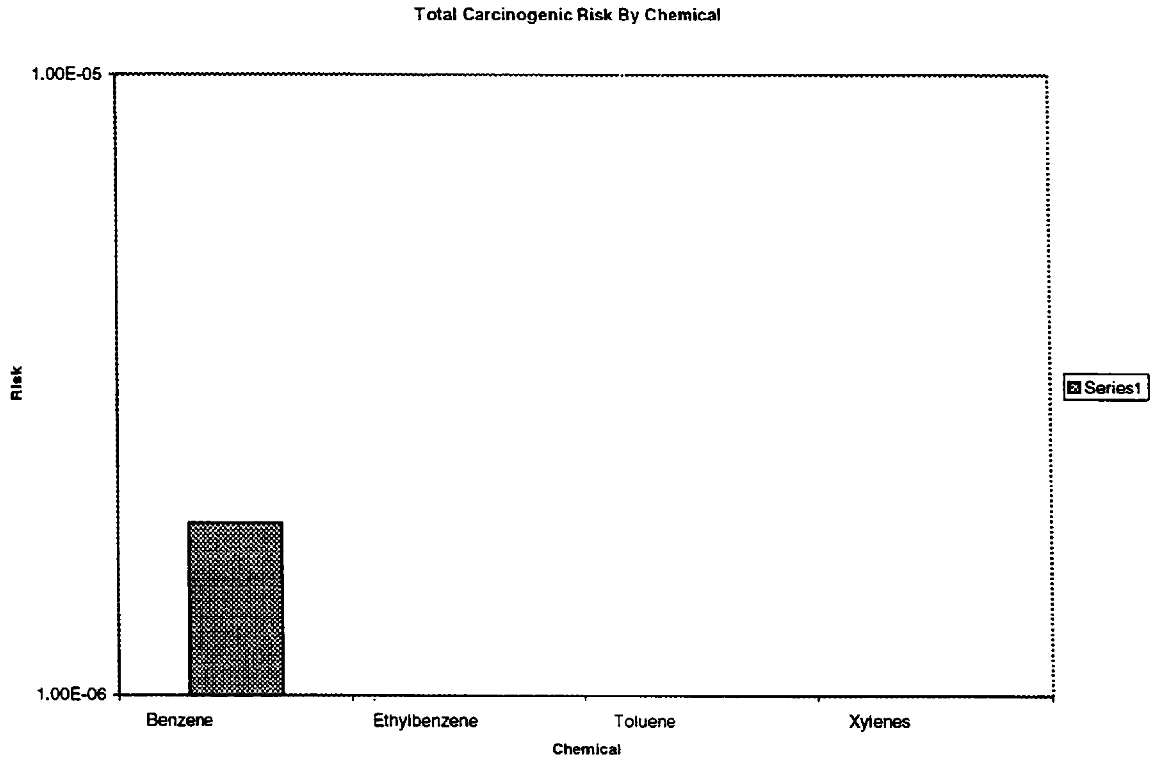


Figure 7-3(a). Example of Chart Obtained by Selecting Deterministic Chart 1.

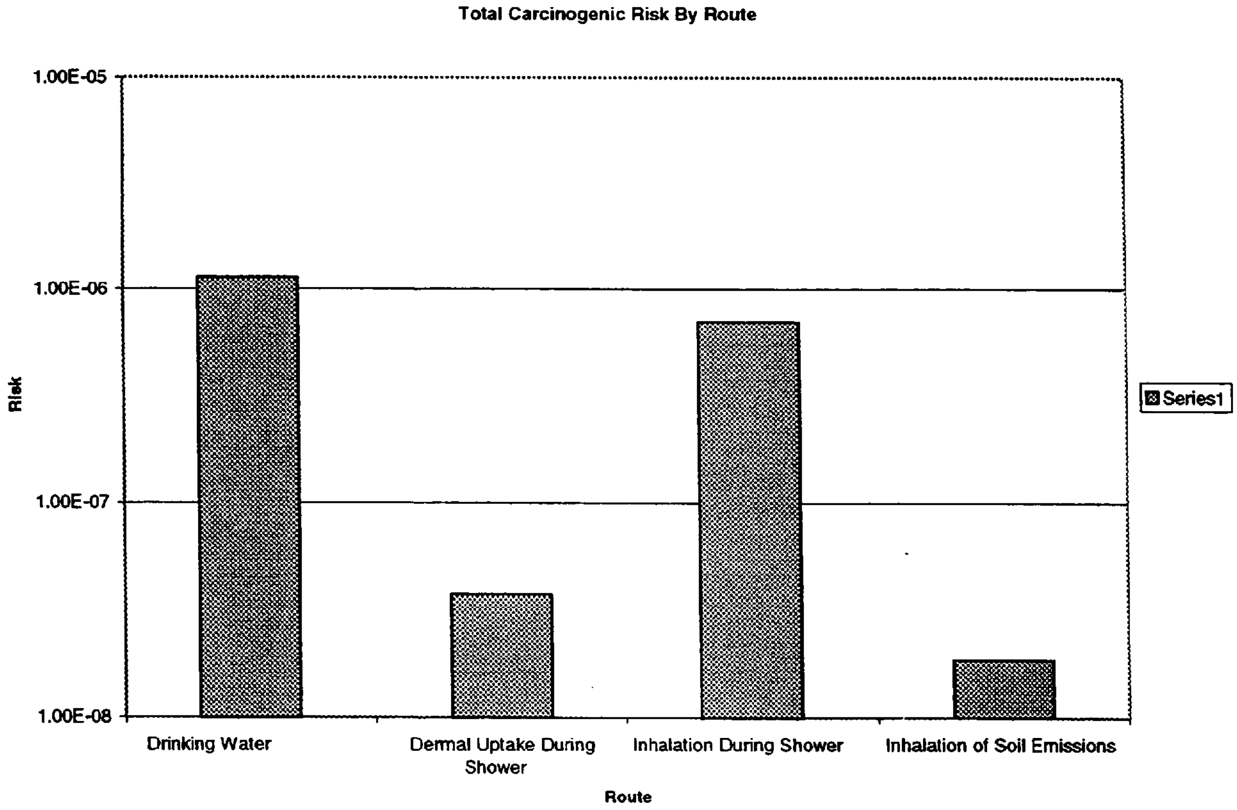


Figure 7-3(b). Example of Chart Obtained by Selecting Deterministic Chart 2.

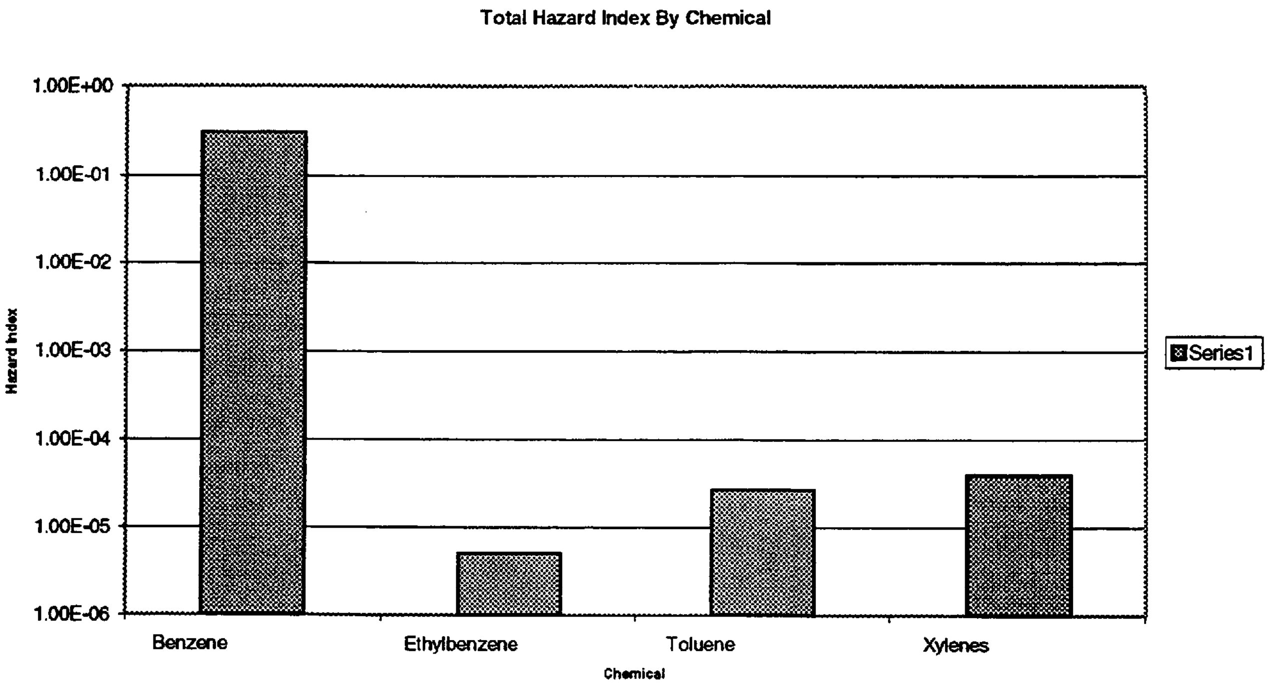


Figure 7-3(c). Example of Chart Obtained by Selecting Deterministic Chart 3.

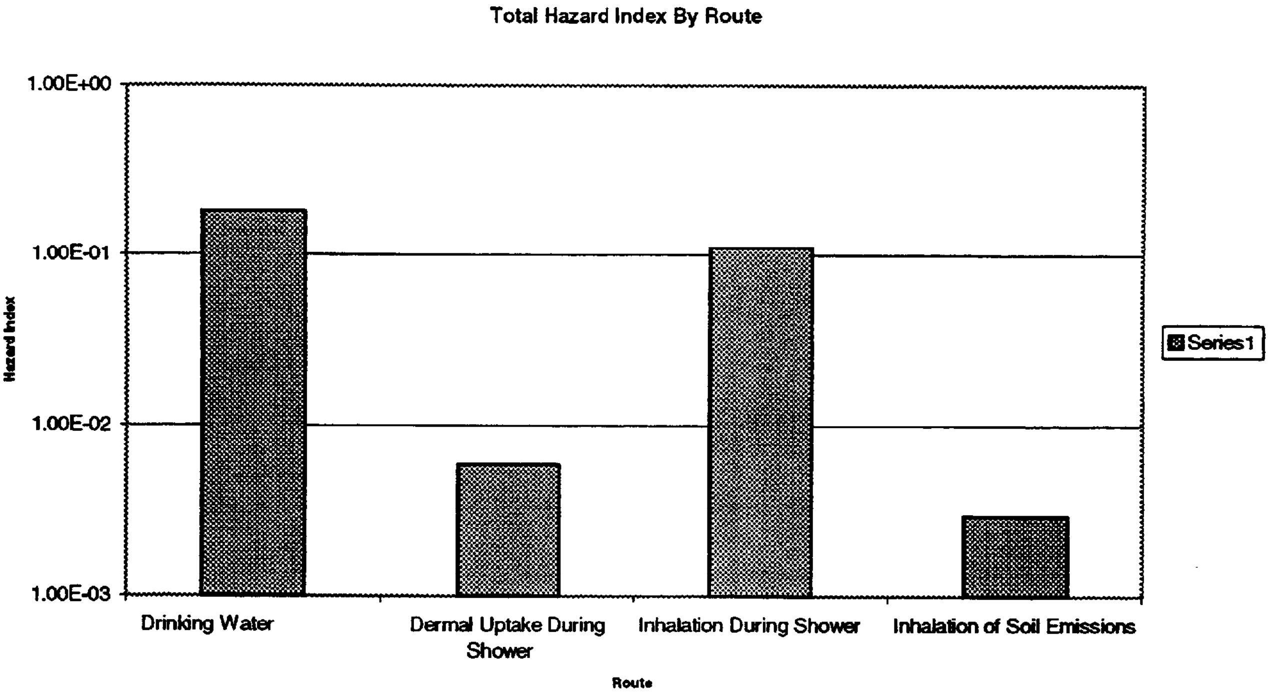


Figure 7-3(d). Example of Chart Obtained by Selecting Deterministic Chart 4.

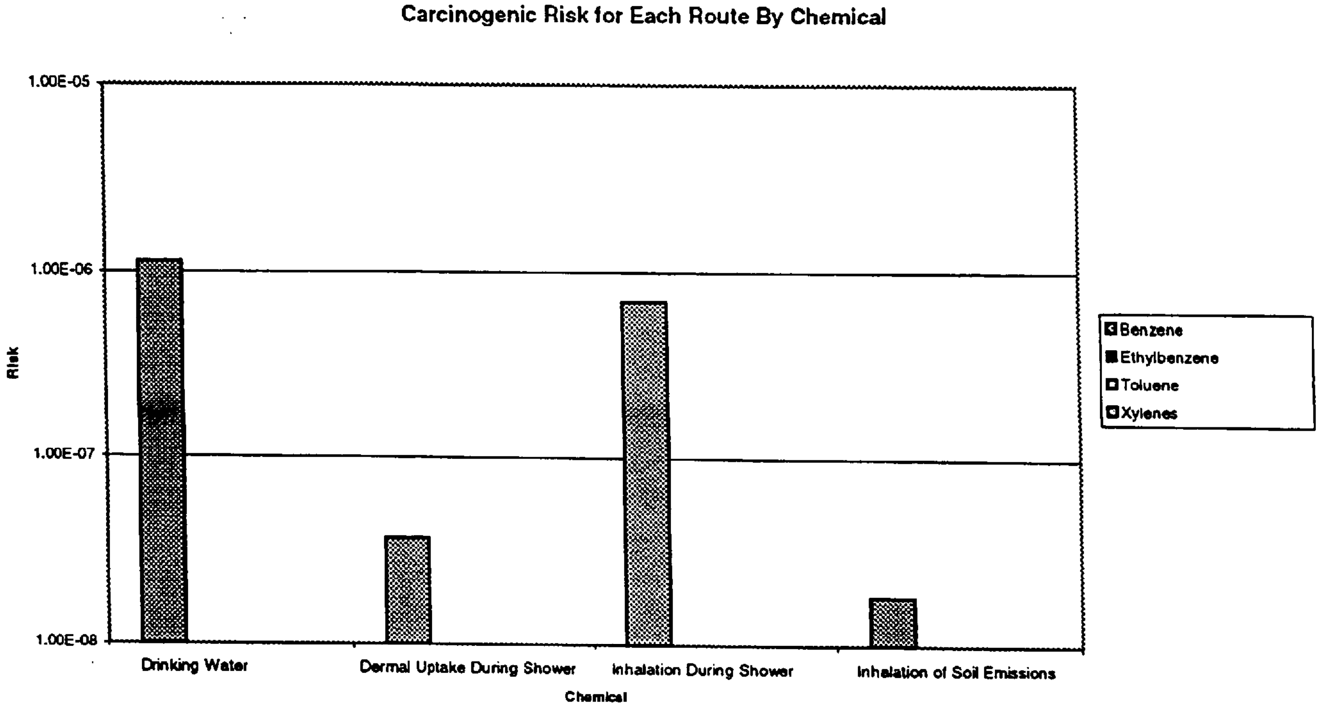


Figure 7-3(e). Example of Chart Obtained by Selecting Deterministic Chart 5.

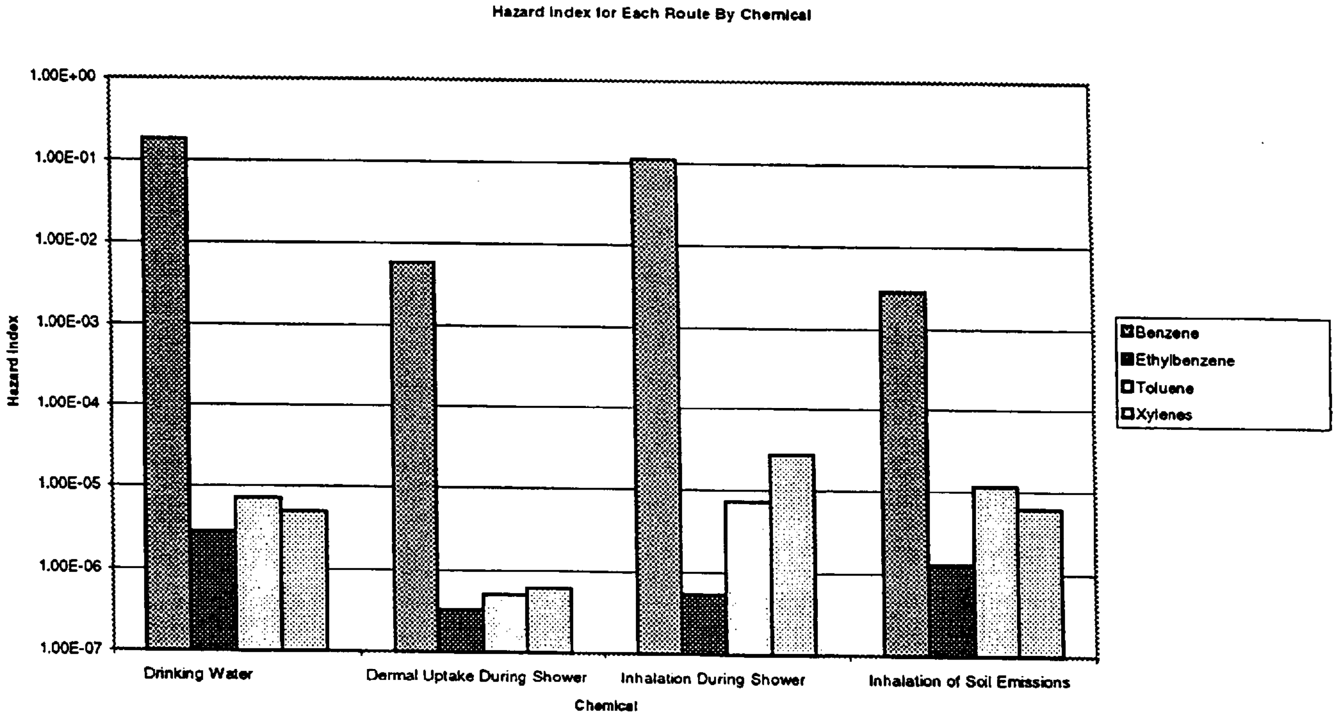
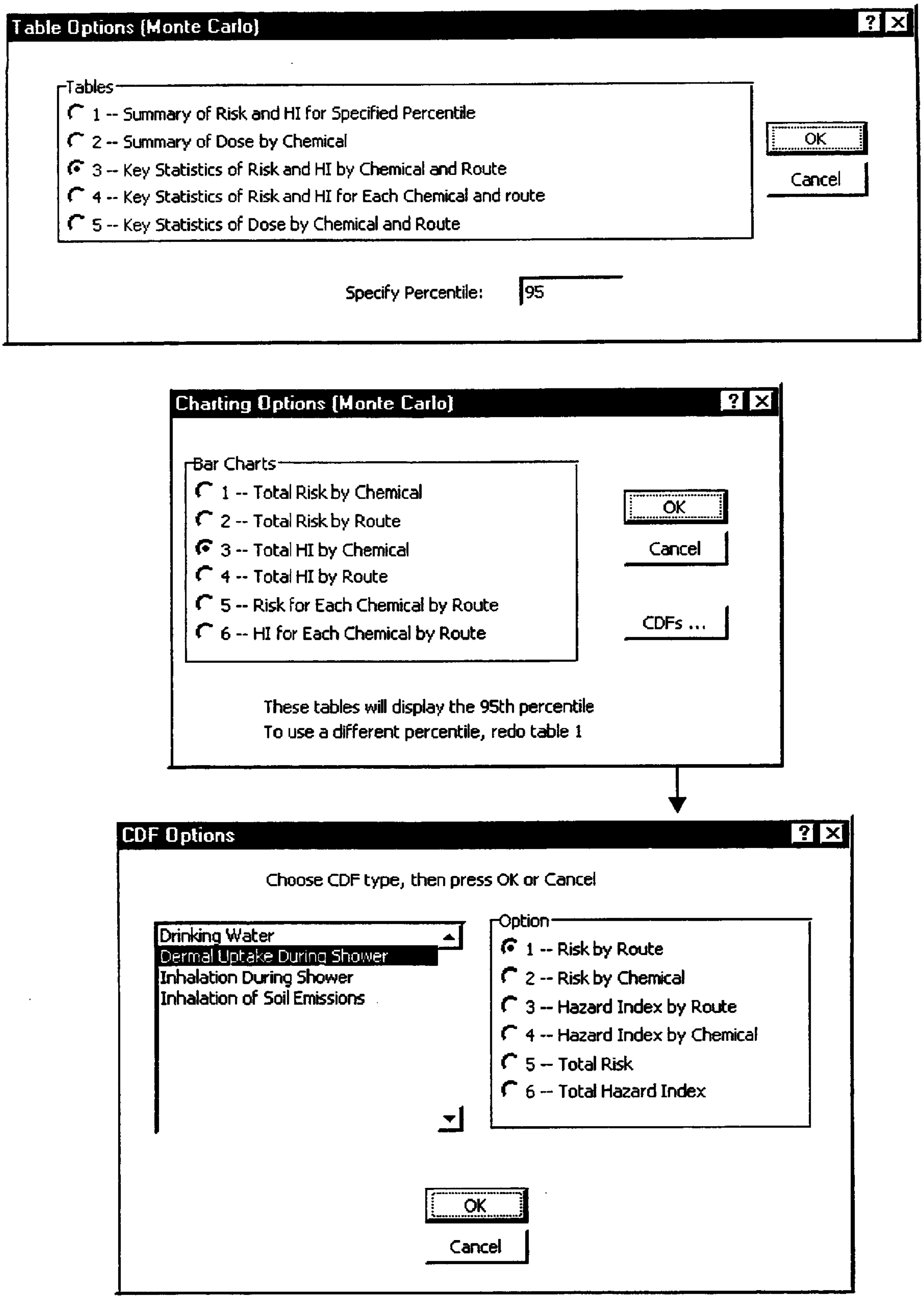


Figure 7-3(f). Example of Chart Obtained by Selecting Deterministic Chart 6.



Tables

○ 1 -- Summary of Risk and HI for Specified Percentile
○ 2 -- Summary of Dose by Chemical
● 3 -- Key Statistics of Risk and HI by Chemical and Route
○ 4 -- Key Statistics of Risk and HI for Each Chemical and route
○ 5 -- Key Statistics of Dose by Chemical and Route

Specify Percentile: 95

Bar Charts

○ 1 -- Total Risk by Chemical
○ 2 -- Total Risk by Route
● 3 -- Total HI by Chemical
○ 4 -- Total HI by Route
○ 5 -- Risk for Each Chemical by Route
○ 6 -- HI for Each Chemical by Route

These tables will display the 95th percentile
To use a different percentile, redo table 1

Choose CDF type, then press OK or Cancel

Drinking Water
Dermal Uptake During Shower
Inhalation During Shower
Inhalation of Soil Emissions

Option

● 1 -- Risk by Route
○ 2 -- Risk by Chemical
○ 3 -- Hazard Index by Route
○ 4 -- Hazard Index by Chemical
○ 5 -- Total Risk
○ 6 -- Total Hazard Index

Figure 7-4. Available Options for Presenting Monte Carlo Results.

85th Percentile Risk by Chemical for Each Route of Concern

Chemical	Ingestion of Drinking Water	Dermal Uptake During Shower	Inhalation During Shower	Inhalation of Soil Emissions	Total
Benzene	1.68E-06	1.19E-07	5.79E-06	9.16E-08	7.68E-06
Ethylbenzene	ND	ND	ND	ND	0.00E+00
Toluene	ND	ND	ND	ND	0.00E+00
Xylenes	ND	ND	ND	ND	0.00E+00
Total	1.68E-06	1.19E-07	5.79E-06	9.16E-08	7.68E-06

85th Percentile Hazard Index by Chemical for Each Route of Concern

Chemical	Ingestion of Drinking Water	Dermal Uptake During Shower	Inhalation During Shower	Inhalation of Soil Emissions	Total
Benzene	3.15E-01	2.39E-02	1.23E+00	2.17E-02	1.59E+00
Ethylbenzene	4.93E-06	1.32E-06	5.97E-06	9.79E-06	2.20E-05
Toluene	1.25E-05	2.04E-06	8.12E-05	8.59E-05	1.82E-04
Xylenes	8.66E-06	2.51E-06	3.04E-04	4.58E-05	3.61E-04
Total	3.15E-01	2.39E-02	1.23E+00	2.19E-02	1.59E+00

Number of Monte Carlo Runs: 500
ND = Not Determined because RfD or Slope Factor not entered
NA = Not Applicable
09/02/98 22:53

Figure 7-5(a). Example of Table Obtained by Selecting Monte Carlo Table 1.

85th Percentile Total Dose for Each Chemical of Concern (mg/kg-day)

Chemical	Daily Intake (DI) [mg/kg-d]	Chronic Daily Intake (CDI) [mg/kg-d]	Lifetime Average Daily Dose (LADD) [mg/kg-d]
Benzene	2.14E-03	2.67E-03	2.48E-04
Ethylbenzene	4.02E-06	4.48E-06	4.11E-07
Toluene	1.65E-05	1.88E-05	1.70E-06
Xylenes	7.34E-05	8.68E-05	8.53E-06

Number of Monte Carlo Runs: 500

NA = Not Applicable
09/02/98 22:53

Figure 7-5(b). Example of Table Obtained by Selecting Monte Carlo Table 2.

Total Carcinogenic Risk by Chemical

Chemical	Median	Standard Deviation	Min	Max	85th Percentile	95th Percentile
Benzene	3.51E-06	3.17E-06	3.42E-07	1.76E-05	7.18E-06	1.10E-05
Ethylbenzene	ND	0.00E+00	ND	ND	ND	ND
Toluene	ND	0.00E+00	ND	ND	ND	ND
Xylenes	ND	0.00E+00	ND	ND	ND	ND
Total	3.51E-06	NA	3.42E-07	1.76E-05	7.18E-06	1.10E-05

Total Hazard Index by Chemical

Chemical	Median	Standard Deviation	Min	Max	85th Percentile	95th Percentile
Benzene	7.84E-01	5.88E-01	2.65E-01	3.19E+00	1.57E+00	2.16E+00
Ethylbenzene	1.32E-05	4.99E-06	4.62E-06	3.24E-05	1.92E-05	2.27E-05
Toluene	9.80E-05	4.90E-05	2.02E-05	2.93E-04	1.54E-04	1.96E-04
Xylenes	1.56E-04	1.42E-04	2.08E-05	7.22E-04	3.42E-04	4.90E-04
Total	7.84E-01	NA	2.65E-01	3.19E+00	1.57E+00	2.16E+00

Total Carcinogenic Risk by Route

Route	Median	Standard Deviation	Min	Max	85th Percentile	95th Percentile
Drinking Water	1.24E-06	4.47E-07	1.21E-07	2.40E-06	1.68E-06	1.93E-06
Dermal Uptake During Show	6.72E-08	4.36E-08	5.21E-09	2.31E-07	1.19E-07	1.58E-07
Inhalation During Shower	2.22E-06	2.92E-06	6.37E-08	1.53E-05	5.79E-06	9.15E-06
Inhalation of Soil Emissions	4.60E-08	3.64E-08	2.38E-09	1.77E-07	9.16E-08	1.24E-07
Total	3.57E-06	NA	1.92E-07	1.81E-05	7.68E-06	1.14E-05

Total Hazard Index by Route

Route	Median	Standard Deviation	Min	Max	85th Percentile	95th Percentile
Drinking Water	2.60E-01	4.65E-02	1.53E-01	3.58E-01	3.15E-01	3.45E-01
Dermal Uptake During Show	1.48E-02	7.58E-03	3.96E-03	3.95E-02	2.39E-02	3.02E-02
Inhalation During Shower	4.87E-01	5.68E-01	3.92E-02	2.83E+00	1.23E+00	1.83E+00
Inhalation of Soil Emissions	1.18E-02	7.72E-03	8.32E-04	3.40E-02	2.19E-02	2.53E-02
Total	7.73E-01	NA	1.97E-01	3.26E+00	1.59E+00	2.23E+00

Number of Monte Carlo Runs: 500
ND = Not Determined because RfD or Slope Factor not entered
NA = Not Applicable
09/02/98 22:53

Figure 7-5(c). Example of Table Obtained by Selecting Monte Carlo Table 3.

Carcinogenic Risk by Chemical for Each Route of Concern

Drinking Water

Chemical	Median	Standard Deviation	Min	Max	85th Percentile	95th Percentile
Benzene	1.24E-06	4.47E-07	1.21E-07	2.40E-06	1.68E-06	1.93E-06
Ethylbenzene	ND	0.00E+00	ND	ND	ND	ND
Toluene	ND	0.00E+00	ND	ND	ND	ND
Xylenes	ND	0.00E+00	ND	ND	ND	ND
Total	1.24E-06	4.47E-07	1.21E-07	2.40E-06	1.68E-06	1.93E-06

Dermal Uptake During Shower

Chemical	Median	Standard Deviation	Min	Max	85th Percentile	95th Percentile
Benzene	6.72E-08	4.36E-08	5.21E-09	2.31E-07	1.19E-07	1.58E-07
Ethylbenzene	ND	0.00E+00	ND	ND	ND	ND
Toluene	ND	0.00E+00	ND	ND	ND	ND
Xylenes	ND	0.00E+00	ND	ND	ND	ND
Total	6.72E-08	4.36E-08	5.21E-09	2.31E-07	1.19E-07	1.58E-07

Inhalation During Shower

Chemical	Median	Standard Deviation	Min	Max	85th Percentile	95th Percentile
Benzene	2.22E-06	2.92E-06	6.37E-08	1.53E-05	5.79E-06	9.15E-06
Ethylbenzene	ND	0.00E+00	ND	ND	ND	ND
Toluene	ND	0.00E+00	ND	ND	ND	ND
Xylenes	ND	0.00E+00	ND	ND	ND	ND
Total	2.22E-06	2.92E-06	6.37E-08	1.53E-05	5.79E-06	9.15E-06

Inhalation of Soil Emissions

Chemical	Median	Standard Deviation	Min	Max	85th Percentile	95th Percentile
Benzene	4.60E-08	3.64E-08	2.38E-09	1.77E-07	9.16E-08	1.24E-07
Ethylbenzene	ND	0.00E+00	ND	ND	ND	ND
Toluene	ND	0.00E+00	ND	ND	ND	ND
Xylenes	ND	0.00E+00	ND	ND	ND	ND
Total	4.60E-08	3.64E-08	2.38E-09	1.77E-07	9.16E-08	1.24E-07

Figure 7-5(d). Example of Table Obtained by Selecting Monte Carlo Table 4 (continued).

Hazard Index by Chemical for Each Route of Concern

Drinking Water

Chemical	Median	Standard Deviation	Min	Max	85th Percentile	95th Percentile
Benzene	2.60E-01	4.65E-02	1.53E-01	3.58E-01	3.15E-01	3.45E-01
Ethylbenzene	4.07E-06	7.26E-07	2.40E-06	5.59E-06	4.93E-06	5.39E-06
Toluene	1.04E-05	1.85E-06	6.10E-06	1.42E-05	1.25E-05	1.37E-05
Xylenes	7.14E-06	1.28E-06	4.21E-06	9.83E-06	8.66E-06	9.47E-06
Total	2.60E-01	4.65E-02	1.53E-01	3.58E-01	3.15E-01	3.45E-01

Dermal Uptake During Shower

Chemical	Median	Standard Deviation	Min	Max	85th Percentile	95th Percentile
Benzene	1.48E-02	7.58E-03	3.96E-03	3.95E-02	2.39E-02	3.02E-02
Ethylbenzene	8.16E-07	4.17E-07	2.18E-07	2.18E-06	1.32E-06	1.66E-06
Toluene	1.26E-06	6.47E-07	3.38E-07	3.37E-06	2.04E-06	2.57E-06
Xylenes	1.55E-06	7.93E-07	4.14E-07	4.13E-06	2.51E-06	3.16E-06
Total	1.48E-02	7.58E-03	3.96E-03	3.95E-02	2.39E-02	3.02E-02

Inhalation During Shower

Chemical	Median	Standard Deviation	Min	Max	85th Percentile	95th Percentile
Benzene	4.86E-01	5.68E-01	3.92E-02	2.83E+00	1.23E+00	1.83E+00
Ethylbenzene	2.37E-06	2.76E-06	1.91E-07	1.38E-05	5.97E-06	8.91E-06
Toluene	3.22E-05	3.75E-05	2.59E-06	1.87E-04	8.12E-05	1.21E-04
Xylenes	1.21E-04	1.40E-04	9.69E-06	7.01E-04	3.04E-04	4.52E-04
Total	4.86E-01	5.68E-01	3.92E-02	2.83E+00	1.23E+00	1.83E+00

Inhalation of Soil Emissions

Chemical	Median	Standard Deviation	Min	Max	85th Percentile	95th Percentile
Benzene	1.18E-02	7.67E-03	8.26E-04	3.38E-02	2.17E-02	2.51E-02
Ethylbenzene	5.29E-06	3.45E-06	3.72E-07	1.52E-05	9.79E-06	1.13E-05
Toluene	4.65E-05	3.03E-05	3.26E-06	1.33E-04	8.59E-05	9.92E-05
Xylenes	2.48E-05	1.62E-05	1.74E-06	7.11E-05	4.58E-05	5.29E-05
Total	1.19E-02	7.72E-03	8.31E-04	3.40E-02	2.19E-02	2.53E-02

Figure 7-5(d). Example of Table Obtained by Selecting Monte Carlo Table 4 (concluded).

Dose by Chemical for Each Route of Concern (mg/kg-day)

Drinking Water

	Intake	Median	Standard Deviation	Min	Max	85th Percentile	95th Percentile
Benzene	DI	3.64E-04	1.28E-04	1.00E-04	6.34E-04	5.07E-04	5.92E-04
	CDI	4.42E-04	7.90E-05	2.61E-04	6.08E-04	5.36E-04	5.86E-04
	LADD	4.27E-05	1.54E-05	4.16E-06	8.26E-05	5.79E-05	6.65E-05
Ethylbenzene	DI	3.28E-07	1.21E-07	8.76E-08	5.83E-07	4.66E-07	5.44E-07
	CDI	4.07E-07	7.26E-08	2.40E-07	5.59E-07	4.93E-07	5.39E-07
	LADD	3.78E-08	1.39E-08	3.83E-09	7.60E-08	5.14E-08	6.01E-08
Toluene	DI	1.63E-06	6.40E-07	4.22E-07	2.97E-06	2.38E-06	2.77E-06
	CDI	2.07E-06	3.70E-07	1.22E-06	2.85E-06	2.51E-06	2.74E-06
	LADD	1.86E-07	6.92E-08	1.95E-08	3.87E-07	2.56E-07	3.06E-07
Xylenes	DI	1.19E-05	3.95E-06	3.48E-06	2.05E-05	1.64E-05	1.91E-05
	CDI	1.43E-05	2.55E-06	8.42E-06	1.97E-05	1.73E-05	1.89E-05
	LADD	1.45E-06	5.17E-07	1.35E-07	2.67E-06	1.90E-06	2.21E-06

Dermal Uptake During Shower

	Intake	Median	Standard Deviation	Min	Max	85th Percentile	95th Percentile
Benzene	DI	1.94E-05	1.25E-05	3.70E-06	7.00E-05	3.51E-05	4.81E-05
	CDI	2.52E-05	1.29E-05	6.73E-06	6.71E-05	4.07E-05	5.13E-05
	LADD	2.32E-06	1.50E-06	1.80E-07	7.95E-06	4.10E-06	5.44E-06
Ethylbenzene	DI	6.17E-08	4.08E-08	1.14E-08	2.27E-07	1.14E-07	1.56E-07
	CDI	8.16E-08	4.17E-08	2.18E-08	2.18E-07	1.32E-07	1.66E-07
	LADD	7.27E-09	4.75E-09	5.82E-10	2.58E-08	1.30E-08	1.71E-08
Toluene	DI	1.89E-07	1.27E-07	3.34E-08	7.03E-07	3.51E-07	4.83E-07
	CDI	2.53E-07	1.29E-07	6.75E-08	6.74E-07	4.09E-07	5.15E-07
	LADD	2.17E-08	1.43E-08	1.80E-09	7.98E-08	3.89E-08	5.08E-08
Xylenes	DI	2.45E-06	1.53E-06	4.89E-07	8.62E-06	4.34E-06	5.92E-06
	CDI	3.10E-06	1.59E-06	8.28E-07	8.27E-06	5.01E-06	6.32E-06
	LADD	2.92E-07	1.92E-07	2.21E-08	9.79E-07	5.23E-07	7.12E-07

Figure 7-5(e). Example of Table Obtained by Selecting Monte Carlo Table 5 (continued).

Inhalation During Shower

	Intake	Median	Standard Deviation	Min	Max	85th Percentile	95th Percentile
Benzene	DI	6.37E-04	8.57E-04	4.04E-05	4.89E-03	1.73E-03	2.75E-03
	CDI	8.27E-04	9.65E-04	6.66E-05	4.82E-03	2.08E-03	3.11E-03
	LADD	7.63E-05	1.01E-04	2.20E-06	5.26E-04	2.00E-04	3.16E-04
Ethylbenzene	DI	5.16E-07	7.09E-07	3.19E-08	4.06E-06	1.40E-06	2.28E-06
	CDI	6.86E-07	8.01E-07	5.53E-08	4.00E-06	1.73E-06	2.58E-06
	LADD	6.13E-08	8.17E-08	1.82E-09	4.37E-07	1.59E-07	2.51E-07
Toluene	DI	2.65E-06	3.77E-06	1.61E-07	2.17E-05	7.32E-06	1.22E-05
	CDI	3.66E-06	4.28E-06	2.95E-07	2.14E-05	9.25E-06	1.38E-05
	LADD	3.12E-07	4.25E-07	9.74E-09	2.33E-06	8.14E-07	1.33E-06
Xylenes	DI	1.94E-05	2.51E-05	1.26E-06	1.42E-04	5.17E-05	8.12E-05
	CDI	2.41E-05	2.81E-05	1.94E-06	1.40E-04	6.07E-05	9.06E-05
	LADD	2.27E-06	3.04E-06	6.39E-08	1.53E-05	5.88E-06	9.73E-06

Inhalation of Soil Emissions

	Intake	Median	Standard Deviation	Min	Max	85th Percentile	95th Percentile
Benzene	DI	1.51E-05	1.32E-05	4.49E-07	5.62E-05	3.39E-05	4.27E-05
	CDI	2.00E-05	1.30E-05	1.40E-06	5.74E-05	3.69E-05	4.27E-05
	LADD	1.59E-06	1.26E-06	8.22E-08	6.09E-06	3.16E-06	4.30E-06
Ethylbenzene	DI	1.16E-06	1.01E-06	3.45E-08	4.32E-06	2.60E-06	3.28E-0
	CDI	1.54E-06	1.00E-06	1.08E-07	4.40E-06	2.84E-06	3.28E-06
	LADD	1.22E-07	9.64E-08	6.31E-09	4.67E-07	2.42E-07	3.29E-07
Toluene	DI	3.98E-06	3.49E-06	1.19E-07	1.49E-05	8.98E-06	1.13E-05
	CDI	5.30E-06	3.45E-06	3.72E-07	1.52E-05	9.80E-06	1.13E-05
	LADD	4.21E-07	3.32E-07	2.18E-08	1.61E-06	8.34E-07	1.14E-06
Xylenes	DI	3.73E-06	3.26E-06	1.13E-07	1.39E-05	8.40E-06	1.06E-05
	CDI	4.96E-06	3.23E-06	3.48E-07	1.42E-05	9.17E-06	1.06E-05
	LADD	3.94E-07	3.13E-07	2.04E-08	1.51E-06	7.87E-07	1.06E-06

Number of Monte Carlo Runs: 500
ND = Not Determined because RfD or Slope Factor not entered
NA = Not Applicable
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Figure 7-5(e). Example of Table Obtained by Selecting Monte Carlo Table 5 (concluded).

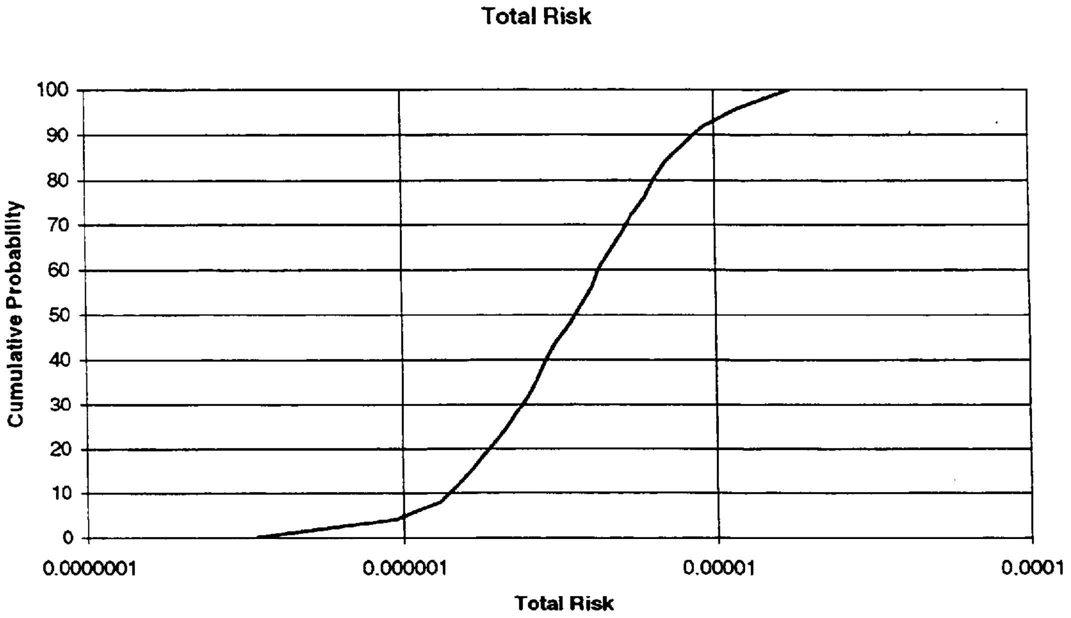

Figure 7-6. Example of Chart Obtained by CDF Chart Option 5: CDF of Total Risk.

8.0

UNCERTAINTY ANALYSIS

The Risk Calculation model may be run in a Monte Carlo mode. Monte Carlo analysis allows the evaluation of uncertainty in input parameters for a given model. In a risk determination, variables such as exposure frequency and duration can vary considerably from one potential receptor to the next. Therefore, it is often more appropriate to express their value in terms of a probability distribution rather than a single deterministic value and to use an uncertainty propagation model to assess the effect of the variability on the output of the models (i.e., to assess the uncertainty in the risk and hazard index values).

This section presents the uncertainty propagation method (Monte Carlo simulation technique) implemented in the DSS. The method allows a quantitative estimate of the uncertainty in the risk/hazard index estimated using the DSS.

8.1 UNCERTAINTY IN THE INPUT VARIABLES

For exposure and risk analysis, input variables can be broadly classified into two categories having different uncertainty characteristics. These are:

(i) Variables that describe the physical and toxicological properties of the chemicals of concern. A few examples of these include parameters such as bioavailability, Henry's law constant, and carcinogenic slope factors.

(ii) Variables that describe the environmental properties of various media, as well as characteristics of human receptors. A few examples of these include groundwater concentrations, skin surface area, and inhalation rate.

Uncertainty in the first set of variables arises primarily due to non-systematic/random laboratory measurement errors or due to the use of empirical and/or theoretical methods used to estimate numerical values. In addition to experimental precision

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and accuracy, errors may arise due to extrapolations from controlled (laboratory) measurement conditions to uncontrolled (field) conditions.

Uncertainty in the second set of variables may include measurement and extrapolation errors, but is predominantly due to inherent natural variability (e.g., spatial, temporal, and interhuman variability). For environmental properties, this can be due to the natural variability of soil, groundwater, and meteorologic properties within the region of interest. For human exposure parameters, uncertainty arises primarily due to the variability of physiological and behavioral characteristics from person to person. This uncertainty will depend upon the scale of the problem, since greater variability will result in an assessment of large-scale regional risks than in an assessment of site-specific local risks.

Whatever the source of the parameter uncertainty, the uncertainty can be quantified using a cumulative probability distribution. Thus, for each parameter to be analyzed as an uncertain variable, the user needs to select and assign a probability distribution for the variable and specify the parameters that describe the distribution. Methods for testing and fitting probability distributions to data are described in Benjamin and Cornell (1970).

The current version of the DSS allows the user to assign one of the following five probability distributions to quantify uncertainty in the chemical intake input variables:

(i) Normal
(ii) Log Normal
(iii) Uniform
(iv) Exponential
(v) Triangular

Alternatively, the DSS allows a constant value to be assigned to any variable. Many environmental data are skewed and bounded by zero (or the method detection limit), and can be represented well by log-normal distributions. A uniform distribution can be used only if the range of possible values is known; if the most likely value (or mode) is also known, a triangular distribution can be used. Appendix K provides a brief discussion of each probability distribution.

In addition to the parameters of the distribution, it is important to specify the upper and lower bounds of each distribution. These bounds may be based on available data or physical considerations (e.g., porosity must be greater than 0 and less than 1.0). Specifying upper and lower bounds will ensure that the randomly generated values from the distributions are not outside these specified bounds.

Having quantified the uncertainty in the input parameters, the Monte Carlo simulation technique is used to propagate the uncertainty through the computational algorithm in the Chemical Intake and Risk Calculation module to estimate the uncertainty in chemical intake, risk and hazard index. The Monte Carlo simulation technique, as well as its specific application for the DSS, is presented below.

8.2 DESCRIPTION OF THE MONTE CARLO METHOD

Figure 8-1 illustrates how the Monte Carlo method performs uncertainty analysis. In the analysis, computation algorithms (equations used to estimate risk in this case) are represented as a function g(X) relating the model output Y to the input parameters $X_1, X_2, \ldots X_n$:

$$Y = g(X_1, X_2, \ldots X_n) \qquad (8\text{-}1)$$

A user-specified number (N_{sim}) of sets of input parameters ($X_1 \ldots X_n$) is randomly generated from the probability distributions that describe the uncertainty in each input parameter. The model is applied N_{sim} times using the randomly generated sets of input parameters, resulting in N_{sim} values of the model output Y. This series of outputs is then statistically analyzed to yield a cumulative probability distribution of Y. The specific steps involved in the application of the method are as follows:

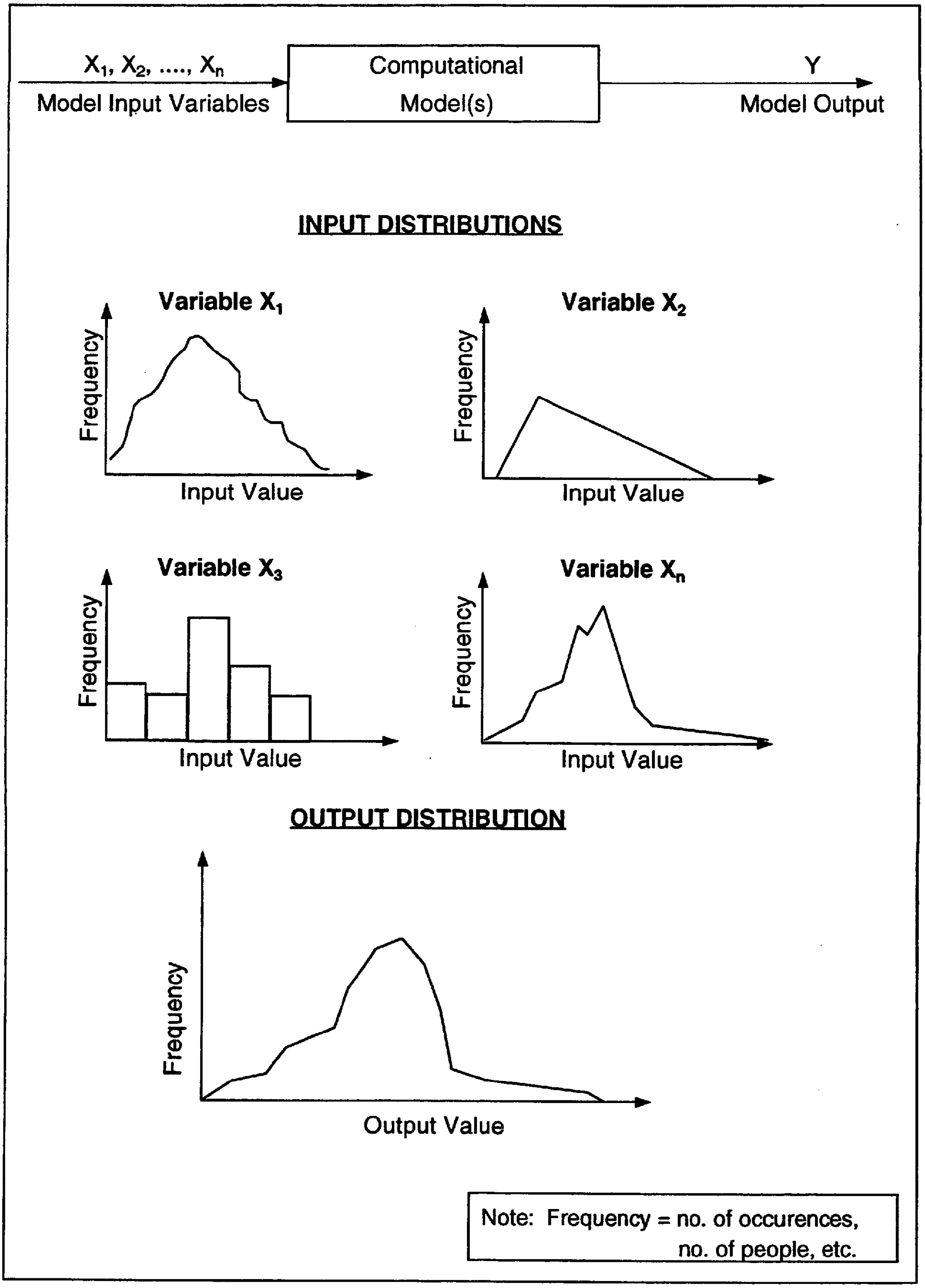

Figure 8-1. Schematic Description of the Monte Carlo Method of Uncertainty Analysis.

(i) Select probability distributions to describe uncertainty in model input variables.

(ii) Generate a set of random values of input variables from the distributions selected in (i) using random number generators.

(iii) Apply the model using the randomly generated input values. Store the calculated output value.

(iv) Repeat steps (ii) and (iii) until a sample of model outputs sufficiently large for statistical analysis is produced.

(v) Use the results from (iv) to develop probability distributions of model outputs for use as a tool in decision making.

Step (i) should be performed by the user prior to using the DSS, and involves statistical analysis of data collected from on-site sampling activities or the open literature. Methods for testing and fitting probability distributions to data are described in Benjamin and Cornell (1970).

Steps (ii), (iii), (iv), and (v) of the uncertainty analysis are performed for the user by the DSS. The number of Monte Carlo runs required in Step (iv) will depend upon the variability of the model inputs, the response of the model output to inputs, and the percentile (or confidence level) in which the user is interested. There is no way of knowing beforehand how many runs are sufficient; a common approach is to try different numbers of runs (e.g., 50, 100, 500, 1000, and 5000) and observe the convergence in the confidence bounds about the estimated percentile as the number of runs increases. Generally, 1000 or more runs are required for accurate estimation of low-frequency parameters such as the 90th or 95th percentile of the model output. **The DSS allows a maximum of 10,000 Monte Carlo simulations.**

The output of the Monte Carlo simulation is the N_{sim} number of model output (Y) values which are used in Step (v) to develop a cumulative probability distribution of

Y. This distribution quantitatively describes the uncertainty in the model output and can be used for decision making.

8.3 APPLICATION OF THE MONTE CARLO METHOD IN THE DECISION SUPPORT SYSTEM

The DSS performs Monte Carlo analyses of the Risk Calculation module only. This analysis may use the results of a deterministic fate and transport model run. As explained in Section 5.0, implementation of the contaminant fate and transport models results in the breakthrough curve, (i.e., estimate of receptor point concentration as a function of time). (In the event that the fate and transport models are time invariant these concentrations do not vary over time.) The breakthrough curves are analyzed by the DSS to compute the maximum receptor-point chemical concentrations in each medium for a series of averaging periods ranging from 5 years to 75 years at 5-year intervals (see Figure 5-3). These data are stored on the computer's hard drive and are then used in the Chemical Intake and Risk Calculation module.

If the Chemical Intake and Risk Calculation module is implemented in the Monte Carlo mode, the estimated concentration distributions are internally read by the risk calculation FORTRAN code as an empirical distribution for the specific exposure period. Selection of the concentration distribution is approximate if the exposure time is not a multiple of five. For example, if the exposure period is 37 years, the model uses concentrations corresponding to 35-year averaging periods. This applies for both the Monte Carlo and deterministic cases.

Following are the specific steps used in Monte Carlo analysis of the risk assessment process:

(i) In the Chemical Intake and Risk Calculation module, select frequency distributions for relevant input parameters. At least one input parameter must have a non-constant distribution.

(ii) Perform a Monte Carlo analysis (run the risk code) using a maximum of 10,000 model runs.

(iii) Run the Risk Presentation module to review the results and print charts and tables as explained in Section 7.0.

Output of the Monte Carlo analysis results in cumulative frequency distributions of intake, carcinogenic risk and the hazard index. These distributions reflect a reasonable range of values for the dose, risk and hazard index corresponding to the specified uncertainty in the input parameters and can be used to estimate the most likely (e.g., 50th percentile) or the worst case (e.g., 90th or 95th percentile) value for risk or hazard index. These best and worst case risk estimates are more realistic since they explicitly account for the uncertainty in the inputs. The estimates obtained in a deterministic analysis using the combination of most likely and/or the worst case values for each input parameter may not necessarily result in the most likely and worst case risk and/or hazard index values.

8.4 ANALYSIS OF MONTE CARLO OUTPUT

The following outputs are available when the Chemical Intake and Risk Calculation module is implemented in the Monte Carlo mode.

(i) A statistical summary file for the variables used in the Chemical Intake and Risk Calculation module (INTAKE.SUM).

(ii) A number of ASCII files (DOSEI.DAT, RISK1.DAT, RISK2.DAT, etc.) that are read by the EXCEL® macro in the Risk Presentation module and used to present the results discussed in Section 7.0.

9.0

THE CHEMICAL DATABASE

The DSS uses a chemical database containing physical/chemical properties relating to fate and transport characteristics and human toxicity for 85 chemicals.

Properties contained in the database for each chemical include molecular weight, saturation vapor pressure, solubility in water, Henry's Law constant, organic carbon partition coefficient, diffusion coefficients in air and water, dermal permeability coefficients, and toxicity parameters. These properties are required by the fate and transport models and the risk calculation codes included in the API DSS.

9.1 FATE AND TRANSPORT PROPERTIES

Table 9-1 (at the end of this section) lists the chemical property values pertaining to both fate and transport and toxicity. These values were derived from the following sources: EPA (1996), Howard and Meylan (1997), Verschueren (1983), EPA guidance documents (EPA, 1986a and 1988), and Lyman et al. (1982). The database currently contains data for 85 chemicals. The user may add additional chemicals and their properties in the Development of Risk Scenario module.

9.1.1 Vapor Pressure

All of the values for vapor pressure in the DSS database are from Howard and Meylan (1997). The values listed in Table 9-1 are at a reference temperature of 20 degrees C.

Saturation vapor pressure may be corrected for temperature using the following relationship (Lyman et al., 1982):

$$\ln(P_{vT}) = \ln(P_{vR})\,[1/(T_b\text{-}C) - 1/(T\text{-}C)]/[1/(T_b\text{-}C) - 1/(T_R\text{-}C)] \qquad (9\text{-}1)$$

where

$\ln$ = natural logarithm

P_{vT} = vapor pressure at temperature T (atm)

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P_{vR} = vapor pressure at the reference temperature (atm)
T_b = boiling point (K)
T = temperature (K)
T_R = reference temperature (K)
C = $0.19T_b - 18$

Equation 9-1 is derived from the Clapeyron and the Antoine equations. The latter is a purely empirical expression that works well over a wide range of vapor pressures.

9.1.2 Solubility

Solubility values were obtained from EPA (1996). The values listed in Table 9-1 are at a reference temperature of 20 degrees C.

The relationship between solubility and temperature varies from chemical to chemical; the solubility of some chemicals in water increases with temperature, while other chemicals become less soluble as temperature increases. The system does not provide a temperature correction for solubility, and it is the user's responsibility to ensure that the solubility used is sufficiently accurate for the simulated conditions. Lyman et al. (1982) provides a discussion of alternative ways for estimating solubilities in water.

Contamination at underground fuel storage tanks typically consists of complex mixtures of several hydrocarbons. For mixtures of liquid chemicals the dissolved phase concentration at equilibrium with non-aqueous phase liquid (NAPL) (the effective solubility) can be estimated as the product of pure phase solubility of the chemical and the mole fraction of that chemical in the mixture. This is based on Raoult's Law and is strictly valid only for ideal mixtures. The VADSAT model is the only model in the DSS that calculates the effective solubility internally.

On a site-specific basis the mole fraction of individual chemicals in the hydrocarbon mixture may vary depending on the composition of the original product, the age of the leak, etc. Thus, the chemical database in the API DSS provides pure phase solubilities of each chemical and not effective solubilities nor immiscible phase mole fractions. The API DSS gives the user the option to override this 'default value' for site-specific analysis. The effective solubility should be used in all models except VADSAT as the VADSAT model calculates effective solubility from the pure phase solubility and the chemical's mole fraction in the mixture.

9.1.3 Henry's Law Constant

Henry's Law constant relates the concentration in the vapor phase to the concentration in the liquid phase at equilibrium, as the liquid phase concentration goes to zero (infinite dilution). The values contained in the database for this parameter were obtained from EPA (1996).

For chemicals where a published value for Henry's Law constant cannot be found, the value can be estimated as the ratio of the saturation vapor pressure to the solubility (Lyman et al., 1982):

$$H = (P_v / S)/(RT) \tag{9-2}$$

where

P_v = saturation vapor pressure (atm)
S = solubility (mol/m^3)
R = universal gas constant (atm-m^3/mol-$^\circ$K)
T = absolute temperature ($^\circ$K)
H = Henry's Law constant (mg/L)/(mg/L)

Since Henry's Law applies as infinite dilution is approached, Equation 9-2 assumes a linear vapor liquid equilibrium relationship at concentration values ranging from zero to the solubility. This assumption is most valid at low concentrations. Thus, the estimate of Henry's Law constant using Equation 9-2 is reasonably valid for relatively insoluble compounds.

9.1.4 Organic Carbon Partition Coefficient (K_{oc})

The organic carbon partition coefficient describes the chemical's affinity for sorbing to organic carbon in the soil. The higher the K_{oc} value, the more the chemical sorbs to the soil. The organic carbon partition coefficient values contained in the database were obtained from EPA (1996).

The organic carbon partition coefficient may be estimated from the octanol-water partition coefficient (K_{ow}) using the following empirical relationship (Lyman et al., 1982):

$$\text{Log}(K_{oc}) = \text{Log}(K_{ow}) - 0.32 \qquad (9\text{-}3)$$

where

K_{oc} = normalized organic carbon partition coefficient (cm^3/g)
K_{ow} = octanol-water partition coefficient (cm^3/g)

The normalized organic carbon partition coefficient is used to estimate the soil-water distribution coefficient using:

$$K_d = f_{oc} K_{oc} \qquad (9\text{-}4)$$

where

K_d = soil-water distribution coefficient (cm^3/g)
f_{oc} = fractional organic carbon content in soil (g/g)

Equation 9-4 only yields the chemical-specific adsorption to organic carbon in the soil but does not account for the adsorption onto the mineral or soil particles.

Equations 9-3 and 9-4 are not rigorous expressions but are based on simplifications that are valid for and typically used in most environmental contaminant fate and transport models.

9.1.5 Diffusion Coefficients

Diffusion coefficients in air and water were obtained from EPA (1996). The values listed in Table 9-1 are based on a reference temperature of 20 degrees C. To compute the air diffusion coefficient at temperatures other than 20 degrees C, the DSS uses the following relationship (Lyman et al., 1982):

$$D_{aT} = D_{aR} (T/T_R)^{1.75} \qquad (9\text{-}5)$$

where

D_{aT} = air diffusion coefficient at temperature T (cm^2/s)
D_{aR} = air diffusion coefficient at the reference temperature T_R (cm^2/s)

T = temperature (°K)
T_R = reference temperature (°K)

Please note that the temperature is expressed in degrees Kelvin. The temperature correction for the diffusion coefficient in water is based on the Hayduk and Laudie method described in Lyman et al. (1982):

$$D_{wT} = D_{wR} \left(\mu_{TR}/\mu_T\right)^{1.14} \tag{9-6}$$

where

D_{wT} = water diffusion coefficient at temperature T (cm^2/s)
D_{wR} = water diffusion coefficient at the reference temperature T_R (cm^2/s)
μ_{TR} = viscosity of water at temperature T_R (g/m-s)
μ_T = viscosity of water at temperature T (g/m-s)

Water viscosities are estimated within the fate and transport models as a function of temperature using the empirical relationships listed in Appendix I.

9.1.6 Decay Rate Constants

Several of the contaminant fate and transport models (SESOIL, AT123D, etc.) are capable of simulating contaminant decay using a first order decay process and require the user to enter a decay rate constant for the chemical. This overall decay rate should be considered a lumped parameter that accounts for biodegradation, hydrolysis, natural attenuation, etc. Since chemical-specific values of this parameter can vary significantly due to site-specific factors, no general values are available. Hence chemical-specific values of the decay rate constants are set to zero in the data base.

9.1.7 Dermal Permeability Coefficient

The aqueous permeability coefficient is a key parameter used to estimate dermal absorption. This parameter is used in the Chemical Intake and Risk Calculation module by the dermal intake while showering route. EPA's Dermal Exposure Assessment: Principles and Applications (1992) has tabulated values of permeability coefficients for many chemicals. When published values are not available, the permeability coefficient can be estimated using the following equation (EPA, 1992):

$$\log K_p = -2.72 + 0.71 \log K_{ow} - 0.0061 \text{ MW} \qquad (9\text{-}7)$$

where

K_p = skin permeability coefficient (cm/hour) of the chemical
K_{ow} = octanol water partition coefficient
MW = molecular weight

When published values of K_{ow} were not readily available, the following regression equation was used to estimate K_{ow} (Verschueren, 1983):

$$\log K_{ow} = 4.5 - 0.75 \log S \qquad (9\text{-}8)$$

where

S = solubility of the chemical [mg/l]

The chemicals having estimated values for K_{ow} are noted in Table 9-1.

9.2 TOXICITY PARAMETERS

The chemical database also contains quantitative data on the potential toxic effects of chemicals, and is accessed by the Chemical Intake and Risk Calculation module. Included in these parameters are the EPA cancer group classifications (defined in Table 9-2), the Slope Factor (also referred to as the Potency Factor for carcinogenic effects), and the Reference Dose (for noncarcinogenic effects) for each of the chemicals currently in the DSS. Toxicity data are provided for the inhalation and oral exposure routes. (The dermal toxicity values default to the oral value; however, the user may change the dermal toxicity if necessary.) Details on the use of these parameters in risk characterization are given in Section 6.0.

The RfDs and Slope Factors contained in the database were taken directly from EPA's Integrated Risk Information System (IRIS) database (EPA, 1997). This online database is updated monthly, and represents the current consensus from EPA's

Office of Health and Environmental Assessment on the toxicity of chemicals. Data not available in IRIS were obtained from EPA's Health Effects Assessment Summary Tables (HEAST; EPA, 1991b). This document is updated periodically (about every quarter), and contains interim toxicity values that may not yet be available in IRIS. The values in the database are current as of August 1997. It is recommended that the user check these against the most current IRIS values to ensure that current toxicological information is used in risk characterization.

9.3 RISK ASSESSMENTS WITH LEAD

Lead is not included in the database. EPA recommends the use of the EPA Uptake Biokinetic (UBK) model as a risk assessment tool to evaluate risks from soil contaminated with lead, rather than the method outlined in Section 6. The UBK calculates a total blood lead level (from background and incremental site contributions) and then compares this blood level with the currently accepted level. More information can be found on calculating risk from lead at the EPA's Lead and Human Health Web Page at:

http://www.epa.gov/oerrpage/superfnd/web/oerr/ini_pro/lead/lead.htm

The UBK guidance and spreadsheets are available for purchase from NTIS (see the EPA web page for pointers.)

Table 9-1. The Chemical Properties Database.

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CHEMICAL	CAS Number [-]	Molecular Weight [g/mole]	Density [g/cc]	Vapor Pressure [mmHg]	Solubility [mg/l]	Henry's Law Constant [(mg/l)/(mg/l)]	K_{oc} [ml/g]	Diffusion Coeff. in Air [cm^2/s]	Diffusion Coeff. in Water [cm^2/s]	K_d [-]
Acenaphthene	83-32-9	154.2	1.07	2.30E-03	4.24E+00	6.36E-03	7.08E+03	4.21E-02	7.69E-06	ND
Acenaphthylene	208-96-8	152.2	0.90	9.12E-04	3.93E+00	4.67E-03	4.79E+03	5.40E-02	6.60E-06	ND
Acetone	67-64-1	58.08	0.79	2.31E+02	1.00E+06	1.59E-03	5.75E-01	1.24E-01	1.14E-05	ND
Anthracene	120-12-7	178.2	1.25	2.67E-04	4.34E-02	2.67E-03	2.95E+04	3.24E-02	7.74E-06	ND
Arsenic	7440-38-2	74.9	ND	0.00E+00	ND	0.00E+00	ND	ND	ND	2.90E+01
Barium	7440-39-3	137.3	ND	0.00E+00	ND	0.00E+00	ND	ND	ND	3.00E+01
Benz(a)anthracene	56-55-3	228.0	1.27	3.05E-08	9.40E-03	1.37E-04	3.98E+05	5.10E-02	9.00E-06	ND
Benzene	71-43-2	78	0.88	9.52E+01	1.75E+03	2.28E-01	5.89E+01	8.80E-02	9.80E-06	ND
Benzo(a)pyrene	50-32-8	252.3	1.35	5.49E-09	1.62E-03	4.63E-05	1.02E+06	4.30E-02	9.00E-06	ND
Benzo(b)fluoranthene	205-99-2	252.3	1.35	5.00E-07	1.50E-03	4.55E-03	1.23E+06	2.26E-02	5.56E-06	ND
Benzo(g,h,i)perylene	191-24-2	276.3	1.35	1.01E-10	2.60E-04	1.09E-05	7.76E+06	4.10E-02	4.90E-06	ND
Benzo(k)fluoranthene	207-08-9	252.3	1.35	9.65E-10	8.00E-04	3.40E-05	1.23E+06	2.26E-02	5.56E-06	ND
Beryllium	7440-41-7	9.0	ND	0.00E+00	ND	0.00E+00	ND	ND	ND	8.20E+01
Bis(2-ethylhexyl)phthalate	117-81-7	390.6	0.99	9.75E-06	3.40E-01	4.18E-06	1.51E+07	3.51E-02	3.66E-06	ND
Butyl benzyl phthalate	85-68-7	312.4	1.10	8.25E-06	2.69E+00	5.17E-05	5.75E+04	3.90E-02	7.03E-06	ND
Cadmium	7440-43-9	112.4	ND	0.00E+00	ND	0.00E+00	ND	ND	ND	3.70E+01
Carbon Disulfide	75-15-0	76.1	1.26	3.58E+02	1.19E+03	5.92E-01	4.57E+01	1.04E-01	1.00E-05	ND
Carbon Tetrachloride	56-23-5	76.7	1.59	1.15E+02	7.93E+02	1.25E+00	1.74E+02	7.80E-02	8.80E-06	ND
Chlorobenzene	108-90-7	112.6	1.11	1.20E+01	4.72E+01	1.52E-01	2.19E+01	7.30E-01	8.70E-06	ND
Chloroform	67-66-3	119.4	1.49	1.97E+02	7.92E+03	1.50E-01	3.98E+01	1.04E-01	1.00E-05	ND
Chromium (III)	7440-47-2	52.0	ND	0.00E+00	ND	0.00E+00	ND	ND	ND	2.00E+05
Chromium (VI)	7440-47-3	52.0	ND	0.00E+00	ND	0.00E+00	ND	ND	ND	2.30E+01
Chrysene	218-01-9	228.3	1.27	6.23E-09	1.60E-03	3.88E-03	3.98E+05	2.48E-02	6.21E-06	ND
Copper	7440-50-8	63.5	ND	0.00E+00	ND	0.00E+00	ND	ND	ND	2.47E+00
Cresol(-m)	108-39-4	108.1	1.04	1.38E-01	2.27E+04	3.55E-05	8.71E+01	7.40E-02	1.00E-05	ND
Cresol(-o)	95-48-7	108.1	1.04	2.99E-01	2.60E+04	4.92E-05	9.12E+01	7.40E-02	8.30E-06	ND
Cresol(-p)	106-44-5	108.1	1.03	1.10E-01	3.53E+04	4.10E-05	8.13E+01	7.40E-02	1.00E-05	ND
Cyanide	57-12-5	ND	ND	ND	ND	0.00E+00	ND	ND	ND	9.90E+00
Dibenz(a,h)anthracene	53-70-3	278.4	1.28	1.00E-10	[illegible].49E-03	6.03E-07	3.80E+06	2.02E-02	5.18E-06	ND

Table 9-1. The Chemical Properties Database.

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CHEMICAL	CAS Number [-]	Molecular Weight [g/mole]	Density [g/cc]	Vapor Pressure [mmHg]	Solubility [mg/l]	Henry's Law Constant [(mg/l)/(mg/l)]	K_{oc} [ml/g]	Diffusion Coeff. In Air [cm^2/s]	Diffusion Coeff. In Water [cm^2/s]	K_d [-]
Dichloroethane (1,1-)	75-34-3	99.0	1.17	2.27E+02	5.06E+03	2.30E-01	3.16E+01	7.42E-02	1.05E-05	ND
Dichloroethane (1,2-) (EDC)	107-06-2	99.0	1.17	7.89E+01	8.52E+03	4.01E-02	1.74E+01	1.04E-01	9.90E-06	ND
Dichloroethylene (1,1-)	75-34-4	96.9	1.22	6.00E+02	2.25E+03	1.07E+00	5.89E+01	9.00E-02	1.04E-05	ND
Dichloroethylene (cis 1,2-)	156-59-2	96.9	1.21	2.01E+02	3.50E+03	1.67E-01	3.55E+01	7.36E-02	1.13E-05	ND
Dichloroethene (trans 1,2)	156-60-5	96.9	1.26	3.31E+02	6.30E+03	3.85E-01	5.25E+01	7.07E-02	1.19E-05	ND
Dimethylbenza(a) anthracene (7,1	57-97-6	147	1.30	5.63E-09	6.10E-02	1.28E-06	4.80E+05	4.60E-02	5.00E-06	ND
Dimethyl phenol (2,4)	105-67-9	122.2	1.04	9.80E-02	7.87E+03	8.20E-05	2.09E+02	5.84E-02	8.69E-06	ND
di-n-Butyl phthalate	84-74-2	178.3	1.05	7.30E-05	1.12E+01	3.85E-08	8.32E+07	1.51E-02	3.58E-06	ND
di-n-octyl phthalate	117-84-0	390.6	1.00	2.60E-06	2.90E-01	7.50E-09	1.10E+05	3.70E-02	4.00E-05	ND
Dinitrotoluene (2,4)	121-14-2	182.1	1.31	1.47E-04	2.70E+02	3.80E-06	9.55E+01	2.03E-01	7.06E-06	ND
Dioxane (1,4)	123-91-1	88.1	1.03	3.81E+01	1.10E-02	1.10E-02	1.70E+01	2.30E-01	1.00E-05	ND
Ethylbenzene	100-41-4	106.2	0.87	9.60E+00	1.69E+02	3.23E-01	3.63E+02	7.50E-02	7.80E-06	ND
Ethylene Dibromide	106-93-4	187.9	2.18	1.12E+01	4.30E+03	2.89E-02	4.37E+01	5.00E-02	9.60E-06	ND
Flouranthene	206-44-0	202.3	1.25	1.23E-08	2.06E-01	6.60E-04	1.07E+05	3.02E-02	6.35E-06	ND
Fluorene	86-73-7	166.2	1.20	8.42E-03	1.98E+00	2.61E-03	1.38E+04	3.63E-02	7.88E-06	ND
Indeno(1,2,3-CD)pyrene	193-39-5	276.3	1.35	1.00E-10	2.20E-05	6.56E-05	3.47E+06	1.90E-02	5.66E-06	ND
Mercury	7439-97-6	200.6	ND	1.30E-03	ND	4.67E-01	ND	3.07E-02	6.30E-06	8.20E+01
Methanol	67-56-1	32	0.80	1.27E+02	1.00E+06	1.87E-04	0.00E+00	1.55E-01	1.64E-05	ND
Methyl ethyl ketone	78-93-3	72.1	0.82	9.53E+01	2.12E+05	2.33E-03	4.50E+00	8.08E-02	9.80E-06	ND
Methylene Chloride	75-09-2	84.93	1.34	4.35E+02	1.30E+04	8.98E-02	1.17E+01	1.01E-01	1.17E-05	ND
Methylnapthalene (2-)	91-57-6	142.2	0.99	8.30E-03	2.46E+01	2.12E-02	8.50E+03	5.80E-02	7.37E-06	ND
MTBE	1634-04-4	88.17	0.74	2.49E+02	4.80E+04	2.04E-02	1.20E+01	7.10E-02	9.04E-06	ND
Naphthalene	91-20-3	128.2	1.16	8.50E-02	3.10E+01	1.98E-02	2.00E+03	5.90E-02	7.50E-06	ND
Nickel	7440-02-0	58.7	ND	0.00E+00	1.73E+05	0.00E+00	ND	ND	ND	8.80E+01
Nitrobenzene	98-95-3	123.1	1.20	2.45E-01	2.09E+03	9.84E-04	6.46E+01	7.60E-02	8.60E-05	ND
PCBs	1336-36-3	225.1	1.10	8.00E-05	4.20E-01	1.11E-02	3.09E+05	1.04E-01	1.00E-05	ND
Phenanthrene	85-01-8	178.2	1.18	1.12E-04	1.29E+00	1.60E-03	2.29E+04	5.17E-02	5.90E-06	ND
Phenol	108-95-2	94.1	1.07	3.50E-01	8.28E+04	1.63E-05	2.88E+01	8.20E-02	9.10E-06	ND
Pyrene	129-00-0	202.3	1.27	2.45E-06	1.35E-01	4.51E-04	1.05E+05	2.72E-02	7.24E-06	ND

Table 9-1. The Chemical Properties Database.

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CHEMICAL	CAS Number [-]	Molecular Weight [g/mole]	Density [g/cc]	Vapor Pressure [mmHg]	Solubility [mg/l]	Henry's Law Constant [(mg/l)/(mg/l)]	K_{oc} [ml/g]	Diffusion Coeff. In Air [cm^2/s]	Diffusion Coeff. In Water [cm^2/s]	K_d [-]
Pyridine	110-86-1	79.1	0.98	2.00E+01	1.00E+06	4.51E-04	5.38E+01	9.10E-02	7.60E-06	ND
Selenium	7782-49-2	79.0	ND	0.00E+00	ND	0.00E+00	ND	ND	ND	4.30E+00
Silver	7440-22-4	107.9	ND	0.00E+00	ND	0.00E+00	ND	ND	ND	1.30E+01
Stryene	100-42-5	104.2	0.90	6.40E+00	3.10E+02	1.13E-01	7.76E+02	7.10E-02	8.00E-06	ND
Tetrachloroethane (1,1,2,2 -)	79-34-5	167.9	1.60	4.62E+00	2.97E+03	1.41E-02	9.33E+01	7.10E-02	7.90E-06	ND
Tetrachloroethylene (PCE)	127-18-4	165.8	1.63	1.86E+01	2.00E+02	7.54E-01	1.55E+02	7.20E-02	8.20E-06	ND
Tetraethyl Lead	78-00-2	323	1.66	3.90E-01	2.10E-01	2.33E+01	4.90E+03	5.70E-02	6.40E-06	ND
Toluene	108-88-3	92.1	0.87	2.84E+01	5.26E+02	2.72E-01	1.82E+02	8.70E-02	8.60E-06	ND
TPH Aliphatic C5-6	NA	81	0.64	3.50E-01	3.60E+01	3.40E+01	7.94E+02	1.00E-01	1.00E-05	ND
TPH Aliphatic C6-8	NA	100	0.68	6.30E-02	5.40E+00	5.10E+01	3.98E+03	1.00E-01	1.00E-05	ND
TPH Aliphatic C8-10	NA	130	0.72	6.30E-03	4.30E-01	8.20E+01	3.16E+04	1.00E-01	1.00E-05	ND
TPH Aliphatic C10-12	NA	160	0.74	6.40E-04	3.40E-02	1.30E+02	2.51E+05	1.00E-01	1.00E-05	ND
TPH Aliphatic C12-16	NA	200	0.76	4.80E-05	7.60E-04	5.40E+02	5.01E+06	1.00E-01	1.00E-05	ND
TPH Aliphatic C16-35	NA	270	0.79	7.60E-06	1.30E-06	6.40E+03	1.00E+09	1.00E-01	1.00E-05	ND
TPH Aromatic C5-7	NA	78	0.88	1.30E-01	1.80E+03	2.30E-01	7.94E+01	1.00E-01	1.00E-05	ND
TPH Aromatic C7-8	NA	92	0.87	3.80E-02	5.20E+02	2.70E-01	2.51E+02	1.00E-01	1.00E-05	ND
TPH Aromatic C8-10	NA	120	0.88	6.30E-03	6.50E+01	4.90E-01	1.58E+03	1.00E-01	1.00E-05	ND
TPH Aromatic C10-12	NA	130	0.88	6.30E-04	2.50E+01	1.40E-01	2.51E+03	1.00E-01	1.00E-05	ND
TPH Aromatic C12-16	NA	150	1.00	4.80E-05	5.80E+00	5.40E-02	5.01E+03	1.00E-01	1.00E-05	ND
TPH Aromatic C16-21	NA	190	1.10	7.60E-06	5.10E-01	1.30E-02	1.58E+04	1.00E-01	1.00E-05	ND
TPH Aromatic C21-35	NA	240	1.20	4.40E-09	6.60E-03	6.80E-04	1.26E+05	1.00E-01	1.00E-05	ND
Trichloroethane (1,1,1-)	71-55-6	133.4	1.35	1.24E+02	1.33E+03	7.05E-01	1.10E+02	7.80E-02	8.80E-06	ND
Trichloroethane (1,1,2-)	79-00-5	133.4	1.35	2.30E+01	4.42E+03	3.74E-02	5.01E+01	7.80E-02	8.80E-06	ND
Trichloroethylene (TCE)	79-01-6	131.4	1.46	6.90E+01	1.10E+03	4.22E-01	1.66E+02	7.90E-02	9.10E-06	ND
Vanadium	7440-62-2	50.9	ND	0.00E+00	ND	0.00E+00	ND	ND	ND	1.00E+03
Vinyl Chloride	75-01-4	62.5	0.91	2.98E+03	2.67E+03	1.11E+00	1.86E+01	1.06E-01	1.23E-05	ND
Xylenes	1330-20-7	106.2	0.87	8.84E+00	1.98E+02	2.90E-01	2.40E+02	7.20E-02	8.50E-06	ND
Zinc	7440-66-6	65.38	ND	0.00E+00	ND	0.00E+00	ND	ND	ND	7.50E+01

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CHEMICAL	EPA Toxicity Classification [-]	Inhalation RfD [mg/kg*d]	Inhalation Slope Factor [1/(mg/kg*d)]	Oral RfD [mg/kg*d]	Oral Slope Factor [1/(mg/kg*d)]	Absorption Coeff. from Soil [-]	Skin Permeability Constant [cm/hour]
Acenaphthene	ND	6.00E-02	ND	6.00E-02	ND	1.00E+00	1.50E-01
Acenaphthylene	ND	ND	ND	ND	ND	1.00E+00	9.60E-02
Acetone	D	1.00E-01	ND	1.00E-01	ND	1.00E+00	5.69E-04
Anthracene	ND	3.00E-01	ND	3.00E-01	ND	1.00E+00	2.20E-01
Arsenic	A	ND	1.51E+00	3.00E-04	1.50E+00	1.00E+00	1.00E-03
Barium	ND	1.43E-04	ND	7.00E-02	ND	1.00E+00	1.00E-03
Benz(a)anthracene	B2	ND	7.30E-01	ND	7.30E-01	1.00E+00	8.10E-01
Benzene	A	1.70E-03	2.90E-02	1.70E-03	2.90E-02	1.00E+00	2.10E-02
Benzo(a)pyrene	B2	ND	7.30E+00	ND	7.30E+00	1.00E+00	1.20E+00
Benzo(b)fluoranthene	B2	ND	7.30E-01	ND	7.30E-01	1.00E+00	1.20E+00
Benzo(g,h,i)perylene	ND	ND	ND	ND	ND	1.00E+00	1.66E+00
Benzo(k)fluoranthene	B2	ND	7.30E-02	ND	7.30E-02	1.00E+00	1.10E+00
Beryllium	B2	ND	8.40E+00	5.00E-03	4.30E+00	1.00E+00	1.00E-03
Bis(2-ethylhexyl)phthalate	B2	2.20E-02	1.40E-02	2.00E-02	1.40E-02	1.00E+00	3.30E-02
Butyl benzyl phthalate	C	ND	ND	2.00E-01	ND	1.00E+00	7.40E-02
Cadmium	B1	5.00E-04	6.30E+00	5.00E-04	ND	1.00E+00	1.00E-03
Carbon Disulfide	NA	2.90E-03	ND	1.00E-01	ND	1.00E+00	2.40E-02
Carbon Tetrachloride	B2	5.71E-04	5.30E-02	7.00E-04	1.30E-01	1.00E+00	2.20E-02
Chlorobenzene	D	5.70E-03	ND	2.00E-02	ND	1.00E+00	4.10E-02
Chloroform	B2	1.00E-02	8.10E-02	1.00E-02	6.10E-03	1.00E+00	8.90E-03
Chromium (III)	ND	5.70E-07	ND	1.00E+00	ND	1.00E+00	1.30E-03
Chromium (VI)	A	ND	2.90E+02	5.00E-03	ND	1.00E+00	1.30E-03
Chrysene	B2	ND	7.30E-03	ND	7.30E-03	1.00E+00	8.10E-01
Copper	D	ND	ND	3.70E-02	ND	1.00E+00	1.00E-03
Cresol(-m)	NA	5.00E-02	ND	5.00E-02	ND	1.00E+00	1.50E-02
Cresol(-o)	NA	5.00E-02	ND	5.00E-02	ND	1.00E+00	1.60E-02
Cresol(-p)	NA	5.00E-03	ND	5.00E-03	ND	1.00E+00	1.80E-02
Cyanide	NA	ND	ND	4.00E-02	ND	1.00E+00	1.00E-02
Dibenz(a,h)anthracene	B2	ND	7.30E+00	ND	7.30E+00	1.00E+00	2.70E+00

Table 9-1. The Chemical Properties Database.
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CHEMICAL	EPA Toxicity Classification [-]	Inhalation RfD [mg/kg*d]	Inhalation Slope Factor [1/(mg/kg*d)]	Oral RfD [mg/kg*d]	Oral Slope Factor [1/(mg/kg*d)]	Absorption Coeff. from Soil [-]	Skin Permeability Constant [cm/hour]
Dichloroethane (1,1-)	NA	1.40E-01	ND	1.00E-01	ND	1.00E+00	8.90E-03
Dichloroethane (1,2-) (EDC)	B2	2.90E-03	9.10E-02	2.90E-03	9.10E-02	1.00E+00	5.30E-03
Dichloroethylene (1,1-)	C	9.00E-03	1.80E-01	9.00E-03	6.00E-01	1.00E+00	1.60E-02
Dichloroethylene (cis 1,2-)	C	1.00E-02	ND	1.00E-02	ND	1.00E+00	1.00E-02
Dichloroethene (trans 1,2)	C	2.00E-02	ND	2.00E-02	ND	1.00E+00	1.00E-02
Dimethylbenza(a) anthracene (7,1	NA	ND	ND	3.00E-02	ND	1.00E+00	1.20E+00
Dimethyl phenol (2,4)	NA	ND	2.00E-02	ND	2.00E-02	1.00E+00	1.50E-02
di-n-Butyl phthalate	D	1.00E-01	ND	1.00E-01	ND	1.00E+00	3.30E-02
di-n-octyl phthalate	NA	2.00E-02	ND	2.00E-02	ND	1.00E+00	2.70E+01
Dinitrotoluene (2,4)	NA	ND	2.00E-03	ND	2.00E-03	1.00E+00	3.80E-03
Dioxane (1,4)	B2	ND	1.10E-01	ND	1.10E-01	1.00E+00	3.60E-04
Ethylbenzene	D	2.90E-01	ND	1.00E-01	ND	1.00E+00	7.40E-02
Ethylene Dibromide	B2	5.70E-05	7.70E-01	5.70E-05	8.50E+01	1.00E+00	3.30E-03
Flouranthene	D	4.00E-02	ND	4.00E-02	ND	1.00E+00	3.60E-01
Fluorene	D	4.00E-02	ND	4.00E-02	ND	1.00E+00	3.60E-01
Indeno(1,2,3-CD)pyrene	B2	ND	7.30E-01	ND	7.30E-01	1.00E+00	1.90E+00
Mercury	D	8.57E-05	ND	3.04E-04	ND	1.00E+00	1.67E-03
Methanol	ND	5.00E-01	ND	5.00E-01	ND	1.00E+00	3.50E-04
Methyl ethyl ketone	ND	2.90E-01	ND	6.00E-01	ND	1.00E+00	5.00E-03
Methylene Chloride	B2	8.60E-01	1.60E-03	6.00E-02	7.50E-03	1.00E+00	4.50E-03
Methylnapthalene (2-)	ND	4.00E-02	ND	4.00E-02	ND	1.00E+00	1.80E-01
MTBE	ND	8.57E-01	ND	5.00E-03	ND	1.00E+00	3.08E-03
Naphthalene	D	4.00E-02	ND	4.00E-02	ND	1.00E+00	6.90E-02
Nickel	A	ND	8.40E-01	2.00E-02	ND	1.00E+00	1.00E-03
Nitrobenzene	D	ND	5.70E-04	ND	5.00E-04	1.00E+00	7.00E-03
PCBs	B2	2.00E-05	7.70E+00	2.00E-05	7.70E+00	1.00E+00	1.30E+00
Phenanthrene	ND	ND	ND	ND	ND	1.00E+00	2.70E-01
Phenol	D	6.00E-01	ND	6.00E-01	ND	1.00E+00	5.50E-03
Pyrene	D	3.00E-02	ND	3.00E-02	ND	1.00E+00	3.24E-01

Table 9-1. The Chemical Properties Database.
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CHEMICAL	EPA Toxicity Classification [-]	Inhalation RfD [mg/kg*d]	Inhalation Slope Factor [1/(mg/kg*d)]	Oral RfD [mg/kg*d]	Oral Slope Factor [1/(mg/kg*d)]	Absorption Coeff. from Soil [-]	Skin Permeability Constant [cm/hour]
Pyridine	ND	ND	1.00E-03	ND	1.00E-03	1.00E+00	1.80E-03
Selenium	D	ND	ND	5.00E-03	ND	1.00E+00	1.00E-03
Silver	D	ND	ND	5.00E-03	ND	1.00E+00	6.00E-04
Stryene	ND	2.86E-01	ND	2.00E-01	ND	1.00E+00	5.50E-02
Tetrachloroethane (1,1,2,2 -)	C	ND	2.00E-01	ND	2.00E-01	1.00E+00	9.00E-03
Tetrachloroethylene (PCE)	B2	1.00E-02	ND	1.00E-02	ND	1.00E+00	4.80E-02
Tetraethyl Lead	ND	ND	ND	1.00E-07	ND	1.00E+00	3.60E-02
Toluene	D	1.14E-01	ND	2.00E-01	ND	1.00E+00	4.50E-02
TPH Aliphatic C5-6	D	5.04E+00	ND	5.00E+00	ND	1.00E+00	1.42E-01
TPH Aliphatic C6-8	D	5.04E+00	ND	5.00E+00	ND	1.00E+00	2.99E-01
TPH Aliphatic C8-10	D	2.74E-01	ND	1.00E-01	ND	1.00E+00	7.54E-01
TPH Aliphatic C10-12	D	2.74E-01	ND	1.00E-01	ND	1.00E+00	1.91E+00
TPH Aliphatic C12-16	D	2.74E-01	ND	1.00E-01	ND	1.00E+00	8.24E+00
TPH Aliphatic C16-35	D	ND	ND	2.00E+00	ND	1.00E+00	9.17E+01
TPH Aromatic C5-7	D	1.10E-01	ND	2.00E-01	ND	1.00E+00	1.84E-02
TPH Aromatic C7-8	D	1.10E-01	ND	2.00E-01	ND	1.00E+00	2.93E-02
TPH Aromatic C8-10	D	5.50E-02	ND	4.00E-02	ND	1.00E+00	5.99E-02
TPH Aromatic C10-12	D	5.50E-02	ND	4.00E-02	ND	1.00E+00	8.66E-02
TPH Aromatic C12-16	D	5.50E-02	ND	4.00E-02	ND	1.00E+00	1.42E-01
TPH Aromatic C16-21	D	ND	ND	3.00E-02	ND	1.00E+00	2.96E-01
TPH Aromatic C21-35	D	ND	ND	1.03E+00	ND	1.00E+00	1.49E+00
Trichloroethane (1,1,1-)	D	2.90E-01	ND	3.50E-02	ND	1.00E+00	1.70E-02
Trichloroethane (1,1,2-)	C	4.00E-03	5.60E-02	4.00E-03	5.70E-02	1.00E+00	8.40E-03
Trichloroethylene (TCE)	B2	6.00E-03	6.00E-03	6.00E-03	1.10E-02	1.00E+00	2.30E-01
Vanadium	ND	ND	ND	7.00E-03	ND	1.00E+00	1.00E-03
Vinyl Chloride	A	ND	3.00E-01	ND	1.90E+00	1.00E+00	7.30E-03
Xylenes	D	2.00E-01	ND	2.00E+00	ND	1.00E+00	8.00E-02
Zinc	D	ND	ND	3.00E-01	ND	1.00E+00	6.00E-04

Table 9-2. EPA Weight-of-Evidence Classifications for Carcinogenicity.

EPA CLASSIFICATION	DESCRIPTION
A	Human carcinogen
B1	Probable human carcinogen, based on limited human data
B2	Probable human carcinogen, based on sufficient evidence in animals and inadequate evidence in humans
C	Possible human carcinogen
D	Not classifiable as to human carcinogenicity
E	Evidence of noncarcinogenicity for humans

10.0
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APPENDIX A
THE SESOIL MODEL

The Seasonal Soil (SESOIL) model (Bonazountas and Wagner, 1984, as updated by Hetrick, 1994) is a one-dimensional vertical transport model for the unsaturated zone. The DSS is used to estimate (i) volatilization flux to the atmosphere, and (ii) contaminant mass loading to the water table.

The original SESOIL model (available from Oak Ridge National Laboratory, ORNL) consists of three calculation modules: a hydrologic module, a pollutant transport module, and a sediment erosion module.

The hydrologic module (or cycle) uses a water budget approach to estimate infiltration and soil moisture content in the unsaturated zone. The pollutant transport module estimates the volatilization, mass loading to groundwater, and pollutant migration between layers in the soil column. A brief description of the hydrogeologic and the pollutant transport modules is presented below. The sediment erosion module is not included in the API DSS and is not discussed below.

The reader is encouraged to obtain "The New SESOIL User's Guide" (Hetrick et al., 1994) for more detailed information on the SESOIL model.

The Soil Column

The SESOIL model simulates water and contaminant transport in a vertical soil compartment, or column, extending from the ground surface to the water table. This soil column is treated differently by the hydrologic cycle and the pollutant cycle in SESOIL. In the hydrologic cycle, the soil column is assumed to be homogenous with respect to soil properties. In the pollutant transport module, the soil column is simulated using different vertical layers. Each layer is treated as a separate compartment with unique soil properties. Up to four layers with different soil characteristics can be simulated with SESOIL. Each of these layers can be divided into up to 10 sublayers for purposes of pollutant transport. The sublayers have the same soil properties as the layer in which they reside.

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The Hydrologic Module

The purpose of the hydrologic cycle is to estimate the infiltration rate and moisture content in the soil column. These results are then passed to the pollutant transport module. Since the hydrologic cycle assumes a uniform soil column (no layers), a single soil moisture content is calculated for the entire soil column.

The hydrologic cycle is based on the annual water balance algorithm described by Eagleson (1978). (Please note that the model is run in a monthly mode, that is, the inputs such as precipitation vary for each month.) The annual water balance algorithm couples the climatic and soil systems through a statistical description of each of the hydrologic parameters. SESOIL hydrology is based upon the following water balance equations (expressed per unit horizontal area):

$$P = E + MR + S + G \tag{A-1a}$$

$$I = P - S \tag{A-1b}$$

$$Y = S + G \tag{A-1c}$$

where

P = precipitation (cm)
E = evapotranspiration (cm)
MR = moisture retention (cm)
S = surface runoff (cm)
G = groundwater runoff or recharge (cm) (includes term for capillary rise)
Y = yield (cm)
I = infiltration (cm)

In Eagleson's (1978) theory, evapotranspiration, surface runoff, groundwater runoff, moisture retention, precipitation, and infiltration are all functions of soil moisture. Since soil moisture is initially unknown, SESOIL makes an initial estimate of the soil moisture. This estimate and the user-specified inputs are used to estimate the terms on the right hand side of Equation (A-1a), the sum of which provides an estimate of precipitation. If this value differs by more than 1% from the user specified value (for precipitation), the soil moisture estimate is corrected and the calculations repeated.

The standalone SESOIL model (ORNL, 1995) provides three options for simulating hydrology: user specified hydrology, annual hydrology and monthly hydrology. The following discussion is primarily concerned with the monthly hydrology that is used by the API DSS (and is the most common mode for running SESOIL).

Computation of various elements in Equation (A-1) are all based upon relationships between precipitation and the climatic parameters entered by the user. The processes used in estimating precipitation are briefly discussed in the following sections.

Precipitation

SESOIL assumes that precipitation can be represented by arrivals of square pulses that have random depth and duration. The model assumes that the length of rainy season is constant from year to year. The use of a Poisson process implies the following assumptions:

- An event can occur at random and at any time.
- The occurrence of an event in a given time interval is independent of that in any other time interval.
- The probability of occurrence of an event in a small interval "dt" is proportional to "dt", and can be given by the product of the mean rate of occurrence of the event (assumed to be constant) and "dt". The probability of two or more occurrences in the same interval is negligible.

The last assumption requires that the average storm duration be much smaller than the average time between storms.

The assumption of rainfall occurring in square pulses yields a rainfall distribution of the form depicted in Figure A-1.

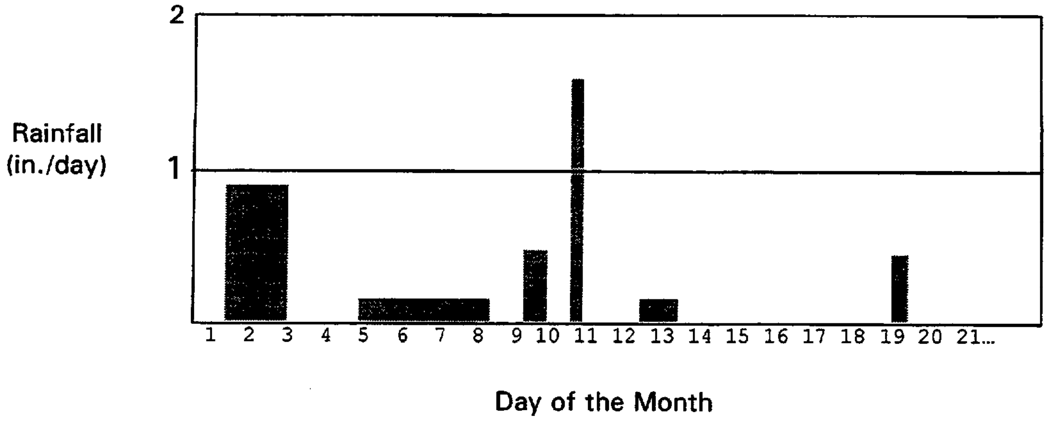


Figure A-1. Example of a SESOIL Storm Occurrence and Rainfall Distribution.

Infiltration

Infiltration is calculated using the Philip equation (Philip, 1969) which assumes that the surface soil is semi-infinite, and the internal soil moisture content at the beginning of each storm and inter-storm period is uniform, equal to its long-term average.

Percolation

Percolation to the groundwater is assumed to be constant within each time step, however, the percolation rate may vary from month to month. The net percolation to groundwater is estimated from the long-term average soil moisture content, the effective hydraulic conductivity, and the capillary rise. The hydraulic conductivity of the soil is a function of the soil moisture that is estimated using Brooks and Corey's (1966) relationship:

$$K = K_{sat} S^{c} \tag{A-2}$$

where:

K = hydraulic conductivity at S (cm/s)
K_{sat} = saturated hydraulic conductivity (cm/s)
S = soil saturation (cm^3 water/cm^3 pore space)
c = soil (or pore) disconnectedness index (unitless) (a user input)

The hydrologic cycle in SESOIL assumes a uniform soil column with respect to soil properties. The user can enter different hydraulic permeability values for each layer.

SESOIL estimates a depth-weighted average for use in the hydrologic cycle from the following equation:

$$k_z = \frac{d}{\sum_{i=1}^{n} \frac{d_i}{k_i}} \qquad \text{(A-3)}$$

where:

k_z = vertically average permeability (cm^2)
k_i = permeability for layer i (cm^2)
d = depth from surface to groundwater (cm)
d_i = thickness of layer i (cm)
n = number of layers in the SESOIL model

SESOIL should be applied with caution at sites with large vertical variability in soil properties because of this assumption of uniform moisture content.

Overall Water Balance—Monthly Cycle

In the monthly mode of the SESOIL model, the user enters long-term average monthly values of rainfall, number of storms, storm length, and evapotranspiration (or the terms required to calculate it). These monthly parameters are then used for each year of simulation creating a sequence of "identical hydrologic years."

The overall water balance is obtained by combining the expressions for precipitation, infiltration, moisture retention, evapotranspiration, surface runoff and percolation in Equation (A-1). The initial value for soil moisture content is calculated in SESOIL by summing the appropriate monthly climatic input data to obtain annual values and then by running the hydrology module in an annual mode. Because of this rough estimate of the initial soil moisture content, the results of the hydrology cycle will be different for the first two years, thereafter the results will be the same year to year.

The monthly cycle in SESOIL accounts for the change in moisture storage from month to month; however, the change is not accounted for from year to year (each new year starts over).

Evapotranspiration

SESOIL has two options as far as evapotranspiration is concerned: The user may enter monthly values, or, the user may enter information on solar radiation capacity and SESOIL will calculate evapotranspiration. For both cases the following assumptions are made:

1. The surface retention capacity of the soil is zero. That is, water does not pond on the surface. Thus, only water that has already infiltrated is subject to evaporation.
2. Vegetation does not bring water to the surface for evaporation. The only mechanism available to account for plant transpiration is for the user to specify the evapotranspiration rate.
3. Soil moisture is the same at the beginning and the end of the storm. This assumption eliminates the necessity of tracking soil moisture during and between storms. This constant soil moisture value represents a spatial and temporal average moisture content.
4. The variance in the average annual rate of potential evapotranspiration is negligible.
5. Potential evaporation is much greater than the rate of capillary rise from the water table.

The rate of evaporation is a trade off between the maximum potential evaporation rate, and the exfiltration capacity, i.e., the rate at which soil can deliver moisture to the surface. Evaporation initially occurs from the thin surface-retained film at the maximum rate. Next evaporation occurs from soil moisture. Immediately following a storm, soil moisture is high, water moves up readily to satisfy the evaporation demand, and evaporation will occur at the potential rate. As soil moisture is depleted, the exfiltration capacity of the soil decreases until it equals the potential rate of evaporation. Beyond this point, the rate of evaporation and the exfiltration capacity both decrease as soil moisture decreases.

Eagleson (1978) derived an expression for the expected value of annual evapotranspiration that is a function of the maximum evapotranspiration effectiveness, the vegetative cover, the ratio of capillary rise to potential evaporation and the surface retention capacity. Evapotranspiration effectiveness is a function of the average time between storms, potential evapotranspiration, velocity of capillary rise, soil moisture, and the soil physical parameters including effective porosity, hydraulic conductivity, saturated matrix potential of the soil (suction), exfiltration diffusivity, pore size distribution index, and diffusivity index.

The maximum potential evapotranspiration rate can be either user-specified (as a fraction of total rainfall) or estimated by SESOIL using the modified Penman energy balance and is required to calculate the actual evapotranspiration rates used in the model. The input parameters that affect evapotranspiration are: porosity, saturated hydraulic conductivity and pore disconnectedness index; the other parameters are internally calculated.

Surface Runoff

Surface runoff is calculated from the distribution of rainfall intensity and duration, and by use of the Philip equation. The input parameters that affect surface runoff are: number of storms per month, monthly rainfall, porosity, hydraulic conductivity of the top layer and soil disconnectedness index.

Major Assumptions and Limitations for the Hydrology Module

SESOIL does not use a time series of climatic data to calculate infiltration rate and soil moisture. Rather, it uses average annual climatic data to directly calculate the average infiltration rate and soil moisture. A list of assumptions used by SESOIL's hydrology module is contained in Appendix HY in Bonazountas (1984). Some of the major limitations to the use of the SESOIL hydrology are:

- Only one-dimensional flow can be simulated.
- The average interstorm period is assumed to be much greater than the average storm duration. This may limit the use of SESOIL in areas with frequent storm events.
- SESOIL assumes only a single homogeneous soil layer. SESOIL allows the user to specify a different intrinsic permeability for each layer (up to four allowed layers); however, the depth-weighted value is used in the hydrology computations.

Hydrology Module Outputs and Coupling with Fate and Transport Module

The outputs of the hydrology component of SESOIL are the infiltration rate at the ground surface, the groundwater recharge rate at the water table, and the average soil moisture in the unsaturated zone. These results from the hydrology module are used by the contaminant transport module as discussed below.

Chemical Fate and Transport Module

SESOIL simulates pollutant transport by dividing the soil column into a maximum of four layers. A few fate and transport properties can be different for each layer. For computation purposes, these layers can be further subdivided into a maximum of ten equal sublayers with the same properties as those specified for the layer. A mass balance is then applied to each sublayer independently. Communication between layers is through advection and diffusion, i.e., advection out of an upper layer becomes advection into an adjacent lower layer. Diffusion takes place from the layer with higher concentration to an adjacent layer with lower concentration and can be in the upward direction only.

Chemical transport in SESOIL is based upon the following mass balance equation:

$$M_{rem}(t) = M_{orig}(t\text{-}1) + M_{inp}(t) - M_{out}(t) - M_{trans}(t) \qquad \text{(A-4)}$$

where:

$M_{orig}(t\text{-}1)$ = initial mass in the compartment at beginning of time step

$M_{inp}(t)$ = mass coming into compartment during time step

$M_{trans}(t)$ = pollutant transformation (or loss) within compartment during time step

$M_{rem}(t)$ = pollutant remaining in compartment at end of time step (dt)

$M_{out}(t)$ = exported pollutant during time step

The above equation is applied to three phases in the soil matrix (i) liquid phase (soil moisture), (ii) solid, (iii) soil air. Thus, SESOIL partitions the chemicals between different phases assuming all phases are in equilibrium at all times. An overview of the solution of the transport model is provided in the New SESOIL User's Guide (Hetrick *et al.*, 1994) and the SESOIL manual in Appendix PT (Bonazountas and Wagner, 1984).

Equilibrium Partitioning

For pollutant concentrations below the residual (free phase) level, SESOIL assumes that all phases of the contaminant (liquid, vapor, and sorbed) are in equilibrium at all times.

$$C_T = \theta_a C_v + \theta_w C_w + \rho_b C_s \tag{A-5}$$

where:

C_T = total pollutant concentration in soil ($\mu g/cm^3$)
C_v = vapor phase concentration ($\mu g/cm^3$)
C_w = liquid phase concentration ($\mu g/cm^3$)
C_s = sorbed concentration ($\mu g/cm^3$)
θ_a = air-filled porosity (cm^3/cm^3)
θ_w = water-filled porosity (cm^3/cm^3)
ρ_b = soil bulk density (g/cm^3)

Equation A-4 assumes equilibrium partitioning among three phases only. When the fourth phase, residual phase (free-phase), is present, SESOIL limits the liquid phase concentration to the user-entered solubility. This in turn limits the vapor phase concentration and the amount of contaminant leached and volatilized. SESOIL checks the dissolved phase concentrations with the user-entered solubility so that the leachate from one layer to a lower layer cannot exceed the entered solubility. When the fourth phase is present the output from SESOIL includes a "Pure Phase" concentration.

Concentration in the Vapor Phase

Concentration in the vapor phase (C_v) is estimated from the liquid phase concentration using Henry's law modified for temperature:

$$C_v = \frac{C_w H}{R(T+273)} \tag{A-6}$$

where:

C_v = vapor phase concentration ($\mu g/cm^3$)
C_w = liquid phase concentration, or solubility, whichever is less ($\mu g/cm^3$)

H = Henry's law constant (m^3 atm/mol)
R = universal gas constant [8.2E-5 m^3atm/(mol °K)]
T = soil temperature (°C)

Concentration in the Sorbed Phase

Concentration in the sorbed phase (C_s) is estimated using the Freundlich isotherm equation.

$$C_s = K_d C_w^{\frac{1}{n}} \tag{A-7}$$

where:

n = Freundlich exponent

See the section on "Adsorption" in this appendix for more information on the Freundlich exponent.

Cation Exchange

Cation exchange is another process modeled by SESOIL that accounts for adsorption. Cation exchange is the exchange of a cation in solution (e.g., dissolved metals) with another cation in the soil. The exchange of cations causes the dissolved phase constituent to become physically sorbed onto the soil. The cation exchange process is modeled by SESOIL using:

$$MCEC = \frac{10.0 \cdot CEC \cdot MW}{Val} \tag{A-8}$$

where:

MCEC = maximum pollutant cation mass exchanged by the soil (μg/g soil)
CEC = cation exchange capacity of the soil (meq/100 g dry wt. soil)
MW = molecular weight of the pollutant (g/mol)
Val = valence of the cation (-)

The variables defined above are user inputs to the SESOIL model. There are defaults in the chemical database for molecular weight.

Contaminant Mass Loading and Transport

Contaminant mass can enter a layer in two ways: (i) an input specified by the user or (ii) mass transported from an adjacent layer. Mass enters the sublayers through advective transport in the liquid phase or from diffusive transport in the gaseous phase.

Diffusion and Volatilization

When volatile emissions are calculated, SESOIL assumes the air above the soil surface has zero concentration and calculates volatile emissions as the diffusive flux over the source area to the air. The algorithm used is the Farmer's model (Farmer et al., 1980) which is discussed in more detail in Appendix E. However, the Farmer's algorithm differs from the standalone Farmer's model because the SESOIL code conserves mass, the volatilization is calculated (and updated) at each time step, and the SESOIL code accounts for other loss terms, such as degradation. The Millington and Quirk (1961) adjustments are made to estimate the effective diffusion coefficient based on moisture content. The vapor diffusion flux is estimated by

$$J_a = -D_a \left(\frac{\theta_a^{\frac{10}{3}}}{\theta_T^{2}} \right) \frac{dC_v}{dz} \qquad \text{(A-9)}$$

where:

J_a	=	diffusion flux (ug/cm^{2}s)
D_a	=	diffusion coefficient in air for the compound (cm^2/s)
θ_a	=	air-filled porosity (cm^3/cm^3)
θ_T	=	total porosity (cm^3/cm^3)
C_v	=	concentration of the compound in the soil vapor (ug/cm^3)
z	=	depth (cm)

The user has the option to “turn off” or “dial down” the amount of volatilization allowed from each layer. For example, specifying a value of 0.0 for the volatilization index means that no volatilization will be allowed for that layer. A value of 0.5 means that 50% of the calculated volatilization will be allowed. This feature was included in SESOIL because volatilization routines that assume uniform moisture content tend to greatly overestimate volatilization. In reality, the soil moisture content would contain some regions with a higher moisture content than the long-term average and some regions with lower moisture content. The regions of higher moisture content (and hence lower air content) will tend to greatly reduce volatilization. Since these are not accounted for in the model, SESOIL will tend to over estimate the amount of volatilization occurring. This is a common problem with analytical or semi-analytical vadose zone models.

Some state agencies have understood this concern and have specified that when SESOIL is used for risk assessments the volatilization should be limited to a certain value. For example, the Hawaii state UST guidance recommends that the volatilization be limited to 0.2 for all layers. This volatilization index is specified in the "Soil Data for Each Layer" group (see Figure A-2).

Adsorption

SESOIL uses the Freundlich equation to estimate concentrations in the solid phase. The Freundlich isotherm is defined as

$$C_s = K_d C_w^{\frac{1}{n}} \qquad \text{(A-10)}$$

where:

C_s = pollutant adsorbed concentration (ug/g)

K_d = pollutant partitioning coefficient (ug/g)/(ug/ml)

C_w = pollutant concentration in soil water (ug/ml)

n = Freundlich exponent

For most organic chemicals, adsorption is assumed to occur mainly on the organic carbon found in the soil. In this case, K_d is assumed to equal the product of K_{oc} and F_{oc} (the fraction organic carbon). In the DSS, the default value of the Freundlich exponent is set to 1.0 which assumes a linear model for sorption. According to "The New SESOIL User's Guide" (Hetrick et al., 1994) values for n generally range from 0.9 and 1.4 and if the value is not known a value of 1.0 should be used. Lyman et al. (1992) states that there is a lack of reported values for the Freundlich exponent for petroleum hydrocarbons. Rao and Davidson (1980) have compiled a list of mean values of n for several pesticides and pesticide related compounds. These values were derived from sorption experiments and ranged from 0.70 to 1.18 with an overall mean value of 0.87.

The Freundlich exponent and organic carbon content (F_{oc}) are entered in the "Soil Data for Each Layer" group (see Data Requirements). The user may enter an overall partitioning coefficient, K_d, for the chemical (in the chemical database or in the SESOIL chemical inputs). This K_d value will override the K_d that would have been calculated from F_{oc} and K_{oc}. If K_d is zero (the default value), it will be calculated from F_{oc} and K_{oc}.

Cation exchange is primarily used to simulate the complexation of metals. Cation exchange, as modeled in SESOIL, is not an equilibrium reaction. It is irreversible and the mass of pollutant "exchanged" is unavailable for further reactions. This is in contrast to the adsorption discussed above which is an equilibrium reaction and is reversible. Cation exchange and adsorption are two mechanisms that remove pollutants from the liquid phase. These two mechanisms may both remove the same pollutant. The user is advised to simulate only one of these mechanisms unless the user-specified coefficients are chosen such that there is no "double counting" of adsorbed pollutant. The molecular weight and valence of the chemical are used in the cation calculations. These are entered in either the chemical database or the SESOIL chemical parameters group.

SESOIL calculates the mass of pollutant exchanged before simulating other processes. This means that cation exchange precedes the other processes and pollutants involved in cation exchange are not available to other processes.

Mass Transformations

Mass transformations contribute to the loss of contaminant mass through a number of processes. These include (i) user-specified losses (or gains), (ii) degradation in the liquid phase, (iii) degradation in the solid phase, (iv) transformation by hydrolysis in the liquid phase, (v) transformation by hydrolysis in the solid phase, and (vi) contaminant transformation by cation exchange. Each of these processes is discussed below.

In the standalone version of SESOIL, the user can specify the mass of pollutant that is transformed in each time step (monthly or annually). The user-specified value is considered a loss to the system. This option is not available in the DSS (the decay rates should be used instead).

In addition to the user-specified mass transformations, SESOIL estimates first order decay of contaminant mass in the solid and the liquid phase. If concentrations are quite high, it may be reasonable to set the solid phase decay rate to zero, thereby assuming degradation only takes place after the contaminant solubilizes and migrates away from the source.

SESOIL simulates neutral, base and acid catalyzed hydrolysis of organic compounds. It is assumed that the rate of hydrolysis is the same for the adsorbed, the dissolved and the cation exchanged pollutants. These chemical-specific parameters are entered in the "Chemical Parameters" section (see Figure A-2).

Mass Out

Mass can leave a layer in SESOIL through three mechanisms: (i) advection of the dissolved phase, (ii) volatilization or diffusion, and (iii) a user-specified sink. The API DSS version of the SESOIL code does not allow the user to specify a sink.

Diffusion occurs only in the upward direction between sublayers. Diffusion is calculated from a sublayer with a higher concentration to an adjacent layer with lower concentration. The mass diffused is considered an input to the layer with the lower concentration. For the uppermost sublayer, diffusion loss to the atmosphere is calculated assuming zero concentration in the atmosphere. The user-specified sink is mass that the user specifies as leaving a layer and not moving to any other layer. Thus this mass is lost to the system. The user-specified sink is not an option in the DSS.

Assumptions and Limitations of the Contaminant Transport Module

Following are the key assumptions that are used to estimate the fate and transport of contaminants by SESOIL:

1. Compositional equilibrium among phases is assumed at all locations at all times.
2. SESOIL can only provide the average concentration for a layer. It does not have the capability to estimate concentrations at arbitrary depths; however, SESOIL can calculate concentrations for up to 40 different sublayers.
3. Each layer in SESOIL is defined by its depth, pH, intrinsic permeability, organic

carbon content, cation exchange capacity, Freundlich exponent and adsorption coefficient. All other model parameters are constant with depth.

4. SESOIL assumes no dispersion in the liquid phase. This will cause the model to underestimate travel times. For cases with shallow water tables and short travel times, dispersion may be small. For large depths and/or long travel times dispersion may be large and ignoring dispersion could be a significant omission.

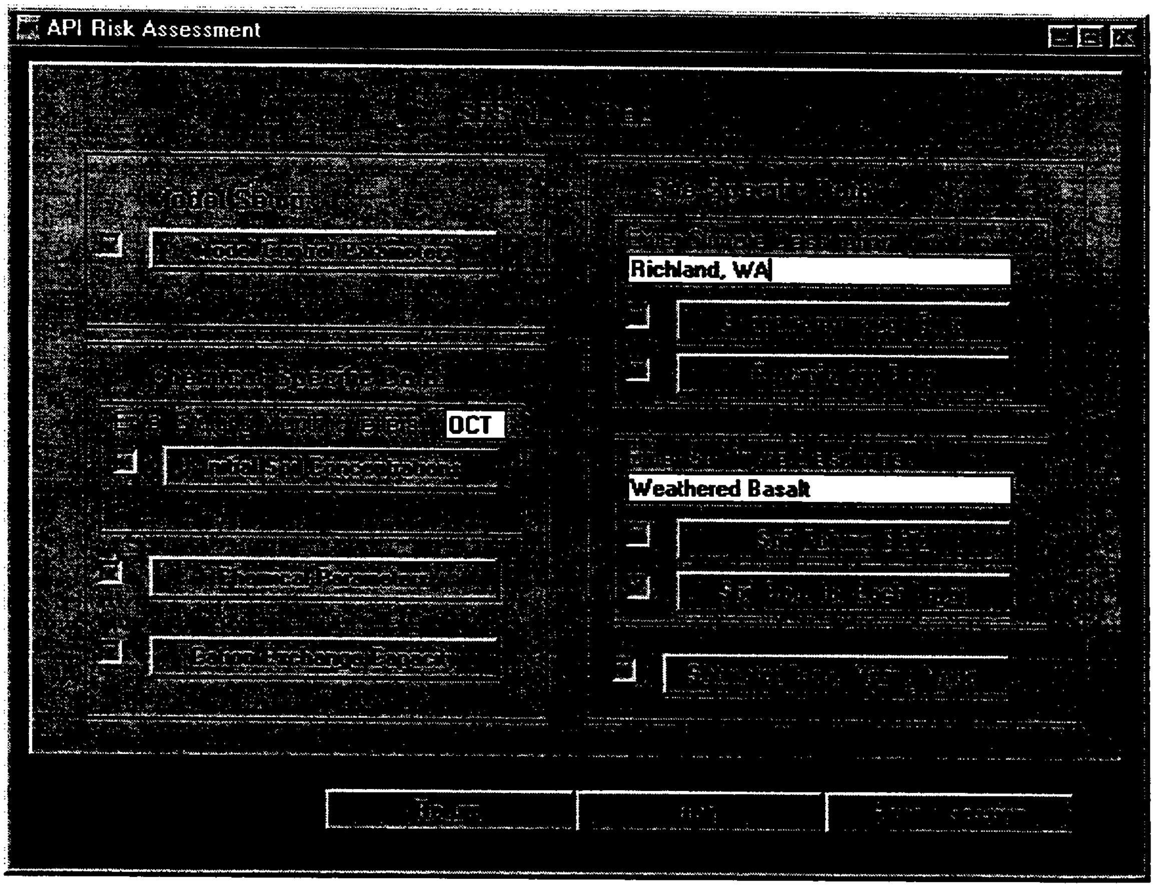
5. The soil moisture is a key parameter that usually varies with depth in the unsaturated zone. This parameter has a significant effect on pollutant transport and is considered to be constant with depth in SESOIL.

Data Requirements for the SESOIL Model

Table A-1 shows the data required to run the hydrology and contaminant fate and transport modules of SESOIL. Figure A-2 shows the main SESOIL input screen in the DSS. The following sections are organized around the buttons in this figure.

TABLE A-1. DATA REQUIRED TO IMPLEMENT THE SESOIL MODEL

	PARAMETER DEFINITION	UNITS	API DSS UNITS
Model Control Parameters			
	Simulation Time	[yrs]	[yrs]
	No. of Layers	[-]	[-]
	No. of Sublayers/Layer	[-]	[-]
Chemical Data			
	Solubility	[ug/ml]	[mg/L]
	Diffusion Coefficient in Air	[cm^2/sec]	[cm^2/sec]
	Henry's Law Constant	[mg^3 atm/mole]	[(mg/L)/(mg/L)]
	K_{oc}	[ug/g oc /ug/ml]	[ug/g oc /ug/ml]
	Overall Decay Rate	[1/day]	[1/day]
Climate Data			
	Surface Temperature	[C]	[C]
	Evapotranspiration	[cm/day]	[cm/day]
	Annual Precipitation	[cm/year]	[cm/year]
	Storm Duration	[days]	[days]
	Storm Events	[no. events/year]	[no. events/year]
	Length of Rainy Season	[months]	[months]
	Surface Runoff	[cm/yr]	[cm/yr]
Unsaturated Zone Data for the Entire Soil Column:			
	Effective Porosity	[-]	[-]
	Soil Bulk Density	[g/cm^3]	[g/cm^3]
	X-dimension of the source	[m]	[m]
	Y-dimension of the source	[m]	[m]
Unsaturated Zone Data for Each Layer:			
	Thickness of the layer	[m]	[m]
	Intrinsic Permeability	[cm^2]	[cm^2]
	Fraction Organic Carbon	[mg/mg]	[mg/mg]
	Pollutant load to the layer for each chemical of concern	[kg]	[kg]



Richland, WA

OCT

Weathered Basalt

Figure A-2. Main SESOIL Screen of the DSS.

Initial Soil Concentrations

At the start of the simulation (i.e., time = 0) the user may specify initial total contaminant concentrations in soil (in mg/kg) for each sublayer of each layer. The concentrations specified are for the individual contaminant being modeled. If the individual contaminant being modeled is part of a contaminant mixture (such as benzene in a gasoline spill) the effective solubility should be modified to account for the effects of the mixture. For more information, see the section on chemical-specific parameters.

Starting Month for Simulation

The first three letters of the starting month for the transport model must be entered. SESOIL operates on a hydrologic year—that is the hydrologic simulations always start at the beginning of the hydrologic year (October). The initial mass however need not be assumed to be present in October. In this variable the user has the opportunity to enter the actual month in which fate and transport simulation begins. For example, if initial concentrations in soil were measured in January, the user would enter "JAN" in this option. The SESOIL output would show zero concentration input for the first three months of simulation and then the mass loading would occur in January of the first year of simulation.

Chemical-Specific Properties

The following chemical-specific properties are required to run SESOIL:

- effective solubility (mg/l)
- diffusion coefficient in air (cm^2/s)
- Henry's law coefficient (mg/l)/(mg/l)
- K_{oc} (organic carbon partition coefficient) (μg/goc)/(μg/ml)
- molecular weight (g/mol)
- K_d (soil adsorption coefficient) (μg/g)/(μg/ml)
- nuetral hydrolysis coefficient (1/day)
- acid hydrolysis coefficient (L/mol/day)
- base hydrolysis coefficient (L/mol/day)
- degradation rate in liquid (1/day)
- degradation rate in solid (1/day)

Effective Solubility (mg/l)

The default value that appears in this box is the chemical's *pure phase* solubility from the API DSS chemical database. If the chemical is part of a chemical mixture (such as benzene in a gasoline mixture) the user should calculate the chemical's effective solubility and enter it in this box. The effective solubility is calculated from the chemical's mole fraction in the solution and its pure phase solubility.

$$S_{eff} = x_i S_i \qquad \text{(A-11)}$$

where:

S_i = aqueous solubility of pure component [g/l]

x_i = mole fraction of component in the hydrocarbon mixture [mol/mol]

The mole fraction of the individual component is calculated from:

$$x_i = \frac{m_i}{m_{TPH}} \qquad \text{(A-12)}$$

$$x_i = \frac{C_{si} MW_{TPH}}{MW_i C_{sTPH}} \qquad \text{(A-13)}$$

where:

m_i = total moles of component [mol]
m_{TPH} = total moles of TPH [mol]
C_{si} = total concentration of component i in soil [mg/kg]
C_{sTPH} = total concentration of TPH in soil [mg/kg]
MW_i = molecular weight of component i [g/mol]
MW_{TPH} = molecular weight of TPH [g/mol]

For components that have similar molecular weights as TPH (92 to 105 g/mol) the mole fraction can be roughly estimated from the concentration of the individual constituent divided by the TPH concentration, and the equation for effective solubility reduces to:

$$S_{eff} = \frac{C_{si}}{C_{TPH}} S_i \qquad \text{(A-14)}$$

Diffusion Coefficient in Air (cm^2/s)

Default values for the diffusion coefficient in air are located in the API DSS chemical database. For chemicals not included in the database, EPA's Soil Screening Guidance (1996) provides a large database with values for diffusion coefficient in air.

Henry's Law Coefficient (mg/l)/(mg/l)

Default values for Henry's Law coefficients are located in the API DSS chemical database. To estimate the Henry's Law coefficient (H´) in units of (mg/m^3 vapor)/(mg/m^3 water) from a Henry's Law value in units of atm-cm^3/mol use:

$$H' = \frac{H}{RT} \qquad \text{(A-15)}$$

where:

H' = Henry's law coefficient (mg/m^3 vapor)/(mg/m^3 water)
H = Henry's law coefficient (atm-cm^3/mol)
R = Universal gas constant (82.1 atm-cm^3/mol)
T = temperature (K)

Organic Carbon Partition Coefficient [K_{oc}] (μg/g soil)/(μg/ml water)

The default values for K_{oc} in the API DSS database are from EPA's Soil Screening Guidance (USEPA, 1996). If the K_{oc} value entered is non-zero, then the partition coefficient (K_d) is calculated from:

$$K_d = K_{oc} F_{oc} \tag{A-16}$$

where:

K_d = partition coefficient (μg/g soil)/(μg/ml water)
F_{oc} = fraction organic carbon in soil (mg oc/mg soil)
K_{oc} = organic carbon partition coefficient (μg/g soil)/(μg/ml water)

If K_{oc} is entered as a non-zero value the user should make sure that the K_d input parameter is equal to zero to avoid "double counting" sorption. Only one or the other sorption mechanism should be used for any one chemical.

Soil Sorption Coefficient [K_d] (μg/g)/(μg/ml)

The soil sorption coefficient is used for non-organic constituents for which a sorption coefficient is known. This value can be measured in the lab. If K_d is non-zero the user should make sure that the K_{oc} input parameter is equal to zero to avoid "double counting" (or predicting more sorption than was intended). The default value for K_d in the DSS database is zero.

Nuetral Hydrolysis Coefficient (1/day)

The default value for the nuetral hydrolysis coefficient in the DSS database is zero.

Acid Hydrolysis Coefficient (L/mol/day)

The default value for the acid hydrolysis coefficient in the DSS database is zero.

Base Hydrolysis Coefficient (L/mol/day)

The default value for the base hydrolysis coefficient in the DSS database is zero.

Degradation Rate in Liquid (1/day)

This degradation rate (decay rate) describes the rate at which the chemical degrades in the dissolved phase. The degradation rate can be calculated from the half-life using:

$$\text{Degradation Rate} = -\ln(0.5)/\text{Half-Life} = 0.693\,/\text{Half-Life} \tag{A-17}$$

where the half-life is in days. SESOIL does not model the creation of daughter products.

Degradation Rate in Solid (1/day)

This degradation rate describes the rate at which the chemical degrades in the solid (sorbed) phase.

Cation Exchange Capacity (CEC)

The cation exchange capacity function is used as an alternative way to estimate adsorption in SESOIL. When cation exchange occurs, positively charged atoms or molecules (cations such as heavy metals) are exchanged with the cations of minerals and other soil constituents. The CEC is a measure of the amount of cations per unit of soil that is available for exchange with the chemical. The user is referred to the "New SESOIL User's Guide" (Hetrick et al., 1994) for more information. The use of the cation exchange capacity function is optional and the default values in SESOIL are zero.

Evapotranspiration Data Group

Depending on the option chosen in "Model Control Parameters," the user will either specify the amount of evapotranspiration occurring, or the user will enter values for parameters used by SESOIL to calculate the evapotranspiration.

Evapotranspiration (fraction of rainfall)
("Enter Evapotranspiration" option only)

Evapotranspiration represents the amount of water leaving the soil column (through the soil surface). In the SESOIL input parameters, the amount of evapotranspiration occurring is specified as a fraction of rainfall for the given time period. For example, if 2 inches of rain were specified for January and the evapotranspiration was set at 0.3, the amount of water that SESOIL will attempt to have leave the soil column via evapotranspiration is 0.3 x 2 = 0.6 inches. SESOIL may not be able to meet this goal since depending on other input parameters and soil moisture conditions, less than 0.6 inches may enter the soil column for that month. The input parameters that affect the amount of water infiltrating are: precipitation, hydraulic conductivity (especially of the top sublayer), porosity, and soil disconnectedness index.

Mean Air Temperature (°C)

The mean air temperature is used to estimate evapotranspiration rates and soil temperatures. If the evapotranspiration rates are specified then the mean air temperature is not used to estimate evapotranspiration but is still used to calculate soil temperature.

Albedo (fraction)
("Calculate Evapotranspiration" option only)

The short wave albedo fraction ranges from 0 to 1 and is used to calculate evapotranspiration rates. It represents the fraction of light (or solar radiation) reflected by the soil surface.

Relative Humidity (fraction)
("Calculate Evapotranspiration" option only)

This value is readily available from basic weather data. If the humidity is presented as a percent value, convert it to a fraction before entering in the DSS.

Cloud Cover (fraction)
("Calculate Evapotranspiration" option only)

This value represents the fraction of the time that the site is in cloud cover.

Precipitation Data Group

Precipitation (cm/yr or cm/month)

The precipitation value should include all forms of precipitation, including snow.

Storm Duration (days)

This value should represent the average length of storms during the month. This type of information is available from weather station data.

Number of Storms per month (#/month)

This value represents the average number of storms during the month. This type of information is available from weather station data.

Soil Column Data Group

This data group contains the input parameters that are constant for the entire soil column.

Effective Porosity

The effective porosity is the volume of void spaces available to transmit water in the soil. Eagleson (1978) defines effective porosity as

$$N=(1-s_r)n_t \tag{A-18}$$

where:

N = effective porosity (cm^3 voids/cm^3 soil)
n_t = total porosity (cm^3 voids/cm^3 soil)
s_r = residual saturation (cm^3 water/cm^3 soil)

The residual saturation is the volume of water unmoved by gravity drainage/volume of voids. The New SESOIL User's Guide (Hetrick et al., 1994) presents the following table showing default values of effective porosity.

Table A-2. Effective Porosity by Soil Class.

USDA Textural Soil Class	Effective Porosity (Bonazountas and Wagner, 1994)
Clay (very fine)	0.20
Clay (medium fine)	0.20
Clay (fine)	0.22
Silty clay	0.25
Silty clay loam	0.27
Clay loam	0.30
Loam	0.30
Silt loam	0.35
Silt	0.27
Sandy clay	0.24
Sandy clay loam	0.26
Sandy loam	0.25
Loamy sand	0.28
Sand	0.30

Soil Disconnectedness Index

The soil pore disconnectedness index typically ranges from 3.7 for sand to 12.0 for fine clay. It relates the soil permeability to the soil moisture content.

Table A-3. Disconnectedness Index by Soil Class.

USDA Textural Soil Class	Disconnectedness Index (Bonazountas and Wagner, 1994)
Clay (very fine)	12
Clay (medium fine)	12
Clay (fine)	12
Silty clay	12
Silty clay loam	10
Clay loam	7.5
Loam	6.5
Silt loam	5.5
Silt	12
Sandy clay	6
Sandy clay loam	4
Sandy loam	4
Loamy sand	3.9
Sand	3.7

Soil Bulk Density (g/cm^3)

The average dry weight soil bulk density should be entered. Measured as average dry density of soil (including pore spaces)—g of soil/cm^3 *bulk* volume. General ranges used: sand (1.18 to 1.58), silt (1.29 to 1.80), and clay (1.40 to 2.2).

X-Dimension of Source (m)

The x-dimension of the source represents the length of the source in the direction of groundwater flow *in the aquifer* beneath the soil column.

Y-Dimension of Source (m)

The y-dimension of the source represents the length of the source perpendicular to the direction of groundwater flow *in the aquifer* beneath the soil column.

Latitude (degree)

This value is used to calculate evapotranspiration rates. If evapotranspiration rates are specified by the user then this value is not used.

Soil Data For Each Layer Data Group

The following input parameters are entered for each layer in the model. The values may differ between layers.

Thickness of Layer (m)

The thickness of each layer is entered for this input parameter. The sum of all the thicknesses should represent the distance from the soil surface to the water table.

Intrinsic Permeability (cm²)

To obtain intrinsic permeability from hydraulic conductivity, use the following equation:

$$k = K\frac{\mu}{\rho g} \qquad \text{(A-19)}$$

where:

k = intrinsic permeability (cm^2)
K = hydraulic conductivity (cm/s)
μ = dynamic viscosity of fluid (usually water) (g/cm-s)
ρ = density of fluid (usually water) (g/cm^3)
g = gravitational acceleration (cm/s^2)

For water at 20 °C, in the units presented above, the value of $\mu/\rho g$ is equal to 1.0E-5 cm^2. See table for default values.

Table A-4. Intrinsic Permeability by Soil Class.

USDA Textural Soil Class	Intrinsic Permeability (cm^2) (Bonazountas and Wagner, 1994)
Clay (very fine)	7.5E-11
Clay (medium fine)	2.5E-10
Clay (fine)	6.0E-10
Silty clay	5.0E-11
Silty clay loam	8.5E-11
Clay loam	6.5E-10
Loam	8.0E-10
Silt loam	3.5E-10
Silt	5.0E-11
Sandy clay	1.5E-9
Sandy clay loam	2.5E-9
Sandy loam	2.0E-9
Loamy sand	5.0E-8
Sand	1E-8

Fraction Organic Carbon (g oc/g soil)

Fraction organic carbon (F_{oc}) is easy to measure by a soil laboratory. The F_{oc} is used to estimate retardation and sorption rates for organic chemicals (having a non-zero K_{oc}). The higher the F_{oc}, the greater the sorption to soil by the chemical, and the greater the retardation with respect to average groundwater flow.

pH

This value should describe the soil's pH value for the given sublayer. The pH value is used in the cation exchange processes and for deriving the hydrolysis degradation rates.

Fraction of Emissions Allowed (fraction)

SESOIL allows the user to "dial down" the amount of emissions occurring between each layer and between the top layer and the ambient air. The SESOIL code first calculates what the emission rate should be and then if a value less than 1.0 is entered for this fraction, the actual emission rate from the given layer is adjusted accordingly. This option was included because the volatile emission algorithms used in SESOIL (and many other codes using a Farmer's type algorithm) tend to overestimate emissions. (See explanation in the section entitled "Diffusion and Volatilization".) Since SESOIL conserves mass, the more emissions that exit the soil column from the top, the less mass there is in the soil column available to transport to the water table.

Fruendlich Equation Exponent (-)

The Freundlich equation exponent is used to determine chemical sorption. Values of this exponent typically range from 0.9 to 1.4. If the value is not known, use a value of 1.0 (Hetrick et al., 1994).

Saturated Zone Mixing Model Data Group

This data group only appears if 'SESOIL linked with a mixing zone model' is chosen in Step 1.

Saturated Conductivity of the Aquifer (m/d)

The hydraulic conductivity of the aquifer just beneath the soil column is entered here. The units used for the saturated hydraulic conductivity are different than for intrinsic permeability which is used for the soil column.

Hydraulic Gradient (m/m)

The hydraulic gradient of the aquifer beneath the soil column.

Thickness of the Aquifer (m)

This value represents the thickness of the saturated zone beneath the soil column.

SESOIL Options Not Available from the API DSS Interface

1. The standalone SESOIL model provides three options for implementing the hydrologic module - user specified hydrology, annual hydrology and monthly hydrology. The API DSS allows the user to implement SESOIL using the monthly hydrology option only.
2. The sediment erosion module cannot be accessed from the API DSS version.
3. Ligand complexation cannot be modeled using the API DSS version.

Example Problem

In this hypothetical example problem a former gas station located in San Francisco, California, has been closed and is for sale.

When the USTs were excavated, a spill was discovered in the vadose zone. The spill appears to have occurred underground, there is no evidence of surface spills. Soil samples were collected from the bottom of the excavation and around the sides. It appears that the geologic media beneath the site is predominantly sandy clay. The soil contamination appears to not have reached groundwater in any great quantity, based on relatively clean soil samples taken just above the water table and groundwater samples. The excavation will be backfilled with clean silty clay. The native soil has been characterized as a sandy clay.

The site geology and soil concentration data are shown below.

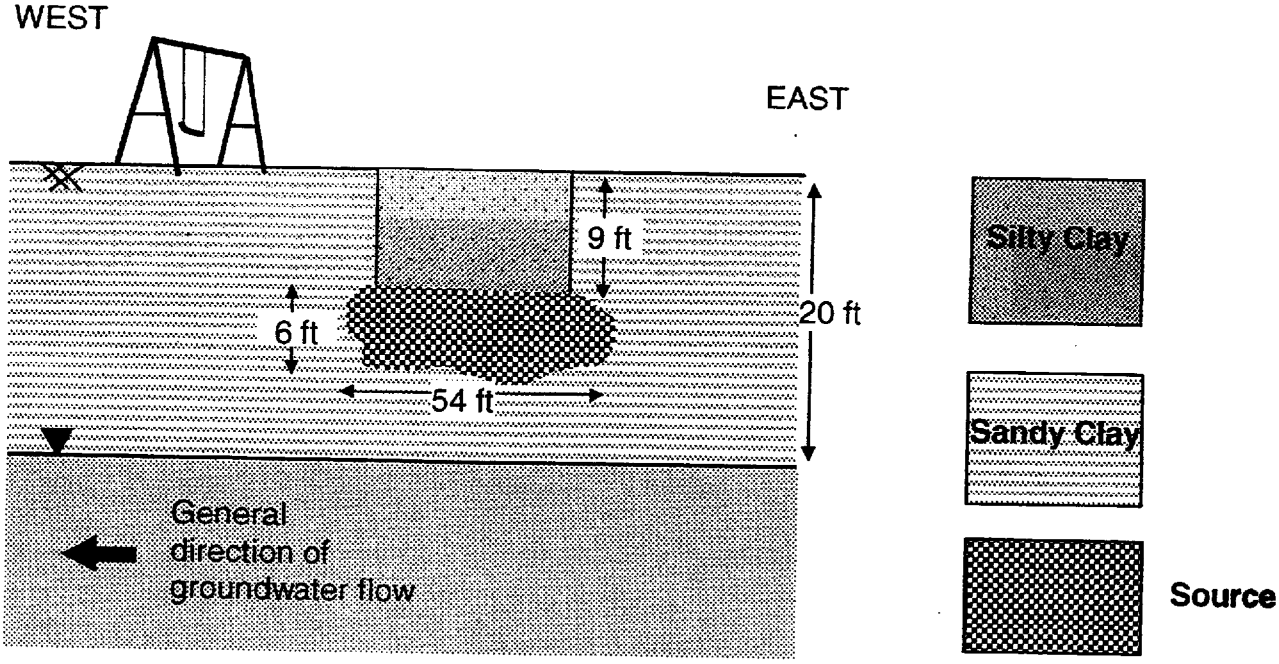


Figure A-3. Site Hydrogeology for Example Problem.

In this example, SESOIL will be run with the mixing zone model to estimate concentration in groundwater directly underneath the source. The aquifer gradient is 0.008 ft/ft. From Bonazountas and Wagner (see Table A-4) the intrinsic permeability of sandy clay is estimated to be 1.5E-9 cm^2. This intrinsic permeability value translates to a hydraulic conductivity of 1.5E-4 cm/s, or, 0.13 m/d (see equation A-19). The mixing zone height for the aquifer will be set at an (arbitrary) value of 2 m.

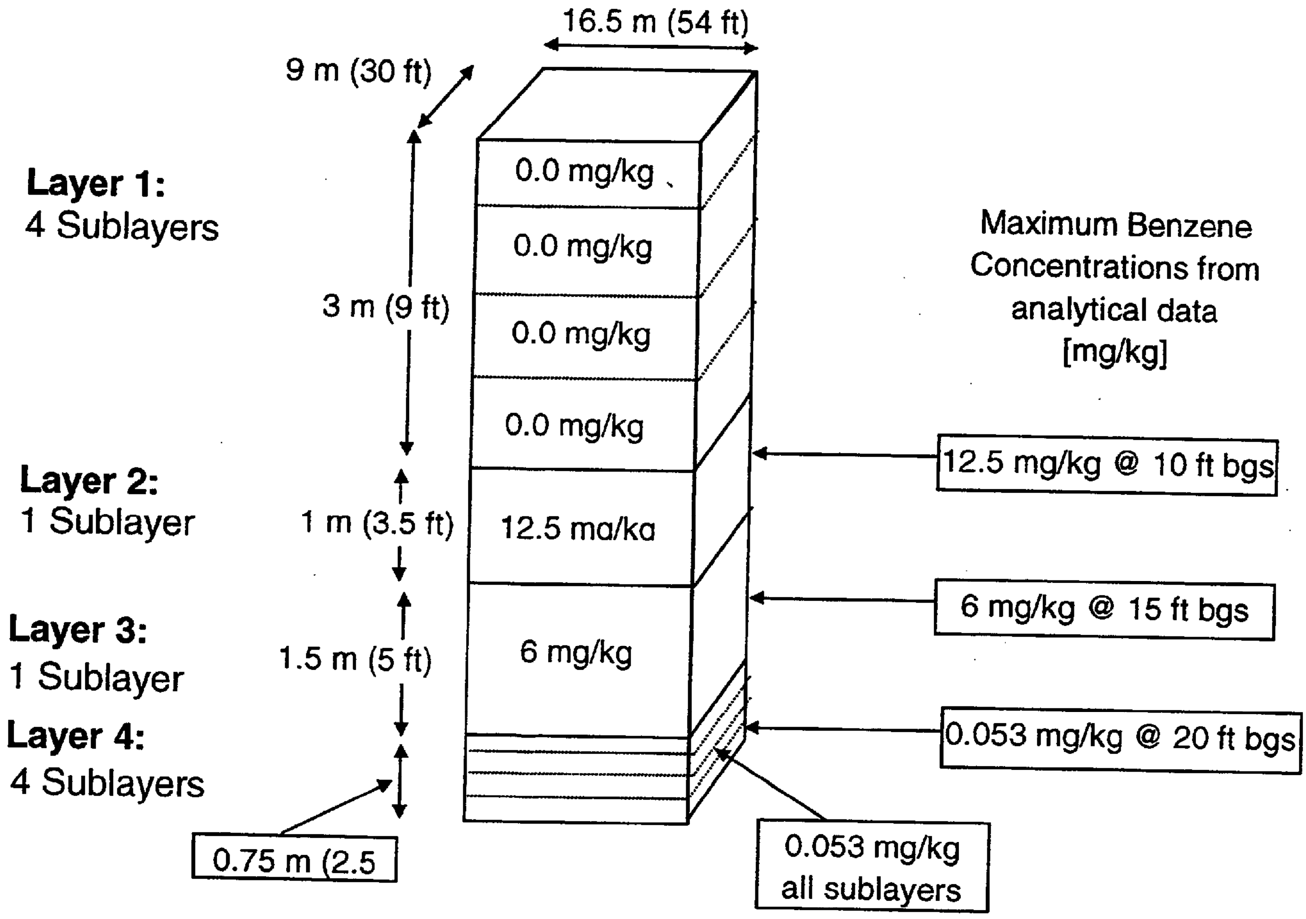
Table A-5. Soil Concentration Results for Example Problem.
Sampling Date: Jan 6, 1997

Sample Description	Units	Benzene Concentration
Soil Boring 1	mg/kg soil	
10 ft depth		ND (0.05)
15 ft depth		4.5
20 ft depth		0.053
Soil Boring 2	mg/kg soil	
10 ft depth		12.5
15 ft depth		6
20 ft depth		ND (0.05)
Soil Boring 3	mg/kg soil	
10 ft depth		1.2
15 ft depth		3.4
20 ft depth		ND (0.05)

In the SESOIL model, the maximum number of layers is four with a maximum of 10 sublayers for each layer. SESOIL will have a much better “resolution of the solution” if the maximum number of layers and sublayers are used. Each additional layer causes the code to run slower, however.

For this example problem, the number of sublayers will be kept to a minimum to reduce runtime. The SESOIL model geometry used is shown in Figure A-4 (the benzene concentrations for each layer are also given.)

Note: Layer 1 corresponds to the silty clay placed into the excavation.



Rationale

Layer 1 represents the clean soil to be placed back in the excavation. It should be subdivided into as many layers as possible to slow down the volatile emissions. This layer is assumed to be "clean" (zero concentrations).

Layer 2 represents an estimated volume of soil corresponding to the sample taken at 10 ft bgs. The layer was assigned a thickness of 3.5 ft roughly corresponding to the distance from the bottom of the tank pit to halfway in between the 10 and 15 ft samples. The maximum concentration found at 10 ft was assigned to this layer.

Layer 3 represents an estimated volume of soil corresponding to the sample taken at 15 ft bgs. The thickness of the layer corresponds to half of the distance between the 15 ft and 10 ft samples added to half of the distance between the 15 ft and 20 ft samples (5 ft thickness).

Layer 4 represents an estimated volume of soil corresponding to the 20 ft sample. Since the 20 ft sample was at the water table the thickness of the layer was assumed to be equal to one half the distance from the water table to the 15 ft sample.

Figure A-4. Model Geometry Chosen and Rationale.

Running the API DSS for this Example

Step 1: Development of Risk Scenario.

In this step, the chemicals of concern and the exposure pathways are selected—the risk scenario is defined.

- Select the benzene as the chemical of concern.
- For the exposure pathways, choose a groundwater route (e.g. "Drinking water"; it doesn't matter which one since this is just a fate and transport example).
- Select "SESOIL with Mixing Zone" for the groundwater fate and transport model.

Step 2: Receptor Point Concentrations

Entering SESOIL data

Tables A-6 and A-7 summarize the input parameter values for SESOIL for this example problem. The initial soil concentrations for benzene for each layer are shown in Figure A-4.

Table A-6. Parameter Values for SESOIL for the Example Problem (continued).

	Units	Value	Layer 1	Layer 2	Layer 3	Layer 4
Model Control Parameters						
Simulation Time	yrs					
No. of Layers	-	4				
No. of Sublayers/Layer	-		4	1	1	4
Climatic Data: Annual or Monthly?	-	monthly values				
Enter Evapotranspiration?	-	yes				
Chemical Data						
Solubility	mg/L	use default				
Diffusion Coefficient in Air	cm^2/sec	"				
Henry's Law Constant	(mg/L)/(mg/L)	"				
Koc	ug/g oc /ug/ml	"				
Overall Decay Rate	1/day	0				
Climate Data (See separate table for values)						
Unsaturated Zone Data for the Entire Soil Column:						
Effective Porosity	-	0.25				
Soil Bulk Density	g/cm^3	1.7				
Soil Disconnectedness Index	-	6				
Latitude	degrees	39				
X-dim. of the source	m	16.5				
Y-dim. of the source	m	9				
Unsaturated Zone Data for Each Layer:						
Thickness of each layer	m		3	1	1.5	0.75
Intrinsic Permeability	cm^2		5E-11	1.5E-9	1.5E-9	1.5E-9
Fraction Volatile Emissions Allowed*	-		0.2	0.2	0.2	0.2
Fraction Organic Carbon	mg/mg		0.005	0.005	0.005	0.005
Chemical concentration	mg/kg	chem-specific				
Saturated Zone Mixing Model:						
Hydraulic Conductivity	m/d	0.13				
Hydraulic gradient	m/m	0.008				
Depth of mixing zone	m	2				

*See discussion in model input section of this appendix.

Table A-7. Monthly Climatic Values for SESOIL Example Problem. San Francisco

Month	Mean Air Temp.[1] F	Mean Air Temp. C	Evapo-transpiration[2] fraction	Precipitation[1] in/mo	Precipitation cm/mo	Storm Duration[3] days	Storm Events[3] #/mo
October	71	22	0.3	1.09	2.8	0.1	3
November	65	18	0.3	2.49	6.3	0.25	5
December	60	16	0.3	3.52	8.9	0.25	5
January	55	13	0.3	4.48	11.4	0.25	8
February	55	13	0.3	2.83	7.2	0.25	9
March	60	16	0.3	2.58	6.6	0.25	5
April	64	18	0.3	1.48	3.8	0.1	3
May	68	20	0.3	0.35	0.9	0.1	2
June	68	20	0.3	0.15	0.4	0.1	2
July	72	22	0.3	0.04	0.1	0.1	1
August	71	22	0.3	0.08	0.2	0.1	1
September	71	22	0.3	0.24	0.6	0.1	2
Annual Totals or Annual Average	65	18	0.3	19.3	49.1	0.2	46.0

[1] *The Water Encyclopedia*, van der Leeden, et al., Lewis Publishers, 1991.

[2] This value was chosen by running the model and adjusting the evapotranspiration input value until the groundwater runoff predicted was in the range of 10 to 20% of the total precipitation.

[3] These input values were based on professional judgment.

Example Problem Results

The first two years of the SESOIL output file are at the end of this appendix (blank lines have been deleted to save paper). Figure A-5 shows the hydrologic cycle components from the annual summary report contained in the SESOIL output. The first hydrology may vary a little but from the second year until the end of the simulation the same hydrologic parameters are used in the model.

Figure A-5 shows one of the very important sections of the SESOIL output. This section summarizes the model-calculated values for soil moisture content for the entire soil column, infiltration (across the ground surface—not the amount of water reaching groundwater), surface runoff, and groundwater runoff (called GRW RUNOFF in the output). These values should be checked for reasonableness for every SESOIL run. This table is summarized in the "SESOIL Hydrology Summary" option under the "View Model Output" button.

```
1      YEAR -    2 ANNUAL SUMMARY REPORT

      ==================================
        -- TOTAL INPUTS (UG) --

 UPPER SOIL ZONE                 0.000E+00
 SOIL ZONE 2                     0.000E+00
 SOIL ZONE 3                     0.000E+00
 LOWER SOIL ZONE                 0.000E+00

           -- HYDROLOGIC CYCLE COMPONENTS --

 AVERAGE SOIL MOISTURE ZONE 1 (%)                 17.766
 AVERAGE SOIL MOISTURE BELOW ZONE 1 (%)           17.766
 TOTAL PRECIPITATION (CM)                         49.047
 TOTAL INFILTRATION (CM)                          22.656
 TOTAL EVAPOTRANSPIRATION (CM)                    14.760
 TOTAL SURFACE RUNOFF (CM)                        26.387
 TOTAL GRW RUNOFF (CM)                             7.896
 TOTAL MOISTURE RETENTION (CM)                      .000
 TOTAL YIELD (CM)                                 34.288
```

Figure A-5. Hydrologic Summary from SESOIL Output for Year 2.

Figure A-6 shows the first 20 years of simulation from the groundwater concentration chart in EXCEL®. The chart shows the seasonality of the SESOIL output. The wet months are assumed to produce higher groundwater runoff rates and hence higher mass loading rates.

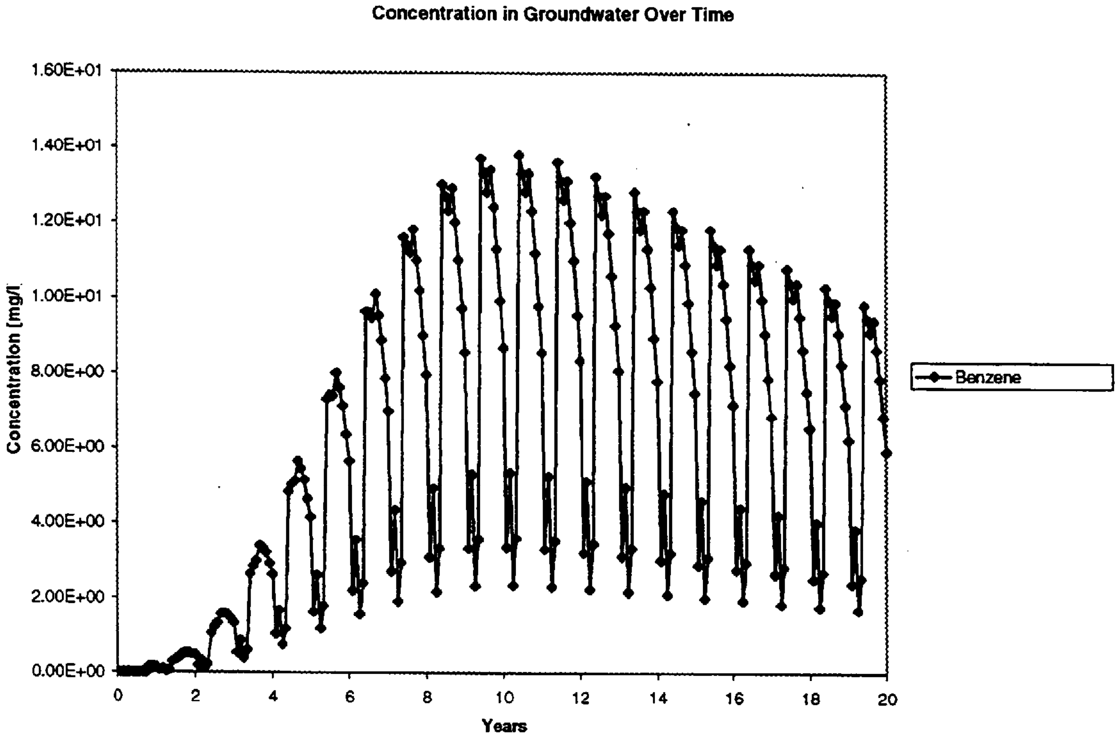


Figure A-6. Groundwater Concentrations for the First 20 Years.

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```
*********************************************************************************************************
*****                                                                                             *****
***** SESOIL-84 :  SEASONAL CYCLES OF WATER, SEDIMENT, AND POLLUTANTS IN SOIL ENVIRONMENTS        *****
*****                                                                                             *****
***** DEVELOPERS:  M. BONAZOUNTAS,ARTHUR D. LITTLE INC.   ,(617)864-5770,X5871                    *****
*****              J. WAGNER     ,DIS/ADLPIPE, INC.       ,(617)492-1991,X5820                    *****
*****                                                                                             *****
***** MODIFIED EXTENSIVELY BY:                                                                    *****
***** D.M. HETRICK                                                                                *****
***** OAK RIDGE NATIONAL LABORATORY                                                               *****
***** (615) 576-7556                                                                              *****
***** VERSION    :  JANUARY, 1995                                                                 *****
*****                                                                                             *****
*********************************************************************************************************

                        ****** MONTHLY SESOIL MODEL OPERATION ******
                               MONTHLY SITE SPECIFIC SIMULATION
RUN:    1

REGION          : (     1)          Enter Site Description Here
SOIL TYPE       : (     1)         Default soil type
COMPOUND        : (     1)         Benzene
WASHLOAD DATA   : (     0)
APPLICATION AREA: (     1)         DSS Fate and Transport

WARNING- SOIL PERMEABILITY VARYS CONSIDERABLY AMONG LAYERS
SESOIL MAY NOT BE ACCURATE FOR SUCH AN INHOMOGENEOUS COLUMN

     GENERAL INPUT PARAMETERS
     ========================

     -- SOIL INPUT PARAMETERS --

SOIL DENSITY (G/CM**3):                                       1.70
INTRINSIC PERMEABILITY (CM**2):                               .500E-10
DISCONNECTEDNESS INDEX (-):                                   6.00
POROSITY (-):                                                 .250
ORGANIC CARBON CONTENT (%):                                   .500
CATION EXCHANGE CAPACITY (MILLI EQ./100G DRY SOIL):           .000
FREUNDLICH EXPONENT (-):                                      1.00

     -- CHEMICAL INPUT PARAMETERS --

SOLUBILITY (UG/ML):                                           .175E+04
DIFFUSION COEFFICIENT IN AIR (CM**2/SEC):                     .880E-01
HENRYS LAW CONSTANT (M**3-ATM/MOLE):                          .548E-02
ADSORPTION COEFFICIENT ON ORGANIC CARBON(KOC):                58.9
ADSORPTION COEFFICIENT ON SOIL (K):                           .000
MOLECULAR  WEIGHT (G/MOL):                                    78.0
VALENCE (-):                                                  .000
NEUTRAL HYDROLYSIS CONSTANT (/DAY):                           .000
```

SESOIL Output for Example problem (Page 1 of 16)

```
BASE HYDROLYSIS CONSTANT (L/MOL-DAY):                        .000
ACID HYDROLYSIS CONSTANT (L/MOL-DAY):                        .000
DEGRADATION RATE IN MOISTURE (/DAY):                         .000
DEGRADATION RATE ON SOIL (/DAY):                             .000
LIGAND-POLLUTANT STABILITY CONSTANT (-):                     .000
NO. MOLES LIGAND/MOLE POLLUTANT (-):                         .000
LIGAND MOLECULAR WEIGHT (G/MOL):                             .000

    -- APPLICATION INPUT PARAMETERS --

NUMBER OF SOIL LAYERS:                                        4
YEARS TO BE SIMULATED:                                        2
AREA (CM**2):                                               .149E+07
APPLICATION AREA LATITUDE (DEG.):                           39.0
SPILL (1) OR STEADY APPLICATION (0):                         1
MODIFIED SUMMERS MODEL USED (1) OR NOT (0) FOR GWR. CONC.:   1
INITIAL CHEMICAL CONCENTRATIONS GIVEN (1) OR NOT GIVEN (0)   1
DEPTHS (CM):                                                .30E+03  .10E+03  .15E+03  75.
NUMBER OF SUBLAYERS/LAYER                                        4        1        1        4
PH (CM):                                                    7.0      7.0      7.0      7.0
INTRINSIC PERMEABILITIES (CM**2):                           .50E-10  .15E-08  .15E-08  .15E-08
KDEL RATIOS (-):                                            1.0      1.0      1.0
KDES RATIOS (-):                                            1.0      1.0      1.0
OC RATIOS (-):                                              1.0      1.0      1.0
CEC RATIOS (-):                                             1.0      1.0      1.0
FRN RATIOS(-):                                              1.0      1.0      1.0
ADS RATIOS(-):                                              1.0      1.0      1.0
1
    YEAR - 1     MONTHLY INPUT PARAMETERS
    =========    ========================

    -- CLIMATIC INPUT PARAMETERS --
                     OCT      NOV      DEC      JAN      FEB      MAR      APR      MAY      JUN      JUL      AUG      SEP
TEMP. (DEG C)      22.000   18.000   16.000   13.000   13.000   16.000   18.000   20.000   20.000   22.000   22.000   22.000
CLOUD CVR (FRAC.)    .000     .000     .000     .000     .000     .000     .000     .000     .000     .000     .000     .000
REL. HUM.(FRAC.)     .000     .000     .000     .000     .000     .000     .000     .000     .000     .000     .000     .000
ALBEDO (-)           .000     .000     .000     .000     .000     .000     .000     .000     .000     .000     .000     .000
EVAPOT. (CM/DAY)     .028     .062     .088     .112     .071     .065     .038     .009     .004     .001     .002     .006

PRECIP. (CM)        2.800    6.300    8.900   11.400    7.200    6.600    3.800     .900     .400     .100     .200     .600
M.TIME RAIN(DAYS)    .100     .250     .250     .250     .250     .250     .100     .100     .100     .100     .100     .100
M. STORM NO. (-)    3.000    5.000    5.000    8.000    9.000    5.000    3.000    2.000    2.000    1.000    1.000    2.000
M. SEASON (DAYS)   30.400   30.400   30.400   30.400   30.400   30.400   30.400   30.400   30.400   30.400   30.400   30.400

    INITIAL POLLUTANT CONCENTRATIONS IN UG/ML, INPUT FOR MONTH  4 OF YEAR 1
LAYER 1:
   SUBLAYER              1         2         3         4
INITIAL CONC. (UG/ML)  0.00E+00  0.00E+00  0.00E+00  0.00E+00

LAYER 2:
```

SESOIL Output for Example problem (Page 2 of 16)

```
     SUBLAYER              1
 INITIAL CONC. (UG/ML)  2.13E+01

 LAYER 3:
     SUBLAYER              1
 INITIAL CONC. (UG/ML)  1.02E+01

 LAYER 4:
     SUBLAYER              1        2        3        4
 INITIAL CONC. (UG/ML)  9.01E-02 9.01E-02 9.01E-02 9.01E-02

      -- POLLUTANT INPUT PARAMETERS --

                           OCT      NOV      DEC      JAN      FEB      MAR      APR      MAY      JUN      JUL      AUG      SEP
 POL. INP-1 (UG/CM**2)  0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00
 TRNSFORMD-1 (UG/CM**2) 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00
 SINKS-1 (UG/CM**2)     0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00
 LIG.INPUT-1 (UG/CM**2) 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00
 VOLATILIZATION MULT.-1 2.00E-01 2.00E-01 2.00E-01 2.00E-01 2.00E-01 2.00E-01 2.00E-01 2.00E-01 2.00E-01 2.00E-01 2.00E-01 2.00E-01
 SURFACE RUNOFF MULT.   0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00
 POL. IN RAIN (FRAC-SL) 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00

 POL. INP-2 (UG/CM**2)  0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00
 TRNSFORMD-2 (UG/CM**2) 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00
 SINKS-2 (UG/CM**2)     0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00
 LIG.INPUT-2 (UG/CM**2) 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00
 VOLATILIZATION MULT.-2 2.00E-01 2.00E-01 2.00E-01 2.00E-01 2.00E-01 2.00E-01 2.00E-01 2.00E-01 2.00E-01 2.00E-01 2.00E-01 2.00E-01

 POL. INP-3 (UG/CM**2)  0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00
 TRNSFORMD-3 (UG/CM**2) 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00
 SINKS-3 (UG/CM**2)     0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00
 LIG.INPUT-3 (UG/CM**2) 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00
 VOLATILIZATION MULT.-3 2.00E-01 2.00E-01 2.00E-01 2.00E-01 2.00E-01 2.00E-01 2.00E-01 2.00E-01 2.00E-01 2.00E-01 2.00E-01 2.00E-01

 POL. INP-L (UG/CM**2)  0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00
 TRNSFORMD-L (UG/CM**2) 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00
 SINKS-L (UG/CM**2)     0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00
 LIG.INPUT-L (UG/CM**2) 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00
 VOLATILIZATION MULT.-L 2.00E-01 2.00E-01 2.00E-01 2.00E-01 2.00E-01 2.00E-01 2.00E-01 2.00E-01 2.00E-01 2.00E-01 2.00E-01 2.00E-01
1
      YEAR -  2     MONTHLY INPUT PARAMETERS
      =========     ========================
      -- CLIMATIC INPUT PARAMETERS ARE SAME AS LAST YEAR
      -- POLLUTANT INPUT PARAMETERS ARE SAME AS LAST YEAR
      -- MODIFIED SUMMERS MODEL PARAMETERS --
 (INPUT FOR CALCULATION OF CONTAMINANT IN GROUNDWATER)

 SATURATED HYDRAULIC CONDUCTIVITY (CM/DAY):                  1.30E+01
 HORIZONTAL HYDRAULIC GRADIENT:                              8.00E-03
 THICKNESS OF SATURATED ZONE (CM):                           2.00E+02
 WIDTH OF CONTAMINATED ZONE PERPENDICULAR TO FLOW (CM):      9.00E+02
```

SESOIL Output for Example problem (Page 3 of 16)

```
BACKGROUND CONTAMINANT CONCENTRATION IN AQUIFER (UG/ML):   0.00E+00

**** WARNING - PROBLEM IN HYDRO CYCLE: W EQUALS OR  EXCEEDS EP
    W SET TO EP
**** WARNING (MONTH 1) - PROBLEM IN HYDRO CYCLE: W EQUALS OR EXCEEDS EP
    W SET TO EP
**** WARNING (MONTH 2) - PROBLEM IN HYDRO CYCLE: W EQUALS OR EXCEEDS EP
    W SET TO EP
**** WARNING (MONTH 3) - PROBLEM IN HYDRO CYCLE: W EQUALS OR EXCEEDS EP
    W SET TO EP
**** WARNING (MONTH 4) - PROBLEM IN HYDRO CYCLE: W EQUALS OR EXCEEDS EP
    W SET TO EP
**** WARNING (MONTH 5) - PROBLEM IN HYDRO CYCLE: W EQUALS OR EXCEEDS EP
    W SET TO EP
**** WARNING (MONTH 6) - PROBLEM IN HYDRO CYCLE: W EQUALS OR EXCEEDS EP
    W SET TO EP
**** WARNING (MONTH 7) - PROBLEM IN HYDRO CYCLE: W EQUALS OR EXCEEDS EP
    W SET TO EP
**** WARNING (MONTH 8) - PROBLEM IN HYDRO CYCLE: W EQUALS OR EXCEEDS EP
    W SET TO EP
**** WARNING (MONTH 9) - PROBLEM IN HYDRO CYCLE: W EQUALS OR EXCEEDS EP
    W SET TO EP
**** WARNING (MONTH10) - PROBLEM IN HYDRO CYCLE: W EQUALS OR EXCEEDS EP
    W SET TO EP
**** WARNING (MONTH11) - PROBLEM IN HYDRO CYCLE: W EQUALS OR EXCEEDS EP
    W SET TO EP
**** WARNING (MONTH12) - PROBLEM IN HYDRO CYCLE: W EQUALS OR EXCEEDS EP
    W SET TO EP
1
     YEAR -  1     MONTHLY RESULTS (OUTPUT)
     =========     ========================

     -- HYDROLOGIC CYCLE COMPONENTS --
                        OCT      NOV      DEC      JAN      FEB      MAR      APR      MAY      JUN      JUL      AUG      SEP
MOIS. IN L1 (%)       17.964   19.264   19.839   20.814   21.039   20.264   18.789   17.389   16.289   15.214   14.589   14.639
MOIS. BELOW L1 (%)    17.964   19.264   19.839   20.814   21.039   20.264   18.789   17.389   16.289   15.214   14.589   14.639
PRECIPATION (CM)       2.785    6.295    8.902   11.318    7.187    6.609    3.796     .913     .417     .118     .206     .602
NET INFILT. (CM)       1.467    3.227    3.200    4.080    3.914    2.880    1.423     .717     .403     .118     .202     .566
EVAPOTRANS. (CM)        .840    1.890    2.670    3.420    2.160    1.980    1.140     .270     .120     .030     .060     .180
MOIS. RETEN (CM)       -.378     .677     .299     .508     .117    -.404    -.768    -.729    -.573    -.560    -.326     .026
SUR. RUNOFF (CM)       1.318    3.068    5.702    7.238    3.273    3.729    2.374     .196     .013     .000     .000     .037
GRW. RUNOFF (CM)       1.005     .660     .230     .153    1.637    1.304    1.051    1.176     .856     .648     .468     .360
YIELD (CM)             2.323    3.728    5.932    7.391    4.910    5.032    3.425    1.372     .870     .648     .472     .396

PAU/MPA (GZU)           .995     .999    1.000     .993     .998    1.001     .999    1.014    1.042    1.184    1.031    1.004
PA/MPA (GZ)             .995     .999    1.000     .993     .998    1.001     .999    1.014    1.042    1.184    1.031    1.004
```

SESOIL Output for Example problem (Page 4 of 16)

```
1                      -- POLLUTANT MASS INPUT TO COLUMN (UG) - INCLUDES INITIAL POLLUTANT CONCENTRATIONS --
                       -------------------------------------------------------------------------------------
                  OCT        NOV        DEC        JAN        FEB        MAR        APR        MAY        JUN        JUL        AUG        SEP
 PRECIP.      0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00
 LOAD UPPER   0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00
 LOAD ZONE 2  0.000E+00 0.000E+00 0.000E+00 3.163E+09 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00
 LOAD ZONE 3  0.000E+00 0.000E+00 0.000E+00 2.272E+09 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00
 LOAD LOWER   0.000E+00 0.000E+00 0.000E+00 1.003E+07 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00

 TOTAL INPUT 0.000E+00 0.000E+00 0.000E+00 5.445E+09 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00
0            -- POLLUTANT MASS DISTRIBUTION IN COLUMN (UG) -- NOTE: IF COMPONENT IS ZERO EACH MONTH, IT IS NOT PRINTED
             ---------------------------------------------------------------------------------------------------------

      UPPER SOIL ZONE:
           SUBLAYER  1
 VOLATILIZED 0.000E+00 0.000E+00 0.000E+00 7.503E-06 7.201E-06 1.297E-05 3.126E-05 7.641E-03 1.813E-01 2.254E+00 1.542E+01 5.342E+01
 IN SOIL MOI 0.000E+00 0.000E+00 0.000E+00 2.318E-03 2.343E-03 2.257E-03 2.093E-03 7.011E-01 8.008E+00 5.750E+01 2.700E+02 8.119E+02
 ADS ON SOIL 0.000E+00 0.000E+00 0.000E+00 5.576E-03 5.576E-03 5.576E-03 5.576E-03 2.019E+00 2.461E+01 1.892E+02 9.267E+02 2.777E+03
 IN SOIL AIR 0.000E+00 0.000E+00 0.000E+00 1.097E-04 1.038E-04 1.232E-04 1.577E-04 6.945E-02 9.693E-01 8.283E+00 4.315E+01 1.287E+02

           SUBLAYER  2
 DIFFUSED UP 0.000E+00 0.000E+00 0.000E+00 1.847E-05 6.330E-04 8.877E-03 1.884E-01 3.248E+00 3.316E+01 2.363E+02 1.046E+03 2.624E+03
 IN SOIL MOI 0.000E+00 0.000E+00 0.000E+00 3.709E-02 4.686E-01 3.074E+00 2.746E+01 2.187E+02 1.217E+03 5.167E+03 1.614E+04 3.647E+04
 ADS ON SOIL 0.000E+00 0.000E+00 0.000E+00 8.922E-02 1.115E+00 7.594E+00 7.316E+01 6.296E+02 3.741E+03 1.700E+04 5.539E+04 1.247E+05
 IN SOIL AIR 0.000E+00 0.000E+00 0.000E+00 1.755E-03 2.075E-02 1.678E-01 2.069E+00 2.166E+01 1.473E+02 7.443E+02 2.580E+03 5.780E+03

           SUBLAYER  3
 DIFFUSED UP 0.000E+00 0.000E+00 0.000E+00 3.284E-01 1.722E+00 1.012E+01 9.866E+01 8.179E+02 4.486E+03 1.881E+04 5.403E+04 9.831E+04
 IN SOIL MOI 0.000E+00 0.000E+00 0.000E+00 2.616E+02 8.887E+02 2.795E+03 1.147E+04 4.432E+04 1.355E+05 3.451E+05 7.205E+05 1.227E+06
 ADS ON SOIL 0.000E+00 0.000E+00 0.000E+00 6.292E+02 2.115E+03 6.906E+03 3.057E+04 1.276E+05 4.164E+05 1.136E+06 2.473E+06 4.196E+06
 IN SOIL AIR 0.000E+00 0.000E+00 0.000E+00 1.237E+01 3.936E+01 1.526E+02 8.645E+02 4.391E+03 1.640E+04 4.971E+04 1.151E+05 1.945E+05

           SUBLAYER  4
 DIFFUSED UP 0.000E+00 0.000E+00 0.000E+00 9.836E+02 2.283E+03 7.302E+03 3.501E+04 1.406E+05 4.115E+05 1.011E+06 1.878E+06 2.469E+06
 IN SOIL MOI 0.000E+00 0.000E+00 0.000E+00 5.216E+05 9.377E+05 1.613E+06 3.145E+06 5.934E+06 9.995E+06 1.534E+07 2.150E+07 2.772E+07
 ADS ON SOIL 0.000E+00 0.000E+00 0.000E+00 1.255E+06 2.231E+06 3.984E+06 8.381E+06 1.708E+07 3.072E+07 5.047E+07 7.378E+07 9.481E+07
 IN SOIL AIR 0.000E+00 0.000E+00 0.000E+00 2.467E+04 4.153E+04 8.804E+04 2.370E+05 5.878E+05 1.210E+06 2.209E+06 3.436E+06 4.394E+06

      SOIL ZONE 2:
           SUBLAYER  1
 DIFFUSED UP 0.000E+00 0.000E+00 0.000E+00 1.902E+06 1.532E+06 2.697E+06 6.444E+06 1.250E+07 1.935E+07 2.778E+07 3.329E+07 3.164E+07
 IN SOIL MOI 0.000E+00 0.000E+00 0.000E+00 8.958E+08 8.727E+08 8.250E+08 7.630E+08 7.038E+08 6.563E+08 6.104E+08 5.792E+08 5.704E+08
 ADS ON SOIL 0.000E+00 0.000E+00 0.000E+00 2.155E+09 2.077E+09 2.038E+09 2.033E+09 2.026E+09 2.017E+09 2.009E+09 1.988E+09 1.951E+09
 IN SOIL AIR 0.000E+00 0.000E+00 0.000E+00 4.238E+07 3.865E+07 4.504E+07 5.749E+07 6.972E+07 7.944E+07 8.792E+07 9.256E+07 9.041E+07

      SOIL ZONE 3:
           SUBLAYER  1
 IN SOIL MOI 0.000E+00 0.000E+00 0.000E+00 6.739E+08 6.977E+08 6.900E+08 6.565E+08 6.209E+08 5.910E+08 5.599E+08 5.417E+08 5.449E+08
 ADS ON SOIL 0.000E+00 0.000E+00 0.000E+00 1.621E+09 1.660E+09 1.705E+09 1.749E+09 1.788E+09 1.816E+09 1.842E+09 1.859E+09 1.863E+09
 IN SOIL AIR 0.000E+00 0.000E+00 0.000E+00 3.188E+07 3.090E+07 3.767E+07 4.947E+07 6.151E+07 7.153E+07 8.065E+07 8.656E+07 8.636E+07
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SESOIL Output for Example problem (Page 5 of 16)

```
       LOWER SOIL ZONE:
          SUBLAYER  1
   IN SOIL MOI 0.000E+00 0.000E+00 0.000E+00 4.482E+06 1.531E+07 2.237E+07 2.594E+07 2.874E+07 3.004E+07 3.025E+07 3.051E+07 3.174E+07
   ADS ON SOIL 0.000E+00 0.000E+00 0.000E+00 1.078E+07 3.643E+07 5.527E+07 6.911E+07 8.274E+07 9.234E+07 9.956E+07 1.047E+08 1.086E+08
   IN SOIL AIR 0.000E+00 0.000E+00 0.000E+00 2.120E+05 6.780E+05 1.221E+06 1.954E+06 2.847E+06 3.636E+06 4.358E+06 4.876E+06 5.031E+06

          SUBLAYER  2
   IN SOIL MOI 0.000E+00 0.000E+00 0.000E+00 8.051E+05 2.027E+06 3.703E+06 5.085E+06 6.607E+06 7.643E+06 8.246E+06 8.720E+06 9.414E+06
   ADS ON SOIL 0.000E+00 0.000E+00 0.000E+00 1.937E+06 4.822E+06 9.150E+06 1.355E+07 1.902E+07 2.349E+07 2.713E+07 2.992E+07 3.219E+07
   IN SOIL AIR 0.000E+00 0.000E+00 0.000E+00 3.809E+04 8.974E+04 2.022E+05 3.832E+05 6.546E+05 9.251E+05 1.188E+06 1.393E+06 1.492E+06

          SUBLAYER  3
   IN SOIL MOI 0.000E+00 0.000E+00 0.000E+00 7.338E+05 8.182E+05 9.990E+05 1.205E+06 1.520E+06 1.786E+06 1.975E+06 2.134E+06 2.344E+06
   ADS ON SOIL 0.000E+00 0.000E+00 0.000E+00 1.765E+06 1.947E+06 2.468E+06 3.211E+06 4.375E+06 5.490E+06 6.500E+06 7.324E+06 8.017E+06
   IN SOIL AIR 0.000E+00 0.000E+00 0.000E+00 3.471E+04 3.623E+04 5.454E+04 9.081E+04 1.505E+05 2.162E+05 2.845E+05 3.411E+05 3.715E+05

          SUBLAYER  4
   DIFFUSED UP 0.000E+00 0.000E+00 0.000E+00 2.398E+02 1.419E+03 4.124E+02 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00
   IN SOIL MOI 0.000E+00 0.000E+00 0.000E+00 7.412E+05 8.439E+05 9.089E+05 9.429E+05 1.005E+06 1.059E+06 1.041E+06 1.042E+06 1.079E+06
   ADS ON SOIL 0.000E+00 0.000E+00 0.000E+00 1.783E+06 2.008E+06 2.246E+06 2.512E+06 2.893E+06 3.255E+06 3.426E+06 3.574E+06 3.692E+06
   IN SOIL AIR 0.000E+00 0.000E+00 0.000E+00 3.506E+04 3.737E+04 4.962E+04 7.105E+04 9.955E+04 1.282E+05 1.500E+05 1.664E+05 1.711E+05
   GWR. RUNOFF 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 2.320E+05 1.750E+05 1.392E+05


     -- POLLUTANT CONCENTRATIONS (UG/ML) OR (UG/G) -- NOTE: IF CONCENTRATIONS ARE ZERO FOR EACH MONTH, THEY ARE NOT PRINTED --
     ---------------------------------------------------------------------------------------------------------------------------

       UPPER SOIL ZONE:
          SUBLAYER  1
   MOISTURE     0.000E+00 0.000E+00 0.000E+00 1.000E-10 1.000E-10 1.000E-10 1.000E-10 3.620E-08 4.414E-07 3.394E-06 1.662E-05 4.980E-05
   %SOLUBILITY  0.000E+00 0.000E+00 0.000E+00 5.714E-12 5.714E-12 5.714E-12 5.714E-12 2.069E-09 2.522E-08 1.939E-07 9.497E-07 2.846E-06
   ADSORBED     0.000E+00 0.000E+00 0.000E+00 2.945E-11 2.945E-11 2.945E-11 2.945E-11 1.066E-08 1.300E-07 9.994E-07 4.894E-06 1.467E-05
   SOIL AIR     0.000E+00 0.000E+00 0.000E+00 2.352E-11 2.352E-11 2.336E-11 2.280E-11 8.193E-09 9.990E-08 7.600E-07 3.722E-06 1.115E-05

          SUBLAYER  2
   MOISTURE     0.000E+00 0.000E+00 0.000E+00 1.600E-09 2.000E-08 1.362E-07 1.312E-06 1.129E-05 6.710E-05 3.050E-04 9.934E-04 2.237E-03
   %SOLUBILITY  0.000E+00 0.000E+00 0.000E+00 9.143E-11 1.143E-09 7.783E-09 7.497E-08 6.452E-07 3.834E-06 1.743E-05 5.677E-05 1.278E-04
   ADSORBED     0.000E+00 0.000E+00 0.000E+00 4.712E-10 5.890E-09 4.011E-08 3.864E-07 3.325E-06 1.976E-05 8.981E-05 2.926E-04 6.588E-04
   SOIL AIR     0.000E+00 0.000E+00 0.000E+00 3.763E-10 4.704E-09 3.182E-08 2.991E-07 2.556E-06 1.519E-05 6.829E-05 2.225E-04 5.009E-04

          SUBLAYER  3
   MOISTURE     0.000E+00 0.000E+00 0.000E+00 1.128E-05 3.793E-05 1.239E-04 5.482E-04 2.289E-03 7.467E-03 2.037E-02 4.434E-02 7.525E-02
   %SOLUBILITY  0.000E+00 0.000E+00 0.000E+00 6.448E-07 2.167E-06 7.078E-06 3.133E-05 1.308E-04 4.267E-04 1.164E-03 2.534E-03 4.300E-03
   ADSORBED     0.000E+00 0.000E+00 0.000E+00 3.323E-06 1.117E-05 3.648E-05 1.615E-04 6.740E-04 2.199E-03 5.998E-03 1.306E-02 2.216E-02
   SOIL AIR     0.000E+00 0.000E+00 0.000E+00 2.654E-06 8.921E-06 2.893E-05 1.250E-04 5.180E-04 1.690E-03 4.561E-03 9.930E-03 1.685E-02

          SUBLAYER  4
   MOISTURE     0.000E+00 0.000E+00 0.000E+00 2.250E-02 4.002E-02 7.145E-02 1.503E-01 3.064E-01 5.509E-01 9.051E-01 1.323E+00 1.700E+00
   %SOLUBILITY  0.000E+00 0.000E+00 0.000E+00 1.286E-03 2.287E-03 4.083E-03 8.589E-03 1.751E-02 3.148E-02 5.172E-02 7.561E-02 9.716E-02
   ADSORBED     0.000E+00 0.000E+00 0.000E+00 6.626E-03 1.179E-02 2.104E-02 4.426E-02 9.023E-02 1.622E-01 2.666E-01 3.897E-01 5.007E-01
   SOIL AIR     0.000E+00 0.000E+00 0.000E+00 5.293E-03 9.413E-03 1.669E-02 3.426E-02 6.934E-02 1.247E-01 2.027E-01 2.963E-01 3.808E-01
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SESOIL Output for Example problem (Page 6 of 16)

```
        SOIL ZONE 2:
             SUBLAYER  1
MOISTURE      0.000E+00 0.000E+00 0.000E+00 2.898E+01 2.793E+01 2.742E+01 2.735E+01 2.726E+01 2.713E+01 2.702E+01 2.673E+01 2.624E+01
%SOLUBILITY 0.000E+00 0.000E+00 0.000E+00 1.656E+00 1.596E+00 1.567E+00 1.563E+00 1.558E+00 1.550E+00 1.544E+00 1.528E+00 1.499E+00
ADSORBED      0.000E+00 0.000E+00 0.000E+00 8.536E+00 8.226E+00 8.074E+00 8.053E+00 8.027E+00 7.990E+00 7.957E+00 7.873E+00 7.728E+00
SOIL AIR      0.000E+00 0.000E+00 0.000E+00 6.817E+00 6.570E+00 6.404E+00 6.234E+00 6.169E+00 6.141E+00 6.050E+00 5.987E+00 5.876E+00

        SOIL ZONE 3:
             SUBLAYER  1
MOISTURE      0.000E+00 0.000E+00 0.000E+00 1.454E+01 1.489E+01 1.529E+01 1.569E+01 1.603E+01 1.629E+01 1.652E+01 1.667E+01 1.671E+01
%SOLUBILITY 0.000E+00 0.000E+00 0.000E+00 8.306E-01 8.507E-01 8.735E-01 8.964E-01 9.160E-01 9.307E-01 9.441E-01 9.525E-01 9.548E-01
ADSORBED      0.000E+00 0.000E+00 0.000E+00 4.281E+00 4.384E+00 4.502E+00 4.620E+00 4.721E+00 4.797E+00 4.866E+00 4.909E+00 4.921E+00
SOIL AIR      0.000E+00 0.000E+00 0.000E+00 3.419E+00 3.502E+00 3.571E+00 3.576E+00 3.628E+00 3.686E+00 3.700E+00 3.733E+00 3.742E+00

        LOWER SOIL ZONE:
             SUBLAYER  1
MOISTURE      0.000E+00 0.000E+00 0.000E+00 7.735E-01 2.613E+00 3.965E+00 4.957E+00 5.935E+00 6.624E+00 7.142E+00 7.511E+00 7.787E+00
%SOLUBILITY 0.000E+00 0.000E+00 0.000E+00 4.420E-02 1.493E-01 2.266E-01 2.833E-01 3.392E-01 3.785E-01 4.081E-01 4.292E-01 4.450E-01
ADSORBED      0.000E+00 0.000E+00 0.000E+00 2.278E-01 7.697E-01 1.168E+00 1.460E+00 1.748E+00 1.951E+00 2.103E+00 2.212E+00 2.293E+00
SOIL AIR      0.000E+00 0.000E+00 0.000E+00 1.819E-01 6.147E-01 9.262E-01 1.130E+00 1.343E+00 1.499E+00 1.599E+00 1.682E+00 1.744E+00

             SUBLAYER  2
MOISTURE      0.000E+00 0.000E+00 0.000E+00 1.389E-01 3.459E-01 6.564E-01 9.720E-01 1.365E+00 1.685E+00 1.946E+00 2.147E+00 2.310E+00
%SOLUBILITY 0.000E+00 0.000E+00 0.000E+00 7.939E-03 1.977E-02 3.751E-02 5.554E-02 7.798E-02 9.630E-02 1.112E-01 1.227E-01 1.320E-01
ADSORBED      0.000E+00 0.000E+00 0.000E+00 4.091E-02 1.019E-01 1.933E-01 2.863E-01 4.019E-01 4.963E-01 5.732E-01 6.322E-01 6.802E-01
SOIL AIR      0.000E+00 0.000E+00 0.000E+00 3.268E-02 8.137E-02 1.533E-01 2.216E-01 3.089E-01 3.814E-01 4.359E-01 4.807E-01 5.172E-01

             SUBLAYER  3
MOISTURE      0.000E+00 0.000E+00 0.000E+00 1.266E-01 1.397E-01 1.770E-01 2.303E-01 3.139E-01 3.938E-01 4.663E-01 5.254E-01 5.751E-01
%SOLUBILITY 0.000E+00 0.000E+00 0.000E+00 7.235E-03 7.981E-03 1.012E-02 1.316E-02 1.793E-02 2.250E-02 2.665E-02 3.002E-02 3.286E-02
ADSORBED      0.000E+00 0.000E+00 0.000E+00 3.729E-02 4.113E-02 5.214E-02 6.784E-02 9.243E-02 1.160E-01 1.373E-01 1.547E-01 1.694E-01
SOIL AIR      0.000E+00 0.000E+00 0.000E+00 2.978E-02 3.285E-02 4.136E-02 5.251E-02 7.104E-02 8.914E-02 1.044E-01 1.177E-01 1.288E-01

             SUBLAYER  4
MOISTURE      0.000E+00 0.000E+00 0.000E+00 1.279E-01 1.441E-01 1.611E-01 1.802E-01 2.075E-01 2.335E-01 2.458E-01 2.564E-01 2.648E-01
%SOLUBILITY 0.000E+00 0.000E+00 0.000E+00 7.308E-03 8.232E-03 9.205E-03 1.030E-02 1.186E-02 1.334E-02 1.404E-02 1.465E-02 1.513E-02
ADSORBED      0.000E+00 0.000E+00 0.000E+00 3.766E-02 4.242E-02 4.744E-02 5.308E-02 6.112E-02 6.878E-02 7.238E-02 7.551E-02 7.799E-02
SOIL AIR      0.000E+00 0.000E+00 0.000E+00 3.008E-02 3.388E-02 3.763E-02 4.109E-02 4.697E-02 5.286E-02 5.504E-02 5.742E-02 5.930E-02

POL DEP CM    0.000E+00 0.000E+00 0.000E+00 6.162E+02 6.186E+02 6.206E+02 6.221E+02 6.238E+02 6.250E+02 6.250E+02 6.250E+02 6.250E+02

        -- POLLUTANT CONCENTRATION IN GROUNDWATER (UG/ML) --

GWR. CONC.    0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 1.545E-01 1.409E-01 1.282E-01

1                         YEAR -    1 ANNUAL SUMMARY REPORT
                          ==================================
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SESOIL Output for Example problem (Page 7 of 16)

```
        -- TOTAL INPUTS (UG) --

UPPER SOIL ZONE                0.000E+00
SOIL ZONE 2                    3.163E+09
SOIL ZONE 3                    2.272E+09
LOWER SOIL ZONE                1.003E+07

           -- HYDROLOGIC CYCLE COMPONENTS --

AVERAGE SOIL MOISTURE ZONE 1 (%)                18.008
AVERAGE SOIL MOISTURE BELOW ZONE 1 (%)          18.008
TOTAL PRECIPITATION (CM)                        49.149
TOTAL INFILTRATION (CM)                         22.197
TOTAL EVAPOTRANSPIRATION (CM)                   14.760
TOTAL SURFACE RUNOFF (CM)                       26.948
TOTAL GRW RUNOFF (CM)                            9.546
TOTAL MOISTURE RETENTION (CM)                   -2.109
TOTAL YIELD (CM)                                36.499
```

SESOIL Output for Example problem (Page 8 of 16)

```
0           -- POLLUTANT MASS DISTRIBUTION IN COLUMN (UG) -- NOTE: IF COMPONENT IS ZERO EACH MONTH, IT IS NOT PRINTED
               -----------------------------------------------------------------------------------------
 FOR FINAL MASS IN SOIL MOI., ADS. ON SOIL, SOIL AIR, IMMOBIL CEC, COMPLEXED, AND PURE PHASE FOR EACH SUBLAYER, SEE ABOVE (MONTH SEP)
 ----------------------------------------------------------------------------------------------------------------------------------

    UPPER SOIL ZONE:
         SUBLAYER  1
              TOTAL VOLATILIZED                  7.128E+01
         SUBLAYER  2
              TOTAL DIFFUSED (UP)                3.942E+03
         SUBLAYER  3
              TOTAL DIFFUSED (UP)                1.766E+05
         SUBLAYER  4
              TOTAL DIFFUSED (UP)                5.955E+06

    SOIL ZONE 2:
         SUBLAYER  1
              TOTAL DIFFUSED (UP)                1.371E+08

    SOIL ZONE 3:
         SUBLAYER  1

    LOWER SOIL ZONE:
         SUBLAYER  1

         SUBLAYER  2

         SUBLAYER  3

         SUBLAYER  4

              TOTAL DIFFUSED (UP)                2.071E+03
              TOTAL IN GROUNDWATER RUNOFF        5.461E+05
1                         -- AVERAGE POLLUTANT CONCENTRATIONS --  NOTE: ONLY NON-ZERO VALUES ARE PRINTED --
                          ------------------------------------------------------------------------------

    UPPER SOIL ZONE:
         SUBLAYER  1
                                   SOIL MOISTURE (UG/ML)  5.857E-06
                                   ADSORBED SOIL (UG/G)   1.725E-06
                                   SOIL AIR (UG/ML)       1.312E-06
         SUBLAYER  2
                                   SOIL MOISTURE (UG/ML)  3.013E-04
                                   ADSORBED SOIL (UG/G)   8.872E-05
                                   SOIL AIR (UG/ML)       6.748E-05
         SUBLAYER  3
                                   SOIL MOISTURE (UG/ML)  1.254E-02
                                   ADSORBED SOIL (UG/G)   3.692E-03
                                   SOIL AIR (UG/ML)       2.810E-03
         SUBLAYER  4
```

SESOIL Output for Example problem (Page 9 of 16)

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                                        SOIL MOISTURE (UG/ML)  4.225E-01
                                        ADSORBED SOIL (UG/G)   1.244E-01
                                        SOIL AIR (UG/ML)       9.495E-02
   SOIL ZONE 2:
        SUBLAYER  1
                                        SOIL MOISTURE (UG/ML)  2.050E+01
                                        ADSORBED SOIL (UG/G)   6.039E+00
                                        SOIL AIR (UG/ML)       4.687E+00
   SOIL ZONE 3:
        SUBLAYER  1
                                        SOIL MOISTURE (UG/ML)  1.188E+01
                                        ADSORBED SOIL (UG/G)   3.500E+00
                                        SOIL AIR (UG/ML)       2.713E+00
   LOWER SOIL ZONE:
        SUBLAYER  1
                                        SOIL MOISTURE (UG/ML)  3.942E+00
                                        ADSORBED SOIL (UG/G)   1.161E+00
                                        SOIL AIR (UG/ML)       8.934E-01
        SUBLAYER  2
                                        SOIL MOISTURE (UG/ML)  9.638E-01
                                        ADSORBED SOIL (UG/G)   2.838E-01
                                        SOIL AIR (UG/ML)       2.178E-01
        SUBLAYER  3
                                        SOIL MOISTURE (UG/ML)  2.457E-01
                                        ADSORBED SOIL (UG/G)   7.235E-02
                                        SOIL AIR (UG/ML)       5.563E-02
        SUBLAYER  4
                                        SOIL MOISTURE (UG/ML)  1.518E-01
                                        ADSORBED SOIL (UG/G)   4.470E-02
                                        SOIL AIR (UG/ML)       3.452E-02

                                        MAX. POLL. DEPTH (M)   6.250E+00

  AVE. CONTAMINANT CONCENTRATION IN GROUNDWATER (UG/ML)        3.530E-02

**** WARNING (MONTH 1) - PROBLEM IN HYDRO CYCLE: W EQUALS OR EXCEEDS EP
    W SET TO EP
**** WARNING (MONTH 2) - PROBLEM IN HYDRO CYCLE: W EQUALS OR EXCEEDS EP
    W SET TO EP
**** WARNING (MONTH 3) - PROBLEM IN HYDRO CYCLE: W EQUALS OR EXCEEDS EP
    W SET TO EP
**** WARNING (MONTH 4) - PROBLEM IN HYDRO CYCLE: W EQUALS OR EXCEEDS EP
    W SET TO EP
**** WARNING (MONTH 5) - PROBLEM IN HYDRO CYCLE: W EQUALS OR EXCEEDS EP
    W SET TO EP
**** WARNING (MONTH 6) - PROBLEM IN HYDRO CYCLE: W EQUALS OR EXCEEDS EP
    W SET TO EP
**** WARNING (MONTH 7) - PROBLEM IN HYDRO CYCLE: W EQUALS OR EXCEEDS EP
    W SET TO EP
**** WARNING (MONTH 8) - PROBLEM IN HYDRO CYCLE: W EQUALS OR EXCEEDS EP
    W SET TO EP
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SESOIL Output for Example problem (Page 10 of 16)

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**** WARNING (MONTH 9) - PROBLEM IN HYDRO CYCLE: W EQUALS OR EXCEEDS EP
    W SET TO EP
**** WARNING (MONTH10) - PROBLEM IN HYDRO CYCLE: W EQUALS OR EXCEEDS EP
    W SET TO EP
**** WARNING (MONTH11) - PROBLEM IN HYDRO CYCLE: W EQUALS OR EXCEEDS EP
    W SET TO EP
**** WARNING (MONTH12) - PROBLEM IN HYDRO CYCLE: W EQUALS OR EXCEEDS EP
    W SET TO EP


     YEAR -  2    MONTHLY RESULTS (OUTPUT)
     =========    ========================

     -- HYDROLOGIC CYCLE COMPONENTS --

                        OCT      NOV      DEC      JAN      FEB      MAR      APR      MAY      JUN      JUL      AUG      SEP
MOIS. IN L1 (%)       16.014   18.589   19.639   20.764   21.014   20.264   18.789   17.389   16.289   15.214   14.589   14.639
MOIS. BELOW L1 (%)    16.014   18.589   19.639   20.764   21.014   20.264   18.789   17.389   16.289   15.214   14.589   14.639
PRECIPATION (CM)       2.776    6.263    8.880   11.299    7.138    6.639    3.796     .913     .417     .118     .206     .602
NET INFILT. (CM)       1.646    3.404    3.278    4.108    3.900    2.893    1.423     .717     .403     .118     .202     .566
EVAPOTRANS. (CM)        .840    1.890    2.670    3.420    2.160    1.980    1.140     .270     .120     .030     .060     .180
MOIS. RETEN (CM)        .716    1.341     .547     .586     .130    -.391    -.768    -.729    -.573    -.560    -.326     .026
SUR. RUNOFF (CM)       1.130    2.859    5.603    7.192    3.238    3.746    2.374     .196     .013     .000     .000     .037
GRW. RUNOFF (CM)        .090     .172     .061     .102    1.610    1.304    1.051    1.176     .856     .648     .468     .360
YIELD (CM)             1.220    3.032    5.664    7.293    4.848    5.049    3.425    1.372     .870     .648     .472     .396

PAU/MPA (GZU)           .991     .994     .998     .991     .991    1.006     .999    1.014    1.042    1.184    1.031    1.004
PA/MPA (GZ)             .991     .994     .998     .991     .991    1.006     .999    1.014    1.042    1.184    1.031    1.004
1                                         -- POLLUTANT MASS INPUT TO COLUMN (UG) --
                                          ----------------------------------------

                OCT        NOV        DEC        JAN        FEB        MAR        APR        MAY        JUN        JUL        AUG        SEP
PRECIP.     0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00
LOAD UPPER  0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00
LOAD ZONE 2 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00
LOAD ZONE 3 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00
LOAD LOWER  0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00

TOTAL INPUT 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00

0         -- POLLUTANT MASS DISTRIBUTION IN COLUMN (UG) -- NOTE: IF COMPONENT IS ZERO EACH MONTH, IT IS NOT PRINTED
          ----------------------------------------------------------------------------------------------------

     UPPER SOIL ZONE:
          SUBLAYER  1
VOLATILIZED 6.989E+01 3.016E+01 1.770E+01 8.183E+00 6.458E+00 1.132E+01 2.937E+01 6.951E+01 1.493E+02 3.368E+02 6.854E+02 1.078E+03
IN SOIL MOI 1.490E+03 1.886E+03 2.038E+03 2.073E+03 2.021E+03 1.975E+03 2.071E+03 2.464E+03 3.337E+03 5.074E+03 8.172E+03 1.266E+04
ADS ON SOIL 4.660E+03 5.079E+03 5.195E+03 4.998E+03 4.814E+03 4.880E+03 5.519E+03 7.095E+03 1.026E+04 1.670E+04 2.804E+04 4.331E+04
IN SOIL AIR 1.882E+02 1.484E+02 1.278E+02 9.947E+01 9.016E+01 1.078E+02 1.561E+02 2.441E+02 4.039E+02 7.309E+02 1.306E+03 2.007E+03
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          SUBLAYER  2
DIFFUSED UP 2.823E+03 1.121E+03 6.423E+02 2.948E+02 2.325E+02 4.051E+02 1.027E+03 2.304E+03 4.539E+03 9.092E+03 1.612E+04 2.227E+04
IN SOIL MOI 5.808E+04 7.087E+04 7.547E+04 7.676E+04 7.471E+04 7.230E+04 7.330E+04 8.156E+04 1.002E+05 1.343E+05 1.889E+05 2.606E+05
ADS ON SOIL 1.816E+05 1.909E+05 1.924E+05 1.851E+05 1.780E+05 1.786E+05 1.953E+05 2.348E+05 3.081E+05 4.420E+05 6.482E+05 8.914E+05
IN SOIL AIR 7.334E+03 5.577E+03 4.734E+03 3.683E+03 3.333E+03 3.947E+03 5.523E+03 8.079E+03 1.213E+04 1.935E+04 3.019E+04 4.131E+04

          SUBLAYER  3
DIFFUSED UP 8.700E+04 3.181E+04 1.778E+04 8.096E+03 6.373E+03 1.103E+04 2.736E+04 5.837E+04 1.059E+05 1.898E+05 2.955E+05 3.606E+05
IN SOIL MOI 1.698E+06 1.997E+06 2.094E+06 2.127E+06 2.065E+06 1.977E+06 1.940E+06 2.024E+06 2.265E+06 2.685E+06 3.307E+06 4.071E+06
ADS ON SOIL 5.308E+06 5.378E+06 5.339E+06 5.129E+06 4.919E+06 4.885E+06 5.170E+06 5.827E+06 6.963E+06 8.834E+06 1.135E+07 1.392E+07
IN SOIL AIR 2.144E+05 1.571E+05 1.314E+05 1.021E+05 9.211E+04 1.080E+05 1.462E+05 2.005E+05 2.742E+05 3.867E+05 5.285E+05 6.452E+05

          SUBLAYER  4
DIFFUSED UP 1.792E+06 6.035E+05 3.295E+05 1.490E+05 1.171E+05 2.016E+05 4.898E+05 9.968E+05 1.674E+06 2.692E+06 3.687E+06 3.976E+06
IN SOIL MOI 3.344E+07 3.796E+07 3.925E+07 3.985E+07 3.860E+07 3.663E+07 3.486E+07 3.423E+07 3.503E+07 3.686E+07 3.990E+07 4.391E+07
ADS ON SOIL 1.045E+08 1.022E+08 1.001E+08 9.607E+07 9.196E+07 9.050E+07 9.290E+07 9.854E+07 1.077E+08 1.213E+08 1.369E+08 1.502E+08
IN SOIL AIR 4.222E+06 2.987E+06 2.462E+06 1.912E+06 1.722E+06 2.000E+06 2.627E+06 3.390E+06 4.240E+06 5.309E+06 6.376E+06 6.960E+06

     SOIL ZONE 2:
          SUBLAYER  1
DIFFUSED UP 1.889E+07 5.897E+06 3.172E+06 1.436E+06 1.141E+06 1.974E+06 4.728E+06 9.191E+06 1.425E+07 2.049E+07 2.461E+07 2.343E+07
IN SOIL MOI 6.044E+08 6.684E+08 6.865E+08 7.028E+08 6.875E+08 6.519E+08 6.038E+08 5.577E+08 5.206E+08 4.847E+08 4.605E+08 4.541E+08
ADS ON SOIL 1.890E+09 1.800E+09 1.750E+09 1.695E+09 1.638E+09 1.611E+09 1.609E+09 1.606E+09 1.600E+09 1.595E+09 1.580E+09 1.553E+09
IN SOIL AIR 7.632E+07 5.259E+07 4.306E+07 3.372E+07 3.067E+07 3.559E+07 4.550E+07 5.525E+07 6.301E+07 6.982E+07 7.359E+07 7.197E+07

     SOIL ZONE 3:
          SUBLAYER  1
IN SOIL MOI 5.908E+08 6.754E+08 7.142E+08 7.569E+08 7.742E+08 7.594E+08 7.186E+08 6.765E+08 6.419E+08 6.069E+08 5.862E+08 5.886E+08
ADS ON SOIL 1.847E+09 1.819E+09 1.821E+09 1.825E+09 1.844E+09 1.876E+09 1.915E+09 1.948E+09 1.973E+09 1.997E+09 2.012E+09 2.013E+09
IN SOIL AIR 7.460E+07 5.315E+07 4.480E+07 3.632E+07 3.454E+07 4.146E+07 5.415E+07 6.702E+07 7.769E+07 8.742E+07 9.368E+07 9.329E+07

     LOWER SOIL ZONE:
          SUBLAYER  1
IN SOIL MOI 3.514E+07 4.176E+07 4.542E+07 4.982E+07 5.650E+07 5.929E+07 5.863E+07 5.749E+07 5.602E+07 5.395E+07 5.280E+07 5.360E+07
ADS ON SOIL 1.099E+08 1.125E+08 1.158E+08 1.201E+08 1.346E+08 1.465E+08 1.562E+08 1.655E+08 1.722E+08 1.775E+08 1.812E+08 1.833E+08
IN SOIL AIR 4.437E+06 3.286E+06 2.849E+06 2.390E+06 2.521E+06 3.237E+06 4.418E+06 5.695E+06 6.781E+06 7.772E+06 8.438E+06 8.495E+06

          SUBLAYER  2
IN SOIL MOI 1.061E+07 1.305E+07 1.453E+07 1.644E+07 2.133E+07 2.455E+07 2.586E+07 2.696E+07 2.738E+07 2.714E+07 2.711E+07 2.797E+07
ADS ON SOIL 3.317E+07 3.514E+07 3.704E+07 3.964E+07 5.083E+07 6.065E+07 6.890E+07 7.763E+07 8.415E+07 8.932E+07 9.303E+07 9.567E+07
IN SOIL AIR 1.340E+06 1.027E+06 9.114E+05 7.889E+05 9.518E+05 1.340E+06 1.948E+06 2.671E+06 3.314E+06 3.909E+06 4.332E+06 4.434E+06

          SUBLAYER  3
IN SOIL MOI 2.645E+06 3.267E+06 3.638E+06 4.136E+06 6.004E+06 7.532E+06 8.470E+06 9.455E+06 1.006E+07 1.031E+07 1.054E+07 1.107E+07
ADS ON SOIL 8.269E+06 8.798E+06 9.275E+06 9.972E+06 1.430E+07 1.861E+07 2.257E+07 2.722E+07 3.091E+07 3.392E+07 3.617E+07 3.787E+07
IN SOIL AIR 3.340E+05 2.570E+05 2.282E+05 1.985E+05 2.679E+05 4.112E+05 6.383E+05 9.367E+05 1.217E+06 1.485E+06 1.684E+06 1.755E+06

          SUBLAYER  4
IN SOIL MOI 1.182E+06 1.378E+06 1.474E+06 1.593E+06 2.025E+06 2.430E+06 2.719E+06 3.082E+06 3.341E+06 3.485E+06 3.611E+06 3.830E+06
ADS ON SOIL 3.694E+06 3.712E+06 3.759E+06 3.841E+06 4.824E+06 6.004E+06 7.246E+06 8.875E+06 1.027E+07 1.147E+07 1.239E+07 1.310E+07
IN SOIL AIR 1.492E+05 1.085E+05 9.248E+04 7.645E+04 9.034E+04 1.327E+05 2.049E+05 3.054E+05 4.043E+05 5.020E+05 5.771E+05 6.071E+05
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SESOIL Output for Example problem (Page 12 of 16)

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GWR. RUNOFF 3.505E+04 6.706E+04 2.401E+04 4.097E+04 7.389E+05 7.536E+05 7.474E+05 1.017E+06 8.791E+05 7.556E+05 5.968E+05 4.885E+05

      -- POLLUTANT CONCENTRATIONS (UG/ML) OR (UG/G) -- NOTE: IF CONCENTRATIONS ARE ZERO FOR EACH MONTH, THEY ARE NOT PRINTED --
      -------------------------------------------------------------------------------------------------------------------------

      UPPER SOIL ZONE:
           SUBLAYER  1
MOISTURE     8.357E-05 9.109E-05 9.317E-05 8.963E-05 8.634E-05 8.752E-05 9.898E-05 1.272E-04 1.840E-04 2.995E-04 5.029E-04 7.767E-04
%SOLUBILITY 4.775E-06 5.205E-06 5.324E-06 5.122E-06 4.934E-06 5.001E-06 5.656E-06 7.271E-06 1.051E-05 1.711E-05 2.874E-05 4.438E-05
ADSORBED     2.461E-05 2.683E-05 2.744E-05 2.640E-05 2.543E-05 2.577E-05 2.915E-05 3.747E-05 5.417E-05 8.819E-05 1.481E-04 2.287E-04
SOIL AIR     1.880E-05 2.078E-05 2.141E-05 2.108E-05 2.031E-05 2.044E-05 2.256E-05 2.880E-05 4.164E-05 6.706E-05 1.126E-04 1.739E-04

           SUBLAYER  2
MOISTURE     3.257E-03 3.423E-03 3.451E-03 3.319E-03 3.192E-03 3.203E-03 3.503E-03 4.211E-03 5.525E-03 7.926E-03 1.163E-02 1.599E-02
%SOLUBILITY 1.861E-04 1.956E-04 1.972E-04 1.897E-04 1.824E-04 1.831E-04 2.002E-04 2.406E-04 3.157E-04 4.529E-04 6.643E-04 9.135E-04
ADSORBED     9.591E-04 1.008E-03 1.016E-03 9.775E-04 9.400E-04 9.434E-04 1.032E-03 1.240E-03 1.627E-03 2.334E-03 3.424E-03 4.708E-03
SOIL AIR     7.328E-04 7.810E-04 7.928E-04 7.807E-04 7.508E-04 7.483E-04 7.985E-04 9.531E-04 1.251E-03 1.775E-03 2.603E-03 3.580E-03

           SUBLAYER  3
MOISTURE     9.519E-02 9.645E-02 9.575E-02 9.198E-02 8.821E-02 8.762E-02 9.272E-02 1.045E-01 1.249E-01 1.584E-01 2.035E-01 2.497E-01
%SOLUBILITY 5.439E-03 5.511E-03 5.471E-03 5.256E-03 5.041E-03 5.007E-03 5.298E-03 5.972E-03 7.135E-03 9.053E-03 1.163E-02 1.427E-02
ADSORBED     2.803E-02 2.840E-02 2.820E-02 2.709E-02 2.598E-02 2.580E-02 2.730E-02 3.078E-02 3.677E-02 4.666E-02 5.994E-02 7.353E-02
SOIL AIR     2.142E-02 2.201E-02 2.200E-02 2.163E-02 2.075E-02 2.047E-02 2.114E-02 2.365E-02 2.826E-02 3.548E-02 4.558E-02 5.591E-02

           SUBLAYER  4
MOISTURE     1.875E+00 1.834E+00 1.795E+00 1.723E+00 1.649E+00 1.623E+00 1.666E+00 1.767E+00 1.931E+00 2.175E+00 2.455E+00 2.693E+00
%SOLUBILITY 1.071E-01 1.048E-01 1.026E-01 9.845E-02 9.424E-02 9.274E-02 9.520E-02 1.010E-01 1.103E-01 1.243E-01 1.403E-01 1.539E-01
ADSORBED     5.521E-01 5.400E-01 5.285E-01 5.074E-01 4.857E-01 4.780E-01 4.906E-01 5.204E-01 5.687E-01 6.406E-01 7.231E-01 7.932E-01
SOIL AIR     4.219E-01 4.184E-01 4.124E-01 4.053E-01 3.879E-01 3.791E-01 3.798E-01 4.000E-01 4.371E-01 4.871E-01 5.499E-01 6.032E-01

      SOIL ZONE 2:
           SUBLAYER  1
MOISTURE     2.542E+01 2.421E+01 2.354E+01 2.279E+01 2.203E+01 2.166E+01 2.164E+01 2.160E+01 2.152E+01 2.146E+01 2.126E+01 2.089E+01
%SOLUBILITY 1.452E+00 1.384E+00 1.345E+00 1.302E+00 1.259E+00 1.238E+00 1.237E+00 1.234E+00 1.230E+00 1.226E+00 1.215E+00 1.194E+00
ADSORBED     7.485E+00 7.131E+00 6.932E+00 6.712E+00 6.488E+00 6.380E+00 6.373E+00 6.360E+00 6.338E+00 6.319E+00 6.260E+00 6.152E+00
SOIL AIR     5.719E+00 5.524E+00 5.409E+00 5.361E+00 5.182E+00 5.061E+00 4.933E+00 4.888E+00 4.871E+00 4.805E+00 4.760E+00 4.678E+00

      SOIL ZONE 3:
           SUBLAYER  1
MOISTURE     1.656E+01 1.631E+01 1.633E+01 1.637E+01 1.654E+01 1.682E+01 1.717E+01 1.746E+01 1.769E+01 1.791E+01 1.804E+01 1.805E+01
%SOLUBILITY 9.465E-01 9.321E-01 9.329E-01 9.352E-01 9.451E-01 9.614E-01 9.812E-01 9.980E-01 1.011E+00 1.023E+00 1.031E+00 1.031E+00
ADSORBED     4.878E+00 4.804E+00 4.808E+00 4.820E+00 4.871E+00 4.955E+00 5.057E+00 5.143E+00 5.210E+00 5.274E+00 5.313E+00 5.316E+00
SOIL AIR     3.727E+00 3.722E+00 3.751E+00 3.849E+00 3.890E+00 3.930E+00 3.914E+00 3.953E+00 4.004E+00 4.011E+00 4.040E+00 4.042E+00

      LOWER SOIL ZONE:
           SUBLAYER  1
MOISTURE     7.881E+00 8.068E+00 8.305E+00 8.616E+00 9.657E+00 1.051E+01 1.121E+01 1.187E+01 1.235E+01 1.274E+01 1.300E+01 1.315E+01
%SOLUBILITY 4.504E-01 4.610E-01 4.746E-01 4.924E-01 5.518E-01 6.005E-01 6.404E-01 6.785E-01 7.058E-01 7.278E-01 7.428E-01 7.514E-01
ADSORBED     2.321E+00 2.376E+00 2.446E+00 2.538E+00 2.844E+00 3.095E+00 3.300E+00 3.497E+00 3.638E+00 3.751E+00 3.828E+00 3.872E+00
SOIL AIR     1.773E+00 1.841E+00 1.908E+00 2.027E+00 2.271E+00 2.455E+00 2.555E+00 2.687E+00 2.796E+00 2.852E+00 2.911E+00 2.945E+00
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SESOIL Output for Example problem (Page 13 of 16)

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             SUBLAYER  2
MOISTURE     2.380E+00 2.521E+00 2.657E+00 2.844E+00 3.646E+00 4.351E+00 4.943E+00 5.569E+00 6.037E+00 6.407E+00 6.674E+00 6.863E+00
%SOLUBILITY 1.360E-01 1.441E-01 1.518E-01 1.625E-01 2.084E-01 2.486E-01 2.824E-01 3.182E-01 3.449E-01 3.661E-01 3.814E-01 3.922E-01
ADSORBED     7.008E-01 7.424E-01 7.825E-01 8.375E-01 1.074E+00 1.281E+00 1.456E+00 1.640E+00 1.778E+00 1.887E+00 1.965E+00 2.021E+00
SOIL AIR     5.355E-01 5.752E-01 6.105E-01 6.689E-01 8.576E-01 1.016E+00 1.127E+00 1.261E+00 1.366E+00 1.435E+00 1.494E+00 1.537E+00

             SUBLAYER  3
MOISTURE     5.932E-01 6.311E-01 6.654E-01 7.153E-01 1.026E+00 1.335E+00 1.619E+00 1.953E+00 2.217E+00 2.434E+00 2.595E+00 2.716E+00
%SOLUBILITY 3.390E-02 3.606E-02 3.802E-02 4.088E-02 5.863E-02 7.628E-02 9.252E-02 1.116E-01 1.267E-01 1.391E-01 1.483E-01 1.552E-01
ADSORBED     1.747E-01 1.859E-01 1.960E-01 2.107E-01 3.022E-01 3.931E-01 4.768E-01 5.751E-01 6.530E-01 7.167E-01 7.642E-01 8.000E-01
SOIL AIR     1.335E-01 1.440E-01 1.529E-01 1.683E-01 2.413E-01 3.118E-01 3.691E-01 4.420E-01 5.018E-01 5.450E-01 5.811E-01 6.083E-01

             SUBLAYER  4
MOISTURE     2.650E-01 2.663E-01 2.696E-01 2.756E-01 3.461E-01 4.307E-01 5.198E-01 6.366E-01 7.365E-01 8.227E-01 8.890E-01 9.397E-01
%SOLUBILITY 1.514E-02 1.522E-02 1.541E-02 1.575E-02 1.978E-02 2.461E-02 2.970E-02 3.638E-02 4.209E-02 4.701E-02 5.080E-02 5.370E-02
ADSORBED     7.804E-02 7.843E-02 7.941E-02 8.116E-02 1.019E-01 1.268E-01 1.531E-01 1.875E-01 2.169E-01 2.423E-01 2.618E-01 2.767E-01
SOIL AIR     5.963E-02 6.076E-02 6.196E-02 6.482E-02 8.140E-02 1.006E-01 1.185E-01 1.441E-01 1.667E-01 1.842E-01 1.991E-01 2.104E-01

POL DEP CM   6.250E+02 6.250E+02 6.250E+02 6.250E+02 6.250E+02 6.250E+02 6.250E+02 6.250E+02 6.250E+02 6.250E+02 6.250E+02 6.250E+02

     -- POLLUTANT CONCENTRATION IN GROUNDWATER (UG/ML) --

GWR. CONC.   5.030E-02 8.264E-02 3.685E-02 5.784E-02 2.795E-01 3.328E-01 3.809E-01 4.802E-01 5.088E-01 5.170E-01 4.886E-01 4.549E-01
1                            YEAR -    2 ANNUAL SUMMARY REPORT
                             ==================================

       -- TOTAL INPUTS (UG) --

UPPER SOIL ZONE              0.000E+00
SOIL ZONE 2                  0.000E+00
SOIL ZONE 3                  0.000E+00
LOWER SOIL ZONE              0.000E+00

          -- HYDROLOGIC CYCLE COMPONENTS --

AVERAGE SOIL MOISTURE ZONE 1 (%)          17.766
AVERAGE SOIL MOISTURE BELOW ZONE 1 (%)    17.766
TOTAL PRECIPITATION (CM)                  49.047
TOTAL INFILTRATION (CM)                   22.656
TOTAL EVAPOTRANSPIRATION (CM)             14.760
TOTAL SURFACE RUNOFF (CM)                 26.387
TOTAL GRW RUNOFF (CM)                      7.896
TOTAL MOISTURE RETENTION (CM)               .000
TOTAL YIELD (CM)                          34.288
```

SESOIL Output for Example problem (Page 14 of 16)

```
0          -- POLLUTANT MASS DISTRIBUTION IN COLUMN (UG) -- NOTE: IF COMPONENT IS ZERO EACH MONTH, IT IS NOT PRINTED
           ----------------------------------------------------------------------------------------------------
  FOR FINAL MASS IN SOIL MOI., ADS. ON SOIL, SOIL AIR, IMMOBIL CEC, COMPLEXED, AND PURE PHASE FOR EACH SUBLAYER, SEE ABOVE (MONTH SEP)
  ----------------------------------------------------------------------------------------------------------------------------------

      UPPER SOIL ZONE:
           SUBLAYER  1
                TOTAL VOLATILIZED                  2.492E+03

           SUBLAYER  2
                TOTAL DIFFUSED (UP)                6.087E+04

           SUBLAYER  3
                TOTAL DIFFUSED (UP)                1.200E+06

           SUBLAYER  4
                TOTAL DIFFUSED (UP)                1.671E+07

      SOIL ZONE 2:
           SUBLAYER  1
                TOTAL DIFFUSED (UP)                1.292E+08

      SOIL ZONE 3:
           SUBLAYER  1

      LOWER SOIL ZONE:
           SUBLAYER  1

           SUBLAYER  2

           SUBLAYER  3

           SUBLAYER  4

                TOTAL IN GROUNDWATER RUNOFF        6.145E+06

1                          -- AVERAGE POLLUTANT CONCENTRATIONS --  NOTE: ONLY NON-ZERO VALUES ARE PRINTED --
                           ---------------------------------------------------------------------------------

      UPPER SOIL ZONE:
           SUBLAYER  1
                                     SOIL MOISTURE (UG/ML)  2.101E-04
                                     ADSORBED SOIL (UG/G)   6.186E-05
                                     SOIL AIR (UG/ML)       4.745E-05
           SUBLAYER  2
                                     SOIL MOISTURE (UG/ML)  5.718E-03
                                     ADSORBED SOIL (UG/G)   1.684E-03
                                     SOIL AIR (UG/ML)       1.296E-03
           SUBLAYER  3
                                     SOIL MOISTURE (UG/ML)  1.241E-01
```

SESOIL Output for Example problem (Page 15 of 16)

```
                                     ADSORBED SOIL (UG/G)    3.654E-02
                                     SOIL AIR (UG/ML)        2.819E-02
        SUBLAYER  4
                                     SOIL MOISTURE (UG/ML)   1.932E+00
                                     ADSORBED SOIL (UG/G)    5.690E-01
                                     SOIL AIR (UG/ML)        4.402E-01
    SOIL ZONE 2:
        SUBLAYER  1
                                     SOIL MOISTURE (UG/ML)   2.233E+01
                                     ADSORBED SOIL (UG/G)    6.578E+00
                                     SOIL AIR (UG/ML)        5.099E+00

    SOIL ZONE 3:
        SUBLAYER  1
                                     SOIL MOISTURE (UG/ML)   1.710E+01
                                     ADSORBED SOIL (UG/G)    5.037E+00
                                     SOIL AIR (UG/ML)        3.903E+00

    LOWER SOIL ZONE:
        SUBLAYER  1
                                     SOIL MOISTURE (UG/ML)   1.061E+01
                                     ADSORBED SOIL (UG/G)    3.125E+00
                                     SOIL AIR (UG/ML)        2.418E+00
        SUBLAYER  2
                                     SOIL MOISTURE (UG/ML)   4.574E+00
                                     ADSORBED SOIL (UG/G)    1.347E+00
                                     SOIL AIR (UG/ML)        1.040E+00
        SUBLAYER  3
                                     SOIL MOISTURE (UG/ML)   1.542E+00
                                     ADSORBED SOIL (UG/G)    4.540E-01
                                     SOIL AIR (UG/ML)        3.499E-01
        SUBLAYER  4
                                     SOIL MOISTURE (UG/ML)   5.331E-01
                                     ADSORBED SOIL (UG/G)    1.570E-01
                                     SOIL AIR (UG/ML)        1.210E-01

                                     MAX. POLL. DEPTH (M)    6.250E+00

   AVE. CONTAMINANT CONCENTRATION IN GROUNDWATER (UG/ML)     3.059E-01

****************************************EXECUTION COMPLETED****************************************
```

SESOIL Output for Example problem (Page 16 of 16)

APPENDIX B
JURY'S UNSATURATED ZONE MODEL

The Jury model, Jury et al. (1990), is a screening level model that estimates the chemical flux volatilizing from soil and the time-varying concentration profile within the unsaturated zone. The latter can be used to estimate the contaminant mass loading to the water table. This model is based on the analytical solution to the differential mass balance equation and the boundary and initial conditions presented below:

$$\frac{\partial C_T}{\partial t} + \mu C_T = D_E \frac{\partial^2 C_T}{\partial z^2} - V_E \frac{\partial C_T}{\partial z} \qquad \text{(B-1)}$$

where

C_T = total soil concentration is defined by equation B-5 (mg of contaminant/cm^3 of soil)

t = time (day)

μ = first order decay rate constant (1/day)

D_E = effective diffusion coefficient estimated by equation B-8 (cm^2/d)

z = depth measured positive downwards from the soil surface (cm)

V_E = effective contaminant velocity estimated by equation B-9 (cm/d)

The initial condition is:

$$C_T(0 < z < L, t=0) = C_o \qquad \text{(B-2a)}$$

$$C_T(z \geq L, t=0) = 0 \qquad \text{(B-2b)}$$

where

C_o = initial total contaminant concentration in soil (mg/cm^3)

L = initial depth of contamination concentration (cm)

Equations B-2(a) and B-2(b) imply that initially the contaminant is uniformly incorporated to a depth L. For the case of a contaminant source buried under a clean fill, the solution is obtained by superposition as discussed further in this section.

$$-D_E \frac{\partial C_T}{\partial z} + V_E C_T = -H_E C_T \qquad \text{at } z = 0 \qquad \text{(B-3)}$$

where

H_E = mass transfer coefficient variable estimated using equation B-10 (cm/d)

Equation B-3 simulates the volatilization of chemical vapor to the atmosphere through a stagnant air boundary layer above which the chemical concentration in air is assumed zero.

The lower boundary condition is:

$$C_T(z = \infty, \mathit{all}\ t) = 0 \qquad \text{(B-4)}$$

In equation B-1, the total soil concentration is assumed to be distributed among the solid, aqueous and vapor phases and is estimated using:

$$C_T = \rho_b C_S + \theta_w C_w + \theta_a C_v \qquad \text{(B-5)}$$

where

ρ_b = bulk density of soil (g of dry soil/cm^3 of wet soil)
C_S = sorbed phase concentration (g of contaminant/g of dry soil)
θ_w = volumetric water content (cm^3 of water/cm^3 of wet soil)
C_w = dissolved phase concentration (g contaminant/cm^3 solution)
θ_a = air porosity (cm^3 gas in soil/cm^3 wet soil)
C_v = vapor phase concentration (g contaminant/cm^3 gas in soil)

The definition of C_T precludes the use of this model in situations where immiscible liquids or precipitates are present.

The three individual phase concentrations C_s, C_l and C_g are related by partition coefficients as follows:

$$C_s = K_d C_w \tag{B-6}$$

and

$$C_v = H C_W \tag{B-7}$$

where

K_d = the chemical-specific soil-water partition coefficient [(mg/g of dry soil)/(g/cm^3 of solution)] ($K_d = K_{oc} f_{oc}$) and

H = Henry's Law constant [(mg/L of vapor)/(mg/L of solution)]

The chemical-specific partition coefficient can be estimated as the product of the fractional organic carbon content and the normalized organic carbon partition coefficient.

The effective diffusion coefficient in equation B-1 is estimated by:

$$D_E = \frac{\left(\theta_a^{\,3.33} D_g^a H + \theta_W^{\,3.33} D_l^w\right)/\theta^2}{\rho_b f_{oc} K_{oc} + \theta_W + \theta_a H} \tag{B-8}$$

where

D_g^a = the chemical-specific gaseous diffusion coefficient in air (cm^2/day)

D_l^w = the chemical-specific liquid diffusion coefficient in water (cm^2/day)

θ_a = air-filled porosity (cm^3 - air/cm^3 - soil)

θ_w = water-filled porosity (cm^3 - water/cm^3 - soil)

f_{oc} = fraction of organic carbon in soil (mg of organic carbon/mg of soil)

All other variables have been defined previously. The effective contaminant velocity in soil in equation B-1 is estimated by:

$$V_E = \frac{J_W}{\rho_b f_{oc} K_{oc} + \theta_W + \theta_a H} \tag{B-9}$$

where

J_w = the volumetric soil-water flux, i.e., percolation rate when J_w is positive, (cm/day)

Finally, the variable H_E is defined as :

$$H_E = \frac{hH}{\rho_b K_d + \theta_W + \theta_a H} \tag{B-10}$$

$$h = D_g^a/d \tag{B-11}$$

where

h = boundary layer transfer coefficient (cm/day)

d = the stagnant air boundary layer thickness (cm)

The solution for equations (B-1) through (B-4) yields the concentration profile and is presented by Jury et al. (1990) as :

$$\begin{aligned} C_T(z,t;L) = {} & \frac{1}{2} C_o \exp(-\mu t) \left\{ erfc\left[\frac{(z-L-V_E t)}{\sqrt{4D_E t}}\right] - erfc\left[\frac{(z-V_E t)}{\sqrt{4D_E t}}\right] \right. \\ & + \left(1+\frac{V_E}{H_E}\right) \exp\left(\frac{V_E z}{D_E}\right) \left[erfc\left(\frac{(z+L+V_E t)}{\sqrt{4D_E t}}\right) - erfc\left(\frac{(z+V_E t)}{\sqrt{4D_E t}}\right)\right] \\ & \left. + \left(2+\frac{V_E}{H_E}\right) \exp\left(\frac{H_E(H_E+V_E)t + (H_E+V_E)z}{D_E}\right) \left[\begin{array}{l} erfc\left(\dfrac{z+(2H_E+V_E)t}{\sqrt{4D_E t}}\right) \\ -\exp\left(\dfrac{H_E L}{D_E}\right) erfc\left(\dfrac{z+L+(2H_E+V_E)t}{\sqrt{4D_E t}}\right) \end{array} \right] \right. \end{aligned} \tag{B-12}$$

Jury et al. (1990) also present the cumulative volatilization flux $V_c(t)$, i.e., mass/unit area volatilized, from the soil surface between the start of volatilization and time t as:

$$\begin{aligned} V_c(t) = {} & -\frac{C_o}{2} \left\{ \frac{V_E}{\mu}[1-\exp(-\mu t)](S_1 - S_2) - \left(\frac{V_E - 2H_E}{\mu - \xi}\right)[1-\exp(-\mu t)[S_3 - S_4]] \right. \\ & + \exp\left[-\frac{P}{2} + \beta(L\sqrt{D_E})\right] \left[\frac{(V_E+2H_E)}{2(\mu-\xi)} - \frac{V_E}{2\mu} - \frac{(V_E+2H_E)^2}{4(\mu-\xi)\beta\sqrt{D_E}} + \frac{V_E^2}{4\mu\beta\sqrt{D_E}}\right] S_5 \\ & + \exp\left[-\frac{P}{2} + \beta(L\sqrt{D_E})\right] \left[\frac{(V_E+2H_E)}{2(\mu-\xi)} - \frac{V_E}{2\mu} - \frac{(V_E+2H_E)^2}{4(\mu-\xi)\beta\sqrt{D_E}} + \frac{V_E^2}{4\mu\beta\sqrt{D_E}}\right] S_6 \\ & + \left[\frac{1}{2\beta\sqrt{D_E}}\right] \left[\frac{(V_E+2H_E)^2}{(\mu-\xi)} - \frac{V_E^2}{\mu}\right] S_7 \end{aligned} \tag{B-13}$$

where

$P = V_E L/D_E$

$\xi = (H_E + V_E)H_E/D_E$

$\beta = (V_E^2/4D_E + \mu)^{1/2}$

$S_1 = \mathrm{erfc}[V_E t/(4D_E t)^{1/2}]$

$S_2 = \mathrm{erfc}[(L + V_E t)/(4D_E t)^{1/2}]$

$S_3 = \exp(\xi\, t)\ \mathrm{erfc}[(V_E + 2H_E)t/(4D_E t)^{1/2}]$

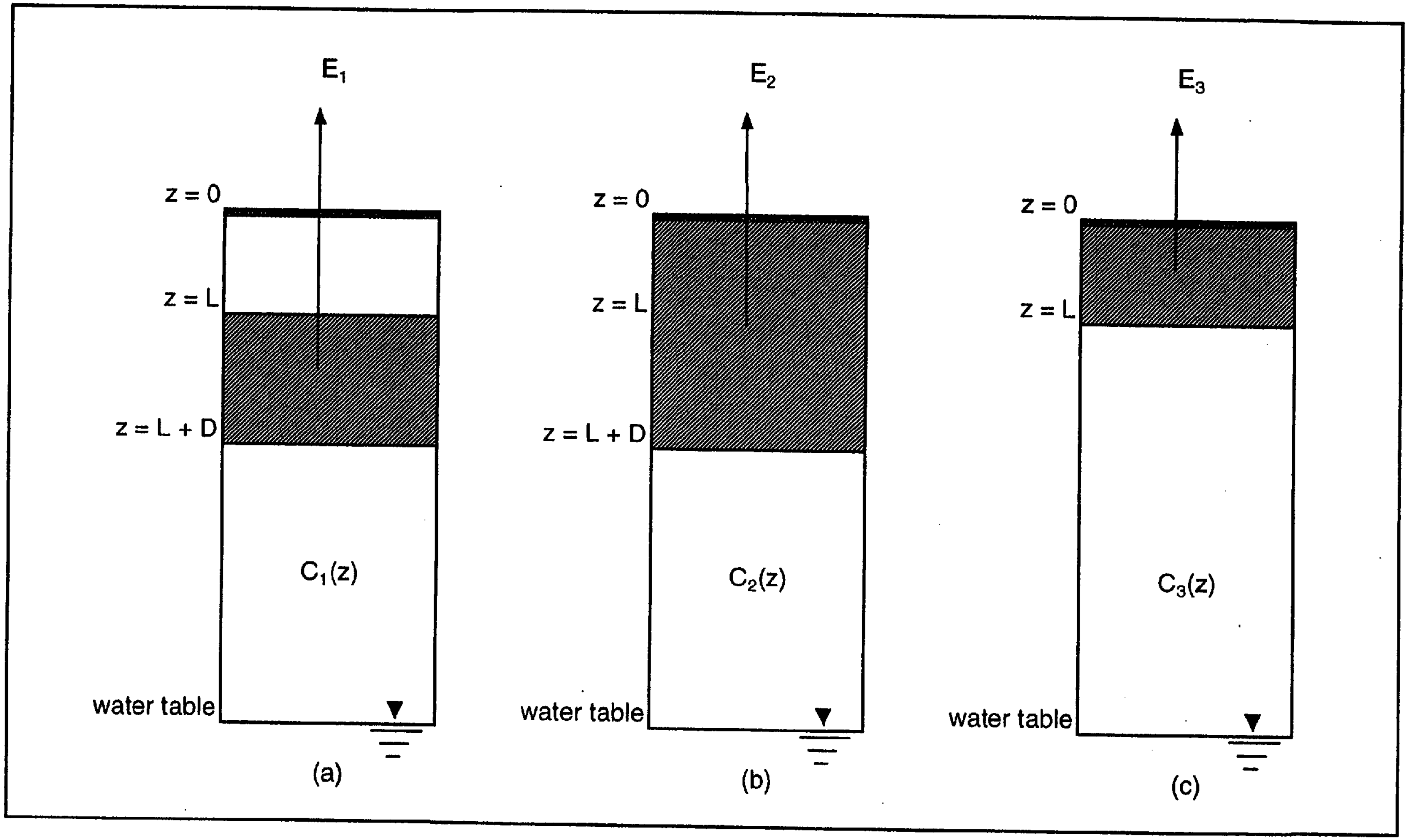
$S_4 = \exp(\xi\, t + H_E L/D_E)\ \mathrm{erfc}[L + (V_E + 2H_E))t/(4D_E t)^{1/2}]$

$S_5 = \mathrm{erfc}[L/(4D_E t)^{1/2} - \beta(t)^{1/2}]$

$S_6 = \mathrm{erfc}[L/(4D_E t)^{1/2} + \beta(t)^{1/2}]$

$S_7 = \mathrm{erf}[\beta(t)^{1/2}]$

Equations B-12 and B-13 present the time varying concentration profile and the cumulative volatilization flux for the case when the contaminant is initially uniformly incorporated over a depth L (see Figure B-1). By using the principle of superposition, Jury's model can be used to estimate the concentration profile and the emissions for the case when the contaminant is buried below a clean layer of soil as shown in figure B-1(a) as discussed below.



NOTE:

$E_1 = E_2 - E_3$ — E_1, E_2 and E_3 are the volatilization fluxes.

$C_1(z) = C_2(z) - C_3(z)$ — $C_1(z)$, $C_2(z)$ and $C_3(z)$ are the computed concentration profiles.

Figure B-1. Schematic of the Jury M and the Principle of Superposition

Assuming that the uniformly contaminated soil of thickness 'D' is buried under a clean cover of thickness 'L', Equations B-12 and B-13 are evaluated for the first hypothetical case figure B-1(b) where the soil is contaminated to a depth (L+D). Equations B-12 and B-13 are then evaluated for the second hypothetical case figure B-1(c) where the soil is contaminated to a depth 'L'. The results of these two hypothetical cases are then subtracted to yield the results for the actual case Figure B-1(a). Concentrations estimated at the water table are used to compute the contaminant fluxes at the water table using:

$$M_{WT} = VC_W A + D\frac{\Delta C}{\Delta z}A \qquad \text{(B-14)}$$

where

M_{WT} = annual mass loading to water table (mg/yr)
V = infiltration rate (m/yr)
A = area of the source (cm^2)
C_w = dissolved phase concentration at the water table (mg/cm^3)
D = hydrodynamic dispersion coefficient (cm^2/yr)
$\frac{\Delta C}{\Delta Z}$ = concentration gradient at the water table ($mg/cm^3/cm$)

Running Jury with Source Concentrations Exceeding Residual Levels

The Jury model assumes that the chemical is in equilibrium in three phases: sorbed, dissolved, and vapor. Residual, or fourth phase free product, are not handled in the Jury equations. The model in DSS checks the following condition to see if residual levels are present:

$$C_w = C_o \frac{\rho_b + \rho_w\theta_w}{\rho_b K_{oc} F_{oc} + \theta_w + H\theta_a} \; \frac{kg}{1000\ mg} \qquad \text{(B-15)}$$

where

H = Henry's constant [(mg/L of vapor)/(mg/L of solution)]
ρ_b = bulk density of soil (g of dry soil/cm^3 of wet soil)
ρ_w = density of water (g /cm^3)
θ_a = air-filled porosity (cm^3 - air/cm^3 - soil)

θ_w = water-filled porosity (cm^3 - water/cm^3 - soil)
f_{oc} = fraction of organic carbon in soil (mg of oc/mg of soil)
C_o = initial total soil concentration (mg of contaminant/kg of wet soil)

If the dissolved phase concentration estimated with Equation B-15 exceeds the solubility entered for the chemical then the following message will be written to the screen and Jury output file:

```
*****************************************
USER INPUT SOIL CONCENTRATION EXCEEDS
CONDITIONS FOR WHICH MODEL IS APPLICABLE
(Jury's model not valid for concentrations
exceeding residual levels.)

SEE USERS MANUAL - APPENDIX B
FOR MORE INFORMATION
*****************************************
```

Data Required

The data required to estimate the time-varying cumulative volatile emissions as well as the concentration profiles are presented in Table B-1. To convert from total mass to initial concentration in the contaminated zone:

$$C_T = \frac{M_T}{V_{soil}} \qquad \text{(B-16)}$$

where

M_T = the total contaminant mass in the soil (mg)
V_{soil} = the volume of wet soil (cm^3)

In Table B-1, the thickness of the boundary layer refers to the thickness of a layer of stagnant air through which vapor must move by molecular diffusion. The thickness of this boundary layer is a complicated function of wind speed, relative humidity, surface roughness, and fetch. Jury et al. (1990) use a value of 0.5 cm for the example problem presented in the paper. Jury et al. (1983) discuss ways of estimating the value of the boundary layer thickness.

TABLE B-1. DATA REQUIRED TO IMPLEMENT THE JURY MODEL

PARAMETER DEFINITION	UNITS	API DSS UNITS
Model Control Parameters		
Simulation Time	[yrs]	[yrs]
Chemical Data		
Total Soil Concentration	[mg/kg]	[mg/kg]
Diffusion Coefficient in Air	[cm^2/sec]	[cm^2/sec]
Diffusion Coefficient in Water	[cm^2/sec]	[cm^2/sec]
Henry's Law Constant	[m^3 Atm/mole]	[(mg/L)/(mg/L)]
K_{oc}	[ug/g oc /ug/ml]	[ug/g oc /ug/ml]
Overall Decay Rate	[1/day]	[1/day]
Solubility	[mg/l]	[mg/l]
Data for the Soil Column		
Volumetric Water Content	[-]	[-]
Effective Porosity	[-]	[-]
Soil Bulk Density	[g/cm^3]	[g/cm^3]
Fractional Organic Carbon Content	[mg/mg]	[mg/mg]
Thickness of Source	[m]	[m]
Thickness of Soil Cover	[m]	[m]
Depth of Unsaturated Zone	[m]	[m]
X-dimension of the Source	[m]	[m]
Y-dimension of the Source	[m]	[m]
Thickness of Boundary Layer	[cm]	[cm]
Infiltration Rate[cm/sec]	[cm/yr]	

Assumptions Underlying the Model and Its Applicability

1. The soil column is assumed to be homogenous and isotropic without any variations with depth.
2. The infiltration rate is assumed to be uniform and steady.
3. The contaminant is initially incorporated uniformly from the top of the soil column to a depth 'L' cm below the surface. Note the case of contaminant incorporated in a thickness of 'D' cm buried below a clean layer of soil is analyzed using the principle of superposition.
4. Contaminant decay is assumed to follow first order decay rate.
5. The partitioning of contaminant concentrations among the three phases, i.e., solid phase, dissolved aqueous phase and the vapor phase, is assumed to be linear. Compositional equilibrium among phases is assumed at all locations at all times.
6. The effective diffusion of contaminant in the vapor and liquid phase within the soil is based on the following relationships:

$$D_g = D_g^{a} \frac{\theta_a^{3.33}}{\theta_T^{2}} \qquad \text{(B-17)}$$

$$D_l = D_l^{w} \frac{\theta_w^{3.33}}{\theta_T^{2}} \qquad \text{(B-18)}$$

It is not possible to quantify the effect of these assumptions on the estimated emission rate or the concentration profile. Depending on the degree of departure between the field situation and the assumptions made above, the Jury model may overestimate or, in some cases, underestimate the emission rate.

Example Problem

Estimate the cumulative emission of benzene over 10 years from an area 10 m by 10 m with an initial total benzene soil concentration of 1 mg/kg in a zone 1 meter thick, 1 meter below the ground surface (covered with 1 m clean fill). The properties of the soil column are shown in Table B-2. The graph of the emissions from the EXCEL® output and the JURY.OUT file are attached at the end of this appendix.

TABLE B-2. PARAMETER VALUES USED FOR THE JURY MODEL EXAMPLE PROBLEM

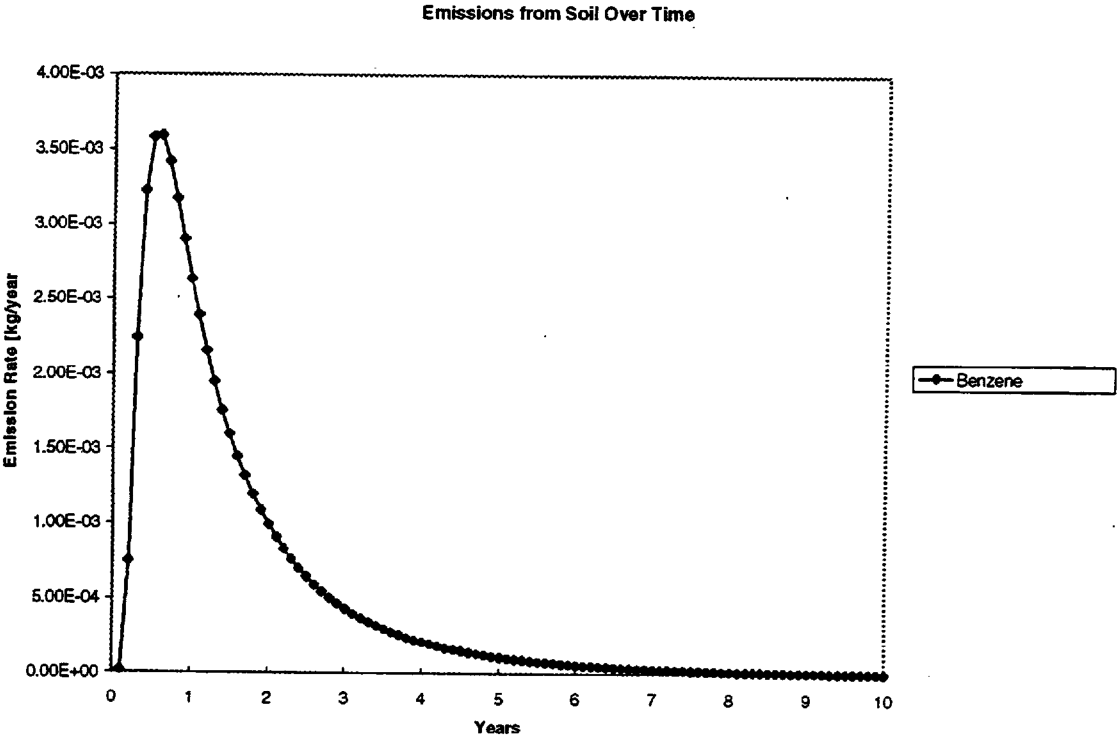
PARAMETER DEFINITION	UNITS	VALUE
Volumetric Water Content	[-]	0.15
Effective Porosity	[-]	0.30
Soil Bulk Density	[g/cm^3]	1.80
Fraction Organic Carbon	[mg/mg]	0.005
Thickness of Source	[m]	1.0
Thickness of Soil Cover	[m]	2.0
Depth of Unsaturated Zone	[m]	5.0
X-dimension of the Source	[m]	10.0
Y-dimension of the Source	[m]	10.0
Thickness of Boundary Layer	[cm]	0.5
Infiltration rate	[cm/yr]	15.0
Chemical Specific Parameters		
Total Concentration in Soil	[mg/kg]	1.0
Air Diffusion Coefficient	[cm^2/s]	0.088
Water Diffusion Coefficient	[cm^2/s]	9.80E-6
Henry's Law Constant	[(mg/L)/(mg/L)]	0.228
KOC	[ug/gOC/ug/ml]	58.9
Solubility	[mg/L]	1750.0
Degradation Rate Constant	[1/days]	0.001

REFERENCES

Jury, W.A., W.F. Spencer, and W.J. Farmer. 1983. Behavior Assessment Model for Trace Organics in Soil - 1. Model Description. J. of Environ. Qual., 12. 558-564.

Jury, W.A., David Russo, Gary Streile, and Hesham El Abd. 1990. Evaluation of Organic Chemicals Residing Below the Soil Surface. Water Resources Research. Vol 26. No. 1, Pages 13-20.

Graph from EXCEL for Example Problem:



```
Jury Output File
DSS Fate and Transport

*** GENERAL INPUT PARAMETERS ***
-------------------------------

PARAMETER NAME                    UNITS    VALUE
--------------------------------------------
Porosity                        (cc/cc)    .3000
Bulk Density                     (g/cc)    1.800
Water Content                   (cc/cc)    .1500
Fraction Organic Carbon         (mg/mg)   5.0000E-03
Incorporation Depth                (cm)    100.0
Clean Soil Thickness               (cm)    200.0
Simulation Time                   (yrs)     10
Length of Soil Column              (cm)    500.0
Infiltration Rate              (cm/day)   4.1096E-02
Source Length                       (m)    10.00
Source Width                        (m)    10.00
Boundary Layer Thickness           (cm)    .5000

Chemical Specific Input Parameters for  Benzene
--------------------------------------------------

Parameter Name                    Units    Value
--------------------------------------------
Total Soil Concentration       (mg/kg)    1.000
Diffusion Coeff. in Air   (cm^2/day)    7603.
Diffusion Coeff. in Water(cm^2/day)    .8467
Henrys Constant       [(mg/L)/(mg/L)]    .2280
Organic Carbon Part. Coeff.   (cc/g)    58.90
Lumped Chemical Decay Rate    (1/day)    .1000E-02


Outputs for  Benzene
----------------------------


          Time =     .10     years
==========================================

Soil Concentration Profile

Depth (cm)      Concentration(mg/kg soil)

      .00                .00
    50.00                .50E-02
   100.00                .41E-01
   150.00                .18
   200.00                .43
   250.00                .58
   300.00                .45
   350.00                .20
   400.00                .48E-01
   450.00                .62E-02
   500.00                .42E-03

     5.00                .20E-03

 Emissions to Air from this time step (g)                          1.952E-02
 Advective Mass Loading Rate to Groundwater (g/day)                4.693E-05
 Diffusive Mass Loading Rate to Groundwater (g/day)                1.084E-02
 Advective & Diffusive Mass Loading Rate to GW (g/day)             1.089E-02

 Cumulative Emissions to Air (g)                                   1.952E-02
 Cumulative Loading to Groundwater (g)                              .398
```

```
          Time =    1.00     years
========================================

Soil Concentration Profile

Depth (cm)      Concentration(mg/kg soil)

     .00               .00
   50.00               .37E-01
  100.00               .73E-01
  150.00               .10
  200.00               .13
  250.00               .14
  300.00               .14
  350.00               .13
  400.00               .12
  450.00               .93E-01
  500.00               .70E-01

    5.00               .37E-02

 Emissions to Air from this time step (g)                      2.63
 Advective Mass Loading Rate to Groundwater (g/day)           7.905E-03
 Diffusive Mass Loading Rate to Groundwater (g/day)           4.315E-02
 Advective & Diffusive Mass Loading Rate to GW (g/day)        5.106E-02

 Cumulative Emissions to Air (g)                               25.5
 Cumulative Loading to Groundwater (g)                         22.9


          Time =    2.00     years
========================================

Soil Concentration Profile

Depth (cm)      Concentration(mg/kg soil)

     .00               .00
   50.00               .14E-01
  100.00               .28E-01
  150.00               .41E-01
  200.00               .51E-01
  250.00               .59E-01
  300.00               .63E-01
  350.00               .64E-01
  400.00               .62E-01
  450.00               .58E-01
  500.00               .52E-01

    5.00               .14E-02

 Emissions to Air from this time step (g)                      .996
 Advective Mass Loading Rate to Groundwater (g/day)           5.779E-03
 Diffusive Mass Loading Rate to Groundwater (g/day)           1.183E-02
 Advective & Diffusive Mass Loading Rate to GW (g/day)        1.760E-02

 Cumulative Emissions to Air (g)                               41.4
 Cumulative Loading to Groundwater (g)                         33.8


          Time =    3.00     years
========================================

Soil Concentration Profile
```

```
 Depth (cm)      Concentration(mg/kg soil)

       .00              .00
     50.00              .62E-02
    100.00              .12E-01
    150.00              .18E-01
    200.00              .23E-01
    250.00              .28E-01
    300.00              .31E-01
    350.00              .33E-01
    400.00              .33E-01
    450.00              .33E-01
    500.00              .31E-01

      5.00              .61E-03

  Emissions to Air from this time step (g)                       .432
  Advective Mass Loading Rate to Groundwater (g/day)           3.514E-03
  Diffusive Mass Loading Rate to Groundwater (g/day)           2.862E-03
  Advective & Diffusive Mass Loading Rate to GW (g/day)        6.376E-03

  Cumulative Emissions to Air (g)                                47.8
  Cumulative Loading to Groundwater (g)                          37.6


           Time =     4.00     years
 ==========================================

 Soil Concentration Profile

 Depth (cm)      Concentration(mg/kg soil)

       .00              .00
     50.00              .30E-02
    100.00              .60E-02
    150.00              .89E-02
    200.00              .12E-01
    250.00              .14E-01
    300.00              .16E-01
    350.00              .17E-01
    400.00              .18E-01
    450.00              .19E-01
    500.00              .18E-01

      5.00              .29E-03

  Emissions to Air from this time step (g)                       .208
  Advective Mass Loading Rate to Groundwater (g/day)           2.070E-03
  Diffusive Mass Loading Rate to Groundwater (g/day)           3.043E-04
  Advective & Diffusive Mass Loading Rate to GW (g/day)        2.375E-03

  Cumulative Emissions to Air (g)                                50.8
  Cumulative Loading to Groundwater (g)                          39.0


           Time =     5.00     years
 ==========================================

 Soil Concentration Profile

 Depth (cm)      Concentration(mg/kg soil)

       .00              .00
     50.00              .15E-02
    100.00              .31E-02
    150.00              .47E-02
    200.00              .61E-02
```

```
    250.00              .75E-02
    300.00              .86E-02
    350.00              .96E-02
    400.00              .10E-01
    450.00              .11E-01
    500.00              .11E-01

      5.00              .15E-03

  Emissions to Air from this time step (g)                    .107
  Advective Mass Loading Rate to Groundwater (g/day)         1.219E-03
  Diffusive Mass Loading Rate to Groundwater (g/day)        -3.342E-04
  Advective & Diffusive Mass Loading Rate to GW (g/day)      8.848E-04

  Cumulative Emissions to Air (g)                             52.2
  Cumulative Loading to Groundwater (g)                       39.5


          Time =     6.00     years
 ==========================================

 Soil Concentration Profile

 Depth (cm)     Concentration(mg/kg soil)

      .00               .00
    50.00               .83E-03
   100.00               .17E-02
   150.00               .25E-02
   200.00               .34E-02
   250.00               .41E-02
   300.00               .48E-02
   350.00               .54E-02
   400.00               .59E-02
   450.00               .62E-02
   500.00               .64E-02

     5.00               .82E-04

  Emissions to Air from this time step (g)                   5.779E-02
  Advective Mass Loading Rate to Groundwater (g/day)         7.233E-04
  Diffusive Mass Loading Rate to Groundwater (g/day)        -4.080E-04
  Advective & Diffusive Mass Loading Rate to GW (g/day)      3.153E-04

  Cumulative Emissions to Air (g)                             53.0
  Cumulative Loading to Groundwater (g)                       39.7


          Time =     7.00     years
 ==========================================

 Soil Concentration Profile

 Depth (cm)     Concentration(mg/kg soil)

      .00               .00
    50.00               .47E-03
   100.00               .95E-03
   150.00               .14E-02
   200.00               .19E-02
   250.00               .24E-02
   300.00               .28E-02
   350.00               .31E-02
   400.00               .34E-02
   450.00               .37E-02
   500.00               .39E-02
```

```
     5.00            .46E-04

  Emissions to Air from this time step (g)                      3.228E-02
  Advective Mass Loading Rate to Groundwater (g/day)            4.335E-04
  Diffusive Mass Loading Rate to Groundwater (g/day)           -3.363E-04
  Advective & Diffusive Mass Loading Rate to GW (g/day)         9.716E-05

  Cumulative Emissions to Air (g)                                53.4
  Cumulative Loading to Groundwater (g)                          39.8


          Time =     8.00     years
==========================================

Soil Concentration Profile

Depth (cm)     Concentration(mg/kg soil)

      .00            .00
    50.00            .27E-03
   100.00            .55E-03
   150.00            .83E-03
   200.00            .11E-02
   250.00            .14E-02
   300.00            .16E-02
   350.00            .18E-02
   400.00            .20E-02
   450.00            .22E-02
   500.00            .23E-02

     5.00            .26E-04

  Emissions to Air from this time step (g)                      1.851E-02
  Advective Mass Loading Rate to Groundwater (g/day)            2.623E-04
  Diffusive Mass Loading Rate to Groundwater (g/day)           -2.459E-04
  Advective & Diffusive Mass Loading Rate to GW (g/day)         1.649E-05

  Cumulative Emissions to Air (g)                                53.7
  Cumulative Loading to Groundwater (g)                          39.8


          Time =     9.00     years
==========================================

Soil Concentration Profile

Depth (cm)     Concentration(mg/kg soil)

      .00            .00
    50.00            .16E-03
   100.00            .32E-03
   150.00            .49E-03
   200.00            .65E-03
   250.00            .81E-03
   300.00            .96E-03
   350.00            .11E-02
   400.00            .12E-02
   450.00            .13E-02
   500.00            .14E-02

     5.00            .15E-04

  Emissions to Air from this time step (g)                      1.083E-02
  Advective Mass Loading Rate to Groundwater (g/day)            1.602E-04
  Diffusive Mass Loading Rate to Groundwater (g/day)           -1.705E-04
  Advective & Diffusive Mass Loading Rate to GW (g/day)        -1.027E-05
```

```
  Cumulative Emissions to Air (g)                               53.8
  Cumulative Loading to Groundwater (g)                         39.8


           Time =   10.00     years
=========================================

Soil Concentration Profile

Depth (cm)     Concentration(mg/kg soil)

     .00               .00
   50.00               .94E-04
  100.00               .19E-03
  150.00               .29E-03
  200.00               .39E-03
  250.00               .49E-03
  300.00               .58E-03
  350.00               .67E-03
  400.00               .75E-03
  450.00               .82E-03
  500.00               .88E-03

    5.00               .00

 Emissions to Air from this time step (g)                     6.435E-03
 Advective Mass Loading Rate to Groundwater (g/day)           9.867E-05
 Diffusive Mass Loading Rate to Groundwater (g/day)          -1.151E-04
 Advective & Diffusive Mass Loading Rate to GW (g/day)       -1.645E-05

 Cumulative Emissions to Air (g)                                53.9
 Cumulative Loading to Groundwater (g)                          39.8
```

APPENDIX C
ANALYTICAL TRANSPORT: ONE-, TWO-, AND THREE-DIMENSIONAL (AT123D) MODEL

The AT123D model is a generalized analytical, transient, one-, two-, and/or three-dimensional code for estimating the transport of wastes (heat, aqueous phase dissolved chemicals, or radioactive waste) in a groundwater porous system. AT123D, developed by Yeh (1981), is a screening-level analytical model that has been used for several applications related to the evaluation of risk at hazardous waste sites.

Figures C-1 and C-2 show schematics of AT123D run by itself and when linked with a vadose zone model, respectively. AT123D solves the differential mass balance (advective-dispersive) equation that describes contaminant fate and transport in the saturated zone. Groundwater flow is assumed to be uniform, one-dimensional, steady and uniform in the downgradient direction. Processes simulated by AT123D include:

- Three-dimensional dispersion (longitudinal, lateral, and vertical).
- One-dimensional uniform advection.
- Linear, reversible equilibrium adsorption.
- Lumped first-order decay.

The saturated zone is assumed to be homogenous and isotropic in terms of its physical properties (porosity, bulk density, etc.). Chemical sources may be simulated as instantaneous injections of mass, or as time-varying mass flux rates into the groundwater system. The saturated zone may be infinite or finite in the lateral and vertical directions. The model has the ability to simulate a variety of contaminant source geometries oriented in different ways along the x, y and z directions. These sources include a point, line, plane, or a volume source. When implemented, AT123D can be used to estimate concentrations as a function of time at any location specified by different values of the x, y, z and t coordinates.

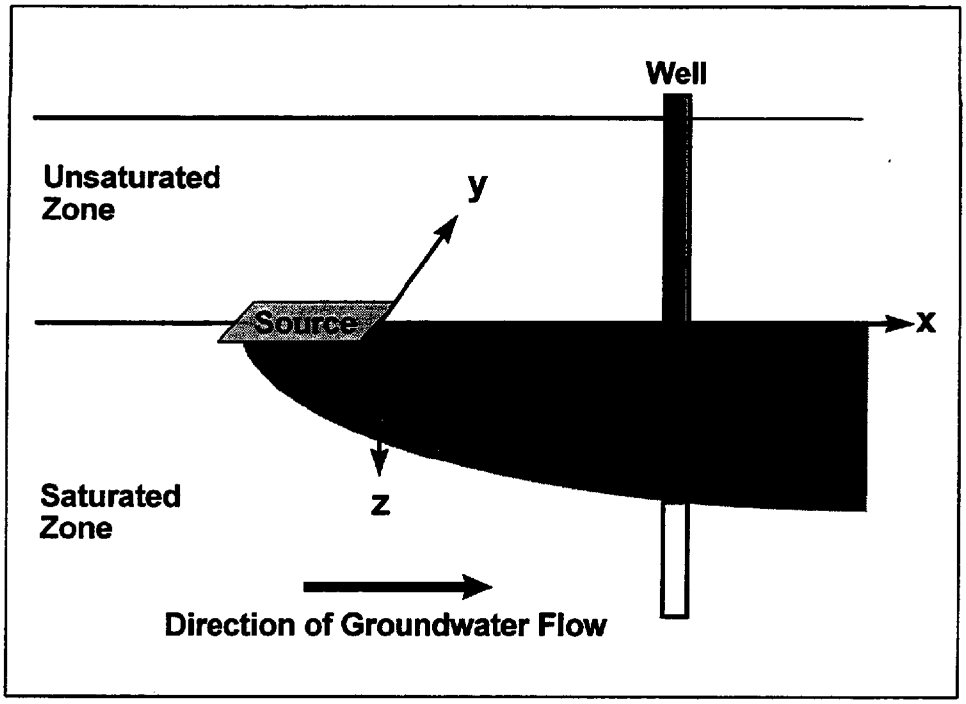


Figure C-1. AT123D by Itself (not linked with a vadose zone model).

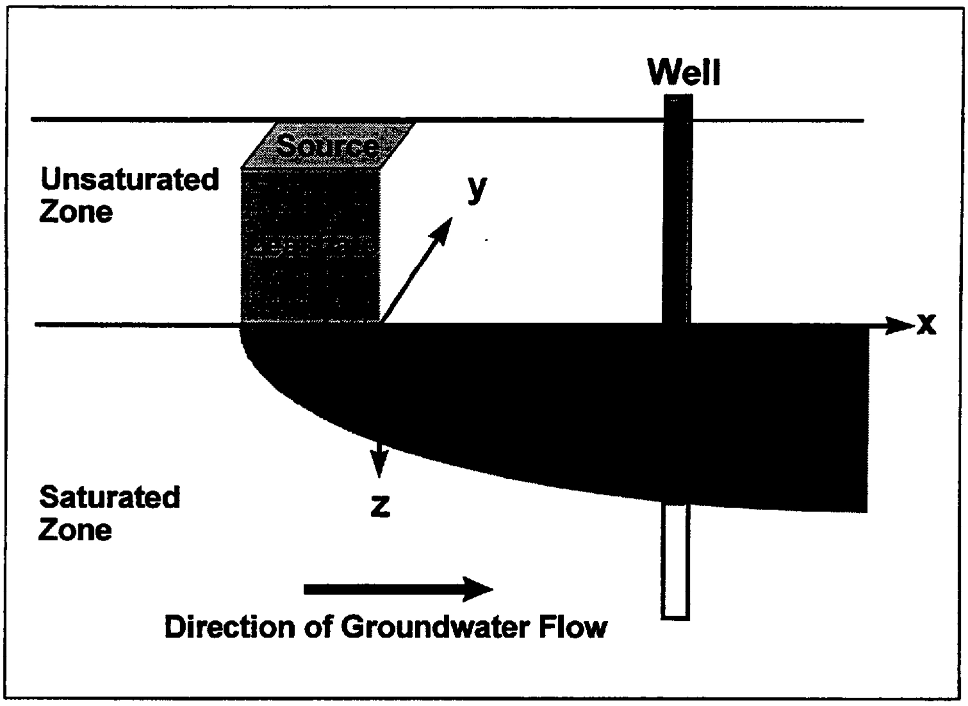


Figure C-2. AT123D Linked with a Vadose Zone Model.

AT123D uses Green's function to solve the advection-dispersion equation for the conditions described above, and a separate solution is used for each type of source and boundary condition. The majority of these are closed-form analytical solutions; however, the solutions for a finite width and/or depth aquifer requires truncation of infinite converging series.

AT123D Coordinate System and Source Configuration

The AT123D model requires the source geometry to be defined by specifying the dimensions of the source in the x, y, and z dimensions (assuming a Cartesian coordinate system). The x-axis or longitudinal axis is the direction of the groundwater flow. The z-axis is the vertical direction measured positive downwards and with a value of zero at the water table. The y-axis is the transverse direction (with respect to groundwater flow).

The AT123D model allows essentially eight different geometric source configurations, a point source, three line sources (one in each direction), three planar sources (one in each axis plane), and a volume source. The model geometry with a volume source is shown in Figure C-3. In more detail the eight sources are:

i) A point source, specified by having an x-length, y-length and z-length equal to zero.

ii) A line source parallel to the x-axis, specified by the length of the line source in the x-direction, and the other two dimensions being zero.

iii) A line source, parallel to the y-axis specified by the length of the line source in the y-direction, and the other two dimensions being zero.

iv) A line source, parallel to the z-axis specified by the length of the source in the z-direction, and the other two dimensions being zero.

v) An area source perpendicular to the x-axis, i.e., perpendicular to the direction of groundwater flow. This area source is specified by specifying lengths for the y- and z- directions and zero for the x direction.

vi) An area source perpendicular to the y-axis, i.e., in the x-z (vertical) plane. This area source is specified by specifying lengths for the x- and z-directions and zero for the y direction.

vii) An area source perpendicular to the z-axis i.e. a horizontal source mapped onto the water table. This area source is specified by specifying lengths for the x- and y- directions and zero for the z direction.

viii) A volume source specified by giving source lengths for the x, y, and z dimensions.

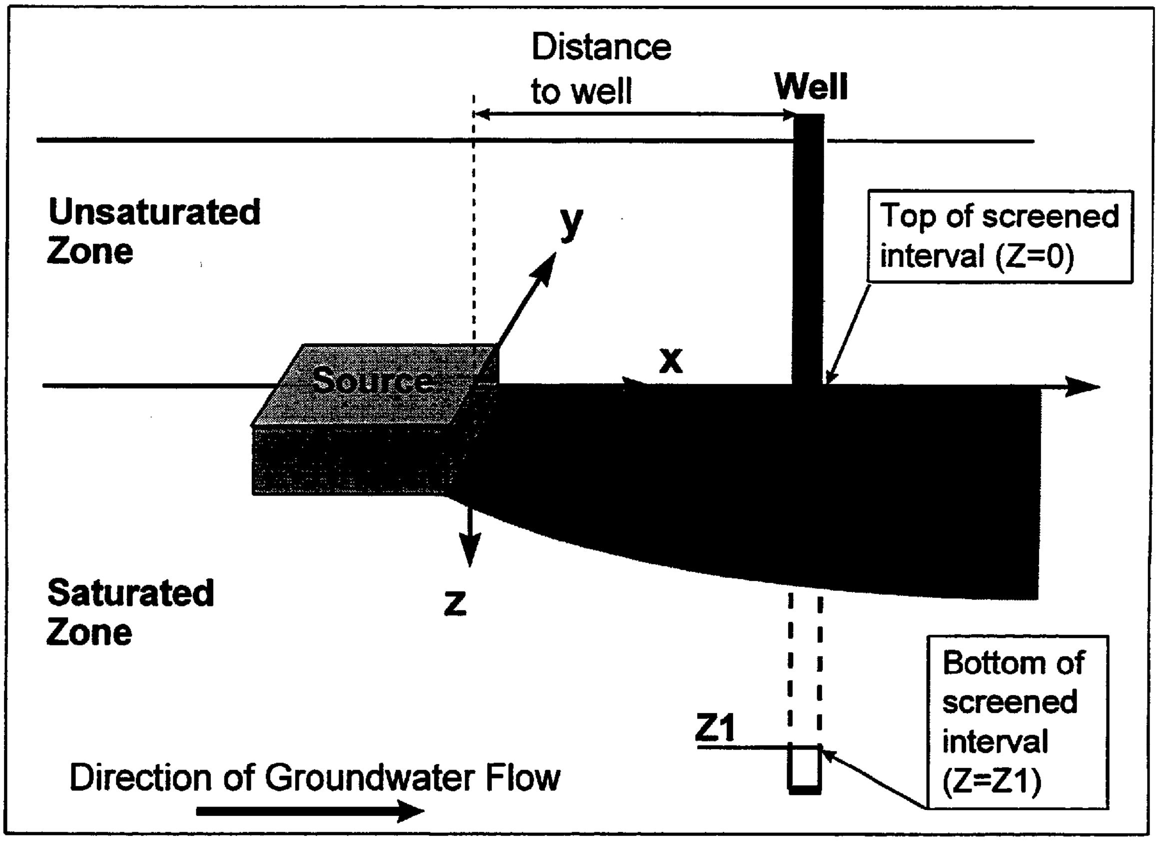


Figure C-3. AT123D Model Geometry with a Volume Source.

The AT123D model is available from and supported by the International Ground Water Modeling Center (IGWMC). A copy of this model was obtained from IGWMC and incorporated with a few modifications discussed below.

AT123D allows three different options for mass release into the aquifer: instantaneous, continuous and finite duration releases. When AT123D is run within the API DSS alone (i.e., not linked to SESOIL or Jury's model), the user may specify any of these three mass release rates and any of the eight different source geometries. In the first source option (instantaneous), the user specifies the mass and volume of the chemical source. This chemical mass is assumed to be instantaneously placed at the source at the beginning of the simulation (time = 0). This option may be applied when a known mass of chemical is present in the saturated zone, and no additional chemical input is expected to occur from the unsaturated zone (e.g., after the unsaturated zone has been remediated). For an ongoing leaking tank or other known discharge into the saturated zone, the user may have an estimate of the mass rate into the saturated zone. In this case, the second or third source option can be used to specify a known chemical mass loading rate. This rate may be specified as a constant over the entire simulation time or as a constant rate for a specified period of time (pulse length) less than the simulation time. Beyond the pulse length, the mass loading is considered to be zero.

When SESOIL or Jury's model is used to simulate chemical transport through the unsaturated zone the rate of chemical mass loading to the water table is used directly as an input for AT123D. This linkage is performed for the user by the API DSS. For this option the user does not have to define the source configuration. The source is assumed to be a horizontal plane with the same x and y dimensions used in SESOIL or Jury's model. A linked SESOIL-AT123D model can thus be used to simulate the transport of chemicals from contaminated soils to a groundwater receptor well. Note, the model estimates concentrations in a monitoring well, not a pumping well. The concentration in a pumping water well is significantly lower than concentrations in a monitoring well due to spatial dilution effects.

Estimating Average Well Concentrations

As shown in Figure C-3, wells are generally screened over a finite vertical interval across the saturated zone. Thus, the concentration of chemicals in water pumped from a well is in reality a vertically and horizontally averaged concentration from the water surrounding the well screen, and cannot be accurately represented by the concentration at a single point in the aquifer. The exact solution to this problem is to determine the flow-weighted average concentration of all water entering the well; however, such a solution has not yet been developed for analytical models such as AT123D. The API DSS therefore employs an approximate method to estimate average well concentrations. Concentrations are estimated by AT123D at a user-specified number of equally-spaced vertical intervals across the well screen; these are then arithmetically averaged to compute the well concentration:

$$C_{well} = \sum_z \frac{C(z)}{N_z} \tag{C-1}$$

where

C_{well} = vertically-averaged well concentration (mg/l)
$C(z)$ = concentration at depth z (mg/l)
N_z = number of intervals between the top and bottom of the well screen (dimensionless)

This method assigns equal weight to all vertical intervals between the top and bottom of the screen, and does not account for well water drawn from below or above the well screen. The method also does not account for lower concentrations in well water drawn radially from the downgradient side of the well.

For certain combinations of parameters, the estimated concentrations in the well may oscillate. If this happens, a number of input parameters should be carefully reviewed, and the time step used should be shortened. The oscillations are caused by the estimated concentrations changing too rapidly with each time step. The input parameters that affect the rapidness of changing concentrations are: gradient, hydraulic conductivity, degradation rate, and time step. This behavior was observed in the stand alone version of AT123D also.

For certain combinations of parameters, the estimated concentrations in the aquifer may exceed the leachate concentrations from the vadose zone model. For example, if a plane source is used and the well is placed at the downgradient edge of the source, the concentrations in groundwater at the very top of the aquifer may exceed the leachate concentrations. The reason for this is that the source is assumed to be a two-dimensional plane with no vertical thickness and all the mass input is assumed to be diluted over that "volume." In reality, leachate from the vadose zone would displace some of the water in the saturated zone so the source would be a volumetric source with a small thickness (equal to the mixing zone thickness). AT123D does not check for this condition so the results should be reviewed carefully and the receptor well should not be placed too close to the source.

Data Required

Table C-1 lists the data requirements for the AT123D model as it is incorporated into the API DSS. The specific differences between the DSS version and the standalone version are:

(i) The API DSS version of AT123D assumes that one of the coordinate points for the source is always at the origin. Thus only the length of the source in each direction needs to be entered.

(ii) The API DSS version of AT123D estimates vertically averaged concentrations at only one monitoring well location (specified values of X and Y). The vertical average is based on the average of ten concentrations estimated at equal distances between the top and bottom of the screen length.

(iii) When the API DSS version of AT123D is run by itself (i.e., without running SESOIL or Jury's model) either the instantaneous source or a constant pulse source of any duration can be specified. A source of varying mass load cannot be specified.

(iv) The API DSS version of AT123D does not allow the user to specify the time(s) at which the output is to be printed.

(v) The API DSS version allows only contaminant transport. The option to simulate heat and radioactive waste has been suppressed.

(vi) The API DSS version estimates the distribution coefficients as the product of the normalized organic carbon partition coefficient and the fractional organic carbon content.

TABLE C-1. DATA REQUIREMENTS FOR AT123D MODEL.

PARAMETER DEFINITION	UNITS/OPTIONS
Model Control Parameters	
Option to indicate if the aquifer is infinitely wide (y-direction)	YES/NO
Option to indicate if the aquifer is infinitely deep (z-direction)	YES/NO
Option to indicate the type of release/source*	Click on selection
instantaneous release	-
constant release rate	-
pulse release rate	-
Time step*	(yr)
Simulation time (max = 100 yrs)*	(yr)
Source Parameters*	
Length in the x-direction	(m)
Length in the y-direction	(m)
Thickness in the z-direction	(m)
Duration of the pulse (only for pulse source)	(yr)
Instantaneous chemical release (only for instantaneous release case)	(kg)
Constant chemical release rate (only for constant release case)	(kg/yr)
Media Parameters	
Effective porosity	(cm^3/cm^3)
Hydraulic conductivity	(m/yr)
Hydraulic gradient	(m/m)
Longitudinal dispersivity	(m)
Transverse dispersivity	(m)
Vertical dispersivity	(m)
Bulk density of soil	(g/cm^3)
Fractional organic carbon content	(g/g)
Thickness of aquifer**	(m)
Width of aquifer**	(m)

TABLE C-1. DATA REQUIREMENTS FOR AT123D MODEL (CONCLUDED)

PARAMETER DEFINITION	UNITS/OPTIONS
Chemical Parameters* **	
Organic carbon partition coefficient	[(mg/g)/(mg/cm^3)]
Overall decay rate	(1/day)
Molecular diffusion coefficient	(cm^2/s)
Receptor Well Data	
x-coordinate of well	(m)
y-coordinate of well	(m)
z-coordinate of top of well	(m)
z-coordinate of bottom of well	(m)

* Not required when AT123D is run in conjunction with the SESOIL or JURY model.

** Required only when aquifer is finite in z- or y- directions respectively.

*** Default values of chemical parameters are available from the database in the APIDSS.

Assumptions Underlying the Model and Its Applicability

AT123D is a semi-analytical model that is based on the following simplifying assumptions:

1) The saturated zone is assumed to be homogenous, isotropic and of uniform geometry, i.e., the thickness and width of the zone are considered to be uniform.
2) The water table is assumed to be steady without any fluctuations.
3) The flow direction is uniform, one-dimensional and steady state.
4) Contaminant decay is assumed to follow a lumped first order decay rate.
5) Contaminant adsorption is considered to follow linear adsorption.
6) Concentrations in the liquid and solid phase of the aquifer are assumed to be in equilibrium at all times.

7) The AT123D model simulates the dissolved phase contaminants only and is not applicable to simulate the transport of free product.
8) The source can be represented as a point, line plane or box.

Example Problem

The media-, chemical-, and receptor-specific properties are shown in Table C-2 for the example problem. The groundwater concentration at the receptor well is shown in the following graph (from the EXCEL® output). The AT123D output file, AT123D.OUT (View Fortran Results) is attached.

Concentration in Receptor Well (EXCEL® output)

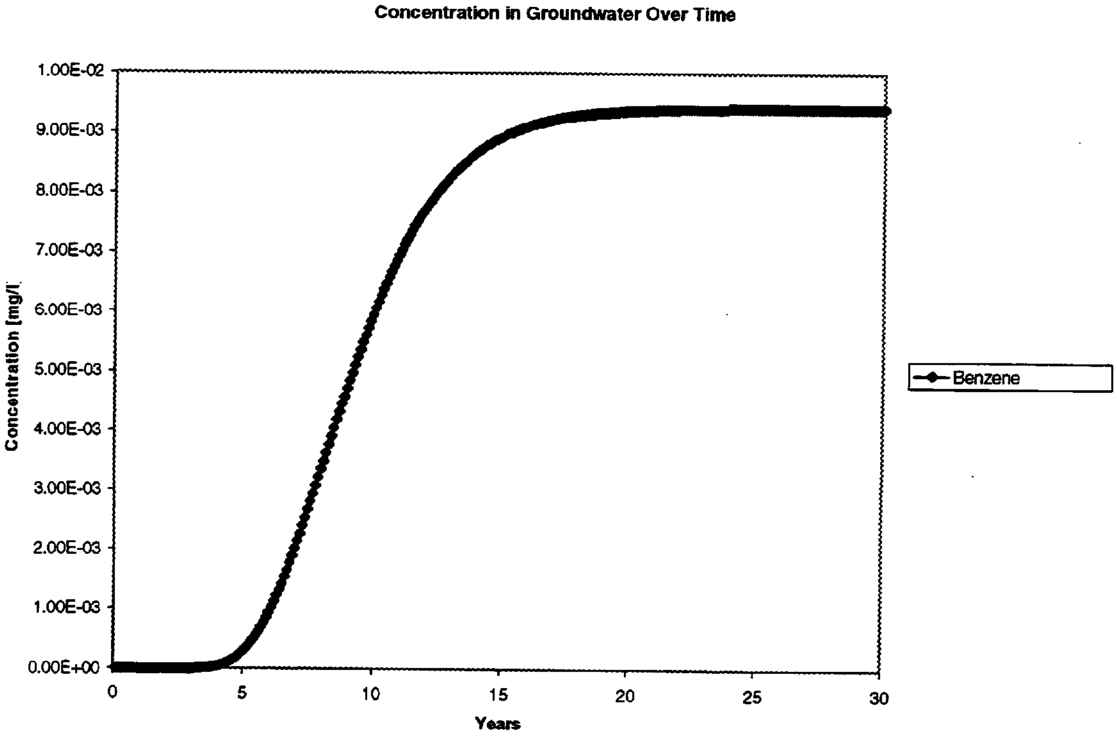


TABLE C-2. PARAMETER VALUES FOR EXAMPLE PROBLEM FOR A 5-YR PULSE SOURCE

PARAMETER DEFINITION	UNITS	VALUES
Model Control Parameters		
Option to indicate if the aquifer is infinitely wide (y-direction)		YES
Option to indicate if the aquifer is infinitely deep (z-direction)		NO
Type of source		Constant
Simulation time (max = 100 yrs)	(yr)	30
Time step	(yr)	0.1
Source Parameters		
Length of source in the direction of groundwater flow	(m)	10
Width of source perpendicular to groundwater flow	(m)	10
Depth to top of source	(m)	1
Depth to bottom of source	(m)	3
Media Parameters		
Porosity	(cm^3/cm^3)	0.3
Hydraulic conductivity	(m/yr)	300
Hydraulic gradient	(m/m)	0.01
Longitudinal dispersivity	(fraction)	0.10
Transverse dispersivity	(fraction)	0.03
Vertical dispersivity	(fraction)	0.01
Bulk density of soil	(g/cm^3)	1.65
Fractional organic carbon content	(g/g)	0.006
Thickness of aquifer	(m)	20
Width of aquifer	(m)	-
Receptor Well Data		
Distance downgradient	(m)	50
Distance off centerline of plume	(m)	0
Top of well screen	(m)	0
Bottom of well screen	(m)	10
Chemical Data for Benzene		
Chemical release rate	(kg/yr)	1
K_{oc}	(ug/gOC/ug/ml)	58.9
Degradation rate	(1/days)	0.001
Diffusion coefficient in water	(cm^2/s)	9.80E-6

References

General Sciences Corporation. 1990. PCGEMS User's Guide. Release 1.0. Prepared for U.S. EPA Office of Pesticides and Toxic Substances.

Yeh, G.T. 1981. AT123D: Analytical Transient One-, Two-, and Three-dimensional Simulation of Waste Transport in the Aquifer System. Oak Ridge National Laboratory, Oak Ride, TN.

```
AT123D Output File
DSS Fate and Transport

Chemicals in the analysis
Benzene

Number of years simulated:          30

GENERAL INPUT DATA
******************

    NO. OF POINTS IN X-DIRECTION ......................     1
    NO. OF POINTS IN Y-DIRECTION ......................     1
    NO. OF POINTS IN Z-DIRECTION ......................     5
    NO. OF ROOTS: NO. OF SERIES TERMS .................   500
    NO. OF BEGINNING TIME STEPS .......................     1
    NO. OF ENDING TIME STEP ...........................   300
    NO. OF TIME INTERVALS FOR PRINTED OUT SOLUTION ....     1
    INSTANTANEOUS SOURCE CONTROL = 0 FOR INSTANT SOURCE     1
    SOURCE CONDITION CONTROL = 0 FOR STEADY SOURCE ....   300
    INTERMITTENT OUTPUT CONTROL = 0 NO SUCH OUTPUT ....     1
    CASE CONTROL =1 THERMAL, = 2 FOR CHEMICAL, = 3 RAD      2

    X-COORDINATE OF RECEPTOR WELL (METERS) ...........   .5000E+02
    Y-COORDINATE OF RECEPTOR WELL (METERS) ...........   .0000E+00
    AQUIFER DEPTH, = 0.0 FOR INFINITE DEEP (METERS) ...  .2000E+02
    AQUIFER WIDTH, = 0.0 FOR INFINITE WIDE (METERS) ...  .0000E+00
    BEGIN POINT OF X-SOURCE LOCATION (METERS) ........  -.1000E+02
    END POINT OF X-SOURCE LOCATION (METERS) ..........   .0000E+00
    BEGIN POINT OF Y-SOURCE LOCATION (METERS) ........  -.5000E+01
    END POINT OF Y-SOURCE LOCATION (METERS) ..........   .5000E+01
    BEGIN POINT OF Z-SOURCE LOCATION (METERS) ........   .1000E+01
    END POINT OF Z-SOURCE LOCATION (METERS) ..........   .3000E+01

    POROSITY .........................................   .3000E+00
    HYDRAULIC CONDUCTIVITY (METER/YEAR) ..............   .3000E+03
    HYDRAULIC GRADIENT ...............................   .1000E-01
    LONGITUDINAL DISPERSIVITY (METER) ................   .5000E+01
    LATERAL DISPERSIVITY (METER) .....................   .1500E+01
    VERTICAL DISPERSIVITY (METER) ....................   .5000E+00

    BULK DENSITY OF THE SOIL (KG/M**3) ...............   .1650E+04
    TIME INTERVAL SIZE FOR THE DESIRED SOLUTION (YR) ..  .1000E+00
    DISCHARGE TIME (YR) ..............................   .3000E+02

INPUT DATA/RESULTS FOR CHEMICAL:  Benzene

    INST. WASTE RELEASE (KG) VALID FOR INST CASE ONLY..  .1000E+01
    DISTRIBUTION COEFFICIENT, KD (M**3/KG) ...........   .3534E-03
    MOLECULAR DIFFUSION COEFFICIENT          (M**2/YR)   .3091E-01
    DECAY CONSTANT ( 1/YR ) ..........................   .3650E+00
    LIST OF TRANSIENT SOURCE RELEASE RATE
        .100E+01    .100E+01    .100E+01    .100E+01    .100E+01
        .100E+01    .100E+01    .100E+01    .100E+01    .100E+01
        .100E+01    .100E+01    .100E+01    .100E+01    .100E+01
        .100E+01    .100E+01    .100E+01    .100E+01    .100E+01
        .100E+01    .100E+01    .100E+01    .100E+01    .100E+01
        .100E+01    .100E+01    .100E+01    .100E+01    .100E+01
        .100E+01    .100E+01    .100E+01    .100E+01    .100E+01
        .100E+01    .100E+01    .100E+01    .100E+01    .100E+01
        .100E+01    .100E+01    .100E+01    .100E+01    .100E+01
        .100E+01    .100E+01    .100E+01    .100E+01    .100E+01
        .100E+01    .100E+01    .100E+01    .100E+01    .100E+01
        .100E+01    .100E+01    .100E+01    .100E+01    .100E+01
        .100E+01    .100E+01    .100E+01    .100E+01    .100E+01
        .100E+01    .100E+01    .100E+01    .100E+01    .100E+01
        .100E+01    .100E+01    .100E+01    .100E+01    .100E+01
        .100E+01    .100E+01    .100E+01    .100E+01    .100E+01
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          .100E+01    .100E+01    .100E+01    .100E+01    .100E+01
          .100E+01    .100E+01    .100E+01    .100E+01    .100E+01
          .100E+01    .100E+01    .100E+01    .100E+01    .100E+01
          .100E+01    .100E+01    .100E+01    .100E+01    .100E+01
          .100E+01    .100E+01    .100E+01    .100E+01    .100E+01
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          .100E+01    .100E+01    .100E+01    .100E+01    .100E+01
          .100E+01    .100E+01    .100E+01    .100E+01    .100E+01
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          .100E+01    .100E+01    .100E+01    .100E+01    .100E+01
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          .100E+01    .100E+01    .100E+01    .100E+01    .100E+01
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          .100E+01    .100E+01    .100E+01    .100E+01    .100E+01
          .100E+01    .100E+01    .100E+01    .100E+01    .100E+01
          .100E+01    .100E+01    .100E+01    .100E+01    .100E+01
          .100E+01    .100E+01    .100E+01    .100E+01    .100E+01
          .100E+01    .100E+01    .100E+01    .100E+01    .100E+01
          .100E+01    .100E+01    .100E+01    .100E+01    .100E+01
          .100E+01    .100E+01    .100E+01    .100E+01
     RETARDATION FACTOR ...............................     .2944E+01
     RETARDED SEEPAGE VELOCITY (M/YR) .................     .3397E+01
     RETARDED LONGITUDINAL DISPERSION COEF. (M**2/YR) ..    .1702E+02
     RETARDED LATERAL DISPERSION COEFFICIENT (M**2/YR) .    .5131E+01
     RETARDED VERTICAL DISPERSION COEFFICIENT (M**2/YR).    .1734E+01

 OUTPUTS
 *******

 OUTPUT FOR CHEMICAL :Benzene

     RETARDATION FACTOR ...............................     .2944E+01
     RETARDED SEEPAGE VELOCITY (M/YR) .................     .3397E+01
     RETARDED LONGITUDINAL DISPERSION COEF. (M**2/YR) ..    .1702E+02
     RETARDED LATERAL DISPERSION COEFFICIENT (M**2/YR) .    .5131E+01
     RETARDED VERTICAL DISPERSION COEFFICIENT (M**2/YR).    .1734E+01

        Time [yr] =     .000
      z [m] =    0.00E+00       conc [mg/l] =  0.000E+00
      z [m] =    2.50E+00       conc [mg/l] =  0.000E+00
      z [m] =    5.00E+00       conc [mg/l] =  0.000E+00
      z [m] =    7.50E+00       conc [mg/l] =  0.000E+00
      z [m] =    1.00E+01       conc [mg/l] =  0.000E+00
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Ave. conc. [mg/l] =  0.000E+00

  Time [yr] =   1.00
z [m] =   0.00E+00      conc [mg/l] =  0.000E+00
z [m] =   2.50E+00      conc [mg/l] =  0.000E+00
z [m] =   5.00E+00      conc [mg/l] =  0.000E+00
z [m] =   7.50E+00      conc [mg/l] =  0.000E+00
z [m] =   1.00E+01      conc [mg/l] =  0.000E+00

Ave. conc. [mg/l] =  0.000E+00

  Time [yr] =   2.00
z [m] =   0.00E+00      conc [mg/l] =  0.000E+00
z [m] =   2.50E+00      conc [mg/l] =  0.000E+00
z [m] =   5.00E+00      conc [mg/l] =  0.000E+00
z [m] =   7.50E+00      conc [mg/l] =  0.000E+00
z [m] =   1.00E+01      conc [mg/l] =  0.000E+00

Ave. conc. [mg/l] =  0.000E+00

  Time [yr] =   3.00
z [m] =   0.00E+00      conc [mg/l] =  4.639E-06
z [m] =   2.50E+00      conc [mg/l] =  3.828E-06
z [m] =   5.00E+00      conc [mg/l] =  2.052E-06
z [m] =   7.50E+00      conc [mg/l] =  6.573E-07
z [m] =   1.00E+01      conc [mg/l] =  1.193E-07

Ave. conc. [mg/l] =  2.259E-06

  Time [yr] =   4.00
z [m] =   0.00E+00      conc [mg/l] =  1.043E-04
z [m] =   2.50E+00      conc [mg/l] =  8.810E-05
z [m] =   5.00E+00      conc [mg/l] =  5.211E-05
z [m] =   7.50E+00      conc [mg/l] =  2.076E-05
z [m] =   1.00E+01      conc [mg/l] =  5.407E-06

Ave. conc. [mg/l] =  5.413E-05

  Time [yr] =   5.00
z [m] =   0.00E+00      conc [mg/l] =  6.102E-04
z [m] =   2.50E+00      conc [mg/l] =  5.254E-04
z [m] =   5.00E+00      conc [mg/l] =  3.323E-04
z [m] =   7.50E+00      conc [mg/l] =  1.514E-04
z [m] =   1.00E+01      conc [mg/l] =  4.892E-05

Ave. conc. [mg/l] =  3.336E-04

  Time [yr] =   6.00
z [m] =   0.00E+00      conc [mg/l] =  1.809E-03
z [m] =   2.50E+00      conc [mg/l] =  1.580E-03
z [m] =   5.00E+00      conc [mg/l] =  1.049E-03
z [m] =   7.50E+00      conc [mg/l] =  5.239E-04
z [m] =   1.00E+01      conc [mg/l] =  1.952E-04

Ave. conc. [mg/l] =  1.032E-03

  Time [yr] =   7.00
z [m] =   0.00E+00      conc [mg/l] =  3.638E-03
z [m] =   2.50E+00      conc [mg/l] =  3.215E-03
z [m] =   5.00E+00      conc [mg/l] =  2.212E-03
z [m] =   7.50E+00      conc [mg/l] =  1.180E-03
z [m] =   1.00E+01      conc [mg/l] =  4.859E-04

Ave. conc. [mg/l] =  2.146E-03

  Time [yr] =   8.00
z [m] =   0.00E+00      conc [mg/l] =  5.767E-03
z [m] =   2.50E+00      conc [mg/l] =  5.140E-03
```

```
z [m] =   5.00E+00      conc [mg/l] =  3.633E-03
z [m] =   7.50E+00      conc [mg/l] =  2.033E-03
z [m] =   1.00E+01      conc [mg/l] =  9.014E-04

Ave. conc. [mg/l] =  3.495E-03

  Time [yr] =    9.00
z [m] =   0.00E+00      conc [mg/l] =  7.841E-03
z [m] =   2.50E+00      conc [mg/l] =  7.033E-03
z [m] =   5.00E+00      conc [mg/l] =  5.073E-03
z [m] =   7.50E+00      conc [mg/l] =  2.944E-03
z [m] =   1.00E+01      conc [mg/l] =  1.379E-03

Ave. conc. [mg/l] =  4.854E-03


  Time [yr] =    10.0
z [m] =   0.00E+00      conc [mg/l] =  9.630E-03
z [m] =   2.50E+00      conc [mg/l] =  8.680E-03
z [m] =   5.00E+00      conc [mg/l] =  6.357E-03
z [m] =   7.50E+00      conc [mg/l] =  3.790E-03
z [m] =   1.00E+01      conc [mg/l] =  1.850E-03

Ave. conc. [mg/l] =  6.061E-03

  Time [yr] =    11.0
z [m] =   0.00E+00      conc [mg/l] =  1.105E-02
z [m] =   2.50E+00      conc [mg/l] =  9.993E-03
z [m] =   5.00E+00      conc [mg/l] =  7.402E-03
z [m] =   7.50E+00      conc [mg/l] =  4.503E-03
z [m] =   1.00E+01      conc [mg/l] =  2.267E-03

Ave. conc. [mg/l] =  7.042E-03

  Time [yr] =    12.0
z [m] =   0.00E+00      conc [mg/l] =  1.210E-02
z [m] =   2.50E+00      conc [mg/l] =  1.097E-02
z [m] =   5.00E+00      conc [mg/l] =  8.196E-03
z [m] =   7.50E+00      conc [mg/l] =  5.062E-03
z [m] =   1.00E+01      conc [mg/l] =  2.608E-03

Ave. conc. [mg/l] =  7.788E-03

  Time [yr] =    13.0
z [m] =   0.00E+00      conc [mg/l] =  1.284E-02
z [m] =   2.50E+00      conc [mg/l] =  1.167E-02
z [m] =   5.00E+00      conc [mg/l] =  8.771E-03
z [m] =   7.50E+00      conc [mg/l] =  5.477E-03
z [m] =   1.00E+01      conc [mg/l] =  2.870E-03

Ave. conc. [mg/l] =  8.327E-03

  Time [yr] =    14.0
z [m] =   0.00E+00      conc [mg/l] =  1.335E-02
z [m] =   2.50E+00      conc [mg/l] =  1.215E-02
z [m] =   5.00E+00      conc [mg/l] =  9.171E-03
z [m] =   7.50E+00      conc [mg/l] =  5.772E-03
z [m] =   1.00E+01      conc [mg/l] =  3.062E-03

Ave. conc. [mg/l] =  8.702E-03

  Time [yr] =    15.0
z [m] =   0.00E+00      conc [mg/l] =  1.369E-02
z [m] =   2.50E+00      conc [mg/l] =  1.247E-02
z [m] =   5.00E+00      conc [mg/l] =  9.441E-03
z [m] =   7.50E+00      conc [mg/l] =  5.974E-03
z [m] =   1.00E+01      conc [mg/l] =  3.198E-03
```

```
Ave. conc. [mg/l] =  8.956E-03

   Time [yr] =    16.0
z [m] =    0.00E+00       conc [mg/l] =  1.391E-02
z [m] =    2.50E+00       conc [mg/l] =  1.268E-02
z [m] =    5.00E+00       conc [mg/l] =  9.618E-03
z [m] =    7.50E+00       conc [mg/l] =  6.110E-03
z [m] =    1.00E+01       conc [mg/l] =  3.292E-03

Ave. conc. [mg/l] =  9.123E-03

  Time [yr] =    17.0
z [m] =    0.00E+00       conc [mg/l] =  1.405E-02
z [m] =    2.50E+00       conc [mg/l] =  1.281E-02
z [m] =    5.00E+00       conc [mg/l] =  9.733E-03
z [m] =    7.50E+00       conc [mg/l] =  6.199E-03
z [m] =    1.00E+01       conc [mg/l] =  3.354E-03

Ave. conc. [mg/l] =  9.231E-03

   Time [yr] =    18.0
z [m] =    0.00E+00       conc [mg/l] =  1.414E-02
z [m] =    2.50E+00       conc [mg/l] =  1.290E-02
z [m] =    5.00E+00       conc [mg/l] =  9.806E-03
z [m] =    7.50E+00       conc [mg/l] =  6.256E-03
z [m] =    1.00E+01       conc [mg/l] =  3.395E-03

Ave. conc. [mg/l] =  9.300E-03

   Time [yr] =    19.0
z [m] =    0.00E+00       conc [mg/l] =  1.420E-02
z [m] =    2.50E+00       conc [mg/l] =  1.295E-02
z [m] =    5.00E+00       conc [mg/l] =  9.851E-03
z [m] =    7.50E+00       conc [mg/l] =  6.293E-03
z [m] =    1.00E+01       conc [mg/l] =  3.421E-03

Ave. conc. [mg/l] =  9.343E-03

  Time [yr] =    20.0
z [m] =    0.00E+00       conc [mg/l] =  1.423E-02
z [m] =    2.50E+00       conc [mg/l] =  1.298E-02
z [m] =    5.00E+00       conc [mg/l] =  9.880E-03
z [m] =    7.50E+00       conc [mg/l] =  6.316E-03
z [m] =    1.00E+01       conc [mg/l] =  3.438E-03

Ave. conc. [mg/l] =  9.369E-03

  Time [yr] =    21.0
z [m] =    0.00E+00       conc [mg/l] =  1.425E-02
z [m] =    2.50E+00       conc [mg/l] =  1.300E-02
z [m] =    5.00E+00       conc [mg/l] =  9.897E-03
z [m] =    7.50E+00       conc [mg/l] =  6.330E-03
z [m] =    1.00E+01       conc [mg/l] =  3.449E-03

Ave. conc. [mg/l] =  9.386E-03

  Time [yr] =    22.0
z [m] =    0.00E+00       conc [mg/l] =  1.426E-02
z [m] =    2.50E+00       conc [mg/l] =  1.301E-02
z [m] =    5.00E+00       conc [mg/l] =  9.908E-03
z [m] =    7.50E+00       conc [mg/l] =  6.338E-03
z [m] =    1.00E+01       conc [mg/l] =  3.456E-03

Ave. conc. [mg/l] =  9.396E-03

  Time [yr] =    23.0
z [m] =    0.00E+00       conc [mg/l] =  1.427E-02
z [m] =    2.50E+00       conc [mg/l] =  1.302E-02
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```
z [m] =    5.00E+00      conc [mg/l] =  9.914E-03
z [m] =    7.50E+00      conc [mg/l] =  6.344E-03
z [m] =    1.00E+01      conc [mg/l] =  3.460E-03

Ave. conc. [mg/l] =  9.402E-03

  Time [yr] =   24.0
z [m] =    0.00E+00      conc [mg/l] =  1.428E-02
z [m] =    2.50E+00      conc [mg/l] =  1.303E-02
z [m] =    5.00E+00      conc [mg/l] =  9.918E-03
z [m] =    7.50E+00      conc [mg/l] =  6.347E-03
z [m] =    1.00E+01      conc [mg/l] =  3.462E-03

Ave. conc. [mg/l] =  9.406E-03

  Time [yr] =   25.0
z [m] =    0.00E+00      conc [mg/l] =  1.428E-02
z [m] =    2.50E+00      conc [mg/l] =  1.303E-02
z [m] =    5.00E+00      conc [mg/l] =  9.920E-03
z [m] =    7.50E+00      conc [mg/l] =  6.349E-03
z [m] =    1.00E+01      conc [mg/l] =  3.464E-03

Ave. conc. [mg/l] =  9.408E-03

  Time [yr] =   26.0
z [m] =    0.00E+00      conc [mg/l] =  1.428E-02
z [m] =    2.50E+00      conc [mg/l] =  1.303E-02
z [m] =    5.00E+00      conc [mg/l] =  9.922E-03
z [m] =    7.50E+00      conc [mg/l] =  6.350E-03
z [m] =    1.00E+01      conc [mg/l] =  3.465E-03

Ave. conc. [mg/l] =  9.409E-03

  Time [yr] =   27.0
z [m] =    0.00E+00      conc [mg/l] =  1.428E-02
z [m] =    2.50E+00      conc [mg/l] =  1.303E-02
z [m] =    5.00E+00      conc [mg/l] =  9.923E-03
z [m] =    7.50E+00      conc [mg/l] =  6.351E-03
z [m] =    1.00E+01      conc [mg/l] =  3.465E-03

Ave. conc. [mg/l] =  9.410E-03

  Time [yr] =   28.0
z [m] =    0.00E+00      conc [mg/l] =  1.428E-02
z [m] =    2.50E+00      conc [mg/l] =  1.303E-02
z [m] =    5.00E+00      conc [mg/l] =  9.923E-03
z [m] =    7.50E+00      conc [mg/l] =  6.351E-03
z [m] =    1.00E+01      conc [mg/l] =  3.466E-03

Ave. conc. [mg/l] =  9.411E-03

  Time [yr] =   29.0
z [m] =    0.00E+00      conc [mg/l] =  1.428E-02
z [m] =    2.50E+00      conc [mg/l] =  1.303E-02
z [m] =    5.00E+00      conc [mg/l] =  9.923E-03
z [m] =    7.50E+00      conc [mg/l] =  6.352E-03
z [m] =    1.00E+01      conc [mg/l] =  3.466E-03

Ave. conc. [mg/l] =  9.411E-03

  Time [yr] =   30.0
z [m] =    0.00E+00      conc [mg/l] =  1.428E-02
z [m] =    2.50E+00      conc [mg/l] =  1.303E-02
z [m] =    5.00E+00      conc [mg/l] =  9.924E-03
z [m] =    7.50E+00      conc [mg/l] =  6.352E-03
z [m] =    1.00E+01      conc [mg/l] =  3.466E-03

Ave. conc. [mg/l] =  9.411E-03
```

APPENDIX D
THIBODEAUX-HWANG MODEL

The Thibodeaux-Hwang model (Thibodeaux-Hwang, 1982) was developed to estimate the time-varying emissions of volatile chemicals from petroleum landfarming operations. The model is applicable both for the case of surface application of the chemical as well as for the case of subsurface injection of waste, i.e., where a zone of contaminated soil is covered by a layer of clean fill as shown in Figure D-1. A modified version of the original model (as discussed below) is also presented in the Superfund Exposure Assessment Manual (EPA, 1988).

Thibodeaux-Hwang (1982) present the following relationship to estimate the volatile chemical flux rate through the soil:

$$E(t) \quad = \quad D_eC_v / [d_1^2 + (2D_eAt(d_2 - d_1)C_v/m_o)]^{0.5} \qquad \text{(D-1)}$$

where

$E(t)$ = the instantaneous volatile flux emission rate (g/cm^2-s)

D_e = effective diffusion coefficient of the chemical in soil vapor (cm^2/s)

C_v = vapor phase concentration of the chemical in soil (g/cm^3)

A = the surface area of the contaminated soil (cm^2)

d_1 = depth to the top of the contaminated soil (cm)

d_2 = depth to the bottom of the contaminated soil (cm)

t = time since the application of contaminants to soil (s)

m_o = the initial mass of contaminant (g)

The original Thibodeaux-Hwang paper has a typographical error and the corrected expression is presented in USEPA (1984). In equation D-1 the initial mass of contaminant can be estimated as:

$$m_o \quad = \quad (d_2 - d_1)\ A\ C_b \qquad \text{(D-2)}$$

where

C_b = the bulk contaminant concentration in soil (g of chemical/cm^3 of wet soil)

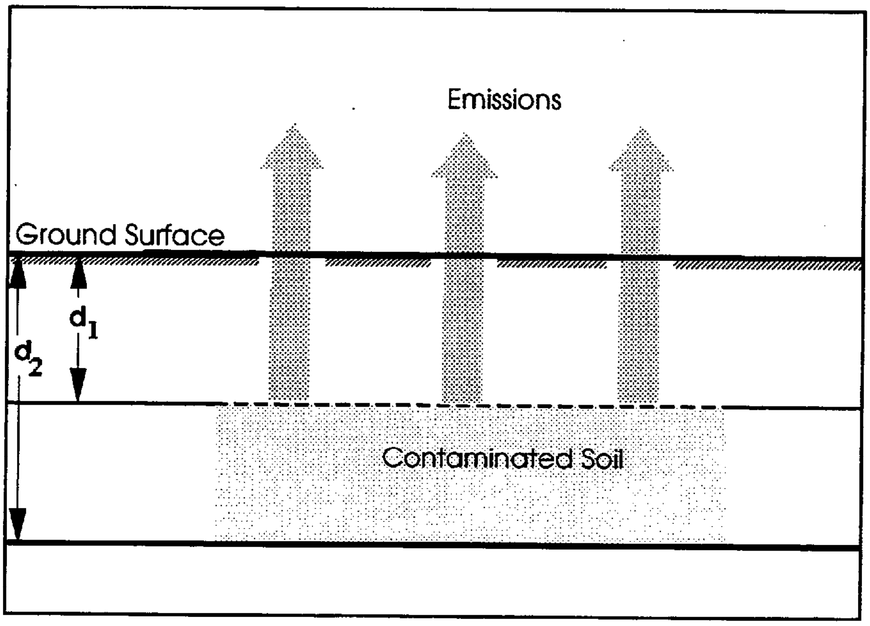

FIGURE D-1. Schematic of the Thibodeaux-Hwang Emission Model.

The relation between the bulk contaminant concentration and the total soil concentration is given by:

$$C_b = C_T (\rho_b + \rho_w \theta_w) \tag{D-3}$$

where

C_T = the total soil concentration (g of chemical/g of soil)

ρ_b = soil bulk density (g/cm^3)

ρ_w = density of water (g/cm^3)

θ_w = volumetric water content (cm^3 of water/cm^3 of soil)

Vapor Phase Concentration

The vapor phase concentration, C_v, is estimated using the following equilibrium partitioning equations:

$$C_v = H\,C_w \tag{D-4}$$

$$C_w = C_T \frac{(\rho_b + \theta_w \rho_w)}{\rho_b K_d + \theta_w + (\theta_T - \theta_w)H} \tag{D-5}$$

where

C_v = the vapor phase concentration of the chemical in soil (g/cm^3)
C_w = the dissolved phase concentration of the chemical (g/cm^3)
H = Henry's Law constant for the chemical [(mg/L)/(mg/L)]
θ_T = total porosity in the soil [cm^3 voids/cm^3 soil]
K_d = chemical-specific partition coefficient [cm^3/g]
$K_d = F_{oc} \bullet K_{oc}$
F_{oc} = fraction organic carbon in the soil [g oc/g soil]
K_{oc} = organic carbon partition coefficient [cm^3/g] or [L/kg]

The total porosity is the sum of air porosity and the water content:

$$\theta_T = \theta_a + \theta_w \tag{D-6}$$

where

θ_a = the volumetric air content of the soil (cm^3 of gas/cm^3 of soil)

If the estimated vapor phase concentration is larger than the saturated vapor concentration for the chemical in soil, the saturated vapor concentration is used in equation D-1 as the soil vapor concentration.

The relationship between the two forms of Henry's constant is

$$H = H'/RT \tag{D-7}$$

where

H' = the dimensional form of the Henry's constant (atm-m^3/mol)
R = the Universal gas constant [(0.0000821 atm-m^3/°K)]
T = the absolute temperature [°K]

Time to Depletion

Thibodeaux-Hwang (1982) also define an 'evaporation diffusion lifetime' (t_d) for the initial mass that is defined as the time taken for the entire contaminant mass to volatilize. This time is estimated as:

$$t_d = [(d_2 - d_1)\, m_o] / (2\, D_e\, A\, C_v) \qquad \text{(D-8)}$$

where

t_d = the time taken for the entire mass to volatilize

By substituting equation D-2 in equation D-8:

$$t_d = [(d_2^2 - d_1^2)/(2D_e)]\, (C_b/C_v) \qquad \text{(D-9)}$$

The instantaneous emission rate presented in equation D-1 can be used to estimate the average emission rate over any time period, i.e.,

$$E'(T) = (1/T) \int_0^T E(t)\, dt \qquad \text{(D-10)}$$

where

$E'(t)$ = the average emission rate of the chemical over time T (g/s)

T = the averaging time (s)

By substituting equation D-1 in equation D-10 and integrating:

$$E'(t) = 2\, D_e C_v A / [d_1 + (2D_e C_v t/C_b + d_1^2)^{0.5}] \qquad \text{(D-11)}$$

The maximum value of time (t) in equation D-11 would be the evaporation diffusion lifetime (t_d) as defined by equation D-8. After this time (t_d) the volatile emission rate would be zero. Thus for exposure assessment purposes, if it is necessary to estimate an average emission rate for periods larger than t_d, the following relationship may be used:

$$E'(t_e) = (t_d/t_e)\, E'(t_d) \qquad \text{(D-12)}$$

where

$E'(t_e)$ = the average emission over the exposure duration t_e (g/s)

$E'(t_d)$ = the average emission over the duration t_d (g/s)

The Effective Diffusion Coefficient

The effective diffusion coefficient for a chemical in soil can be computed using the following relationship presented by Millington and Quirk (1961):

$$D_e = D_{air}\,\theta_a^{10/3}/\theta_T^{2} \qquad \text{(D-13)}$$

where

D_{air} = the molecular diffusion coefficient for the chemical in air (cm^2/s)

For dry soils, the air-filled porosity (volumetric air content) is approximately equal to the total porosity, and equation D-13 reduces to:

$$D_e = D_{air}\,\theta_T^{4/3} \qquad \text{(D-14)}$$

The above relationship is used in the Thibodeaux-Hwang model presented in USEPA (1984). The diffusion coefficient for a chemical in air depends on air temperature based on the following relationship (Lyman et al., 1990):

$$D_{air(T2)} = D_{air(T1)}\,(T_2/T_1)^{1.75} \qquad \text{(D-15)}$$

where

$D_{air(T2)}$, $D_{air(T1)}$ = the diffusion coefficient of the chemical at temperatures T_2 and T_1 respectively (cm^2/s)

T_2 = air (soil vapor) temperature (°K)

T_1 = air temperature at which $D_{air(T1)}$ is known (°K)

Data Requirements

Table D-1 lists the data requirements for the Thibodeaux-Hwang emissions model.

Table D-1. Data Requirements for the Thibodeaux-Hwang Vapor Emissions Model.

PARAMETER DEFINITION	UNITS Used in API DSS
Chemical Data	
Total soil concentration	[mg/kg wet soil]
Henry's Law constant	[(mg/L)/(mg/L)]
Air diffusion coefficient	[cm^2/s]
Soil-water partition coefficient	[(g/g)/(g/cm^3)]
Organic carbon partition coefficient	[(g/g)/(g/cm^3)]
Fractional organic carbon content	[mg/mg]
Soils Data	
Volumetric water content	[cm^3/cm^3]
Total porosity of the soil	[cm^3/cm^3]
Soil dry bulk density	[g/cm^3]
Air-filled porosity	[cm^3/cm^3]
Soil temperature	[°C]
Source Data	
Depth to the top of the contaminated layer	[m]
Depth to the bottom of the contaminated layer	[m]
Source area	[m^2]

Assumptions Underlying the Model and Its Applicability

1. Chemical mass is distributed at a uniform concentration between depths d_1 and d_2 that define the zone of incorporation of the contaminant. Thus, (d_2 - d_1) is the thickness of the contaminated zone. (See Figure D-1.)

2. Contaminant release occurs by molecular diffusion and peeling away of successive layers from the top of the contaminated zone, i.e., the concentration within the contaminated layer is assumed to remain constant, but the thickness of the layer decreases over time. This would tend to underestimate the duration of release (t_d).

3. The concentration in air at the soil surface is zero (or negligible relative to the soil vapor concentration).

4. The model assumes that the entire contaminant mass volatilizes and that none leaks to the water table or degrades. This would tend to overestimate the emission rate.

Example Problem

Estimate the average emission rate of benzene from 10 m by 10 m area of soil contaminated at an average concentration of 5 mg/kg (5.0 E-6 g/g) and buried 0.50 m below clean soil. The thickness of the contaminated zone is 1.0 m. The soil has a bulk density of 1.8 g/cc, total porosity 0.4, air filled porosity of 0.25, and fractional organic carbon content of 0.001. The diffusion coefficient for benzene in air at 20°C is 0.088 cm^2/s, the organic carbon partition coefficient is 58.9 [(g/g)/(g/cm^3)], and the Henry's law constant is 0.228 (mg/l)/(mg/l). Assume temperature of soil is 20°C. Assume the exposure duration to be 75 yrs.

$$D_e = (0.088)\,(0.25)^{10/3} / (0.4)^2$$
$$= 5.414\text{ E-3 cm}^2/\text{s}$$

$$C_b = (5{*}10^{-6})\,(1.8 + 0.15{*}1.0)$$
$$= 9.75\text{ E-06 g/cm}^3$$

$$C_w = (5{*}10^{-6})\,(1.8 + 0.15{*}1.0)/(0.25{*}0.228 + 0.15 + 1.8{*}58.9{*}0.001)$$
$$= 3.115\text{ E-05 g/cm}^3$$

$$C_v = 3.115 * 10^{-5} * 0.228$$
$$= 7.102\text{ E-06 g/cm}^3$$

$$t_d = [(150^2 - 50^2)/(2 * 5.414\text{ E-03})]\,(9.75\text{ E-06}/7.102\text{ E-06})$$
$$= 2.536\text{ E6 s}$$

$$t_e = 75 * 365 * 24 * 3600$$
$$= 2.37\text{ E+09 s}$$

$$E(t_d) = (2 * 5.414\ E\text{-}03 * 7.102\ E\text{-}06 * 100 * 10000)/ [50 + (2 * 5.414\ E\text{-}03 * 7.102\ E\text{-}06 * 2.536\ E6/9.75E\text{-}06 + 50^2)^{0.5}]$$
$$= 3.845\ E\text{-}04\ g/s$$

Since the exposure time is larger than the total duration of release (t_d), the average emission over the exposure duration (t_e) can be estimated using

$$E' = 3.845\ E\text{-}04 * 2.536\ E6/2.37\ E{+}09$$
$$= 4.117\ E\text{-}07\ g/s$$
$$= 1.298\ E\text{-}02\ kg/yr$$

The same problem run using API DSS gave an emission rate of 1.30 E-02 kg/yr (See attached output).

References

Lyman, W.J., W.F. Reehl, and D.H. Rosenblatt. 1990. Handbook of Chemical Property Estimation Methods. American Chemical Society, Washington, D.C.

Millington, R. J., and J. P. Quirk (1961), Permeability of Porous Solids. Trans. Faraday Soc. 57:1200-1207.

Thibodeaux L. J. and Hwang S. T. 1982. Landfarming of Petroleum Wastes - Modeling the air emissions problem. Environmental Progress, Vol. 1, No. 1, Feb. 1982, pp. 42-46.

U.S. Environmental Protection Agency. 1988. Superfund Exposure Assessment Manual. EPA/640/1-88/001.

U.S. Environmental Protection Agency. 1984. Evaluation and Selecton of Models for Estimating Air Emissions from Hazardous Waste Treatment, Storage and Disposal Facilities. EPA-450/3-84-020. Office of Air Quality Planning and Standards, Research Triangle Park, NC 27711.

```
Air Model Output File
DSS Fate and Transport

Chemicals in the analysis
Benzene

Thibodeaux-Hwang volatile emissions
Box Model used for dispersion

  Thibodeaux-Hwang Model Input Parameters:
  ---------------------------------------
  Area of contaminated soil [m^2]             100.
  Depth to top of contamination [m]           .500
  Depth to bottom of contamination [m]        1.00
  Porosity [cm^3/cm^3]                        .400
  Water content [cm^3/cm^3]                   .150
  Soil bulk density [g/cm^3]                  1.80
  Fraction organic carbon [-]                 .100E-02
  Temperature of surface soil [C]             20.0

  Total Soil Concentrations Used for Volatile Emissions [mg/kg]
           Benzene                            5.00

   Box Model Input Parameters:
   --------------------------
  Box height [m]                              2.00
  Box width [m]                               10.0
  Average windspeed [m/s]                     2.00


 //////////////////////////////////////////////////
 Chemical Parameters for :Benzene
    Henrys Law               .228
    Koc                      58.9
    Diffusion in air        8.800E-02
    Vapor pressure           95.2
    Molecular weight         78.0
    Source conc. for emis.   5.00

 ==================================================
      MODEL OUTPUT FOR: Benzene

    Emissions Model:  Thibodeaux-Hwang
    Dispersion Model: Box

Air Model Output:
       Diffusion coef. adjusted for temperature       8.80E-02
       Effective diffusion coefficient cm2/s          5.41E-03
       Total conc. in soil (g/g)                      5.00E-06
       Conc. in the dissolved phase (g/cm3)           3.11E-05
       Calculated vapor concentration (g/cm3)         7.10E-06
       Saturated vapor concentration (g/cm3)          4.06E-04

    Time to depletion (yr):                           3.02E-02
    Averaging Time (yr):                             10
    Vol. Emission Rate Over Averaging Time (kg/yr):   4.87E-02
    Concentration in Air (mg/m^3):                    3.86E-05
```

APPENDIX E
FARMER'S VAPOR EMISSION MODEL

The Farmer's model, Farmer et al. (1980), can be used to estimate the volatile emissions of a chemical from soil. The model treats vapor loss/emission from soil as a diffusion controlled process that is quantified using the Fick's Law for steady state diffusion. The volatile emission rate is expressed as:

$$E = 10^2 * A * D_e * (C_v - C_a) / d \qquad \text{(E-1)}$$

where

E = steady-state emission rate of chemical (g/s)
A = area of the source (m^2)
D_e = effective diffusion coefficient of the chemical in air (cm^2/s)
C_v = vapor phase concentration for the chemical in soil (g/cm^3)
C_a = air concentration of the chemical at the soil surface (g/cm^3)
d = depth of soil cover (m)
10^2 = conversion factor m to cm (cm/m)

Generally when applying the Farmer's model, concentration in the air, C_a, is considered to be significantly less than the soil vapor concentration and often neglected. Thus, equation E-1 is often written as:

$$E = 10^2 * A * D_e * C_v / d \qquad \text{(E-2)}$$

Figure E-1 presents a schematic of the Farmer's emission model.

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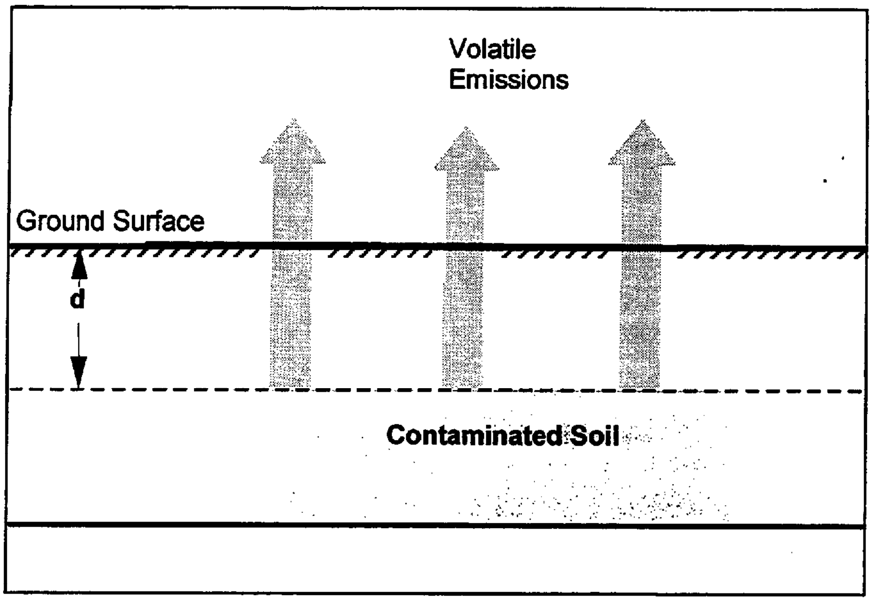

FIGURE E-1. Schematic of the Farmer's Emission Model.

The Effective Diffusion Coefficient

The effective diffusion coefficient for a chemical in soil can be computed using the following relationship presented by Millington and Quirk (1961):

$$D_e = D_{air} * \theta_a^{10/3} / \theta_t^2 \qquad \text{(E-3)}$$

where

D_{air} = the diffusion coefficient for the chemical in air (cm^2/s)

θ_t = the total porosity of soil (cm^3 of gas and liquid/cm^3 of soil)

θ_a = the air-filled porosity of soil (cm^3 of gas/cm^3 of soil)

For dry soils, the air-filled porosity is approximately equal to the total porosity and equation E-3 reduces to:

$$D_e = D_{air} * \theta_t^{4/3} \qquad \text{(E-4)}$$

The diffusion coefficient for a chemical in air depends on air temperature based on the following relationship (Lyman et al., 1990):

$$D_{oi(T2)} = D_{oi(T1)} (T_2/T_1)^{1.75} \qquad \text{(E-5)}$$

where

$D_{oi(T2)}$, $D_{oi(T1)}$ = the diffusion coefficient of chemical i at temperatures T_2 and T_1 respectively (cm^2/s)

T_2 = air (soil vapor) temperature [° K]

T_1 = air temperature at which $D_{air(T1)}$ is known [° K]

Data Required

The data required for estimating emissions using Farmer's model are presented in Table E-1.

The soil vapor concentration can either be directly measured or estimated using the following equilibrium partitioning equations:

$$C_v = H' C_w$$

$$C_w = C_T [\rho_b + \theta_w \rho_w] / [(\theta_t - \theta_w) H' + \theta_w + \rho_b K_d] \qquad \text{(E-6)}$$

where

C_v = the vapor phase concentration of the chemical in soil (g/cm^3)

H' = Henry's Law constant for chemical i [(mg/L)/(mg/L)]

C_w = the aqueous phase concentration of chemical i (g/cm^3)

C_T = total concentration of chemical i in soil (g of contaminant /g of soil)

θ_t = the total porosity of soil (cm^3/cm^3)

ρ_b = soil bulk density (g/cm^3)

ρ_w = density of water (g/cm^3)

θ_w = the volumetric water content (cm^3 of water/cm^3 of soil)

K_d = soil-water partition coefficient for chemical i [$(g/g)/(g/cm^3)$]

In equation (E-6), K_d, is estimated as

$$K_d = K_{oc} f_{oc} \qquad \text{(E-7)}$$

where

K_{oc} = Organic carbon partition coefficient [$(g/g)/(g/cm^3)$]

f_{oc} = fractional organic carbon content [-]

Table E-1. Data Requirements for the Farmer's Emissions Model.

PARAMETER DEFINITION	UNITS	*API DSS UNITS
Chemical Data		
Total soil concentration	[g/g wet soil]	[mg/kg wet soil]
Henry's Law constant	[(mg/L)/(mg/L)]	[(mg/L)/(mg/L)]
Air diffusion coefficient	[cm^2/s]	[cm^2/s]
Soil-water partition coefficient	[(g/g)/(g/cm^3)]	[(g/g)/(g/cm^3)]
Organic carbon partition coefficient	[(g/g)/(g/cm^3)]	[(g/g)/(g/cm^3)]
Fractional organic carbon content	[mg/mg]	[mg/mg]
Above three inputs OR the		
Soil vapor concentration	[g/cm^3]	**
Soils Data		
Volumetric water content	[cm^3/cm^3]	[cm^3/cm^3]
Total porosity of the soil	[cm^3/cm^3]	[cm^3/cm^3]
Soil dry bulk density	[g/cm^3]	[g/cm^3]
Air-filled porosity	[cm^3/cm^3]	[cm^3/cm^3]
Soil temperature	[°K]	[°C]
Source Data		
Depth to the top of the contaminated layer	[cm]	[m]
Source area	[cm^2]	[m^2]

* Conversions handled internally by the API DSS

** This option not available in the API DSS

The relationship between the two forms of Henry's Law constant is

$$H = H'/RT \qquad \text{(E-8)}$$

where

H' = the dimensional form of the Henry's Law constant (atm-m^3/mole)

R = the Universal gas constant [(0.0000821 atm-m^3/° K)]

T = the temperature [° K]

Assumptions Underlying the Model and Its Applicability

1. Farmer's model assumes that the source concentration (C_v) does not decrease as emissions occur. This implies that the amount of contaminant mass in soil available to volatilize is infinite.

2. The contaminant source is considered to be fixed at a depth 'd' below the surface of the soil.

3. Emissions are steady state and constant.

4. The concentration in air at the soil surface is negligible relative to the vapor concentration within the soil.

These assumptions would tend to overestimate the emission rate due to the assumption of infinite mass.

Example Problem

Estimate the steady-state emission of benzene from 10 m by 10 m area of soil contaminated at a concentration of 5 mg/kg (5.0 E-6 g/g) and buried 0.50 m below clean soil. The soil has a bulk density of 1.8 g/cm^3, total porosity of 0.4, air filled porosity of 0.25, and fractional organic carbon content of 0.001. Note the diffusion coefficient for benzene in soil at 20°C is 0.088 cm^2/s, its organic carbon partition coefficient is 58.9 [(g/g)/(g/cm^3)], and the Henry's Law constant is 0.228 (mg/l)/(mg/l). Assume temperature of soil is 20°C.

$$
\begin{aligned}
D_e &= (0.088)\,(0.25)^{10/3} / (0.4)^2 \\
&= 5.414\text{ E-3 cm}^2\text{/s}
\end{aligned}
$$

$$
\begin{aligned}
C_w &= (5{*}10^{-6})\,(1.8 + 0.15{*}1.0)/(0.25{*}0.228 + 0.15 + 1.8{*}58.9{*}0.001) \\
&= 3.115 * 10^{-5}\text{ g/cm}^3
\end{aligned}
$$

$$
\begin{aligned}
C_v &= 3.115 * 10^{-5} * 0.228 \\
&= 7.102\text{ E-6 g/cm}^3
\end{aligned}
$$

$$
\begin{aligned}
E &= 10^2\,(100)\,(5.414\text{ E-3})\,(7.102\text{ E-6})/(0.5) \\
&= 7.690\text{ E-4 g/s} \\
&= 24.25\text{ kg/yr}
\end{aligned}
$$

The same problem run using API DSS gave an emission rate of 24.3 kg/yr (See attached output).

References

Farmer, W.J., M.S. Yang, J. Letey, and W.F. Spencer. 1980. Hexachlorobenzene: Its Vapor Pressure and Vapor Phase Diffusion in Soil. Soil Sci. Soc. Am. J., Vol 44.

Lyman, W.J., W.F. Reehl, and D.H. Rosenblatt. 1990. Handbook of Chemical Property Estimation Methods. American Chemical Society, Washington, D.C.

Millington, R. J., and J. P. Quirk (1961), Permeability of Porous Solids. Trans. Faraday Soc. 57:1200-1207.

AIRMODEL.OUT
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```
Air Model Output File
DSS Fate and Transport

Chemicals in the analysis
Benzene

Farmers volatile emissions
Box Model used for dispersion

     Farmers Model Input Parameters:
  ---------------------------------------
  Area of contaminated soil [m^2]           100.
  Depth to top of contamination [m]         .500
  Porosity [cm^3/cm^3]                      .400
  Water content [cm^3/cm^3]                 .150
  Soil bulk density [g/cm^3]                1.80
  Fraction organic carbon [-]               .100E-02
  Temperature of surface soil [C]           20.0

  Total Soil Concentrations Used for Volatile Emissions [mg/kg]
           Benzene                          5.00

   Box Model Input Parameters:
   --------------------------
  Box height [m]                            2.00
  Box width [m]                             10.0
  Average windspeed [m/s]                   3.00


 //////////////////////////////////////////////////
 Chemical Parameters for :Benzene
    Henrys Law               .228
    Koc                      58.9
    Diffusion in air        8.800E-02
    Vapor pressure           95.2
    Molecular weight         78.0
    Source conc. for emis.   5.00

 ==================================================
    MODEL OUTPUT FOR: Benzene

    Emissions Model:  Farmers
    Dispersion Model: Box


Air Model Output:
       Diffusion coef. adjusted for temperature       8.80E-02
       Effective diffusion coefficient cm2/s          5.41E-03
       Total conc. in soil (g/g)                      5.00E-06
       Conc. in the dissolved phase (g/cm3)           3.11E-05
       Calculated vapor concentration (g/cm3)         7.10E-06
       Saturated vapor concentration (g/cm3)          4.06E-04
       Farmers emission rate (g/s)                    7.69E-04

    Constant Emission Rate (kg/yr):                   2.43E+01
    Concentration in Air (mg/m^3):                    1.28E-02
```

APPENDIX F
COWHERD PARTICULATE EMISSIONS MODEL

Cowherd Particulate Emissions Model

The Cowherd model estimates the emission rate of respirable soil particles, i.e., those particles with a diameter of 10 µm or less. This model, described in EPA (1985) and referred to as the Cowherd model, assumes that there is a limited reservoir of soil available for erosion, and was derived empirically from wind tunnel experiments for mining soils.

$$E_{10} = 0.83\ f\ A\ P(u^{+})(1-V)\ /\ (PE/50)^{2} \qquad \text{(F-1)}$$

where

E_{10} = annual average emission rate of particles less than 10µm in diameter (mg/hr)
f = frequency of disturbance per month (mo^{-1})
A = area of contaminated soils (m^2)
$P(u^{+})$ = $6.7(u^{+} - u^{t})$
u^{+} = fastest mile wind speed (m/s)
u^{t} = erosion threshold wind speed at height of 7 meters (m/s)
V = fraction of vegetative cover (dimensionless)
PE = Thornthwaite's Precipitation Evaporation Index (dimensionless)

For use in Equation (F-1), a disturbance is defined as an action which results in the exposure of fresh surface material and occurs whenever soil material is added to the surface or removed from the old surface. Similarly, breaking of the crust due to vehicular traffic may expose fresh erodible material and would be considered a disturbance.

The emission rate of chemicals due to wind erosion is computed as the product of the concentration of chemicals in soil and the E_{10} soil particle emission rate:

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$$E_I = E_{10}S\,(24*365)/\,1E6 \qquad (F\text{-}2)$$

where

E_{10} = annual average emission rate of particles less than 10μm in diameter (mg/hr)

E_i = annual average emission rate of chemical i (kg/yr).

S = particulate contaminant concentration (kg/kg)

24 = conversion factor (hr/day)

365 = conversion factor (days/yr)

1E6 = conversion factor (kg/mg)

Data Required

Table F-1 lists the data requirements for the Cowherd particulate emissions model. The model requires data on wind speeds, soil erosion potential, vegetative cover, and chemical concentrations.

Wind speed data required by the model include the fastest mile wind speed and the erosion threshold wind speed. The fastest mile wind speed should be obtained from the nearest climatological data station; representative values for selected stations are shown in Table F-2. The erosion threshold wind speed (u^t) is primarily related to the soil particle size distribution, and quantifies the erosion potential.

Thornthwaite's PE Index quantifies average surface soil moisture conditions. Figure F-1 can be used to estimate PE for different regions in the U.S.

The frequency of disturbance f is perhaps the most difficult parameter to estimate in the Cowherd model. A disturbance is defined as an action that results in the exposure of fresh surface material, e.g., a vehicle driving on the surface. The worst case scenario results if a disturbance is assumed to occur every day of the month
($f = 30\ mo^{-1}$).

Table F-1. Data Requirements for the Cowherd Particulate Emissions Model.

	PARAMETER DEFINITION	UNITS	API DSS UNITS
Chemical Data			
	Total concentration in soil	[mg/kg]	[mg/kg]
Soils Data			
	Erosion threshold wind speed	[m/s]	[m/s]
	Frequency of disturbance	[mo^{-1}]	[mo^{-1}]
	Fraction of area with vegetative cover	[fraction]	[fraction]
Source Data			
	Source area	[m^2]	[m^2]
Meteorologic Data			
	Fastest mile wind speed	[m/s]	[m/s]
	Thornthwaite Precipitation evaporation index	[dimensionless]	[dimensionless]

Table F-2. Fastest Mile[a] [U⁺] and Mean Wind Speed[b] [U] for Selected United States Stations.

Page 1 of 3

Station	State	[u⁺] (m/s)	[u] (m/s)	Station	State	[u⁺] (m/s)	[u] (m/s)
Birmingham	AL	20.8	3.3	Detroit	MI	21.8	4.6
Montgomery	AL	20.2	3.0	Grand Rapids	MI	21.6	4.5
Tucson	AZ	23.0	3.7	Lansing	MI	23.7	4.6
Yuma	AZ	21.8	3.5	Sault St. Marie	MI	21.6	4.3
Fort Smith	AR	20.8	3.4	Duluth	MN	22.8	5.1
Little Rock	AR	20.9	3.6	Minneapolis	MN	22.0	4.7
Fresno	CA	15.4	2.8	Jackson	MS	20.5	3.4
Red Bluff	CA	23.3	3.9	Columbia	MO	22.4	4.4
Sacramento	CA	20.6	3.7	Kansas City	MO	22.6	4.6
San Diego	CA	15.4	3.0	St. Louis	MO	21.2	4.2
Denver	CO	22.0	4.1	Springfield	MO	22.4	5.0
Grand Junction	CO	23.6	3.6	Billings	MT	26.6	5.1
Pueblo	CO	28.1	3.9	Great Falls	MT	26.4	5.9
Hartford	CT	20.2	4.0	Havre	MT	25.9	4.5
Washington	DC	21.6	3.4	Helena	MT	24.7	3.5
Jacksonville	FL	21.7	3.8	Missoula	MT	21.6	2.7
Tampa	FL	22.2	3.9	North Platte	NE	27.7	4.6
Atlanta	GA	21.2	4.1	Omaha	NE	24.6	4.8
Macon	GA	20.1	3.5	Valentine	NE	27.1	4.8
Savannah	GA	21.3	3.6	Ely	NV	23.6	4.7
Boise	ID	21.4	4.0	Las Vegas	NV	24.4	4.0
Pocatello	ID	23.8	4.6	Reno	NV	25.2	2.9
Chicago	IL	21.0	4.6	Winnemucca	NV	22.4	3.5

Table F-2. Fastest Mile[a] [U^+] and Mean Wind Speed[b] [U] for Selected United States Stations.

Page 2 of 3

Station	State	[u^+] (m/s)	[u] (m/s)	Station	State	[u^+] (m/s)	[u] (m/s)
Moline	IL	24.5	4.4	Concord	NH	19.2	3.0
Peoria	IL	23.2	4.6	Albuquerque	NM	25.6	4.0
Springfield	IL	24.2	5.1	Roswell	NM	26.0	4.1
Evansville	IN	20.9	3.7	Albany	NY	21.4	4.0
Fort Wayne	IN	23.7	4.6	Binghampton	NY	22.0	4.6
Indianapolis	IN	24.8	4.3	Buffalo	NY	24.1	5.5
Burlington	IA	25.0	4.6	New York	NY	22.5	5.5
Des Moines	IA	25.8	5.0	Rochestor	NY	23.9	4.3
Sioux City	IA	25.9	4.9	Syracuse	NY	22.5	4.4
Concordia	KS	25.7	5.4	Cape Hatteros	NC	25.9	5.1
Dodge City	KS	27.1	6.3	Charlotte	NC	20.0	3.4
Topeka	KS	24.4	4.6	Greensboro	NC	18.9	3.4
Wichita	KS	26.0	5.6	Wilmington	NC	22.3	4.0
Louisville	KY	22.0	3.8	Bismarck	ND	26.1	4.7
Shreveport	LA	19.9	3.9	Fargo	ND	26.6	5.7
Portland	ME	21.7	3.9	Cleveland	OH	23.6	4.8
Baltimore	MD	25.0	4.2	Columbus	OH	22.1	3.9
Boston	MA	25.2	5.6	Dayton	OH	24.0	4.6
Toledo	OH	22.7	4.2	Dallas	TX	21.9	4.9
Oklahoma City	OK	24.1	5.7	El Paso	TX	24.8	4.2
Tulsa	OK	21.4	4.7	Port Arthur	TX	23.7	4.5
Portland	OR	23.5	3.5	San Antonio	TX	21.0	4.2
Harrisburg	PA	20.4	3.4	Salt Lake City	UT	22.6	3.9
Philadelphia	PA	22.1	4.3	Burlington	VT	20.4	3.9

Table F-2. Fastest Mile[a] [U⁺] and Mean Wind Speed[b] [U] for Selected United States Stations.

Page 3 of 3

Station	State	[u⁺] (m/s)	[u] (m/s)	Station	State	[u⁺] (m/s)	[u] (m/s)
Pittsburgh	PA	21.6	4.2	Lynchburg	VA	18.3	3.5
Scranton	PA	19.9	3.8	Norfolk	VA	21.8	4.7
Huron	SD	27.4	5.3	Richmond	VA	18.9	3.4
Rapid City	SD	27.3	5.0	Quillayute	WA	16.3	3.0
Chattanooga	TN	21.4	2.8	Seattle	WA	18.7	4.1
Knoxville	TN	21.8	3.3	Spokane	WA	21.4	3.9
Memphis	TN	20.3	4.1	Green Bay	WI	25.3	4.6
Nashville	TN	20.9	3.6	Madison	WI	24.9	4.4
Abilene	TX	24.4	5.4	Milwaukee	WI	24.0	5.3
Amarillo	TX	27.3	6.1	Cheyenne	WY	27.0	5.9
Austin	TX	20.2	4.2	Lander	WY	27.4	3.1
Brownsville	TX	19.5	5.3	Sheridan	WY	27.5	3.6
Corpus Christi	TX	24.4	5.4	Elkins	WV	22.8	2.8

[a] Data taken from Extreme Wind Speeds at 129 Stations in the Contiguous United States. Simiu, E., Filliben, J.J. and M.J. Changery. NBS Building Science Series 118. U.S. Department of Commerce, National Bureau of Standards, 1979.

[b] Data taken from Local Climatological Data - Annual Summaries for 1977. U.S. Department of Commerce, National Oceanic and Atmospheric Administration/Environmental Data Service/National Climatic Data Center.

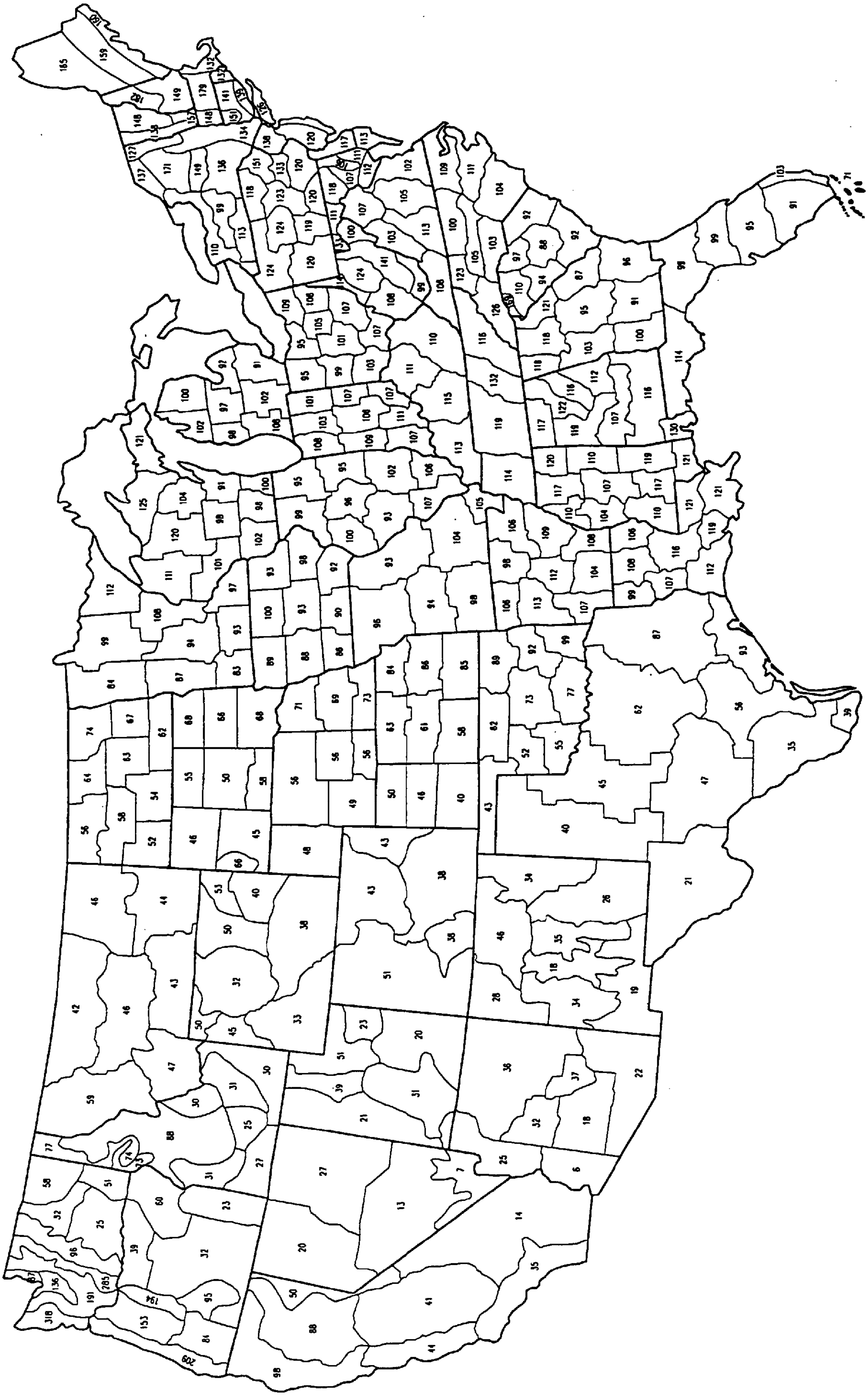

Figure F-1. Map of P-E Index for State Climatic Division

Location: HOUSTON, TX. CAD 4, File name: C:\DWG\93T10BC\93T10B02.DWG Last edited: 07/28/93 @ 14:23

Assumptions Underlying the Model and Its Applicability

1. Cowherd's model can be used for estimating respirable particulate emissions from surfaces due to wind erosion.
2. The model assumes a "limited reservoir" surface whose surface potential is restored after each disturbance.
3. The model was developed based on field measurements using a portable wind tunnel.
4. The model uses the Thornwaite's precipitation-evaporation (P-E) index as a useful indicator of average surface soil moisture conditions.

Example Problem

Estimate the particulate emission rate for benzene at a site 10 m by 10 m with a surface concentration of 5 mg/kg. Assume that the erosion threshold wind speed is 1 m/s, 10% of the area has a vegetative cover and frequency of disturbance is about 50% (15 days per month). Further assume the fastest mile wind speed is 3 m/s and the Thornwaite's precipitation evaporation index is 56.

$$\begin{aligned} E_{10} &= 0.83\ (15)\ (100)\ (6.7)\ [3-1]\ (1-0.1)/(56/50)^2 \\ &= 1.196\ \text{E4 mg/hr} \\ &= 104.769\ \text{kg/yr} \end{aligned}$$

$$\begin{aligned} E_i &= 104.769 * 5 \\ &= 523.84\ \text{kg/yr} \end{aligned}$$

The example problem was run using the API DSS and yielded an emission rate of 5.24 E2 kg/yr (See attached output).

REFERENCES

U. S. Environmental Protection Agency (1985). Rapid Assessment of Exposure to Particulate Emissions from Surface Contaminated Sites. Office of Health and Environmental Assessment. EPA/600/8-85/002.

AIRMODEL.OUT
Page 1 of 1

```
Air Model Output File
DSS Fate and Transport

Chemicals in the analysis
Benzene

Either user specified volatile emissions or    no volatile emissions entered
Particulate emissions
Box Model used for dispersion


  Particulate Emission Input Parameters:
  -----------------------------------------
  Frequency of disturbance [# days/month]     15.0
  Fastest mile windspeed [m/s]                3.00
  Erosion windspeed       [m/s]               1.00
  Fraction of vegetation cover [-]            .100
  PE Index [-]                                56.0
  Area of contaminated soil [m^2]             100.
  Total Soil Concentrations Used for Particulate Emissions [mg/kg]
           Benzene                            5.00


   Box Model Input Parameters:
   --------------------------
  Box height [m]                              2.00
  Box width [m]                               10.0
  Average windspeed [m/s]                     2.00


 //////////////////////////////////////////////////
 Chemical Parameters for :Benzene
    Henrys Law              .228
    Koc                     58.9
    Diffusion in air       8.800E-02
    Vapor pressure          95.2
    Molecular weight        78.0
    Source conc. for dust   5.00

 ==================================================

    MODEL OUTPUT FOR: Benzene

    Emissions Model:  User specified
    Dispersion Model: Box

Air Model Output:
       Emission rate of PM10 dust (mg/hr)              1.20E+04

    Constant Emission Rate (kg/yr):                    0.00E+00
    Dust Emission Rate (kg/yr):                        5.24E+02
    Concentration in Air (mg/m^3):                     4.16E-01
```

APPENDIX G
THE BOX MODEL

The Box Model

The box model can be used to estimate concentrations in the air based on the assumption that the steady-state contaminant emissions completely mix with the air inside the 'box'. As shown in Figure G-1, the box is bounded at the top by the mixing zone and is ventilated by a steady flow of wind across the box. The average air concentration in the box is computed using the following mass balance relationship:

$$C_{air} = 10^3 E / (u * W * H) \qquad \text{(G-1)}$$

where

C_{air} = concentration of the chemical in air (mg/m^3)
E = average volatile chemical emission rate for the exposure period (g/s)
u = mean annual wind speed (m/s)
W = width of the box perpendicular to the predominant wind direction (m)
H = height of the mixing zone (m)
10^3 = conversion factor g to mg

Note Equation (G-1) may be implemented using any consistent set of units.

Data Required

Data required for the box model are shown in Table G-1. For most risk assessment purposes the height of the box is conservatively assumed to be about 2 m, i.e., approximate height of an adult's breathing zone. In the API DSS the emission rate can be estimated using an emissions model or specified by the user.

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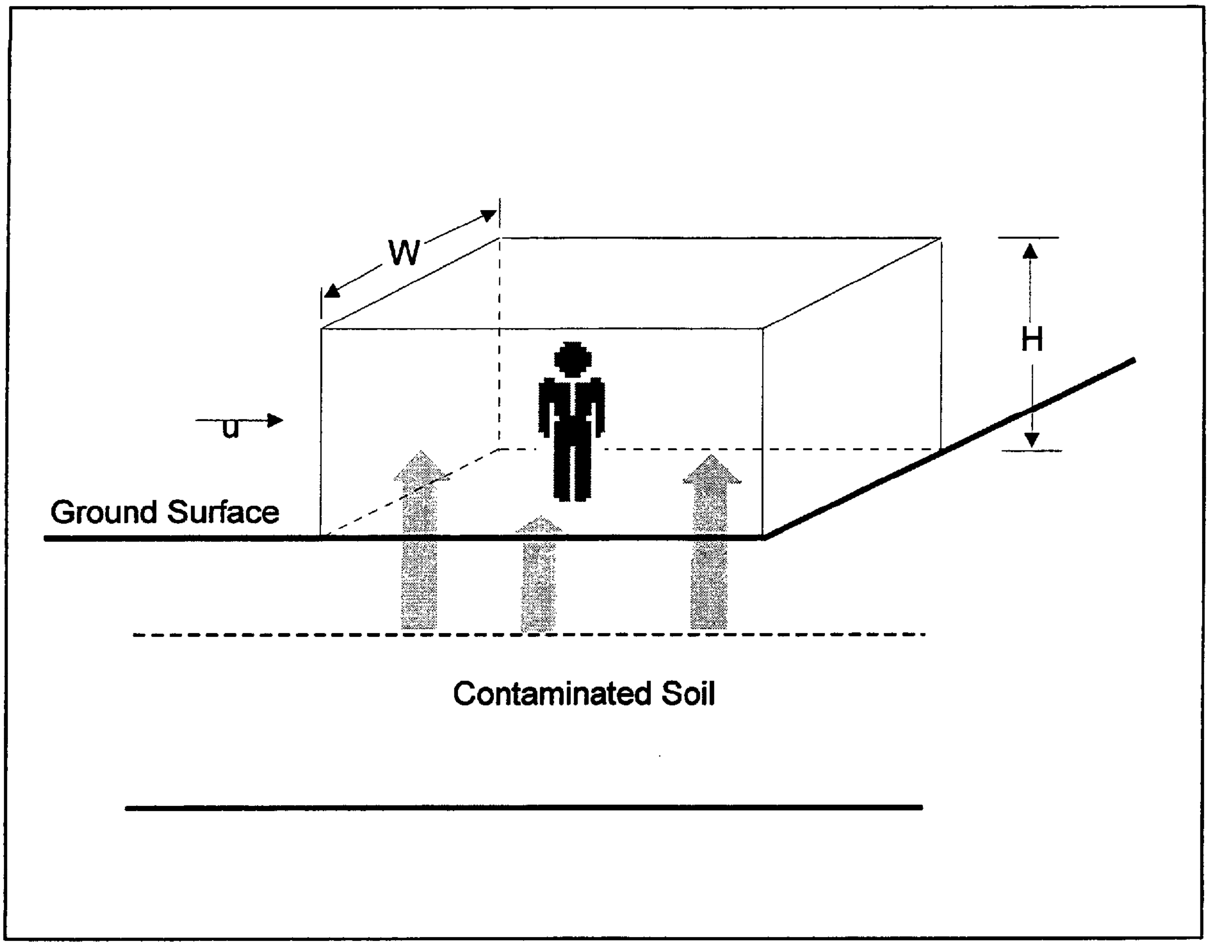


Figure G-1. Schematic of the Box Model.

Table 5-8. Data Requirements for the Box Model.

PARAMETER DEFINITION	UNITS
Emission rate	[g/s]
Mean annual wind speed	[m/s]
Width of site perpendicular to predominant wind direction	[m]
Mixing height	[m]

Assumptions Underlying the Model and Its Applicability

The box model can only be used to estimate the average concentration within a volume of air, and does not account for the decrease in concentration with distance or height from the source. Box model does not include any spatial or temporal variations of concentration.

The model is therefore not appropriate for receptors located at large distances from the source of air emissions. Box models are most applicable for evaluating exposure to receptors living and/or working in the contaminated area and typically result in conservative (higher concentrations) estimates of exposure.

Example Problem

Use the emissions estimated using the example problem in Farmer's model description to estimate air concentrations on-site assuming a wind speed of 3 m/s and a box height of 2 m.

$$\begin{aligned} C_{air} &= (10^3)\,(7.69\text{ E-4})/[(3)\,(10)\,(2)] \\ &= 1.92\text{ E-3 mg/m}^3 \end{aligned}$$

The example problem was run using the API DSS and yielded an air concentration of 1.28 E-2 mg/m^3 (See attached output).

```
Air Model Output File
DSS Fate and Transport

Chemicals in the analysis
Benzene

Farmers volatile emissions
Box Model used for dispersion

     Farmers Model Input Parameters:
  ----------------------------------------
  Area of contaminated soil [m^2]            100.
  Depth to top of contamination [m]          .500
  Porosity [cm^3/cm^3]                       .400
  Water content [cm^3/cm^3]                  .150
  Soil bulk density [g/cm^3]                 1.80
  Fraction organic carbon [-]                .100E-02
  Temperature of surface soil [C]            20.0

  Total Soil Concentrations Used for Volatile Emissions [mg/kg]
           Benzene                           5.00

   Box Model Input Parameters:
   --------------------------
  Box height [m]                             2.00
  Box width [m]                              10.0
  Average windspeed [m/s]                    3.00


//////////////////////////////////////////////////
Chemical Parameters for :Benzene
   Henrys Law              .228
   Koc                     58.9
   Diffusion in air      8.800E-02
   Vapor pressure          95.2
   Molecular weight        78.0
   Source conc. for emis.  5.00

==================================================
   MODEL OUTPUT FOR: Benzene

   Emissions Model:  Farmers
   Dispersion Model: Box


Air Model Output:
      Diffusion coef. adjusted for temperature       8.80E-02
      Effective diffusion coefficient cm2/s          5.41E-03
      Total conc. in soil (g/g)                      5.00E-06
      Conc. in the dissolved phase (g/cm3)           3.11E-05
      Calculated vapor concentration (g/cm3)         7.10E-06
      Saturated vapor concentration (g/cm3)          4.06E-04
      Farmers emission rate (g/s)                    7.69E-04

   Constant Emission Rate (kg/yr):                   2.43E+01
   Concentration in Air (mg/m^3):                    1.28E-02
```

APPENDIX H
GAUSSIAN DISPERSION MODEL

The Gaussian Dispersion Model

Gaussian Dispersion Models are commonly used to estimate the steady-state concentration of chemicals downwind from a source. For atmospheric dispersion modeling, meteorological input consists of wind speed, atmospheric stability that represents the mixing characteristics of the atmosphere, and wind direction. Generally the wind speed is divided into six different classes, the atmospheric stability is classified into one of six different classes, and the wind direction separated into sixteen different wind sectors. This results in a total of (6*6*16) or 576 different combinations of atmospheric conditions. Atmospheric stability represents the effects of thermal (solar radiation) and mechanical (wind) turbulence on the mixing characteristics of the atmosphere. At any receptor location, the long term average concentration is computed by estimating the receptor point concentration for each atmospheric condition and then frequency-weighting these concentrations. This approach requires a complete specification of the joint frequency distribution of atmospheric stability, wind speed and wind direction, termed as the stability array (STAR) data. Because of the large data requirements for the approach discussed above, a simplified screening-level approach was incorporated into the API DSS.

The DSS utilizes the sector-averaged form of the Gaussian dispersion model, but assumes the wind speed is constant in the direction of the receptor for a specified fraction of the year. The steady-state concentration at the receptor is computed for each of the six stability conditions; the annual average concentration is then derived by frequency-weighting the concentrations for each stability class.

The sector-averaged form of the Gaussian model is derived by averaging the concentration profile across a single 22.5 degree wind direction sector. For each stability class, the steady-state ground level concentration is computed by the following equation, Hanna et al. (1982):

$$C_j = (10^3)*(16/2\pi x)*(2)*Q*D*P_j/[u*\sigma_j*(2\pi)^{0.5}] \qquad \text{(H-1)}$$

where

C_j = steady-state concentration at distance x for stability class j (mg/m^3)
x = distance from the source to the receptor (m)
Q = emission rate (g/s)
P_i = fraction of the year wind blows in the direction of the receptor from the source (dimensionless)
u = mean annual wind speed at source release height (m/s)
σ_j = vertical dispersivity for stability class j (m)
10^3 = conversion factor from g to mg
D = factor that accounts for any atmospheric decay (dimensionless)

Vertical dispersion coefficients are computed using the empirical Pasquill-Gifford curves for each stability class as shown in Figure H-1. Their values depend on the distance to the receptor and the atmospheric stability class and are further discussed in the data requirements section.

The factor D accounts for the overall first-order decay of the contaminant as it travels from the source to the receptor:

$$D = \exp(-kx/u) \tag{H-2}$$

where

k = lumped first order decay rate constant (s^{-1})

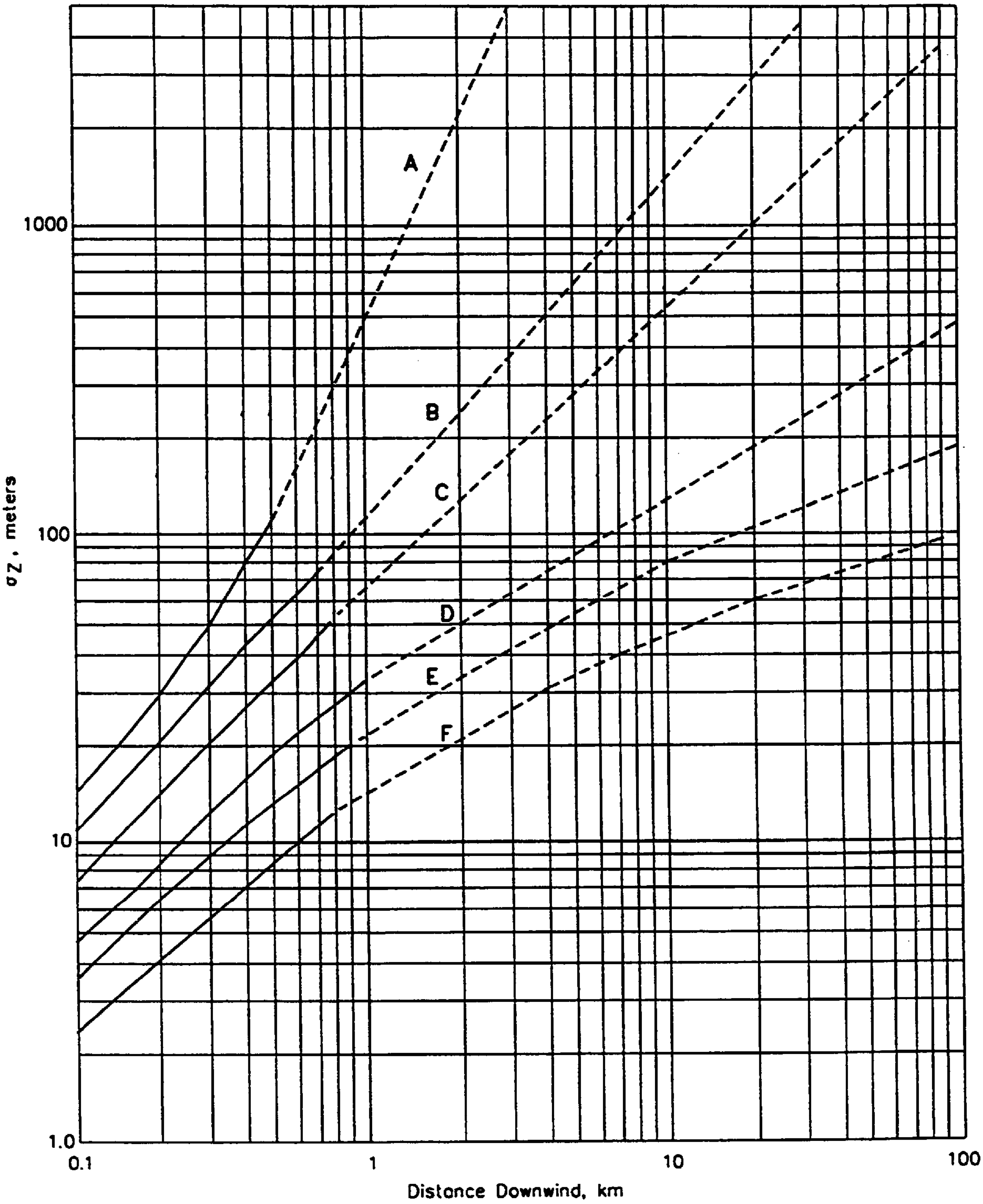
Note that decay in the atmosphere is considered a lumped process that includes all processes that reduce the atmospheric concentration. These processes include photodegradation, downwash, oxidation, etc.

Equation (H-1) computes the steady-state concentration for each stability class. The annual average concentration is then estimated by frequency weighting:

$$C_{avg} = f_j C_j \tag{H-3}$$

where

C_{avg} = annual average concentration (mg/m^3)
f_j = fraction of the year represented by stability class j (dimensionless)



Curves designated A through F represent dispersion coefficient functions for atmospheric stability classes A through F.

Figure H–1. Vertical Dispersion Coefficient as a Function of Downwind Distance from the Source

The Gaussian model assumes that emissions emanate from a point source. This is generally a conservative assumption. To estimate emissions from area sources, a virtual source approximation may be used. This type of source is not implemented in the air dispersion model included in the DSS.

Data Required

Data requirements for the Gaussian dispersion model are listed in Table H-1. The emission rate used by the model is the average emission rate for the exposure period and is estimated using any of the emission models or can be explicitly specified by the user. As mentioned previously, data on mean annual wind speeds are available at climatological stations throughout the country.

Table H-1. Data Requirements for the Gaussian Dispersion Model.

PARAMETER DEFINITION	UNITS
Chemical Data	
Emission rate	[g/s]
First order decay rate in air	[s^{-1}]
Source Data	
Distance from source to receptor	[m]
Width of area source	[m]
Length of area source	[m]
Meteorologic Data	
Mean annual wind speed	[m/s]
Mixing height	[m]
Frequency of occurrence for each stability class	[fraction]
Fraction of the time wind blows in the direction of the receptor	[fraction]

Table H-2 lists the Pasquill-Gifford stability classification scheme used in the model. Frequency data for each stability class can be derived from Stability Array (STAR) files available for airports and other climatological stations. The value of the vertical dispersivity depends on the atmospheric stability class and distance between the source and the receptor as shown in Figure H-1. It is estimated by the DSS using the following regression relationship:

$$\sigma_j \quad = \quad a\,(x)^b + c \qquad \text{(H-4)}$$

where a, b and c are constants associated with the six meteorological classes. The specific values are listed in Table H-3.

Table H-2. Pasquill-Gifford Atmospheric Stability Categories.

CATEGORY	DESCRIPTION
A	Extremely unstable
B	Moderately unstable
C	Slightly unstable
D	Neutral
E	Slightly stable
F	Moderately stable

Table H-3. Constants for Pasquill-Gifford Curves for Each Stability Class.

X 1000 m						
Stability =	A	B	C	D	E	F
a	0.001	0.0476	0.119	2.61	52.6	33.60
b	1.890	1.1100	0.915	0.45	0.15	0.14
c	9.600	2.0000	0.000	-25.50	-126	-75.00

100 m X 1000 m						
Stability =	A	B	C	D	E	F
a	0.001	0.0476	0.119	0.187	0.1345	0.362
b	1.890	1.1100	0.915	0.755	0.745	0.55
c	9.600	2.0000	0.000	-1.4	-1.1	-2.7

X 1000 m						
Stability =	A	B	C	D	E	F
a	0.1742	0.1426	0.1233	0.0804	0.06	0.0434
b	0.936	0.922	0.905	0.881	0.854	0.814
c	0	0	0	0	0	0

Assumptions Underlying the Model and Its Applicability

The model estimates the steady-state sector averaged concentration of airborne chemicals downwind of the source, and is based on the following assumptions:

1. The chemical emissions at the source are steady and continuous.
2. The distribution of chemicals within the plume is Gaussian in the vertical and crosswind direction.
3. Longitudinal (downwind) dispersion is negligible.
4. Wind speed is steady in a constant direction; short-term fluctuations in wind are not accounted for.

5. Atmospheric dispersion can be characterized by six stability classes (A,B,C,D,E, and F) and is used to estimate the dispersivity values.
6. No deposition of chemicals or particles occurs during transport.
7. The model assumes a flat terrain.
8. The model assumes a point source of emission, i.e., a relatively small source area. Thus, the Gaussian model is more appropriate when the distance to the receptor is large relative to the size of the source.

Example Problem

Estimate the annual average concentration at a receptor located 200 m downwind from the source. The emission rate is based on the example presented in the write-up for the Farmer's model. Assume that for 30% of the time during any year wind blows towards the receptor at an annual average speed of 2 m/s. The frequencies for each stability class are given below:

Stability Class	Frequency
A	0.2
B	0.4
C	0.1
D	0.1
E	0.1
F	0.1

$$C_j = (10^3)[16/(2*\pi*200)](2)(7.69\ E\text{-}4)(1)(0.3)/[2*\sigma_j*(2\pi)^{0.5}]$$
$$= 1.172\ E\text{-}3/\sigma_j$$

The values of the vertical dispersivity coefficient for the six stability classes are estimated as 30, 20, 13.5, 8.8, 6.2, and 4 from Figure H-1.

$$C = 1.172\ E\text{-}3\ [(0.2/30)+(0.4/20)+(0.1/13.5)+(0.1/8.8)+(0.1/6.2)+(0.1/4)]$$
$$= 1.02\ E\text{-}4\ mg/m^3$$

This value matches the API DSS estimated value (See attached output).

References

Hanna, S.R., G.A. Briggs and R.P. Hosker, Jr. 1982. Handbook on Atmospheric Diffusion. Report Published by Technical Information Center. U.S. Department of Energy. DOE/TIC-11223 (DE82002045).

U.S. Environmental Protection Agency. 1988. Superfund Exposure Assessment Manual. Page 44 EPA/640/1-88/001.

```
Air Model Output File
DSS Fate and Transport

Chemicals in the analysis
Benzene

Farmers volatile emissions
Gaussian Model used for dispersion


     Farmers Model Input Parameters:
  ----------------------------------------
  Area of contaminated soil [m^2]           100.
  Depth to top of contamination [m]         .500
  Porosity [cm^3/cm^3]                      .400
  Water content [cm^3/cm^3]                 .150
  Soil bulk density [g/cm^3]                1.80
  Fraction organic carbon [-]               .100E-02
  Temperature of surface soil [C]           20.0

  Total Soil Concentrations Used for Volatile Emissions [mg/kg]
           Benzene                          5.00


   Gaussian Dispersion Model Input Parameters:
   ------------------------------------------
  Average windspeed [m/s]                   2.00
  Fraction of time wind blows toward
      the receptor [m/s]                    .300
  Distance to the receptor [m]              200.
  Area for emissions [m^2]                  100.
   Fraction of time spent in each stability class
                       Class 1              .200
                       Class 2              .400
                       Class 3              .100
                       Class 4              .100
                       Class 5              .100
                       Class 6              .100
   Chemical-Specific Decay Rate (1/sec)
           Benzene                          .000


   ///////////////////////////////////////////////////
 Chemical Parameters for :Benzene
    Henrys Law              .228
    Koc                     58.9
    Diffusion in air       8.800E-02
    Vapor pressure          95.2
    Molecular weight        78.0
    Source conc. for emis.  5.00
    Decay coefficient       .000
```

```
==================================================

     MODEL OUTPUT FOR: Benzene

     Emissions Model:  Farmers
     Dispersion Model: Gaussian


 Air Model Output:
        Diffusion coef. adjusted for temperature        8.80E-02
        Effective diffusion coefficient cm2/s           5.41E-03
        Total conc. in soil (g/g)                       5.00E-06
        Conc. in the dissolved phase (g/cm3)            3.11E-05
        Calculated vapor concentration (g/cm3)          7.10E-06
        Saturated vapor concentration (g/cm3)           4.06E-04
        Farmers emission rate (g/s)                     7.69E-04

     Constant Emission Rate (kg/yr):                    2.43E+01
     Concentration in Air (mg/m^3):                     1.02E-04
```

APPENDIX I
ESTIMATION OF CONCENTRATIONS IN SHOWER AIR

Concentrations in the Shower Air

Concentrations in the shower air are estimated assuming that the air in the bathroom or the shower stall (as specified by the user) is fully mixed. Thus, the concentration in the air can be expressed as

$$C_{sh} = M_{sh}/V_{sh} \qquad \text{(I-1)}$$

where

C_{sh} = air concentration in the shower stall or the bathroom (mg/m^3)
M_{sh} = mass of contaminants that volatilize in the shower stall/bathroom from water (mg)
V_{sh} = volume of air in the shower stall/bathroom (m^3)

V_{sh} can be estimated as:

$$V_{sh} = L_{sh} * W_{sh} * H_{sh} \qquad \text{(I-2)}$$

where

L_{sh} = the length of the shower stall/bathroom (m)
W_{sh} = the width of the shower stall/bathroom (m)
H_{sh} = the height of the shower stall/bathroom (m)

The release of contaminant mass from the water used for showering depends on a number of factors that include, but are not limited to, the amount of water consumed, contaminant concentration in the water at the shower head, the volatility of the chemical, and the size of the droplets. The overall effect of these factors can be lumped together and expressed as the efficiency of volatilization that represents the fraction of the total contaminant mass in the water that is released to the air. Thus, the mass of contaminant released can be expressed as:

$$M_{sh} = f_v * Q * t_{sh} * C_w \qquad \text{(I-3)}$$

where

f_v = the fraction of contaminant volatilized (mg/mg)

Q = the volumetric flow rate of water (l/min)
t_{sh} = the duration for which water is flowing (min)
C_w = the concentration of contaminant in water (mg/l)

The API DSS allows the user either to specify the efficiency of contaminant release or to estimate its value using a model. Note, a very conservative estimate of f_v would be unity. This would imply that all the contaminant in the water volatilizes in the bathroom air. A number of models have been proposed to estimate the efficiency of release. The model presented by Foster and Chrostowski (1986) is included in the DSS and is described below.

The Foster and Chrostowski model treats volatilization as a first order process and estimates f_v as:

$$f_v = 1 - \exp\left(\frac{-K_L' \, t}{(d/6)\,3600}\right) \tag{I-4}$$

where

f_v = the efficiency of contaminant release [dimensionless]
K'_L = the overall mass transfer coefficient at the temperature of the shower water (cm/hr)
t = the shower droplet drop time (sec)
d = the representative diameter of the shower droplet (cm)
3600 = conversion factor hr to sec (sec/hr)

In Equation I-4, (6/d) is the specific interfacial area for a hypothetical water droplet of diameter d. The overall mass transfer coefficient is estimated using the two-film boundary theory:

$$K_L = \left(\frac{1}{k_l} + \frac{1}{H k_g}\right)^{-1} \tag{I-5}$$

where

K_L = the overall mass transfer coefficient at a known calibration temperature, T_c, (cm/hr)
k_l = liquid-phase mass transfer coefficient (cm/hr)
k_g = gas-phase mass transfer coefficient (cm/hr)
H = Henry's Law constant [(mg/L)/(mg/L)]

Typical values of the liquid and gas phase mass transfer coefficients measured for carbon dioxide (CO_2) in water (H_2O) are 20 cm/hr and 3,000 cm/hr, respectively.

The following empirical/approximate relations are often used to estimate volatile contaminant-specific mass transfer coefficients:

$$k_g = k_{g(H_2O)} \left(\frac{18}{MW_{voc}} \right)^{0.5} \tag{I-6}$$

$$k_g = k_{g(CO_s)} \left(\frac{44}{MW_{voc}} \right)^{0.5} \tag{I-7}$$

where 18 and 44 are the molecular weights for water and carbon dioxide respectively, and MW_{voc} is the molecular weight of the contaminant. Also refer to Liss and Slater (1974) for additional information on mass transfer coefficients.

Finally, the value of the overall mass transfer coefficient can be adjusted to the temperature of the shower water:

$$K_L' = K_L \left(\frac{T_{sh} \mu_c}{T_c \mu_{sh}} \right)^{0.5} \tag{I-8}$$

where

T_c = the calibration water temperature for K_L, i.e., the temperature at which $k_{g(H_2O)}$ and $k_{g(CO_2)}$ have been estimated (°K)

T_{sh} = temperature of the shower water (°K)

μ_c = viscosity of water at T_c (g/m-s)

μ_{sh} = viscosity of water at T_{sh} (g/m-s)

The following relationship is used to estimate the viscosity of water as a function of temperature. It is based on data presented in the CRC Handbook (CRC Press 1973). Note that in all cases the temperature (T) is expressed in degrees Centigrade.

If T < 20°C

$$\mu_w \text{ [g/m-s]} = 100 * 10^y \tag{I-9}$$

where

$$y = \frac{1301}{998.33 + 8.1855\,(T-20) + 0.00585\,(T-20)^2} - 3.30233 \tag{I-10}$$

If T > 20°C

$$\mu_w = 1.002 * 10^y \qquad (I\text{-}11)$$

where

$$y = (-1.3272 * (T-20) - 0.001053 * (T-20)^2)/(T+105) \qquad (I\text{-}12)$$

Data Required

Table I-1 shows the data required by the shower model. If the value of the fraction that volatilizes (f_v) is zero, the API DSS uses Foster-Chrostowski's model to estimate the volatile emissions. If f_v is non-zero, Foster and Chrostowski's model is not used and hence the values of parameters shown in Table I-1 (except for the value of f_v and the size of the shower stall) are not used.

Assumptions Underlying the Model and Its Applicability

1. The shower model assumes no exchange of air with the outside or the remaining portion of the house. This assumption would tend to over estimate the shower-air concentrations.

2. The model assumes complete and instantaneous mixing of the volatile emissions with the air in the shower stall.

3. For a very conservative screening level analysis, the fraction of contaminant mass in the water used for showering (f_v) would be set equal to unity.

Table I-1. Data Required to Estimate Concentrations in Shower Air Within the DSS.

PARAMETER DEFINITION	UNITS	API DSS UNITS
Chemical Data		
Liquid Phase Gas Transfer Coeff. for CO_2	[cm/hr]	[cm/hr]
Gas Phase Mass Transfer Coeff. for Water	[cm/hr]	[cm/hr]
Henry's Law Constant	[(mg/L)/(mg/L)]	[(mg/L)/(mg/L)]
Molecular Weight of the Contaminant	[g/mole]	[g/mole]
Viscosity of Water	[g/m-s]	[g/m-s]
Concentration of the Contaminant in Water	[mg/L]	[mg/L]
Shower/Source Data		
Volume of Shower Stall/Bathroom	[m^3]	[m^3]
Volumetric Flow Rate of Water	[L/min]	[L/min]
Duration for which Water is Flowing	[min]	[hr]
Shower Droplet Drop Time	[s]	[s]
Representative Diameter of the Shower Droplet	[cm]	[cm]
Fraction of Contaminant Released	[mg/mg]	[mg/mg]*
Temperature of Shower Water	[°K]	[°C]

* If a non-zero value of the fraction of contaminant released (f_v) is entered, the DSS does not use the Foster-Chrostowski's model to estimate the concentration in the shower air.

Example Problem

Estimate the average concentration of benzene in a shower stall/bathroom of volume 3 m^3 using (i) Foster and Chrostowski's model and (ii) assuming the fraction of contaminant volatilized to be 0.7. Assume water flows in the shower for 12 minutes at a rate of 10 liters per minute. The droplet diameter is 0.1 cm and the droplet drop time is 2 sec. The liquid phase mass transfer coefficient for benzene is 20 cm/hr and the gaseous mass transfer coefficient is 3000 cm/hr. Assume the

2 sec. The liquid phase mass transfer coefficient for benzene is 20 cm/hr and the gaseous mass transfer coefficient is 3000 cm/hr. Assume the temperature of the shower water to be 30 °C. The concentration of benzene in the shower water is 0.001 mg/l.

(i) Solution using Foster and Chrostowski's model

Calculate the overall mass transfer coefficient

k_l = $20 * (44/78)^{1/2}$
= 15.02 cm/hr

k_g = $3000 * (18/78)^{1/2}$
= 1441.16 cm/hr

K_L = 1./ (1/15.02 + 1/(.228 * 1441.16))
= 14.36 cm/hr

Adjust the overall mass transfer coefficient for temperature effects (first estimate viscosity of water)

y = -(1.3272 * (T-20) - 0.001053 * (T - 20) ** 2) / (T+ 105)
= -9.75 E-2

μ_{shower} = $1.002 * (10)^y$
= 0.7989 g/m-sec
μ_w(20 °C) = 1.002 g/m-sec

K'_L = $14.42 *[(303 * 1.002) / (293 * 0.7989)]^{1/2}$
= 16.35 cm/hr

Calculate fraction volatilized

f_v = 1 - exp((- 16.35 * 2)/(0.1 * 600))
= 0.42

Calculate the concentration of benzene in the shower air

$$C_{sh} = 0.42 * 10 * 12 * 0.001/3$$
$$= 0.0168 \text{ mg/m}^3$$

(ii) Solution assuming the efficiency of contaminant release to be 0.7

$$C_{sh} = 0.7 * 10 * 12 * 0.001/3$$
$$= 0.028 \text{ mg/m}^3$$

The shower concentrations estimated using the API DSS were 0.0168 mg/m^3 and 0.028 mg/m^3 for cases (i) and (ii), respectively (See attached output).

References

David R. Lide. 1990-1991. CRC Handbook of Chemistry and Physics. 71st Edition, pp. 6-8.

Foster, S.A. and P. C. Chrostowski. 1986. Integrated Household Exposure Model for Use of Tap Water Contaminated with Volatile Organic Chemicals. 79th Annual Meeting of the Air Pollution Control Association, Minneapolis, MN.

Liss, P.S. and P.G. Slater. 1976. Flux of Gases Across the Air-Sea Interface. Nature, Volume 247, pp. 181-186, Jun 25, 1976.

McKone, T.E. 1987. Human Exposure to Volatile Organic Compounds in Household Tap Water: The Indoor Inhalation Pathway. Environmental Science and Technology. Vol. 21. Page 1194.

INTAKE.OUT (using shower model)
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```
Chemicals in the analysis:
Benzene

Chemical Intake Analysis

Deterministic Run

PARAMETER NAME                    UNITS      VALUE
-------------------------------------------------
Body Weight                          kg      7.00E+01
Life Time                            yr      7.00E+01
Exposure Duration Groundwater        yr      9.00E+00
Exposure Frequency Shower         dy/yr      3.50E+02
Shower Duration                      hr      2.00E-01
Inhalation Rate in Shower        m^3/hr      6.30E-01
Fraction Volatilized                (-)      0.00E+00
Shower Flow Rate                   l/hr      1.00E+01
Volume of Bathroom                  m^3      3.00E+00
Temperature of Shower water           C      3.00E+01
Droplet Diameter                     mm      1.00E-01
Droplet Droptime                      s      2.00E+00
Mass Transfer CO2                 cm/hr      2.00E+01
Mass Transfer H2O                 cm/hr      3.00E+03

 Benzene
 -------------
PARAMETER NAME                    UNITS      VALUE
-------------------------------------------------

Henrys constant          (mg/L)/(mg/L)      2.28E-01
Molecular Weight                 g/mol      7.80E+01
Inhal Shower Bioavailibility       (-)      1.00E+00
Inhalation Slope Factor      kg-dy/mg      2.90E-02
Inhalation Reference Dose    mg/kg/dy      1.70E-03
Concentration in Groundwater     mg/l      1.00E-03

 SUMMARY OF THE OUTPUTS
 **********************

    CDI:    Chronic Daily Intake
    LADI:   Lifetime Average Daily Intake


 INHALATION DURING SHOWER
                         Daily        CDI          LADI         Risk      Hazard
                         Intake                                           Quotient
                         (mg/kg-dy)  (mg/kg-dy)  (mg/kg-dy)     (-)        (-)
 --------------------------------------------------------------------------------
Benzene                  3.03E-05    2.91E-05    3.74E-06    1.08E-07    1.71E-02


           Receptor Point Concentrations
=================================================================================
                                        Max. 5-year ave      Ave. over ED
     Shower Air Concentrations:        (non-carcinogens)    (carcinogens)
---------------------------------------------------------------------------------
  Benzene                                1.683E-02            1.683E-02
```

INTAKE.OUT (shower model assuming 0.7 fraction volatilized)

Page 1 of 1

```
 Chemicals in the analysis:
 Benzene

 Chemical Intake Analysis
 Deterministic Run

 PARAMETER NAME                    UNITS      VALUE
 ------------------------------------------------
Body Weight                          kg      7.00E+01
Life Time                            yr      7.00E+01
Exposure Duration Groundwater        yr      9.00E+00
Exposure Frequency Shower         dy/yr      3.50E+02
Shower Duration                      hr      2.00E-01
Inhalation Rate in Shower        m^3/hr      6.30E-01
Fraction Volatilized                (-)      7.00E-01
Shower Flow Rate                   l/hr      1.00E+01
Volume of Bathroom                  m^3      3.00E+00

 Benzene
 -------------
PARAMETER NAME                    UNITS      VALUE
 ------------------------------------------------
Henrys constant         (mg/L)/(mg/L)      2.28E-01
Molecular Weight                 g/mol      7.80E+01
Inhal Shower Bioavailibility       (-)      1.00E+00
Inhalation Slope Factor      kg-dy/mg      2.90E-02
Inhalation Reference Dose   mg/kg/dy      1.70E-03
Concentration in Groundwater     mg/l      1.00E-03


 SUMMARY OF THE OUTPUTS
 **********************
    CDI:   Chronic Daily Intake
    LADI:  Lifetime Average Daily Intake


 INHALATION DURING SHOWER
                               Daily        CDI         LADI        Risk     Hazard
                               Intake                                         Quotient
                            (mg/kg-dy)  (mg/kg-dy)  (mg/kg-dy)      (-)        (-)
 -------------------------------------------------------------------------
Benzene                        5.04E-05    4.83E-05    6.21E-06    1.80E-07    2.84E-02


          Receptor Point Concentrations
 =========================================================================

                                         Max. 5-year ave      Ave. over ED
     Shower Air Concentrations:         (non-carcinogens)    (carcinogens)
 -------------------------------------------------------------------------
  Benzene                                  2.800E-02            2.800E-02
```

APPENDIX J
IMPUT PARAMETERS REQUIRED BY THE DSS AND THE ALLOWABLE RANGES

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Table J-1.
Data Required to Implement the SESOIL Model Within the DSS.

	PARAMETER DEFINITION	UNITS	REMARKS
Chemical Data			
	Solubility	[ug/ml]	See Table 9-1
	Diffusion Coefficient in Air	[cm^2/sec]	See Table 9-1
	Henry's Law Constant	[(mg/L)/(mg/L)]	See Table 9-1
	Koc	[ug/g oc /ug/ml]	See Table 9-1
	Biodegradation Rate in Liquid	[1/day]	See Table 9-1
Climate Data			
	Surface Temperature	[C]	0 - 35
	Evapotranspiration	[cm/day]	+
	Precipitation	[cm/year]	+
	Storm Duration	[days]	<365
	Storm Events	[no. events/year]	<365
	Length of Rainy Season	[months]	<12
Unsaturated Zone Data for the Entire Soil Column			
	Effective Porosity	[-]	0 – 0.5
	Soil Bulk Density	[g/cm^3]	1.5 - 1.85
	X-dimension of the source	[m]	+
	Y-dimension of the source	[m]	+
Unsaturated Zone Data for Each Layer			
	Depth to bottom of the layer	[m]	+
	Intrinsic Permeability	[cm^2]	+
	Fraction Organic Carbon	[-]	0-1
	Pollutant load to the layer for each chemical of concern	[kg]	+

\+ any positive value

Table J-2.
Data Required to Implement the Jury Model Within the DSS.

	PARAMETER DEFINITION	UNITS	REMARKS
Chemical Data			
	Diffusion Coefficient in Air	[cm^2/sec]	See Table 9-1
	Diffusion Coefficient in Water	[cm^2/sec]	See Table 9-1
	Henry's Law Constant	[(mg/L)/(mg/L)]	See Table 9-1
	Koc	[ug/g oc /ug/ml]	See Table 9-1
	Biodegradation Rate in Liquid	[1/day]	See Table 9-1
	Pollutant Load	[kg]	See Table 9-1
Unsaturated Zone Data			
	Volumetric Water Content	[-]	0 - 0.5
	Effective Porosity	[-]	0 - 0.5
	Soil Bulk Density	[g/cm^3]	1.5 - 1.85
	Thickness of Incorporation	[m]	+
	Thickness of Soil Cover	[m]	+
	Fraction Organic Carbon	[g/g]	0 - 1
	Boundary Layer Thickness	[cm]	See Jury's paper
	Infiltration	[cm/yr]	+

+ any positive value

Table J-3.
Data Requirements for the AT123D Model in the DSS.

	PARAMETER DEFINITION	UNITS	REMARKS
Chemical Data			
	Organic carbon partition coefficient	[ug/g oc /ug/ml]	See Table 9-1
	Molecular diffusion coefficient	[m^2/yr]	See Table 9-1
	Lumped first order decay coefficient	[yr^{-1}]	+
Source Data			
	Mass flux of contaminant (flux option)	[kg/yr]	+
	Mass of contaminant (instantaneous release option)	[kg]	+
	Time duration of source flux	[yr]	<100
	X-coordinates of source	[m]	+
	Y-coordinates of source	[m]	+
	Z-coordinates of source	[m]	+
Saturated Zone Data			
	Aquifer width	[m]	+
	Aquifer depth	[m]	+
	Porosity	[cm^3/cm^3]	0 - 0.5
	Hydraulic Conductivity	[m/yr]	+
	Hydraulic gradient	[m/m]	+
	Longitudinal Dispersivity	[m]	+
	Transverse Dispersivity	[m]	+
	Vertical Dispersivity	[m]	+
	Fractional organic carbon content	[g/g]	0 - 1
	Soil Bulk density	[g/cm^3]	1.5 - 1.85
Receptor Data			
	X-coordinate of well	[m]	+
	Y-coordinate of well	[m]	+
	Depth to top of well screen	[m]	< aquifer thickness
	Depth to bottom of well screen	[m]	< aquifer thickness
	Number of intervals for vertical averaging	[dimensionless]	<10

+ any positive value

Table J-4. Data Requirements for the Thibodeaux-Hwang Vapor Emissions Model.

	PARAMETER DEFINITION	UNITS	REMARKS
Chemical Data			
	Total concentration in soil	[mg/kg wet soil]	+
	Henry's Law Constant	[g/cc vapor/g/cc water]	See Table 9-1
	Soil-Water partition coefficient	[g/g dry soil/g/cc water]	See Table 9-1
	Chemical Molecular Weight	[g/mol]	See Table 9-1
	Saturation vapor pressure	[atm]	See Table 9-1
	Air diffusion coefficient	[cm^2/s]	See Table 9-1
	Molecular weight of the residual mixture	[g/mol]	+
	Total concentration of the residual mixture in soil	[mg/kg wet soil]	+
Soils Data			
	Dry bulk density	[g dry soil/cm^3]	1.5 - 1.85
	Porosity	[c/c]	0 - 0.6
	Water content	[c/c]	0-porosity
Source Data			
	Depth to the top of the contaminated layer	[cm]	<unsaturated zone thickness
	Depth to the bottom of the contaminated layer	[cm]	<unsaturated zone thickness
	Source area	[m^2]	+

\+ any positive value

Table J-5.
Data Requirements for the Farmer Vapor Emissions Model.

	PARAMETER DEFINITION	UNITS	
Chemical Data			
	Total concentration in soil	[mg/kg wet soil]	+
	Henry's Law Constant	[g/cc vapor/g/cc water]	See Table 9-1
	Soil-Water partition coefficient	[g/g dry soil/g/cc water]	See Table 9-1
	Chemical Molecular Weight	[g/mol]	See Table 9-1
	Saturation vapor pressure	[atm]	See Table 9-1
	Air diffusion coefficient	[cm^2/s]	See Table 9-1
	Molecular weight of the residual mixture	[g/mol]	+
	Total concentration of the residual mixture in soil	[mg/kg wet soil]	+
Soils Data			
	Dry bulk density	[g dry soil/cm^3]	1.5 - 1.85
	Porosity	[c/c]	0 - 0.6
	Water content	[c/c]	0-porosity
Source Data			
	Depth to the top of the contaminated layer	[cm]	<unsaturated zone thickness
	Source area	[m^2]	+

+ any positive value

Table J-6.
Data Requirements for the Cowherd Particulate Emissions Model.

	PARAMETER DEFINITION	UNITS	REMARKS
Chemical Data			
	Total concentration in soil	[mg/kg wet soil]	+
Soils Data			
	Erosion threshold wind speed	[m/s]	See manual
	Frequency of disturbance	[mo^{-1}]	<30
	Fraction of area with vegetative cover	fraction	0 - 1
Source Data			
	Source area	[m^2]	+
Meteorologic Data			
	Fastest mile wind speed	[m/s]	See Table 5-7
	Thornthwaite Precipitation Evaporation Index	[dimensionless]	See Figure 5-5

+ any positive value

Table J-7.
Data Requirements for the Box Model.

PARAMETER DEFINITION	UNITS	REMARKS
Emission rate	[g/s]	+
Mean annual wind speed	[m/s]	+
Width of site perpendicular to predominant wind direction	[m]	+
Mixing height	[m]	+

+ any positive value

Table J-8.
Data Requirements for the Gaussian Dispersion Model.

	PARAMETER DEFINITION	UNITS	REMARKS
Chemical Data			
	Emission rate	[g/s]	+
	First order decay rate in air	[s^{-1}]	+
Source Data			
	Distance from source to receptor	[m]	+
	Width of area source	[m]	+
	Length of area source	[m]	+
Meteorologic Data			
	Mean annual wind speed	[m/s]	+
	Mixing height	[m]	+
	Frequency of occurrence for each stability class	[fraction]	0 - 1
	Fraction of the time wind blows in the direction of the receptor from the source	[fraction]	0 - 1

+ any positive value

Table J-9.
Data Required to Implement the VADSAT Model Within the DSS.

	PARAMETER DEFINITION	UNITS	REMARKS
Chemical Data			
	Total Concentration in Soil	[mg/kg]	+
	Solubility	[ug/ml]	See Table 9-1
	Diffusion Coefficient in Air	[cm^2/sec]	See Table 9-1
	Diffusion Coefficient in Water	[cm^2/sec]	See Table 9-1
	Henry's Law Constant	[(mg/L)/(mg/L)]	See Table 9-1
	Koc	[ug/g oc /ug/ml]	See Table 9-1
	Molecular Weight	[g/mol]	See Table 9-1
	Biodegradation in Vadose Zone	[1/day]	+
	Biodegradation in Saturated Zone	[1/day]	+
Source Zone Data			
	Saturated Conductivity	[m/day]	+
	Thickness of Waste Zone	[m]	+
	Waste Zone Area	[m^2]	+
	Length to Width Ratio	[m/m]	+
	Thickness of Soil Cover	[m]	+
	Fraction Organic Carbon	[g OC/g soil]	0 - 1
Unsaturated Zone Data			
	Fraction Organic Carbon	[g OC/g soil]	0 - 1
	Saturated Conductivity	[m/day]	+
	Depth to Groundwater	[m]	+
	Effective Porosity	[-]	0 - 0.5
	van Genuchten's n Parameter	[-]	1.01 - 2.8
	Residual Moisture Content	[-]	+
	Net Recharge Rate	[m/day]	+

+ any positive value

(Continued...)

Table J-9.
Data Required to Implement the VADSAT Model Within the DSS. (Concluded)

PARAMETER DEFINITION	UNITS	REMARKS
Saturated Zone Data		
Effective Porosity	[-]	0 - 0.5
Fraction Organic Carbon	[g OC/g soil]	0 - 1
Saturated Conductivity	[m/day]	+
Hydraulic Gradient	[m/m]	+
Aquifer Thickness	[m]	+
Location of Well Downgradient	[m]	+
Location of Well Cross-gradient	[m]	+
Depth of Well	[m]	+
TPH Data		
Concentration of TPH Mixture	[mg/kg]	+
Molecular Weight of TPH	[g/mol]	+
Density of TPH	[g/cm^3]	+

\+ any positive value

Table J-10.
Data Requirements for the Shower Model.

PARAMETER DEFINITION	UNITS	REMARKS
Chemical Data		
Henry's Law Constant	[(mg/L)/(mg/L)]	+
Molecular Weight of the Contaminant	[g/mole]	See Table 9-1
Concentration of the Contaminant in Water	[mg/L]	+
Shower/Source Data		
Volume of Shower Stall/Bathroom	[m^3]	+
Volumetric Flow Rate of Water	[L/min]	+
Duration for which Water is Flowing	[hr]	+
Shower Droplet Drop Time	[s]	+
Representative Diameter of the Shower Droplet	[cm]	+
Temperature of Shower Water	[°C]	+

\+ any positive value

APPENDIX K
BRIEF DESCRIPTION OF PARAMETER DISTRIBUTIONS AND GENERATING ALGORITHMS

The Monte Carlo simulation algorithms included in the DSS have the ability to generate data from a number of probability distributions. These are uniform, normal, log-normal, exponential, triangular, and empirical distributions. A description of each of these distributions, including parameters of the distributions, equations for the probability and cumulative density functions, brief discussion of the properties of these distributions, and the method used to generate/sample a variable from these distributions is provided in this appendix. For additional details refer to any standard textbook in probability and statistics (Benjamin and Correll, 1970; Snedecor and Cochran, 1980).

Uniform Distribution

A uniform distribution is a symmetrical probability distribution in which all values within a given range have an equal chance of occurrence. A uniform distribution is completely described by two parameters: (1) the minimum value (lower bound) A, and (2) the maximum value (upper bound) B. The equation for the uniform probability density distribution of variable x is given by:

$$f_u(x) = \frac{1}{(B-A)} \tag{K-1}$$

where f(x) is the value of the probability density function for x. The cumulative distribution F(x) is obtained by integrating Equation 1. This yields the probability distribution:

$$F_u(x) = \frac{(x-A)}{(B-A)} \tag{K-2}$$

where F(x) is the probability that a value less than or equal to x will occur.

A good uniform (A = 0, B = 1) pseudorandom generator is the basis for generating not only uniform values but also, via transformations, values from all other probability distributions.

Normal Distribution

The term normal distribution refers to the well-known bell-shaped probability distribution. Normal distributions are symmetrical about the mean, are unbounded, and values further from the mean occur less frequently. The spread of the distribution is described by the standard deviation. The normal distribution has only two parameters: the mean and the standard deviation. The probability density function of x is given by:

$$f_n(x) = \frac{1}{S_x\_2\pi} \, exp\left[-0.5 \left(\frac{x - m_x}{S_x} \right)^2 \right] \qquad \text{(K-3)}$$

where

S_x = the standard deviation
m_x = the mean of x

The cumulative distribution is the integral of the probability density function:

$$F_n(x) = \int_{-\infty}^{x} f_n(x)dx \qquad \text{(K-4)}$$

The above integration cannot be performed analytically; however, tables of numerically-integrated values of $F_n(x)$ are widely available in the statistical literature.

The method used in the Monte Carlo shell generates from a standard normal distribution (mean = 0, standard deviation = 1) using the fast but rather complex Marsaglia-Bray composition method discussed by Ripley, 1987, pp. 82-86.

Log-normal Distribution

The log-normal distribution is a skewed distribution in which the natural log of variable x is normally distributed. Thus, if y is the natural log of x, then the probability distribution of y is normal with mean m_y, standard deviation S_y and a probability density function similar to Equation 3. The mean and standard deviation of x (m_x and S_x) are related to the log-normal parameters m_y and S_y as follows:

$$m_x = exp\left[m_y + 0.5(S_y)^2\right] \qquad \text{(K-5)}$$

$$S_x^2 = m_x^2\left[exp\left(S_y^2\right) - 1\right] \qquad \text{(K-6)}$$

where

m_x = the mean of the original, untransformed data

S_x = the standard deviation of the original, untransformed data

m_y = the mean of the log transformed data

S_y = the standard deviation of the log transformed data

To preserve the observed mean and standard deviation of x, the parameters of the log-normal distribution (m_y and S_y) are therefore selected such that the above relationships are satisfied. Note that m_y and S_y do not equal the natural logs of m_x and S_x respectively. Log-normal distributions have a lower bound of 0.0 and no upper bound, and are often used to describe positive data with skewed probability distributions.

The Monte Carlo shell generates log-normal values by exponentiating a normal (m_y, S_y) value generated by the method described in the preceding section.

Exponential Distribution

The probability density function for an exponential distribution is described by an exponential equation:

$$f_e(x) = \frac{exp(-x/m_x)}{m_x} \qquad \text{(K-7)}$$

where m_x is the mean of the random variable x. The cumulative distribution is given by:

$$F_e(x) = 1 - exp(-x/m_x) \qquad \text{(K-8)}$$

The exponential distribution is bounded by zero; the probability density function peaks at zero and decreases exponentially as x increases in magnitude.

Cumulative distribution functions having a closed form such as Equation K-8 are convenient for generation by the simple "inverse" method, which uses the fact that the function F(x) of a random variable x is uniformly distributed on the interval (0,1). Thus, in the exponential case, the uniform (0,1) generator is used to generate a value of $F_e(x)$. The value of the exponentially distributed variable x is then estimated using Equation K-8.

Triangular Distribution

A triangular distribution is a relatively simple probability distribution defined by the minimum value, the maximum value, and the most frequent value (i.e., the mode). Figure K-1 shows an example triangular probability density function. The cumulative distribution for values of x less than the most frequent value x_m is given by:

$$F(x) = \frac{(x - x_1)^2}{(x_m - x_1)(x_2 - x_1)} \qquad \text{(K-9)}$$

where

x_1 = the minimum value

x_2 = the maximum value

x_m = the most frequent value

For values of x greater than the most frequent value, the cumulative distribution is:

$$F(x) = 1. - \frac{\left(1 - \frac{x - x_1}{x_2 - x_1}\right)^2}{\left(1 - \frac{x - x_1}{x_2 - x_1}\right)} \qquad \text{(K-10)}$$

Generation from this distribution is by the inverse method (see Section on Exponential Distribution).

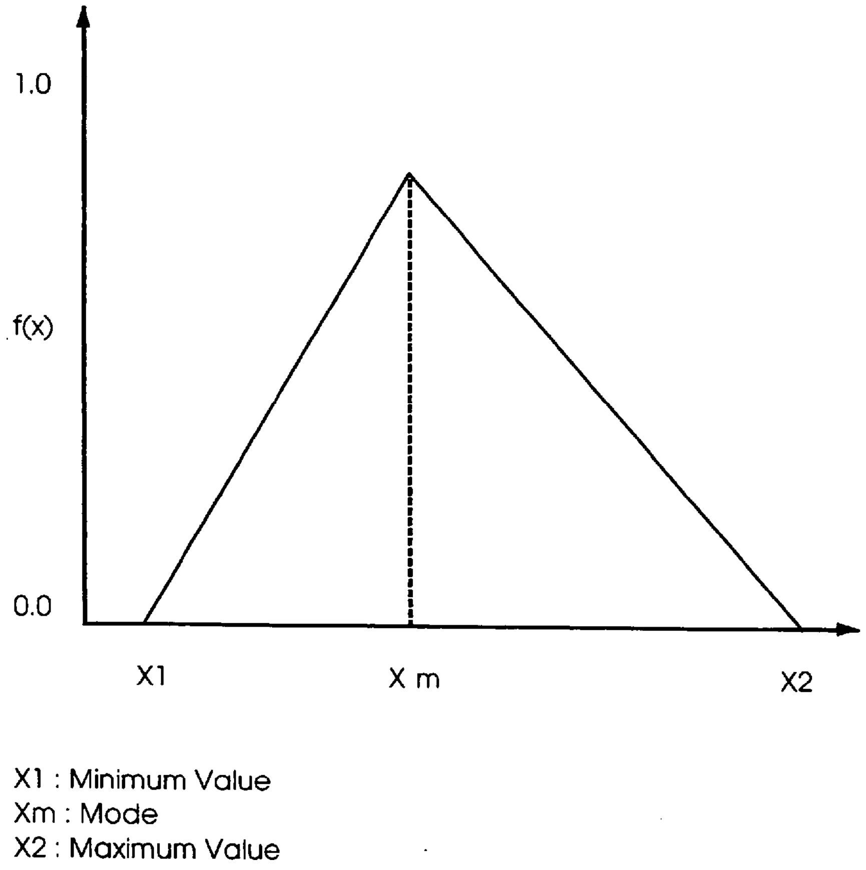

Figure K-1. Schematic of a Triangular Probability Distribution.

Empirical Distribution

At times it may be difficult to fit a standard statistical distribution to observed data. In these cases, it is more appropriate to use an empirical piecewise-linear description of the observed cumulative distribution for the variable of interest. This option is not available in the DSS.

Cumulative probabilities can be estimated from observed data by ranking the data from lowest (rank = 1) to highest (rank = number of samples) value. The cumulative probability associated with a value of x is then calculated as a function of the rank of x and the total number of samples. The cumulative probabilities of values among observed data can be estimated by linear interpolation.

There is no universally accepted formula for computing cumulative probabilities from ranked data. If the number of samples is large (>100), the cumulative probability $F_e(x)$ can be estimated by:

$$F_e(x) = r_x/N \qquad \text{(K-11)}$$

where

r_x = the rank of value x
N = the number of samples

This formula has the disadvantage of assigning a cumulative probability of 1.0 to the highest value, thus requiring the assumption that no higher value can possibly occur. Another formula often used for small samples is the Weibull equation:

$$F_e(x) = r_x/(N + 1) \qquad \text{(K-12)}$$

Numerous other formulae exist; however, it is difficult to test the appropriateness of a given formula without *a priori* knowledge of the true distribution of x. Further, the differences among these formulae decrease as the value of N increases.

Generation from empirical distributions is performed by the inverse method in the Monte Carlo shell. A value uniformly distributed between 0 and 1 is generated by the method presented in the Section on the Uniform Distribution. This value is matched to a bracketing pair of values from the sample distribution function $F_e(x)$. The random value x is then calculated by linear interpolation. Minimum and maximum values of x, corresponding to $F_e(x) = 0$ and $F_e(x) = 1$, should be specified by the user.

References

Benjamin, J.R. and C.A. Cornell. 1970. Probability, Statistics, and Decision for Civil Engineers. McGraw Hill Book Company.

Snedecor, G.S. and W.C. Cochran. 1980. Statistical Methods. The Iowa State University Press, Ames, Iowa.

Ripley, B.D. 1987. Stochastic Simulation. New York. Wiley.

APPENDIX L
CUMULATIVE PROBABILITY DISTRIBUTIONS AVAILABLE IN EPA EXPOSURE FACTORS HANDBOOK

The Exposure Factors Handbook (EPA, 1989b) includes probability distributions for a few parameters required to estimate the intake. These parameters include body weight, drinking water ingestion rate, body surface area and shower duration. The cumulative probability distribution for these parameters are tabulated in Tables L-1, L-2, L-3, and L-4.

Table L-1. Cumulative Distribution of Body Weight.

Percentile	Men (Age : 18 < 75) Body Weight (kg)	Women (Age : 18 < 75) Body Weight (kg)
5	57.7	46.8
10	61.2	49.3
15	64.0	51.2
25	67.8	54.4
50	75.9	61.5
75	84.6	71.1
85	90.4	78.3
90	94.7	83.4
95	101.7	92.3

Table L-2. Cumulative Distribution of Drinking Water Ingestion Rate.

Consumption Rate (L/day)	Cumulative Frequency (%)
0.80	19.2
0.81 - 1.12	39.6
1.13 - 1.44	59.7
1.45 - 1.95	79.9
1.96	100.0

Table L-3. Cumulative Distribution of Body Surface Area.

	Men (Surface Area - sq. m.)			Women (Surface Area - sq. m.)		
Percentile	Total	Upper Extremities	Lower Extremities	Total	Upper Extremities	Lower Extremities
5	1.66	0.321	0.653	1.45	0.260	0.564
10	1.72	0.332	0.676	1.49	0.265	0.582
15	1.76	0.340	0.692	1.53	0.269	0.595
25	1.82	0.350	0.715	1.58	0.274	0.615
50	1.94	0.372	0.761	1.69	0.287	0.657
75	2.07	0.395	0.810	1.82	0.301	0.704
85	2.14	0.408	0.838	1.91	0.311	0.736
90	2.20	0.418	0.858	1.98	0.318	0.757
95	2.28	0.432	0.888	2.09	0.329	0.796

Table L-4. Cumulative Distribution of Shower Duration.

Shower Duration (minutes)	Cumulative Frequency (%)
1	0.20
2	0.80
3	3.20
4	9.80
5	22.60
6	38.20
7	52.60
8	63.80
9	73.40
10	81.00
11	86.20
12	90.20
13	92.40
14	94.20
15	95.60
16	96.80
17	97.60
18	98.60
19	99.40
20	100.00

APPENDIX M
EXAMPLE PROBLEM

Site investigations conducted at an abandoned gas station site revealed the following information.

Background

The former gas station site has a total area of 75 m by 120 m and is located in a small town. The gas station was operational for about 10 years from 1975 to 1985 after which it was closed due to lack of business. Underground tanks and all surface structures were removed. The site was never completely paved but about 10% of the area of the site has asphalt that is heavily cracked on the surface. Review of historic records does not indicate any known spills; however, it is suspected that several small accidental surface spills may have occurred at the site. No visible staining was observed.

The site is surrounded by houses on two sides. A schematic is shown in Figure M-1. A developer intends to use this abandoned site as a neighborhood greenbelt/park area by spreading 1ft of top soil and sod laying. The developer intends to complete this activity within a period of one month. Prior to the city's approval of this project, the developer is required to investigate the nature and extent of contamination and to conduct a human health risk assessment assuming the project is completed as planned.

Pertinent conclusions from a site investigation are presented below.

Site Hydrogeology

As shown in a schematic of the site, five soil borings to a depth of 10 m were made. These borings show the site stratigraphy to be relatively homogenous across the site and consist of sandy silt from surface to 5 m, and silty clay from 5 to 10 m. Consultation with a hydrogeologist indicates that the unsaturated zone has a porosity of 0.3 and an average water content of 0.15. The fraction organic carbon (F_{oc}) in the vadose zone soils was measured to be 0.003 g oc/g soil in one sample.

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Groundwater was encountered in all borings at a depth of approximately 10 m. Evaluation of regional water table maps indicate a regional gradient toward the west of about 0.002 m/m. The hydraulic conductivity and effective porosity of the aquifer are estimated to be 1×10^{-4} m/s and 0.35, respectively. F_{oc} was not measured in the aquifer; it is assumed to be very low based on the type of soil observed in the borings.

Contaminant Concentrations

Soil samples were collected and analyzed for BTEX and TPH from the five soil borings at the surface and at 2 m intervals. The results of these analyses are shown in Table M-1.

Groundwater samples indicated that none of these chemicals has yet reached the water table.

Environmental Conditions

Average annual rainfall in this area is about 126 cm/yr and average annual temperature of 20°C. Twenty percent of the total precipitation was assumed to infiltrate through the vadose zone and reach the water table. The average wind speed in the area is 3 m/s. The climatic data were obtained from a weather station at a nearby airport.

Land Use

As shown in Figure M-1, the site is located in a residential area and the site is planned to be developed as a greenbelt area. Individuals living in this neighborhood are not very mobile and the average stay duration is about 30 years. About 105 m downgradient from the (downgradient) edge of the source is a domestic water supply well.

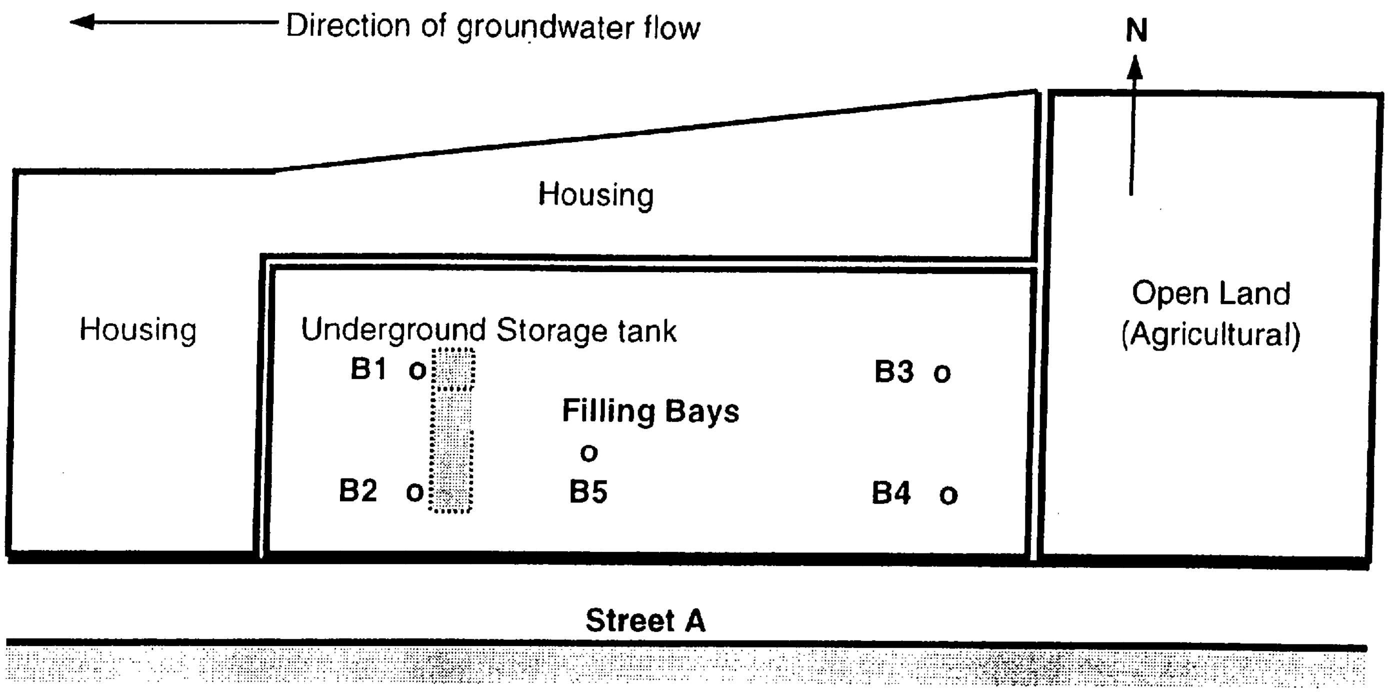


Figure M-1. Schematic of the Abandoned Gas Station Site

Table M-1.
Results of Soil Analysis.
(Total Soil Concentration)

DEPTH (m)	BENZENE (mg/kg)					TOLUENE (mg/kg)					ETHYL BENZENE (mg/kg)					XYLENE (mg/kg)				
	B-1	B-2	B-3	B-4	B-5	B-1	B-2	B-3	B-4	B-5	B-1	B-2	B-3	B-4	B-5	B-1	B-2	B-3	B-4	B-5
0-0	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
2	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
4	200	100	ND	ND	120	100	100	ND	ND	120	25	50	ND	ND	130	50	75	ND	ND	150
6	250	130	ND	ND	130	120	100	ND	ND	130	50	60	ND	ND	120	55	100	ND	ND	97
8	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
10	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
12	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
14	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND

Analysis Required

Use the above example problem to demonstrate the use of the API DSS.

Conceptual Development of the Example Problem

The first step in a risk assessment is to identify all relevant exposure pathways and routes. Based on the information presented above, the following pathways are significant:

Receptor	Pathway
On-site construction workers	Inhalation of volatiles Inhalation of particulates Direct contact with soil
Off-site residents	Ingestion of groundwater Inhalation during shower Dermal contact during shower Inhalation due to volatilization from the site (vapors only)
On-site potential receptors	Inhalation due to volatilization of vapors

Note off-site receptors or on-site potential park users will not be exposed to particulate emissions or direct contact with soils since the surface soils are clean.

For purposes of demonstrating the use of API DSS, the risk to off-site residents will be evaluated. This scenario will use all routes of exposure and will use several fate and transport models. Note for a complete risk assessment, it will be necessary to quantitatively evaluate the risk to the other receptors. The estimation of risk for the off-site resident will require the following concentrations:

- concentration in the well 105 m from the downgradient edge of the source
- concentration in the air (assume same concentration inside and outside the house)
- concentration in the shower air

Concentrations in the well can be estimated using the Jury's model coupled with AT123D model. Concentrations in the air can be estimated by using the emissions from Jury's model with a Gaussian dispersion model. Jury's model is appropriate since the soil column is relatively homogenous and the initial concentrations are fairly low. If residual phase contamination were present, Jury's model would not be appropriate. Concentrations in the shower air are estimated using the shower model (Foster-Chrostowski's model).

In addition to the data required by the models to estimate receptor point concentrations, intake parameters and toxicity values for the four chemicals of concern will be required. These data are shown in Tables M-2 to M-6.

The actual implementation of the API DSS is described below.

Table M-2. Data Required to Implement the Jury Model for the API DSS Example Problem.

	PARAMETER DEFINITION	UNITS	VALUE
Model Control Parameters			
	Simulation time	[yrs]	30
Data for the Soil Column			
	Volumetric water content	[-]	0.15
	Effective porosity	[-]	0.30
	Soil bulk density	[g/cm^3]	1.8
	Fraction organic carbon	[mg/mg]	0.003
	Thickness of source	[m]	2
	Thickness of soil cover	[m]	2.30
	Depth of unsaturated zone	[m]	10
	X-dimension of the source	[m]	75
	Y-dimension of the source	[m]	100
	Thickness of boundary layer	[cm]	0.5
	Infiltration rate	[cm/yr]	24.4
Total Concentration in Soil			
	Benzene	[mg/kg]	155
	Ethyl benzene	[mg/kg]	72.5
	Toluene	[mg/kg]	111.66
	Xylene	[mg/kg]	87.83
Chemical-Specific Degradation Rates			
	Benzene	[1/days]	0.002
	Ethylbenzene	[1/days]	0.003
	Toluene	[1/days]	0.0033
	Xylene	[1/days]	0.002

Table M-3. Data Required to Implement the AT123D Model for API DSS Example Problem.

PARAMETER DEFINITION	UNITS	VALUES
Model Control Parameters		
Option to indicate if the aquifer is infinitely wide (y-direction)-		YES
Option to indicate if the aquifer is infinitely deep (z-direction)-		NO
Media Parameters		
Porosity	cm^3/cm^3	0.35
Hydraulic conductivity	m/yr	3153
Hydraulic gradient	m/m	0.002
Longitudinal dispersivity (as fraction of distance to well)	-	0.1
Transverse dispersivity (as fraction of distance to well)	-	0.03
Vertical dispersivity (as fraction of distance to well)	-	0.01
Bulk density of soil	g/cm^3	1.8
Fractional organic carbon content	g/g	0.0
Thickness of aquifer	m	30
Receptor Well Data		
Distance downgradient	m	105
Distance off centerline of plume	m	0
Top of well screen	m	0.0
Bottom of well screen	m	20
Chemical Specific Degradation Rates		
Benzene	[1/days]	0.002
Ethylbenzene	[1/days]	0.003
Toluene	[1/days]	0.0033
Xylene	[1/days]	0.002

Table M-4. Data Used for the Gaussian Dispersion Model in the API DSS Example Problem.

	PARAMETER DEFINITION	UNITS	VALUE
Source Data			
	Area of source	[m^2]	7500
Chemical Data			
	Emission rate	[g/s]	*
	First order decay rate in air	[1/s]	0
Receptor Data			
	Distance from source to receptor	[m]	150
Meteorologic Data			
	Mean annual wind speed	[m/s]	3
	Frequency of occurrence for Stability Classes A, B, C, D, E, and F, respectively	[-]	0.1,0.2,0.2,0.1, 0.2,0.2
	Fraction of the time wind blows in the direction of the receptor from the source	[-]	0.4
	Vertical dispersivity *	[m]	**

* Estimated using Jury's model

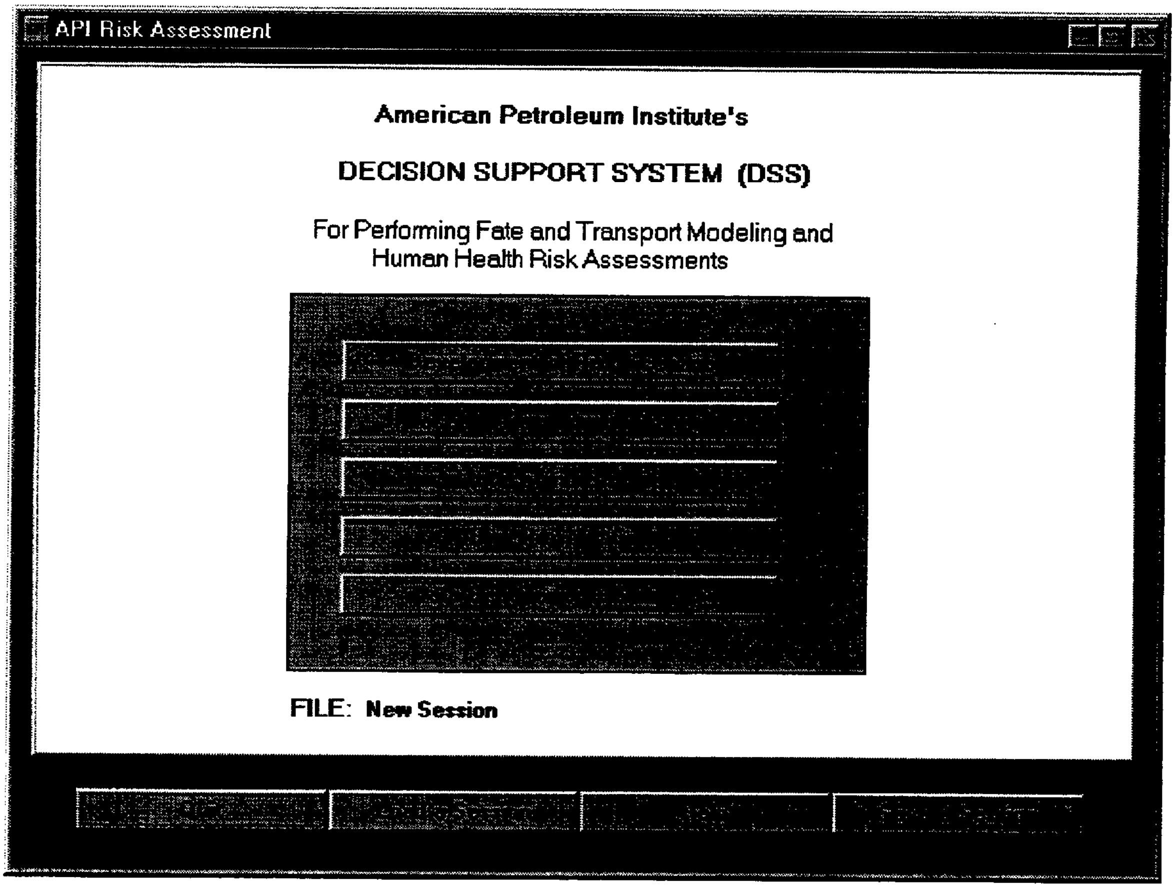
** Estimated based on empirical Pasquill-Gifford relationship

Implementation of the Example Problem Using the API DSS

The main screen of the API DSS software is shown in Figure M-2. The four modules are show in this screen: Development of Risk Scenario, Receptor Point Concentrations, Chemical Intake and Risk Calculation, and Risk Presentation. The fifth button, Data Requirements/Summary summarizes the data contained in the current session, once the routes and chemicals of concern have been selected in the first module.

In the first module, the chemicals and exposure routes of concern are selected. Figure M-3 shows the chemical selection screen with the four chemicals of concern selected. Figure M-4 shows the selection of exposure routes and models used. Jury's model followed by AT123D is selected to estimate groundwater concentrations, and Jury's model coupled with the Gaussian model is to be used to estimate concentrations in off-site air.

After the first module is complete, proceed to the Receptor Point Concentrations module. Figure M-5 shows the main menu for the fate and transport models.



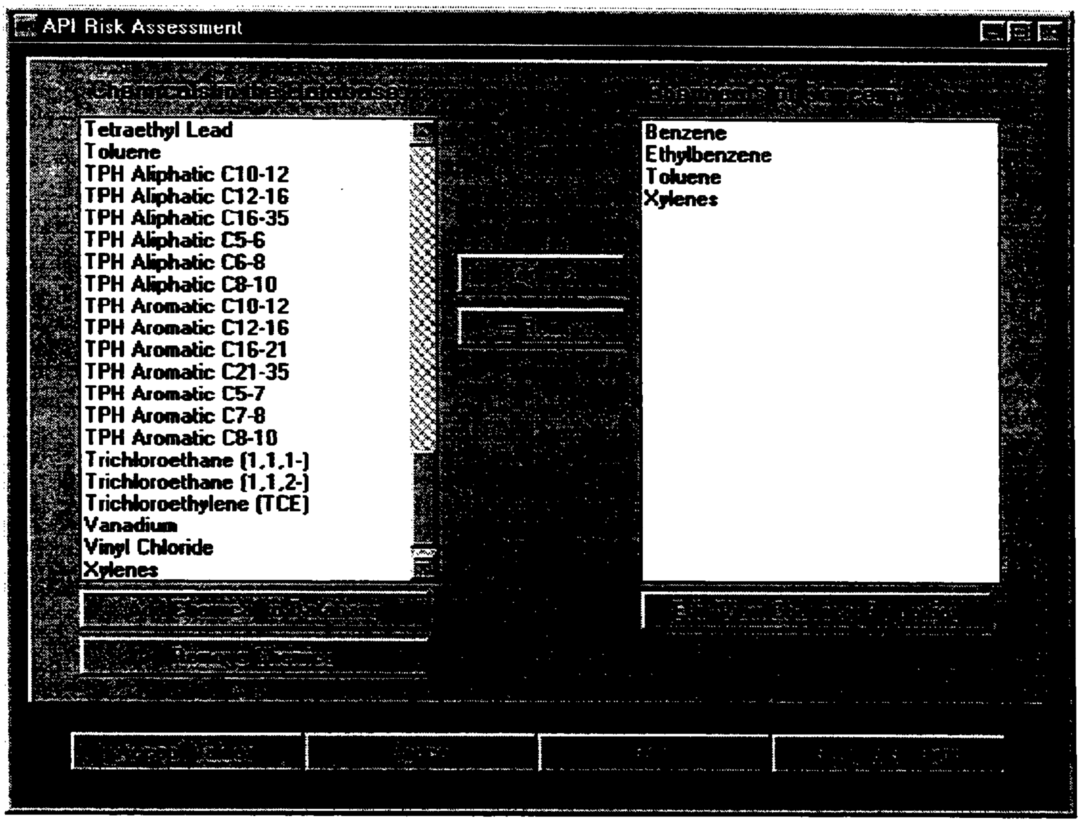
American Petroleum Institute's

DECISION SUPPORT SYSTEM (DSS)

For Performing Fate and Transport Modeling and
Human Health Risk Assessments

FILE: New Session

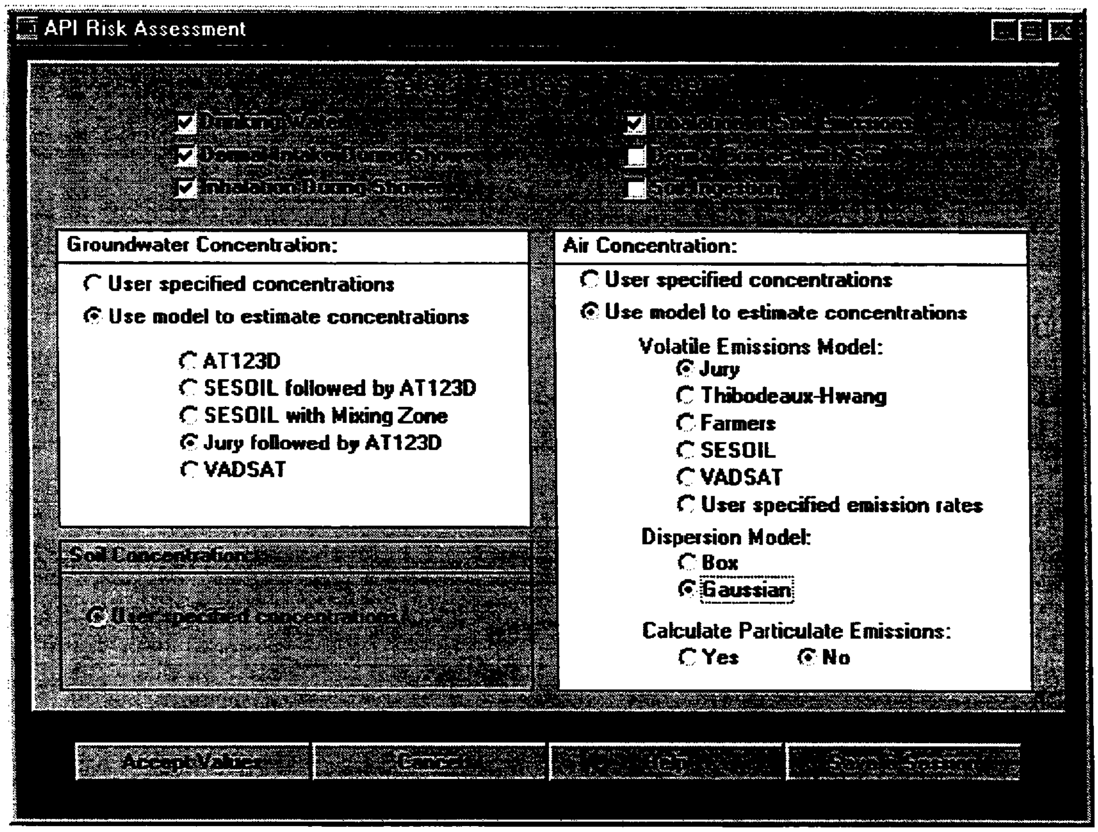
Figure M-2. The Main Screen of the API DSS.



Tetraethyl Lead
Toluene
TPH Aliphatic C10-12
TPH Aliphatic C12-16
TPH Aliphatic C16-35
TPH Aliphatic C5-6
TPH Aliphatic C6-8
TPH Aliphatic C8-10
TPH Aromatic C10-12
TPH Aromatic C12-16
TPH Aromatic C16-21
TPH Aromatic C21-35
TPH Aromatic C5-7
TPH Aromatic C7-8
TPH Aromatic C8-10
Trichloroethane (1,1,1-)
Trichloroethane (1,1,2-)
Trichloroethylene (TCE)
Vanadium
Vinyl Chloride
Xylenes

Benzene
Ethylbenzene
Toluene
Xylenes

Figure M-3. Selecting Chemicals of Concern.



☑ Drinking Water
☑ Dermal Intake During Shower
☑ Inhalation During Shower
☑ Inhalation of Soil Emissions
☐ Dermal Contact with Soil
☐ Soil Ingestion

Groundwater Concentration:

○ User specified concentrations
● Use model to estimate concentrations

○ AT123D
○ SESOIL followed by AT123D
○ SESOIL with Mixing Zone
● Jury followed by AT123D
○ VADSAT

Soil Concentration:

● User specified concentrations

Air Concentration:

○ User specified concentrations
● Use model to estimate concentrations

Volatile Emissions Model:
● Jury
○ Thibodeaux-Hwang
○ Farmers
○ SESOIL
○ VADSAT
○ User specified emission rates

Dispersion Model:
○ Box
● Gaussian

Calculate Particulate Emissions:
○ Yes ● No

Figure M-4. Selecting Exposure Routes and Fate and Transport Models.

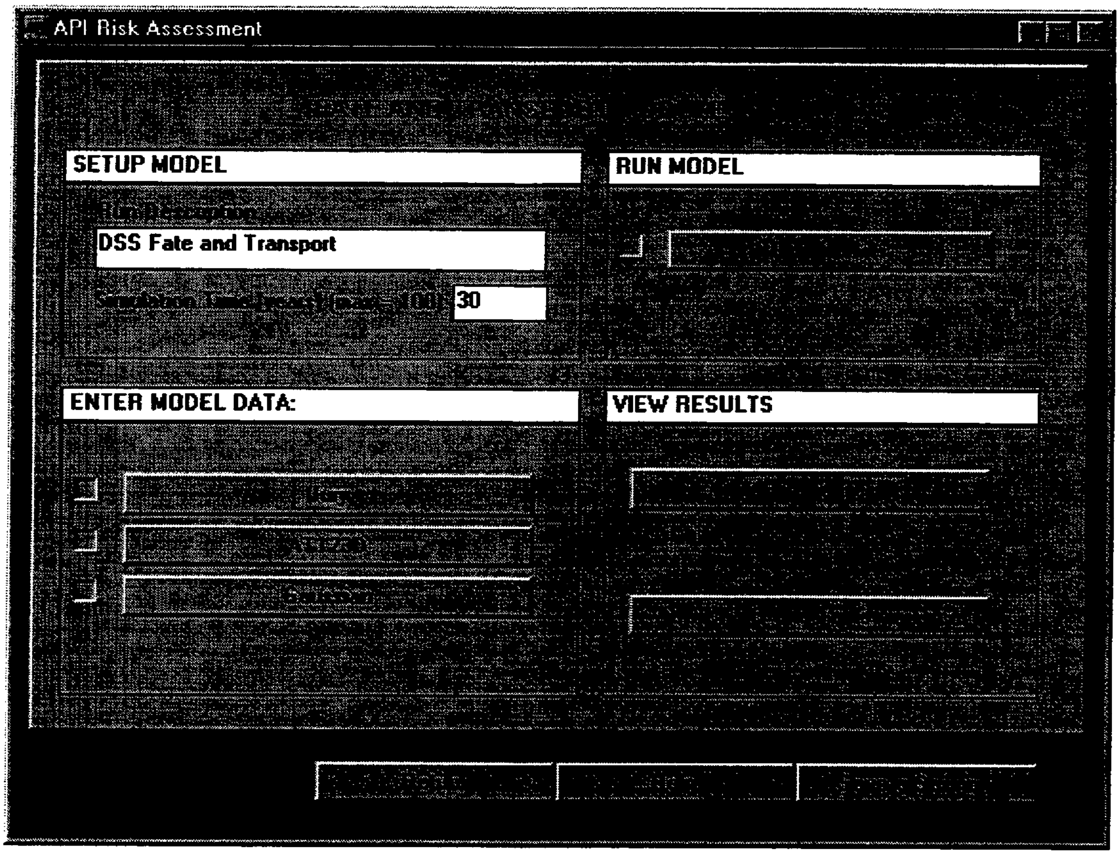
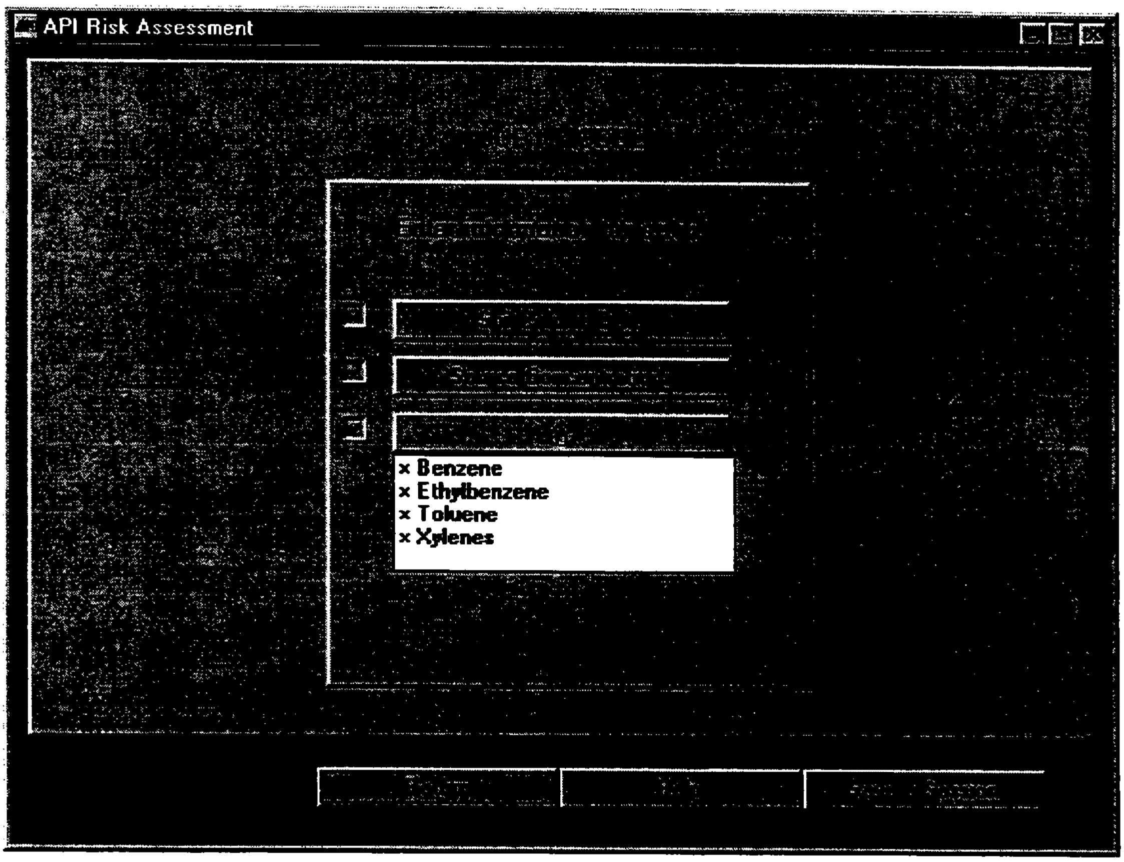


Figure M-5. The Fate and Transport Models Main Screen.

ENTER DATA FOR JURY (LINKED WITH AT123D) MODEL

Select “Jury Model” from the Fate and Transport Module. From the next screen entitled Jury Model, select Soil Column Data, and then on the next screen, type the data from Table M-2. After entering all the values, select Accept Values button. This brings the user back to the Jury Model Screen. Select the Source Concentrations button and enter the soil concentrations for each chemical. The average total soil concentration for each chemical is shown in Table M-2. (Refer to RAGS or relevant state guidance to enter arithmetic, logarithmic or area averaged mean value.) Lastly, select Chemical Parameters and sequentially select each chemical and enter the appropriate data (the only data that need to be changed are the degradation rates). The chemical-specific parameters that appear on the screen are from the API DSS database. Any of these values may be changed by overwriting them if necessary.

After all the data for all the relevant chemicals have been entered, the Jury Model screen should show a check mark in the soil column data box and for each of the chemicals. Figure M-6 shows the Jury model menu once all of the input data have been entered.



× Benzene
× Ethylbenzene
× Toluene
× Xylenes

Figure M-6. Menu for Jury's Model After All Data Have Been Entered.
(Note, chemical parameters are complete.)

Select Return to go back to the Jury Linked with AT123D screen. Note that since data for the Jury Model have been entered, the Enter Jury Model Data box should now have a check mark beside it.

AT123D and Gaussian Models

Continue similarly and enter the input data required for AT123D and the Gaussian models.

RUN THE MODEL

Make sure the simulation time is set to 30 (Figure M-5) years and then select "Run Models." Wait as these models are run once for each chemical. The output screen for Jury will show the time counter to indicate the progress in running the program. Similarly, when AT123D is implemented, the average annual concentration for each year will be displayed on the screen. After all runs have been completed, the user will be asked the question "Program Terminated will exit

Code 0, Exit Windows?". The user should select Yes to return to the Fate and Transport Module screen. This screen will now show two additional options:

- View Fortran Results
- View Charts and Tables in EXCEL

View Fortran Results

If the user makes the first choice, there will be the option of viewing either the Jury, AT123D, or air model results. Depending on the option selected by the user, the appropriate results are displayed on the screen, and the user can select the Print button at the bottom of the screen to print the results followed by the Continue button to go back to the previous screen. These output files are also contained on the hard drive. The output for Jury's model is 'JURY.OUT', for AT123D 'AT123D.OUT', and for the air model 'AIRMODEL.OUT'.

View Charts and Tables in EXCEL

Selecting this button brings the EXCEL spreadsheet to the forefront. From the spreadsheet, the user can view and print the results in several graphical or tabular forms. These can be viewed by clicking on the DSS menu that will be displayed at the top of the screen. After viewing/printing these results, the user may exit the spreadsheet by closing it or by selecting "Return to DSS" from the DSS menu.

Figure M-7 shows a plot of groundwater concentrations for all four chemicals of concern. Note that benzene had a maximum concentration of 2.1E-2 mg/l and the other chemicals were much lower.

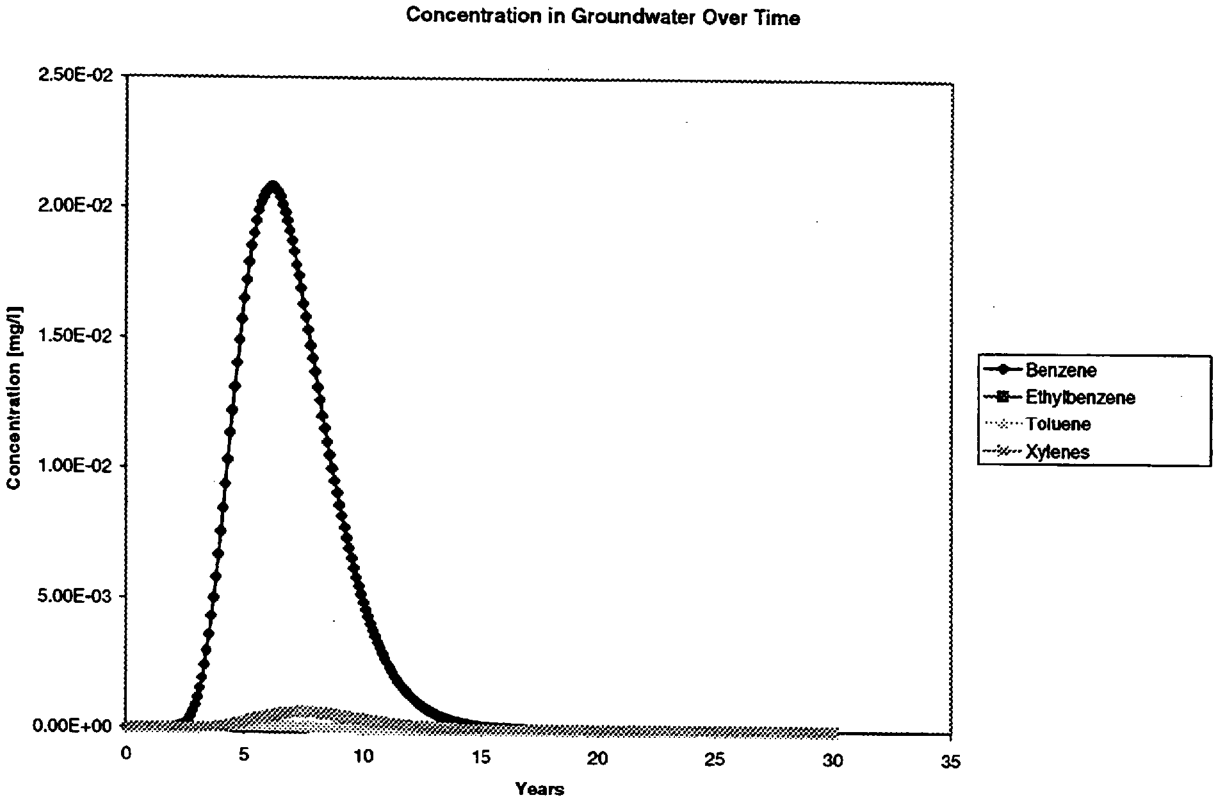


Figure M-7. Groundwater Concentrations for BTEX.

RUN CHEMICAL INTAKE AND RISK CALCULATION

From the Main Menu of the DSS, the user should select the Chemical Intake and Risk Calculation button to enter the data for this module. Figure M-8 shows the Chemical Intake and Risk Calculation Module screen. For the example problem, the user must enter data for the following data groups:

- Body Weight and Lifespan
- Routes of Entry which includes the four exposure routes:
  - Ingestion of drinking water
  - Dermal contact in the shower
  - Inhalation in the shower
  - Inhalation of outdoor air emissions
- Dose Response toxicity data.

The data to be used for this example are shown in Table M-5.

Table M-5. Data Used in the Chemical Intake Module in the API DSS Example Problem.

PARAMETER	VALUE
Drinking Water	
Body Weight [kg]	70.0
Lifetime [years]	70.0
Exposure Frequency [days/yr]	350.0
Exposure Duration [years]	9.0
Ingestion Rate [liters/day]	1.4
For each chemical of concern in groundwater:	
Concentration [mg/l]	*
Oral Reference Dose [mg/kg-d]	**
Oral Slope Factor $[mg/kg\text{-}d]^{-1}$	**
Bioavailability [mg/mg]	**
Inhalation During Shower	
Body Weight [kg]	70.0
Lifetime [years]	70.0
Exposure Frequency [days/yr]	350
Exposure Duration [years]	9
Inhalation Rate $[m^3/hr]$	0.63
Time in Shower [hours/day]	0.12
For each chemical of concern in groundwater:	
Concentration [mg/l]	*
Inhalation Reference Dose [mg/kg-d]	**
Inhalation Slope Factor $[mg/kg\text{-}d]^{-1}$	**
Bioavailability [mg/mg]	**

Table M-5. Data Used in the Chemical Intake Module in the API DSS Example Problem (Continued).

PARAMETER	VALUE
Dermal Exposure in Shower	
Body Weight [kg]	70.0
Lifetime [years]	70.0
Exposure Frequency [days/yr]	350
Exposure Duration [years]	9.0
Total Skin Surface Area [cm^2]	18150
Time in Shower [hours/day]	0.12
For each chemical of concern in groundwater:	
Concentration [mg/l]	*
Dermal Permeability Coefficients [cm/hr]	**
Oral Reference Dose [mg/kg-d]	**
Oral Slope Factor [mg/kg-d]$^{-1}$	**
Inhalation of Volatile Soil Emissions	
Body Weight [kg]	70
Lifetime [years]	70
Exposure Frequency [days/yr]	350
Exposure Duration [years]	9
Inhalation Rate [m^3/hr]	0.833
Time Outdoors [hours/day]	4.0
For each chemical of concern in air:	
Concentration [mg/m^3]	*
Inhalation Reference Dose [mg/kg-d]	**
Inhalation Slope Factor [mg/kg-d]$^{-1}$	**
Bioavailability [mg/mg]	**
For shower volatilization model	**

* These concentrations are calculated in the Fate and Transport Module.

** Use default values from the API DSS in the absence of any additional information.

RISK PRESENTATION

By selecting the Risk Presentation button from the DSS main menu, the user can enter the DSS menu in EXCEL to view/print charts and tables of the results using standard EXCEL commands. This feature is also available from the Chemical Intake and Risk Calculation module.

After printing the results, the user can return to the main screen by selecting the Return to DSS option in the DSS menu.

SAVING THE DATA

At the end of the session, the user may save the data entered and the selections made by selecting Save a Session button or by selecting the Quit button followed by the choice Yes to save the results. The user will be prompted to give a name under which the data will be saved. When restarting a session, the user may load an existing session from the main screen by selecting Load a Session button. This will require the user to select one of several files to be loaded.

SUMMARY

The above discussion would enable the user to conveniently work his or her way once through the API DSS. The API DSS has several other features e.g., Monte Carlo simulation capabilities that the users will learn as they gain experience and familiarity with the system.

The implementation of this example problem generates several files such as JURY.OUT, AT123D.OUT, AIRMODEL.OUT, and INTAKE.OUT. One of these files (INTAKE.OUT) that summarizes the risk to the receptor is attached.

Table M-6 shows the summary risk and hazard index table from EXCEL.

TABLE M-6. Summary of Risk and Hazard Index from the EXCEL Spreadsheet.

Carcinogenic Risk by Chemical for Each Route of Concern

Chemical	Drinking Water	Dermal Uptake During Shower	Inhalation During Shower	Inhalation of Soil Emissions	Total
Benzene	1.14E-06	3.73E-08	7.02E-07	1.84E-08	1.90E-06
Ethylbenzene	ND	ND	ND	ND	0.00E+00
Toluene	ND	ND	ND	ND	0.00E+00
Xylenes	ND	ND	ND	ND	0.00E+00
Total	1.14E-06	3.73E-08	7.02E-07	1.84E-08	1.90E-06

Hazard Index by Chemical for Each Route of Concern

Chemical	Drinking Water	Dermal Uptake During Shower	Inhalation During Shower	Inhalation of Soil Emissions	Total
Benzene	1.80E-01	5.88E-03	1.11E-01	2.91E-03	3.00E-01
Ethylbenzene	2.81E-06	3.24E-07	5.39E-07	1.31E-06	4.98E-06
Toluene	7.15E-06	5.02E-07	7.33E-06	1.15E-05	2.65E-05
Xylenes	4.93E-06	6.16E-07	2.74E-05	6.13E-06	3.91E-05
Total	1.80E-01	5.88E-03	1.11E-01	2.93E-03	3.00E-01

ATTACHMENT: The INTAKE.OUT file.

```
 Chemicals in the analysis:

Benzene
Ethylbenzene
Toluene
Xylenes

Chemical Intake Analysis


 Deterministic Run

 PARAMETER NAME                   UNITS      VALUE
 -----------------------------------------------


Body Weight                          kg     7.00E+01
Life Time                            yr     7.00E+01
Exposure Duration Groundwater        yr     9.00E+00
Exposure Frequency Ingestion      dy/yr     3.50E+02
Water Ingestion Rate              l/day     1.40E+00
Exposure Duration Groundwater        yr     9.00E+00
Exposure Frequency Shower         dy/yr     3.50E+02
Shower Duration                      hr     1.20E-01
Total Skin Surface Area            cm^2     1.82E+04
Exposure Duration Groundwater        yr     9.00E+00
Exposure Duration Groundwater        yr     3.50E+02
Shower Duration                      hr     1.20E-01
Inhalation Rate in Shower        m^3/hr     6.30E-01
Fraction Volatilized                (-)     0.00E+00
Shower Flow Rate                   l/hr     1.00E+01
Volume of Bathroom                  m^3     3.00E+00
Temperature of Shower water           C     4.50E+01
Droplet Diameter                     mm     1.00E-01
Droplet Droptime                      s     2.00E+00
Mass Transfer CO2                 cm/hr     2.00E+01
Mass Transfer H2O                 cm/hr     3.00E+03
Exposure Duration Inhalation         yr     9.00E+00
Exposure Frequency Inhalation     dy/yr     3.50E+02
Exposure Time - Outdoor Air          hr     4.00E+00
Air Inhalation Rate              m^3/hr     8.33E-01

 Benzene
 -------------
PARAMETER NAME                   UNITS      VALUE
 -----------------------------------------------


Water Ingestion Bioavailibility (-)        1.00E+00
Permeability Coefficient        cm/hr      2.10E-02
Henrys constant         (mg/L)/(mg/L)      2.28E-01
Molecular Weight                g/mol      7.80E+01
Inhal Shower Bioavailibility      (-)      1.00E+00
Inhalation Soil Bioavailibility (-)        1.00E+00
Oral Slope Factor           kg-dy/mg       2.90E-02
Oral Reference Dose         mg/kg-dy       1.70E-03
Inhalation Slope Factor     kg-dy/mg       2.90E-02
Inhalation Reference Dose   mg/kg/dy       1.70E-03
Dermal Slope Factor         kg-dy/mg       2.90E-02
Dermal Reference Dose       mg/kg-dy       1.70E-03
```

Ethylbenzene

PARAMETER NAME	UNITS	VALUE
Water Ingestion Bioavailibility	(-)	1.00E+00
Permeability Coefficient	cm/hr	7.40E-02
Henrys constant	(mg/L)/(mg/L)	3.23E-01
Molecular Weight	g/mol	1.06E+02
Inhal Shower Bioavailibility	(-)	1.00E+00
Inhalation Soil Bioavailibility	(-)	1.00E+00
Oral Slope Factor	kg-dy/mg	ND
Oral Reference Dose	mg/kg-dy	1.00E-01
Inhalation Slope Factor	kg-dy/mg	ND
Inhalation Reference Dose	mg/kg/dy	2.90E-01
Dermal Slope Factor	kg-dy/mg	ND
Dermal Reference Dose	mg/kg-dy	1.00E-01

Toluene

PARAMETER NAME	UNITS	VALUE
Water Ingestion Bioavailibility	(-)	1.00E+00
Permeability Coefficient	cm/hr	4.50E-02
Henrys constant	(mg/L)/(mg/L)	2.72E-01
Molecular Weight	g/mol	9.21E+01
Inhal Shower Bioavailibility	(-)	1.00E+00
Inhalation Soil Bioavailibility	(-)	1.00E+00
Oral Slope Factor	kg-dy/mg	ND
Oral Reference Dose	mg/kg-dy	2.00E-01
Inhalation Slope Factor	kg-dy/mg	ND
Inhalation Reference Dose	mg/kg/dy	1.14E-01
Dermal Slope Factor	kg-dy/mg	ND
Dermal Reference Dose	mg/kg-dy	2.00E-01

Xylenes

PARAMETER NAME	UNITS	VALUE
Water Ingestion Bioavailibility	(-)	1.00E+00
Permeability Coefficient	cm/hr	8.00E-02
Henrys constant	(mg/L)/(mg/L)	2.90E-01
Molecular Weight	g/mol	1.06E+02
Inhal Shower Bioavailibility	(-)	1.00E+00
Inhalation Soil Bioavailibility	(-)	1.00E+00
Oral Slope Factor	kg-dy/mg	ND
Oral Reference Dose	mg/kg-dy	2.00E+00
Inhalation Slope Factor	kg-dy/mg	ND
Inhalation Reference Dose	mg/kg/dy	2.00E-01
Dermal Slope Factor	kg-dy/mg	ND
Dermal Reference Dose	mg/kg-dy	2.00E+00

```
SUMMARY OF THE OUTPUTS
**********************

   CDI:   Chronic Daily Intake
   LADI:  Lifetime Average Daily Intake

DRINKING WATER
                    Daily       CDI         LADI        Risk       Hazard
                    Intake                                         Quotient
                 (mg/kg-dy) (mg/kg-dy)  (mg/kg-dy)      (-)          (-)
--------------------------------------------------------------------------
Benzene             3.18E-04   3.05E-04   3.93E-05   1.14E-06    1.80E-01
Ethylbenzene        2.93E-07   2.81E-07   3.61E-08        ND     2.81E-06
Toluene             1.49E-06   1.43E-06   1.84E-07        ND     7.15E-06
Xylenes             1.03E-05   9.87E-06   1.27E-06        ND     4.93E-06

DERMAL INTAKE DURING SHOWER
                    Daily       CDI         LADI        Risk       Hazard
                    Intake                                         Quotient
                 (mg/kg-dy) (mg/kg-dy)  (mg/kg-dy)      (-)          (-)
--------------------------------------------------------------------------
Benzene             1.04E-05   1.00E-05   1.29E-06   3.73E-08    5.88E-03
Ethylbenzene        3.38E-08   3.24E-08   4.17E-09        ND     3.24E-07
Toluene             1.05E-07   1.00E-07   1.29E-08        ND     5.02E-07
Xylenes             1.28E-06   1.23E-06   1.58E-07        ND     6.16E-07

INHALATION DURING SHOWER
                    Daily       CDI         LADI        Risk       Hazard
                    Intake                                         Quotient
                 (mg/kg-dy) (mg/kg-dy)  (mg/kg-dy)      (-)          (-)
--------------------------------------------------------------------------
Benzene             1.96E-04   1.88E-04   2.42E-05   7.02E-07    1.11E-01
Ethylbenzene        1.63E-07   1.56E-07   2.01E-08        ND     5.39E-07
Toluene             8.71E-07   8.35E-07   1.07E-07        ND     7.33E-06
Xylenes             5.72E-06   5.48E-06   7.05E-07        ND     2.74E-05

INHALATION OF SOIL EMISSIONS
                    Daily       CDI         LADI        Risk       Hazard
                    Intake                                         Quotient
                 (mg/kg-dy) (mg/kg-dy)  (mg/kg-dy)      (-)          (-)
--------------------------------------------------------------------------
Benzene             5.16E-06   4.94E-06   6.36E-07   1.84E-08    2.91E-03
Ethylbenzene        3.96E-07   3.79E-07   4.88E-08        ND     1.31E-06
Toluene             1.37E-06   1.31E-06   1.68E-07        ND     1.15E-05
Xylenes             1.28E-06   1.23E-06   1.58E-07        ND     6.13E-06
```

```
          Receptor Point Concentrations
=====================================================================

                                     Max. 5-year ave     Ave. over ED
   Groundwater Concentrations:     (non-carcinogens)   (carcinogens)
---------------------------------------------------------------------
 Benzene                              1.592E-02            1.592E-02
 Ethylbenzene                         1.464E-05            1.464E-05
 Toluene                              7.457E-05            7.457E-05
 Xylenes                              5.146E-04            5.146E-04

                                     Max. 5-year ave     Ave. over ED
    Shower Air Concentrations:     (non-carcinogens)   (carcinogens)
---------------------------------------------------------------------
 Benzene                               .182                 .182
 Ethylbenzene                         1.510E-04            1.510E-04
 Toluene                              8.067E-04            8.067E-04
 Xylenes                              5.294E-03            5.294E-03

                                     Max. 5-year ave      Ave. over ED
           Air Concentrations:     (non-carcinogens)     (carcinogens)
---------------------------------------------------------------------
 Benzene                              1.083E-04            1.083E-04
 Ethylbenzene                         8.312E-06            8.312E-06
 Toluene                              2.869E-05            2.869E-05
 Xylenes                              2.685E-05            2.685E-05
```

APPENDIX N
THE VADSAT MODEL

The VADSAT model is a **VAD**ose zone/**SAT**urated zone model developed by Environmental Systems and Technologies, Inc. (ES&T) for the American Petroleum Institute. The model is available as a standalone model from the API or as part of the API DSS. This appendix summarizes the processes considered in the VADSAT model and the assumptions made. The summary is based on the VADSAT User and Technical Guide, Version 2.1 (ES&T, 1994) and the paper by Ünlü et al. (1992).

Background

VADSAT was originally developed to simulate the movement of inorganic or reactive organic species present in land-disposed exploration and production (E&P) waste. Two source models are available in the standalone VADSAT model, one for salts and one for organic chemicals dissolving from oily wastes. In the API DSS version only the oily source is considered.

The VADSAT model simulates adsorption, biodecay, volatilization, and leaching in the vadose zone. The leaching is coupled with a saturated zone model that considers dispersion, biodecay and adsorption. The source may be composed of "residual" levels of contamination, that is, a hydrocarbon mixture. The model calculates the effective solubility of the species being modeled and adjusts the leaching factor accordingly. This is an important feature of the VADSAT model.

Figure N-1 shows a schematic of the VADSAT model.

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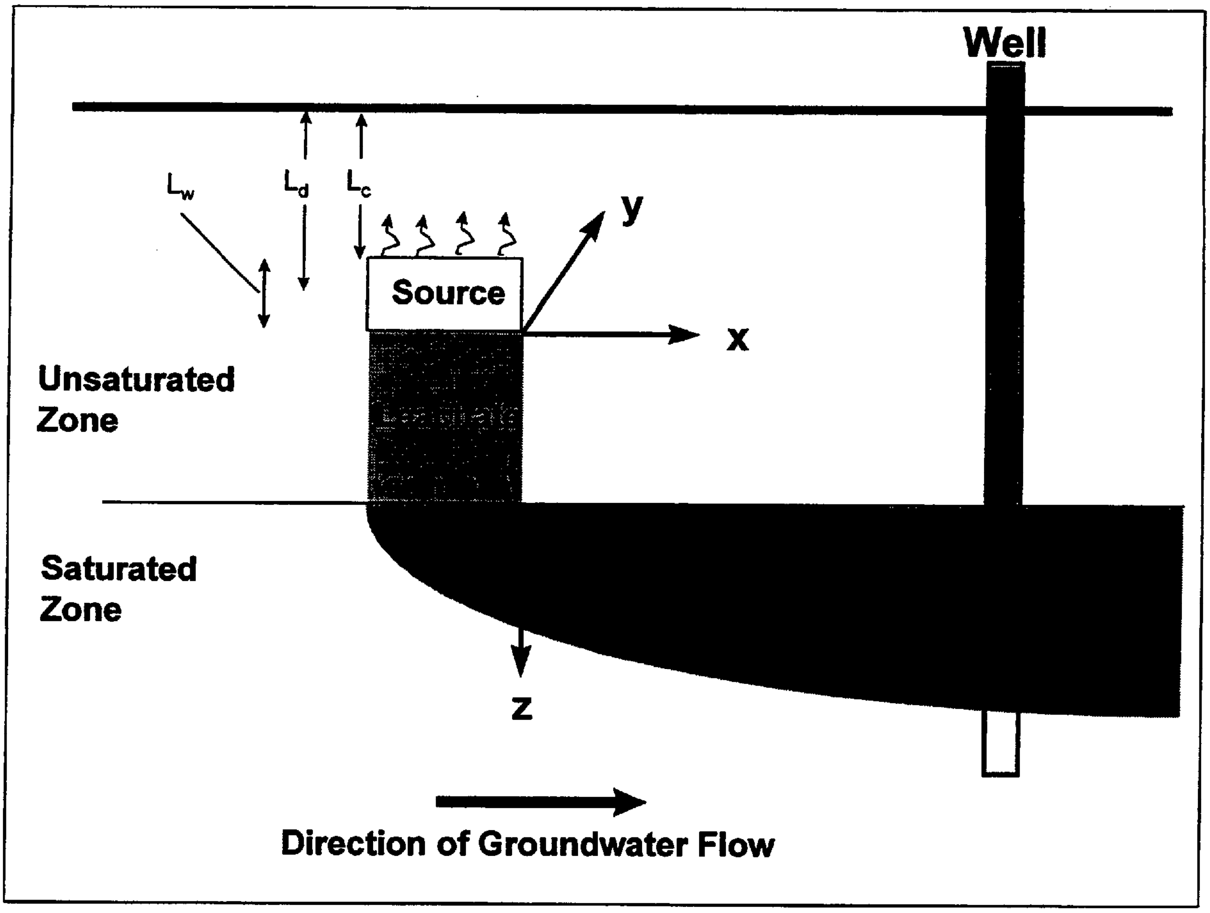

Figure N-1. Geometry of the VADSAT Model.

Hydrocarbon Source

The source is assumed to deplete over time due to the combined effects of water percolating through the waste zone and due to volatilization from the waste zone. The molar balance for a compound i may be written as

$$\frac{dm_i}{dt} = -\frac{J_i^w}{W_i} - \frac{J_i^v}{W_i} \qquad \text{(N-1)}$$

where

m_i = number of moles of i per unit area in the hydrocarbon [moles/L^2]

W_i = molecular weight of i [M moles^{-1}]

J_i^w = rate of dissolved phase mass depletion per area [M/(L^2T)] (due to infiltration through the source)

J_i^v = rate of mass depletion per area due to volatilization $[M/(L^2T)]$
t = time [T]

The dissolved phase loss is assumed to occur only with the percolation of water through the vadose zone (no dispersion from the source):

$$J_i^w = q_u C_i^w \tag{N-2}$$

where

q_u = net recharge rate (infiltration or percolation rate) [L/T]
C_i^w = initial dissolved-phase concentration of i $[M/L^3]$

The initial aqueous concentration, C_i^w, is calculated from the chemical's (i) mole fraction in the hydrocarbon and its solubility:

$$C_i^w = x_i S_i \tag{N-3}$$

where

S_i = aqueous solubility of pure component i $[M/L^3]$
x_i = mole fraction of i in the hydrocarbon [moles/moles]

The mole fraction may be written as

$$x_i = \frac{m_i}{m_H} \tag{N-4}$$

$$x_i = \frac{m_i W_H}{\rho_b L_w F_H} \tag{N-5}$$

where

m_H = total moles of hydrocarbon per unit area $[moles/L^2]$
W_H = average molecular weight of hydrocarbon [M/mole]
ρ_b = soil bulk density in the waste zone $[M/L^3]$
L_w = thickness of the waste zone [L]
F_H = mass of hydrocarbon per mass of soil in the waste zone [M/M] (TPH concentration in dimensionless form)

The diffusive mass loss rate at the soil surface, J_i^v assumes a linear concentration drop from the waste zone to the soil surface (Fick's law), where the concentration is assumed to be equal to zero:

$$J_i^v = D_i^v \frac{C_i^v}{L_d} \qquad \text{(N-6)}$$

where

D_i^v = effective diffusion coefficient of component i in the soil $[L^2/T]$

C_i^v = vapor concentration in the waste zone $[M/L^3]$

L_d = diffusion path length [L]

$L_d = L_c + L_w/2$

L_c = waste cover thickness [L]

L_w = thickness of the waste zone [L]

(Assumed to be the distance from the center of the waste zone to the soil surface.)

The effective diffusion coefficient is estimated from the free gas diffusion coefficient, K_i^{vo}, using Millington-Quirk (1961) model:

$$D_i^v = \frac{(\theta_T - \theta_w)^{10/3}}{\theta_T^{\,2}} D_i^{vo} \qquad \text{(N-7)}$$

where

θ_T = total porosity $[L^3/L^3]$

θ_w = volumetric water content $[L^3/L^3]$

The soil bulk density is calculated from the porosity using

$$\rho_b = 2.65\ (1 - \theta_T)$$

where

ρ_b = soil bulk density $[M/L^3]$

θ_T = total porosity $[L^3/L^3]$

The gas phase concentration in the source is calculated from Henry's law

$$C_i^v = H_i C_i^w \qquad \text{(N-8)}$$

where

H_i = Henry's Law constant for component i (mg/l vapor)/(mg/l water)

Combining equations N-1 through N-8 yields the following relationship summarizing the mass loss rate from the source zone:

$$\frac{dm_i}{dt} = -\beta_i m_i \tag{N-9}$$

where β_i is the depletion coefficient (T^{-1}) given by

$$\beta_i = \frac{q_u W_H S_i}{\rho_b L_w F_H W_i} + \frac{D_i^v H_i W_H S_i}{\rho_b L_d L_w F_H W_i} \tag{N-10}$$

and the variables are as defined previously. The first term in equation N-10 represents the aqueous losses and the second term, the diffusive losses. The VADSAT model assumes that F_H does not change significantly with time (either there are only low solubility compounds in the source or there is a high TPH concentration relative to the concentration of component i). Equation N-9 can then be solved to obtain

$$m_i = m_i^o \exp(-\beta_i t) \tag{N-11}$$

where

m_i^o = initial moles of component i per area [moles/L^2]

The dissolved phase concentration in the source will also decrease exponentially with time:

$$C_i = C_i^w \exp(-\beta_i t) \tag{N-12}$$

where C_i^w is the initial dissolved phase concentration of species i given by (in terms of volume fraction):

$$C_i^w = \frac{f_i^o W_H \rho_i S_i}{W_i \rho_H} \tag{N-13}$$

where

f_i^o = initial volume fraction of component i in the hydrocarbon mixture $[L^3/L^3]$

ρ_i = density of component i $[M/L^3]$

ρ_H = density of hydrocarbon mixture $[M/L^3]$

In the standalone VADSAT code, the initial volume fraction of component i, f_i^o, is a data requirement (input requirement for the model). In the API DSS, f_i^o is calculated from the concentration in soil of component i as follows

$$f_i^o = \frac{C_i^s}{C_H^s}\left(\frac{\rho_H}{\rho_i}\right) \tag{N-14}$$

where

C_i^s = total concentration of component i in soil [mg/kg]

C_H^s = total concentration of hydrocarbon mixture (TPH) in soil [mg/kg]

Unsaturated Zone Transport

The dissolved-phase transport of component i is modeled from the bottom of the source to the water table. Horizontal spreading is considered negligible. Adsorption and first-order decay processes are considered. Therefore, the governing equation (advection-dispersion equation) for the one-dimensional transport in the unsaturated zone is given by:

$$R_{ui}\frac{\partial C_i}{\partial t} = D_u\frac{\partial^2 C_i}{\partial x^2} - V_u\frac{\partial C_i}{\partial x} - \mu_{ui}C_i \tag{N-15}$$

where

C_i = dissolved-phase concentration of component i $[M/L^3]$

D_u = vertical dispersion coefficient in the unsaturated zone $[L^2/T]$

V_u = pore water velocity in the unsaturated zone [L/T]

μ_{ui} = first-order decay coefficient for component i in the unsaturated zone $[T^{-1}]$

x = distance (from the bottom of the source) [L]

t = time [T]

R_{ui} = chemical-specific retardation factor (defined later) [-]

The advection-dispersion equation is solved using the following boundary conditions:

$$\begin{aligned} &C_i(x,0) = 0 \\ &C_i(0,t) = C_i^o \exp(-\beta_i t) \\ &\frac{\partial C}{\partial x} = (\infty, t) = 0 \end{aligned} \qquad \text{(N-16)}$$

Roughly, these boundary conditions specify that (1) at t=0 the area below the source is clean, (2) the source decay is assumed to be exponential with the β_i as defined previously, and (3) the concentration gradient at infinity is zero.

The following sections describe the various components of the advection-dispersion equation.

Pore Water Velocity in Unsaturated Zone

The VADSAT model approximates the water content by assuming a unit hydraulic gradient. The unsaturated hydraulic conductivity is estimated with the Brooks and Corey (1964) model. The unit gradient approach assumes that the pressure (suction) head in the soil profile is constant, as is the moisture content. From the VADSAT manual (ES&T, 1994):

> *"The actual flow behavior in the vadose zone can be quite complicated when one considers the effects of spatial heterogeneity and transient boundary conditions. However, in the present analysis, we are concerned with simulating the average conditions over long term periods. In light of this objective, it was decided to simplify the flow calculations, utilizing a unit hydraulic gradient approximation. This approach has been proven to work reasonable well even in moderately heterogeneous soils under steady flow conditions (Yeh, 1989)."*

It is important to note that the model is suitable only for average conditions over long time periods -- the type of modeling usually done for estimating long term exposure for risk assessments.

Darcy's equation for the unit gradient case can be written as:

$$q = k_r K_{su} \tag{N-17}$$

where

q = net infiltration rate [L/T]
k_r = relative permeability [dimensionless]
K_{su} = hydraulic conductivity of the unsaturated zone if it were fully saturated [L/T]

In the unsaturated zone, the relative permeability depends on the volumetric water content. It is assumed that this relationship can be described by the Brooks and Corey (1964) model:

$$k_r = \left[\frac{\theta_w - \theta_r}{\theta_T - \theta_r}\right]^{\gamma} \tag{N-18}$$

where

θ_T = total porosity in unsaturated zone [L^3 voids/L^3 soil]
θ_w = volumetric water content or water-filled porosity [L^3 water/L^3 soil]
θ_r = irreducible water content [L^3 water/L^3 soil]
γ = pore size.distribution parameter [-]

The pore size distribution parameter is estimated from the van Genuchten *"n"* parameter using the following relationship (Lenhard et al., 1989):

$$\gamma = 3 + \frac{2}{(n-1)(1-0.5^{\frac{n}{(n-1)}})} \tag{N-19}$$

The VADSAT model requires the user to enter the van Genucten parameter, *n*. Carsel and Parrish (1988) have a large database of van Genuchten's *"n"* for various soil types. This database is in the API DSS help system and is reproduced in Table N-1.

The water content is calculated using equations N-17 and N-18. The pore water velocity, V_u is then calculated from:

$$V_u = \frac{q}{\theta_w} \tag{N-20}$$

where

V_u = pore water velocity in the vadose zone [L/T]

Table N-1. Values of van Genucten's "n" Parameter for Various Soil Types.

Soil Type	n
Clay	1.09
Clay loam	1.31
Loam	1.56
Loamy sand	2.28
Silt	1.37
Silt loam	1.41
Silty clay	1.09
Silty clay loam	1.23
Sand	2.68
Sandy clay	1.23
Sandy clay loam	1.48
Sandy loam	1.89

If the infiltration rate entered by the user exceeds the unsaturated zone conductivity, K_{su}, then the infiltration rate is limited to K_{su} assuming that the excess flow will be diverted as runoff. The standalone version of the VADSAT model asks the user to enter a liner hydraulic conductivity in addition to the vadose zone hydraulic conductivity. The liner is assumed to occur beneath the source (waste pit) and the conductivity is only used to limit the infiltration rate in the same manner as the general vadose zone hydraulic conductivity. The API DSS version of VADSAT does not use the liner conductivity input parameter.

Retardation in the Unsaturated Zone

The chemical-specific retardation factor for the unsaturated zone, R_{ui}, is estimated using:

$$R_{ui} = 1 + \frac{\rho_b F_{oc} K_{oc_i}}{\theta_w} \tag{N-21}$$

where

F_{oc} = fraction organic carbon in dry soil [kg/kg]
K_{oc} = organic carbon normalized partition coefficient [m^3/kg]

Degradation in the Unsaturated Zone

Degradation is assumed to be a first-order reaction occurring in the dissolved and adsorbed phase. The decay coefficient is defined by:

$$\mu_{ui} = \mu_{uw_i}\theta_W + F\mu_{uw_i}\rho_b F_{oc} K_{oc_i} \tag{N-22}$$

where

μ_{ui} = overall decay coefficient in vadose zone for chemical i [L^{-1}]
μ_{uwi} = decay coefficient in the aqueous phase for chemical i [L^{-1}]
F = a factor equal to 0 or 1 depending on whether sorbed phase decay is to be considered.
F = 0, no degradation of adsorbed (solid) phase
F = 1, degradation considered in the solid phase

The user specifies whether or not to consider adsorbed phase decay in the model input parameters screen for the VADSAT model.

Dispersion in the Unsaturated Zone

Dispersion is assumed to occur in the direction of infiltration only (no horizontal spreading). The dispersion coefficient is assumed to be a linear function of the pore water velocity, V_u, (defined in Equation N-20)

$$D_u = \alpha_L V_u \tag{N-23}$$

where

α_L = longitudinal dispersivity [L]

The longitudinal dispersivity is calculated using data from Gelhar *et al.* (1985) as a function of the vertical distance from the source

$$ln(\alpha_L) = -4.933 + 3.811\,ln(x) \qquad x \le 2m \qquad \text{(N-24)}$$

$$x \;\le\; 2\;m \qquad x \ge 2m \qquad \text{(N-25)}$$

where

x = distance from the source to the observation location [L]

The distance, x, is measured vertically downward from the bottom of the source zone. Note, for the vadose zone portion of the VADSAT model the dispersion is always calculated using the above algorithms – it is not an option for the user to specify dispersivity in the vadose zone.

Saturated Zone Transport

The saturated zone transport model in VADSAT considers a one-dimensional horizontal flow field and three-dimensional dispersion (very similar to AT123D). The following sections will describe the various components of the saturated zone model, for more details on the mathematical solution the reader is referred to the VADSAT manual (ES&T, 1994) and Galya (1987).

Horizontal Plane Source and Saturated Zone Transport

The VADSAT model assumes that the leachate (and chemicals) from the vadose zone enters the saturated zone via a horizontal plane source. This is the same type of source as is used when SESOIL is coupled with AT123D in the API DSS. The dimensions of the plane source are assumed to be equal to the horizontal dimensions of the source in the vadose zone.

For a uniform velocity field (moving in the x-direction) in an aquifer with uniform hydrogeologic properties, the advection-dispersion equation can be written:

$$R_{si}\frac{\partial C_i}{\partial t} = D_x\frac{\partial^2 C_i}{\partial x^2} + D_y\frac{\partial^2 C_i}{\partial y^2} + D_z\frac{\partial^2 C_i}{\partial z^2} - \frac{q_s \partial C_i}{\theta_{Ts}\partial x} - \mu_{si}C_i + \frac{Q_i(x,y,z)}{\theta_{Ts}} \qquad \text{(N-26)}$$

where

R_{si} = retardation coefficient for species i in saturated zone [-]

C_i = aqueous concentration of species i in saturated zone [M/L^3]

q_s	=	Darcy velocity in the saturated zone [L/T]
D_x, D_y, D_z	=	dispersion coefficients in the x, y, and z directions [L^2/T]
θ_{Ts}	=	total effective porosity in the saturated zone [L^3 water/L^3 soil]
μ_{si}	=	first-order decay coefficient for mass loss in the saturated zone [T^{-1}]
Q_i	=	source term for species i [$M/T/L^3$] (calculated by the unsaturated zone part of the VADSAT model)

Dispersion in the Saturated Zone

Dispersion coefficients in the saturated zone are described by:

$$D_x = \frac{\alpha_x q_s}{\theta_{Ts}}$$

$$D_y = \frac{\alpha_y q_s}{\theta_{Ts}} \qquad \text{(N-27)}$$

$$D_z = \frac{\alpha_z q_s}{\theta_{Ts}}$$

where

$\alpha_x, \alpha_y, \alpha_z$ = dispersivities in the x, y, and z directions [L]

The user has the option to specify or have the VADSAT model calculate the dispersivities in the x, y, and z directions. If the dispersivities are internally calculated by the VADSAT code, the following equations (from Gelhar *et al.*, 1985) are used:

$$ln(\alpha_x) = -3.795 + 1.774\, ln(x) - 0.093[ln(x)]^2 \qquad \text{(N-28)}$$

Remember, x is measured from the downgradient edge of the source in the direction of groundwater flow. The transverse dispersivities, α_y and α_z are estimated using:

$$\alpha_y = \frac{\alpha_x}{\tau_1} \qquad \text{(N-29)}$$

$$\alpha_z = \frac{\alpha_y}{\tau_2} \qquad \text{(N-30)}$$

where τ_1 is assumed to be equal to 3 and τ_2 is 87 (from API, 1987).

Data Requirements

The data requirements for the VADSAT model are shown in Table N-2.

Assumptions/Limitations

1. VADSAT simulates the transport of dissolved phase contaminants downward, and vapor phase contaminants upward, only. It does not simulate the movement of non-aqueous phase liquids (NAPLs).
2. The vadose zone is considered to be homogeneous and uniform below the source. The hydraulic conductivity in the vadose zone is calculated as a function of moisture content, however, this derived moisture content is assumed to be constant for the entire depth of the soil column.
3. The contaminant source in the vadose zone has a uniform concentration across the user-specified source volume.
4. The saturated zone is assumed to be homogenous and isotropic.
5. The water table is assumed to be steady without any fluctuations.
6. The flow direction is uniform, one-dimensional and steady state.
7. Contaminant decay is assumed to follow a lumped first order decay rate.
8. Contaminant adsorption is considered to follow linear adsorption.
9. Concentrations in the liquid and solid phase of the aquifer are assumed to be in equilibrium at all times.

Table N-2. Data Requirements for the VADSAT Model.

INPUT PARAMETER	Units used in API DSS
Model Control Parameters	
Allowing volatilization?	yes/no
Solid phase degradation?	yes/no
Code-calculated dispersivities?	yes/no
Source Zone Parameters	
Saturated conductivity of waste zone	m/day
Thickness of waste zone	m
Waste zone area	m^2
Length to width ratio	m/m
Thickness of soil cover	m
Fraction organic carbon	g OC/g soil
Vadose Zone Soil Parameters	
Fraction organic carbon	g OC/g soil
Saturated conductivity	m/day
Depth to groundwater	m
Effective porosity	cm^3/cm^3
van Genucten's n parameter	-
Residual moisture content	cm^3/cm^3
Net recharge rate	m/day
Saturated Zone (Aquifer) Parameters	
Effective porosity	cm^3/cm^3
Fraction organic carbon	g OC/g soil
Saturated conductivity	m/day
Hydraulic gradient	m/m
Aquifer thickness	m
Location of well-downgradient	m
Location of well--cross-gradient	m
Depth of well	m
TPH Data	
Concentration of TPH mixture	mg/kg
Molecular weight of TPH	g/mole
Density of TPH	g/cm^3
Chemical-Specific Parameters	
Total concentration in soil	mg/kg
Diffusion coeff. in air	cm^2/s
Diffusion coeff. in water	cm^2/s
Henry's Law constant	(mg/L)/(mg/L)
K_{oc}	µg/gOC/µg/ml
Solubility	mg/l
Degradation rate in vadose zone	$days^{-1}$
Degradation rate in aquifer	$days^{-1}$
Molecular weight	g/mole

Example Problem

This example will use the same hypothetical scenario as the SESOIL example (in Appendix A).

VADSAT assumes that the soil above and below the source is clean and that the source is at a uniform concentration. Using the SESOIL example, the source for this problem may be defined as extending from 3 to 5.5 m bgs.

Table N-3 presents the input values for the VADSAT example problem.

The VADSAT output is attached to the end of this appendix. Figures N-2 and N-3 show the concentration in the receptor well over time and the mass loading rate to groundwater.

Table N-3. VADSAT Model Inputs for the Example Problem.

Model Control Parameters	Units	Value	Rationale
Allow volatilization?		yes	
Allow sorbed phase decay?		no	
Have code calculate dispersivity?		yes	
Source Zone Data			
Saturated conductivity of waste zone	[m/day]	8.6E-2	
Thickness of waste zone	[m]	2.5	= second and third layer from SESOIL example
Waste zone area	[m^2]	149	= 16.5 x 9 m
Length to width ratio	[m/m]	1.8	= 16.5/9 m
Thickness of soil cover	[m]	3	
Fraction organic carbon	[-]	0.005	
Vadose Zone Soil Parameters			
Fraction organic carbon	[-]	0.005	
Saturated conductivity	[m/day]	8.6e-2	
Depth to groundwater from bottom of source	[m]	0.75	
Effective porosity	[-]	0.25	
van Genuchten's n parameter	[-]	1.23	Use DSS Help system, parameter for sandy clay
Residual moisture content	[-]	0.12	field capacity (measured)
Net recharge rate	[m/day]	1.34E-4	10% of total precipitation
Saturated Zone (Aquifer) Parameters			
Effective porosity	[-]	0.25	
Fraction organic carbon	[-]	0.005	
Saturated conductivity	[m/day]	8.6e-2	
Hydraulic gradient	[m/m]	0.008	
Aquifer thickness	[-]	30	
Location of well-downgradient	[m]	55	
Location of well--cross-gradient	[m]	0	
Depth of well	[m]	0.5	
TPH Data			
Concentration of TPH mixture	[mg/kg]	845	measured
Molecular Weight of TPH	[g/mole]	95	for gasoline
Density of TPH	[g/cm^3]	0.95	for gasoline
Source Concentrations—Total concentration in soil [mg/kg]			
Benzene	[mg/kg]	12.5	max. conc. sampled

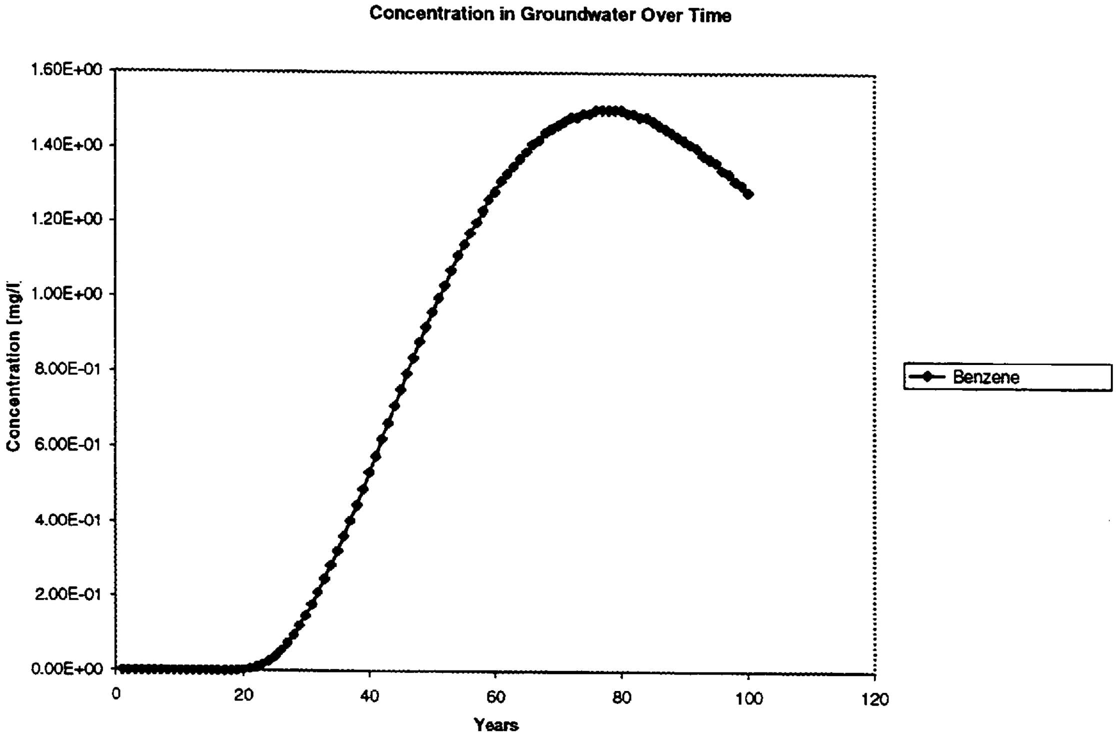

Figure N-2. Concentration in Receptor Well for Example Problem.

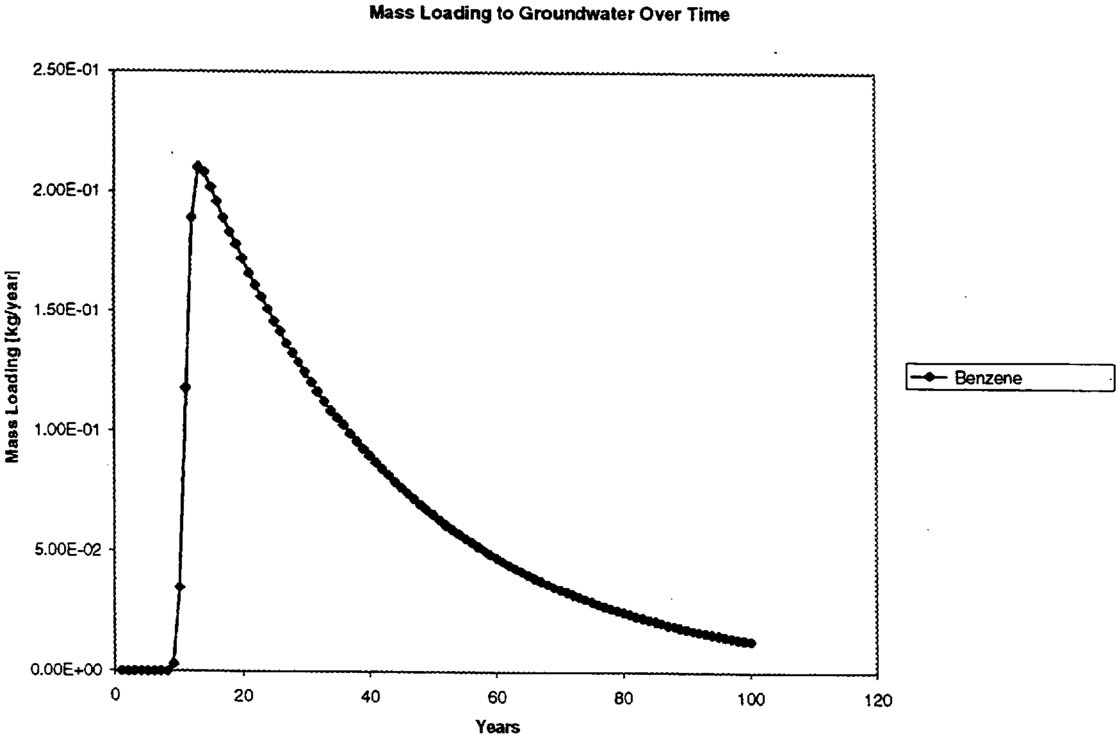

Figure N-3. Mass Loading to Groundwater for Example Problem.

Note: The results of this example are very different than those from the SESOIL example. There are several reasons for this:

- In the SESOIL model the volatilization was "dialed down" using a volatilization fraction of 0.2 and a lower permeability upper layer. In VADSAT the soil column is uniform and there is no easy way to limit volatilization (except to turn it completely off). The chemical parameters may be adjusted in VADSAT to "dial down" the amount volatilized.
- VADSAT limits the amount of each constituent leaching from the source according to the chemicals effective solubility. To duplicate this second process the chemical's effective solubility must explicitly be entered into chemical parameters for the SESOIL model. To run the SESOIL model in a similar fashion, the effective solubility should be entered explicitly in the SESOIL chemical parameters.
- VADSAT is predicting groundwater concentration in a downgradient well; the SESOIL example estimated groundwater concentrations in the mixing zone directly beneath the source.
- VADSAT assumes the source to be at a uniform concentration whereas in SESOIL the three lower layers all had different concentrations of benzene.
- VADSAT assumes a uniform, steady infiltration rate whereas SESOIL is run on a monthly time step with different infiltration rates for each month of the year.
- The infiltration rate entered in this example (5 cm/yr) doesn't match the annual average "groundwater runoff" calculated by SESOIL (~8 cm/yr). (Of course, these values can be adjusted.)
- VADSAT simulates dispersion in the vadose zone so the contaminant "front" is lessened; SESOIL does not consider dispersion so the contaminant "front" is sharper.

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van Genucten, M. Th. and Alves, W.J., 1982. Analytical Solutions of the One-Dimensional Convective-Dispersive Solute Transport Equation, United States Department of Agriculture, Technical Bulletin Number 1661.

```
VADSAT Output File
******************
DSS Fate and Transport

Chemicals in the analysis
Benzene

Number of years simulated:        100

   Volatilization will be considered.
   Degradation on the sorbed phase will not be considered.
   Dispersivity will be calculated.
***************************************************
                     VADSAT 3.0
***************************************************


    PROJECT TITLE:  Benzene

     SOURCE AND CHEMICAL DATA ****
     ----------------------------
    Thickness of waste zone (m)                    =     2.50000
    Waste zone area (m^2)                          =   149.00000
    Length/Width ratio for waste area (-)          =     1.80000
    Cover thickness (depth to waste) (m)           =     3.00000
    Initial volume fraction of contaminant(-)      =  .148E-01
    MASS OF CONTAMINANT PER MASS OF WASTE(mg/kg)=      12.50000
    Hydrocarbon mass fraction in waste (mg/kg)     =  845.

    CHEMICAL SPECIES           Benzene
     ------------------------------------------------
    Organic carbon partition coeff(cm^3/g)         =    58.90000
    Molecular weight of contaminant(g/mole)        =    78.00000
    Density of contaminant(g/cm^3)                 =      .88000
    Solubility of contaminant (g/m^3)              =  1750.00000
    Henry's constant (-)                           =  .228
    Diffusion coeff. in free air (m^2/day)         =  .760

     TPH (Hydrocarbon)
     ----------------
    Average mole. weight of hydrocarbon(g/mole)    =    95.00000
    Average density of hydrocarbon (g/cm^3)        =      .95000

     ** UNSATURATED ZONE INPUT PARAMETERS **
     --------------------------------------
    Unsaturated zone decay coeff(1/day)            =      .00000
    Unsaturated zone fraction organic carbon (-)   =      .00500
    Saturated conductivity (unsat. zone) (m/day)   =      .08600
    Depth to groundwater (m)                       =      .75000
    Unsaturated zone porosity (-)                  =      .25000
    Value of Van Genucten n parameter (-)          =     1.23000
    Residual water content (-)                     =      .12000
```

```
   ** SATURATED ZONE INPUT PARAMETERS **
    -------------------------------------
   Saturated zone decay coefficient (1/day)      =      .00000
   Saturated zone porosity (-)                   =      .25000
   Saturated zone organic carbon fration (-)     =      .00500
   Dispersivity ratio LONG/TRANSV. (-)           =     1.00000
   Dispersivity ratio TRANSV/VERT. (-)           =     1.00000
   Saturated zone hydraulic conductivity(m/day)  =      .08600
   Hydraulic gradient (m/m)                      =      .00800
   Aquifer thickness (m)                         =    30.00000
   Infiltration rate (m/day)                     =      .00013

   LOCATION OF RECEPTORS:

               X (M)           Y (M)           Z (M)
              10.0              .0              1.0

BREAKTHROUGH CURVES

             CONCENTRATIONS (mg/l) AT:

    TIME      THE WATER TABLE          RECEPTOR
   (years)   (below the source)          WELL
      1.00       0.0000E+00          0.0000E+00
      2.00       0.0000E+00          0.0000E+00
      3.00       0.0000E+00          0.0000E+00
      4.00       0.0000E+00          0.0000E+00
      5.00       0.0000E+00          0.0000E+00
      6.00       0.0000E+00          0.0000E+00
      7.00       2.3461E-10          0.0000E+00
      8.00       7.5607E-06          1.1156E-29
      9.00       6.2778E-03          1.9370E-22
     10.00       4.1897E-01          1.1667E-17
     11.00       4.7781E+00          4.5263E-14
     12.00       1.6210E+01          2.3782E-11
     13.00       2.5931E+01          2.8254E-09
     14.00       2.8815E+01          1.1010E-07
     15.00       2.8547E+01          1.8546E-06
     16.00       2.7703E+01          1.6621E-05
     17.00       2.6828E+01          9.2689E-05
     18.00       2.5978E+01          3.6196E-04
     19.00       2.5154E+01          1.0806E-03
     20.00       2.4357E+01          2.6319E-03
     21.00       2.3584E+01          5.4858E-03
     22.00       2.2836E+01          1.0137E-02
     23.00       2.2112E+01          1.7042E-02
     24.00       2.1411E+01          2.6582E-02
     25.00       2.0732E+01          3.9035E-02
     26.00       2.0075E+01          5.4571E-02
     27.00       1.9438E+01          7.3259E-02
     28.00       1.8822E+01          9.5080E-02
     29.00       1.8225E+01          1.1994E-01
     30.00       1.7647E+01          1.4769E-01
     31.00       1.7088E+01          1.7814E-01
     32.00       1.6546E+01          2.1105E-01
     33.00       1.6021E+01          2.4619E-01
```

```
34.00      1.5513E+01      2.8329E-01
35.00      1.5021E+01      3.2210E-01
36.00      1.4545E+01      3.6237E-01
37.00      1.4084E+01      4.0384E-01
38.00      1.3637E+01      4.4626E-01
39.00      1.3205E+01      4.8941E-01
40.00      1.2786E+01      5.3307E-01
41.00      1.2381E+01      5.7702E-01
42.00      1.1988E+01      6.2109E-01
43.00      1.1608E+01      6.6509E-01
44.00      1.1240E+01      7.0884E-01
45.00      1.0884E+01      7.5221E-01
46.00      1.0539E+01      7.9504E-01
47.00      1.0204E+01      8.3721E-01
48.00      9.8808E+00      8.7859E-01
49.00      9.5675E+00      9.1909E-01
50.00      9.2642E+00      9.5860E-01
51.00      8.9704E+00      9.9703E-01
52.00      8.6859E+00      1.0343E+00
53.00      8.4105E+00      1.0704E+00
54.00      8.1438E+00      1.1051E+00
55.00      7.8856E+00      1.1385E+00
56.00      7.6356E+00      1.1706E+00
57.00      7.3935E+00      1.2012E+00
58.00      7.1591E+00      1.2303E+00
59.00      6.9320E+00      1.2579E+00
60.00      6.7122E+00      1.2840E+00
61.00      6.4994E+00      1.3086E+00
62.00      6.2933E+00      1.3317E+00
63.00      6.0938E+00      1.3532E+00
64.00      5.9005E+00      1.3731E+00
65.00      5.7135E+00      1.3915E+00
66.00      5.5323E+00      1.4084E+00
67.00      5.3568E+00      1.4237E+00
68.00      5.1870E+00      1.4376E+00
69.00      5.0225E+00      1.4499E+00
70.00      4.8633E+00      1.4608E+00
71.00      4.7091E+00      1.4702E+00
72.00      4.5598E+00      1.4783E+00
73.00      4.4152E+00      1.4849E+00
74.00      4.2752E+00      1.4901E+00
75.00      4.1396E+00      1.4941E+00
76.00      4.0083E+00      1.4968E+00
77.00      3.8812E+00      1.4982E+00
78.00      3.7582E+00      1.4984E+00
79.00      3.6391E+00      1.4974E+00
80.00      3.5237E+00      1.4953E+00
81.00      3.4119E+00      1.4921E+00
82.00      3.3037E+00      1.4879E+00
83.00      3.1990E+00      1.4826E+00
84.00      3.0975E+00      1.4764E+00
85.00      2.9994E+00      1.4693E+00
86.00      2.9042E+00      1.4612E+00
87.00      2.8121E+00      1.4524E+00
88.00      2.7230E+00      1.4427E+00
89.00      2.6366E+00      1.4323E+00
```

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     90.00        2.5530E+00          1.4212E+00
     91.00        2.4721E+00          1.4094E+00
     92.00        2.3937E+00          1.3969E+00
     93.00        2.3178E+00          1.3839E+00
     94.00        2.2443E+00          1.3703E+00
     95.00        2.1731E+00          1.3562E+00
     96.00        2.1042E+00          1.3416E+00
     97.00        2.0375E+00          1.3265E+00
     98.00        1.9729E+00          1.3110E+00
     99.00        1.9103E+00          1.2952E+00
    100.00        1.8498E+00          1.2790E+00

MASS  OF CONTAMINANT REMAINING IN THE WASTE ZONE

   TIME             MASS/AREA      MASS FRAC. IN WASTE
  (YEARS)           (g/m^2)

       .00        6.2109E+01          1.2500E-05
      1.00        5.8233E+01          1.1720E-05
      2.00        5.6387E+01          1.1348E-05
      3.00        5.4599E+01          1.0988E-05
      4.00        5.2867E+01          1.0640E-05
      5.00        5.1191E+01          1.0303E-05
      6.00        4.9568E+01          9.9759E-06
      7.00        4.7996E+01          9.6596E-06
      8.00        4.6474E+01          9.3533E-06
      9.00        4.5001E+01          9.0568E-06
     10.00        4.3574E+01          8.7696E-06
     11.00        4.2192E+01          8.4915E-06
     12.00        4.0854E+01          8.2223E-06
     13.00        3.9559E+01          7.9616E-06
     14.00        3.8305E+01          7.7091E-06
     15.00        3.7090E+01          7.4647E-06
     16.00        3.5914E+01          7.2280E-06
     17.00        3.4775E+01          6.9988E-06
     18.00        3.3673E+01          6.7769E-06
     19.00        3.2605E+01          6.5620E-06
     20.00        3.1571E+01          6.3539E-06
     21.00        3.0570E+01          6.1524E-06
     22.00        2.9601E+01          5.9574E-06
     23.00        2.8662E+01          5.7685E-06
     24.00        2.7753E+01          5.5856E-06
     25.00        2.6873E+01          5.4085E-06
     26.00        2.6021E+01          5.2370E-06
     27.00        2.5196E+01          5.0709E-06
     28.00        2.4397E+01          4.9101E-06
     29.00        2.3624E+01          4.7544E-06
     30.00        2.2874E+01          4.6037E-06
     31.00        2.2149E+01          4.4577E-06
     32.00        2.1447E+01          4.3164E-06
     33.00        2.0767E+01          4.1795E-06
     34.00        2.0108E+01          4.0470E-06
     35.00        1.9471E+01          3.9186E-06
     36.00        1.8853E+01          3.7944E-06
     37.00        1.8256E+01          3.6741E-06
     38.00        1.7677E+01          3.5576E-06
```

```
    39.00       1.7116E+01       3.4448E-06
    40.00       1.6573E+01       3.3355E-06
    41.00       1.6048E+01       3.2298E-06
    42.00       1.5539E+01       3.1274E-06
    43.00       1.5046E+01       3.0282E-06
    44.00       1.4569E+01       2.9322E-06
    45.00       1.4107E+01       2.8392E-06
    46.00       1.3660E+01       2.7492E-06
    47.00       1.3227E+01       2.6620E-06
    48.00       1.2807E+01       2.5776E-06
    49.00       1.2401E+01       2.4959E-06
    50.00       1.2008E+01       2.4167E-06
    51.00       1.1627E+01       2.3401E-06
    52.00       1.1259E+01       2.2659E-06
    53.00       1.0902E+01       2.1941E-06
    54.00       1.0556E+01       2.1245E-06
    55.00       1.0221E+01       2.0571E-06
    56.00       9.8972E+00       1.9919E-06
    57.00       9.5834E+00       1.9287E-06
    58.00       9.2796E+00       1.8676E-06
    59.00       8.9853E+00       1.8084E-06
    60.00       8.7004E+00       1.7510E-06
    61.00       8.4245E+00       1.6955E-06
    62.00       8.1574E+00       1.6417E-06
    63.00       7.8987E+00       1.5897E-06
    64.00       7.6483E+00       1.5393E-06
    65.00       7.4058E+00       1.4905E-06
    66.00       7.1710E+00       1.4432E-06
    67.00       6.9436E+00       1.3974E-06
    68.00       6.7234E+00       1.3531E-06
    69.00       6.5102E+00       1.3102E-06
    70.00       6.3038E+00       1.2687E-06
    71.00       6.1039E+00       1.2285E-06
    72.00       5.9104E+00       1.1895E-06
    73.00       5.7230E+00       1.1518E-06
    74.00       5.5415E+00       1.1153E-06
    75.00       5.3658E+00       1.0799E-06
    76.00       5.1956E+00       1.0457E-06
    77.00       5.0309E+00       1.0125E-06
    78.00       4.8714E+00       9.8040E-07
    79.00       4.7169E+00       9.4932E-07
    80.00       4.5674E+00       9.1922E-07
    81.00       4.4225E+00       8.9007E-07
    82.00       4.2823E+00       8.6185E-07
    83.00       4.1465E+00       8.3452E-07
    84.00       4.0150E+00       8.0806E-07
    85.00       3.8877E+00       7.8244E-07
    86.00       3.7645E+00       7.5763E-07
    87.00       3.6451E+00       7.3360E-07
    88.00       3.5295E+00       7.1034E-07
    89.00       3.4176E+00       6.8782E-07
    90.00       3.3092E+00       6.6601E-07
    91.00       3.2043E+00       6.4489E-07
    92.00       3.1027E+00       6.2444E-07
    93.00       3.0043E+00       6.0464E-07
    94.00       2.9091E+00       5.8547E-07
```

```
      95.00       2.8168E+00        5.6691E-07
      96.00       2.7275E+00        5.4893E-07
      97.00       2.6410E+00        5.3153E-07
      98.00       2.5573E+00        5.1467E-07
      99.00       2.4762E+00        4.9835E-07

  Mass lost/area (g/m^2)

  Time (years)       Percolation      Volatilization

        .00       0.0000E+00        0.0000E+00
       1.00       2.9870E+00        8.8934E-01
       2.00       4.4098E+00        1.3130E+00
       3.00       5.7875E+00        1.7232E+00
       4.00       7.1215E+00        2.1204E+00
       5.00       8.4133E+00        2.5050E+00
       6.00       9.6640E+00        2.8774E+00
       7.00       1.0875E+01        3.2380E+00
       8.00       1.2048E+01        3.5872E+00
       9.00       1.3183E+01        3.9252E+00
      10.00       1.4283E+01        4.2526E+00
      11.00       1.5348E+01        4.5696E+00
      12.00       1.6378E+01        4.8766E+00
      13.00       1.7377E+01        5.1738E+00
      14.00       1.8343E+01        5.4615E+00
      15.00       1.9279E+01        5.7402E+00
      16.00       2.0185E+01        6.0100E+00
      17.00       2.1063E+01        6.2713E+00
      18.00       2.1913E+01        6.5243E+00
      19.00       2.2735E+01        6.7692E+00
      20.00       2.3532E+01        7.0064E+00
      21.00       2.4303E+01        7.2361E+00
      22.00       2.5050E+01        7.4585E+00
      23.00       2.5773E+01        7.6738E+00
      24.00       2.6474E+01        7.8824E+00
      25.00       2.7152E+01        8.0843E+00
      26.00       2.7808E+01        8.2798E+00
      27.00       2.8444E+01        8.4691E+00
      28.00       2.9060E+01        8.6523E+00
      29.00       2.9656E+01        8.8298E+00
      30.00       3.0233E+01        9.0017E+00
      31.00       3.0792E+01        9.1681E+00
      32.00       3.1333E+01        9.3292E+00
      33.00       3.1857E+01        9.4853E+00
      34.00       3.2365E+01        9.6363E+00
      35.00       3.2856E+01        9.7826E+00
      36.00       3.3332E+01        9.9243E+00
      37.00       3.3792E+01        1.0061E+01
      38.00       3.4238E+01        1.0194E+01
      39.00       3.4670E+01        1.0323E+01
      40.00       3.5089E+01        1.0447E+01
      41.00       3.5493E+01        1.0568E+01
      42.00       3.5886E+01        1.0685E+01
      43.00       3.6265E+01        1.0798E+01
      44.00       3.6633E+01        1.0907E+01
      45.00       3.6989E+01        1.1013E+01
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46.00     3.7334E+01     1.1116E+01
47.00     3.7667E+01     1.1215E+01
48.00     3.7991E+01     1.1311E+01
49.00     3.8303E+01     1.1405E+01
50.00     3.8606E+01     1.1495E+01
51.00     3.8900E+01     1.1582E+01
52.00     3.9184E+01     1.1667E+01
53.00     3.9459E+01     1.1749E+01
54.00     3.9725E+01     1.1828E+01
55.00     3.9983E+01     1.1905E+01
56.00     4.0233E+01     1.1979E+01
57.00     4.0475E+01     1.2051E+01
58.00     4.0709E+01     1.2121E+01
59.00     4.0936E+01     1.2188E+01
60.00     4.1155E+01     1.2254E+01
61.00     4.1368E+01     1.2317E+01
62.00     4.1574E+01     1.2378E+01
63.00     4.1773E+01     1.2438E+01
64.00     4.1966E+01     1.2495E+01
65.00     4.2153E+01     1.2551E+01
66.00     4.2334E+01     1.2605E+01
67.00     4.2509E+01     1.2657E+01
68.00     4.2679E+01     1.2707E+01
69.00     4.2843E+01     1.2756E+01
70.00     4.3002E+01     1.2804E+01
71.00     4.3156E+01     1.2849E+01
72.00     4.3305E+01     1.2894E+01
73.00     4.3450E+01     1.2937E+01
74.00     4.3589E+01     1.2978E+01
75.00     4.3725E+01     1.3019E+01
76.00     4.3856E+01     1.3058E+01
77.00     4.3983E+01     1.3096E+01
78.00     4.4106E+01     1.3132E+01
79.00     4.4225E+01     1.3168E+01
80.00     4.4340E+01     1.3202E+01
81.00     4.4452E+01     1.3235E+01
82.00     4.4560E+01     1.3267E+01
83.00     4.4664E+01     1.3298E+01
84.00     4.4766E+01     1.3329E+01
85.00     4.4864E+01     1.3358E+01
86.00     4.4959E+01     1.3386E+01
87.00     4.5051E+01     1.3414E+01
88.00     4.5140E+01     1.3440E+01
89.00     4.5226E+01     1.3466E+01
90.00     4.5310E+01     1.3491E+01
91.00     4.5390E+01     1.3515E+01
92.00     4.5469E+01     1.3538E+01
93.00     4.5545E+01     1.3561E+01
94.00     4.5618E+01     1.3582E+01
95.00     4.5689E+01     1.3604E+01
96.00     4.5758E+01     1.3624E+01
97.00     4.5824E+01     1.3644E+01
98.00     4.5889E+01     1.3663E+01
99.00     4.5951E+01     1.3682E+01
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