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INTERACTIVE SIMULATION OF THE FATE OF HAZARDOUS CHEMICALS DURING LAND TREATMENT OF OILY WASTES: RITZ USER'S GUIDE

by

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ABSTRACT

An interactive software system was developed to enable decision-makers to simulate the movement and fate of hazardous chemicals during land treatment of oily wastes. The mathematical model known as the Regulatory and Investigative Treatment Zone Model or RITZ was developed and published earlier by Short (1985). The model incorporates the influence of oil in the sludge, water movement, volatilization, and degradation upon the transport and fate of a hazardous chemical. This manual describes the conceptual framework and assumptions used by Short (1985) in developing the model. It then explains the micro-computer hardware and software requirements, the input parameters for the model, and the graphical and tabular outputs which can be selected. Illustrations of the use of the software are also included. The computational equations developed by Short (1985) are presented for completeness but are not derived.

FOREWORD

EPA is charged by Congress to protect the Nation's land, air and water systems. Under a mandate of national environmental laws focused on air and water quality, solid waste management and the control of toxic substances, pesticides, noise and radiation, the Agency strives to formulate and inplement actions which lead to a compatible balance between human activities and the ability of natural systems to support and nurture life.

The Robert S. Kerr Environmental Research Laboratory is the Agency's center of expertise for investigation of the soil and subsurface environment. Personnel at the Laboratory are responsible for management of research programs to: (a) determine the fate, transport and transformation rates of pollutants in the soil, the unsaturated and the saturated zones of the subsurface environment; (b) define the processes to be used in characterizing the soil and subsurface environment as a receptor of pollutants; (c) develop techniques for predicting the effect of pollutants on ground water, soil, and indigenous organisms; and (d) define and demonstrate the applicability and limitations of using natural processes, indigenous to the soil and subsurface environment, for the protection of this resource.

This user's guide serves the purpose of instructing the user to the execution of a software package based on the Regulatory and Investigative Treatment Zone (RITZ) model. The guide should allow easy access to information critical to the development of an understanding of the transport and fate of hazardous chemicals applied during land treatment.

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INTRODUCTION

The Regulatory and Investigative Treatment Zone Model, RITZ, (Short, 1985) was developed to help decision-makers systematically estimate the movement and fate of hazardous chemicals during land treatment of oily wastes. The model considers the downward movement of the pollutant with the soil solution, volatilization and loss to the atmosphere, and degradation. The model incorporates the influence of oil upon the transport and fate of the pollutant. This RITZ model forms the basis of this interactive software system. The software enables users to conveniently enter the required soil, chemical, environmental, and management parameters and checks the validity of these entries. The user may then select graphical and tabular outputs of the quantities of interest.

This manual describes the basic concepts of RITZ and lists the inherent assumptions. The manual, also, describes the use of the interactive software and the hardware and software requirements for it. Illustrative examples of the software are presented. The appendix includes a list of the mathematical equations used in the software.

BASIC CONCEPTS, ASSUMPTIONS, AND LIMITATIONS

A land treatment site is illustrated in Figure 1. The treatment site consists of two soil layers called the plow zone and the treatment zone. The sludge (waste material) containing oil and pollutant is applied to the plow zone. It is thoroughly mixed with the soil in that layer. As time passes the pollutant and oil are degraded. Some of the pollutant is carried down through the soil with percolating water. Some of the pollutant is volatilized and moves into the air above the treatment site.

Figure 1. Diagram of land treatment site.

The following assumptions were made by Short (1985) in developing this model.

1. Waste material is uniformly mixed in the plow zone.

2. The oil in the waste material is immobile. It never leaves the plow zone. Only the pollutant moves with the soil water.

3. The soil properties are uniform from the soil surface to the bottom of the treatment zone. This assumption will rarely, if ever, be met in the field. The user can estimate the impact of non-uniform soils by comparing results for several simulations covering the range of soil properties present at the site.

4. The flux of water is uniform throughout the treatment site and throughout time. This assumption will rarely be met in the field.

5. Hydrodynamic dispersion is insignificant and can be neglected. This assumption gives rise to sharp leading and trailing edges in the pollutant slug. These sharp fronts will not exist in soils. As a result, the pollutant will likely reach any depth in the treatment zone before the time predicted and it will remain at that depth longer than predicted by the model.

6. Linear isotherms describe the partitioning of the pollutant between the liquid, soil, vapor, and oil phases. Local equilibrium between phases is assumed.

7. First order degradation of the pollutant and oil are assumed. Degradation constants do not change with soil depth or time. This assumption ignores changes in biological activity with soil depth. It also ignores the influence of loading rate, temperature, and the quality of the environment for microorganisms upon the degradation rate.

8. The pollutant partitions between the soil, oil, water, and soil vapor and does not partition to the remaining fractions of the sludge.

9. The sludge does not measurably change the properties of the soil water or the soil so the pore liquid behaves as water.

10. The water content of the soil is related to the hydraulic conductivity as described by Clapp and Hornberger (1978). That is,

$$\frac{k}{k_s} = \left(\frac{\theta}{\theta_s}\right)^{2b+3}$$

where k is the hydraulic conductivity at a volumetric water content of θ, k_s is the saturated hydraulic conductivity or the conductivity of the soil at the saturated water content, θ_s, and b is the Clapp and Hornberger constant for the soil.

Field validation of the model is in progress. The user is cautioned to consider the assumptions in the model and to apply the model only where appropriate. The writers are aware the assumptions are only simplistic approximations to the continuum of nature. Many of the assumptions were made to either simplify the mathematical solution or because there was insufficient experimental data to permit more realistic descriptions of the system.

The model presents results for the specific parameters entered without any measure of uncertainty in the calculated values. The user is encouraged to compare results for a series of simulations using parameters in the expected ranges for the site to obtain an estimate of this uncertainty. For example, if the site contains two soil layers, the user may want to run the simulation twice, once for the soil properties of each Layer.

SOFTWARE OVERVIEW

The software can be divided functionally into the following three parts.

1. Parameter Entry — This part of the program enables the user to define the land treatment system to be modeled. This includes specification of the soil parameters, properties of the pollutant and oil, and environmental and management parameters. These user inputs can be made by means of a data entry editor which allows the user to move the cursor around the screen to enter or modify parameters in any sequence. These inputs may be saved in disk files for use at a later time. The values entered are verified as much as possible as they are entered. When the user has finished entering the parameters, a final check is made to determine if the set of parameters is consistent as a whole.

2. Output Selection — This part of the program enables the user to specify the desired graphs and tables. The user may also specify the desired output device. Tabular outputs from the model may be directed to the screen, printer, or a text file. These entries are also made by means of the data entry editor.

   Graphical outputs available in this software include the following:

   1. A circle graph of mass balance indicating the portions of the pollutant leached, volatilized, and degraded.

   2. A line graph of the pollutant volatilized as a function of time.

   3. A line graph of the pollutant leached below the treatment zone as a function of time.

   4. A line graph of the position of the top and bottom of the pollutant as a function of time.

   5. A line graph of the concentration of pollutant as a function of time for selected depths.

   6. A line graph of the concentration of pollutant as a function of depth at selected times.

   7. Bar graphs of the concentration of pollutant in different phases as functions of time and depth.

Tabular outputs include:

1. Input soil, pollutant, oil, environmental, and operational parameters.

2. Calculated parameters relating to the treatment system.

3. The amount of pollutant volatilized, leached, and degraded and the computational mass balance error.

4. The quantity of pollutant volatilized as a function of time.

5. The quantity of pollutant leached below the treatment zone as a function of time.

6. The position of the top and bottom of the pollutant as a function of time.

7. The concentration of pollutant in different phases as a function of time at selected depths.

8. The concentration of pollutant in different phases as a function of depth at selected times.

3. Computations/Display This part of the software performs the specified calculation and displays the desired results.

When the software is executed, an introductory screen is displayed followed by the parameter entry screens. When the user has finished entering the parameters and the entries are verified, the output selection screen is selected. When the desired outputs have been specified, the computations and outputs are displayed. When all of the outputs have been displayed the system returns to the output selection screen. This provides the user with the opportunity to obtain additional outputs for the same input parameters. If no additional outputs are desired, the user may return to the parameter entry screen by pressing the <Esc> key. Each time the user returns to the data entry editor, the values selected most recently are displayed. Thus, only the parameters to be changed need to be entered. Thus if a series of pollutants are to be simulated for one treatment site, the soil, environmental, and management parameters need to be entered only once. Repeated simulations can be made easily by simply modifying the properties of the pollutant.

Illustrations of the operation of the software follow a description of the operating conventions.

HARDWARE AND SOFTWARE REQUIREMENTS

This software requires an IBM® with at least 256K bytes of random access memory, one floppy disk drive, and an 8087 or 80287 math coprocessor. An IBM color/graphics board and a compatible monitor are required to fully utilize the software with graphics. A monochrome card and monitor can be used for tabular output only. A printer is useful but not essential. If the printer is compatible with the IBM graphics printer, copies of the graphics may be printed.

The operating system must be PC-DOS or MS-DOS version 2.0 or later. The GRAPHICS.COM file from your DOS diskette must be executed before executing this software to obtain copies of the graphics on the printer.

OPERATING CONVENTIONS

The following conventions are used throughout this software.

1. Program Interruption: The user may interrupt the program at any time the system is asking for an input by pressing the <Esc> key. Control in the program reverts to the previous data entry screen. If the <Esc> key is pressed from within the parameter entry option, the program is terminated and control is returned to the disk operating system.

2. Special Keys: Cursor control keys and function keys are used in the data entry editor. The keys and their functions are listed below.

   <Up Arrow> This key is used to move up one line in the editor. If the cursor is already on the first entry on the screen, the cursor moves to the last entry on the screen.

   <Down Arrow> This key is used to move down one line in the editor. If the cursor is already in the last entry on the screen, the cursor moves to the first entry.

   <Right Arrow> This key is used to move the cursor one character to the right. If the cursor is at the right end of the entry on the line, this key does nothing.

   <Left Arrow> This key is used to move the cursor one character to the left. If the cursor is under the left character in the entry, this key does nothing.

   <End> This key moves the cursor from its present position to the beginning of the last entry on the screen.

   <Home> This key moves the cursor from its present position to the beginning of the first entry on the screen.

<PgDn>	The parameter entry process requires three screens. One screen is for soil properties, one for pollutant and oil properties, and one for environmental and operational parameters. In this case, the <PgDn> key moves to the next screen in thee series. For example, if the screen for soil properties is displayed, pressing this key will display the pollutant and oil properties screen. Pressing it again will display the operational and environmental screen.
<PgUp>	This key is used to move to the previous screen when entering the land treatment site parameters.
<F1>	This key is used to obtain brief help messages relating to the parameter being entered.
<F2>	This key is used to enter and calculate a weighted average value of a soil parameter from values for different soil depths. See the Appendix for details.
<F7>	If the parameters entered into this model at one time have been saved in a file, those values can be input to the system from the file. The <F7> key enables the user to specify the name of the input file. If the file exists, its values are input and displayed by the editor. If the file is not found, the values in the editor remain unchanged. The user may view the directory of a disk by pressing <F1> when the file name is requested.
<F8>	Parameters entered into the system can be saved in disk files for use at another time. Pressing the <F8> key enables the user to specify the name of an output file. After the file is specified, the present soil, chemical and environmental parameters are written to disk. Pressing <F1> when the output file is requested enables the user to view a disk directory.
<F10>	This key is used to terminate data entry on a particular screen and to proceed to the next phase of the program.
<Esc>	This key is used to interrupt the present process and to return to the previous data entry screen.
<Enter>	This key is used to terminate entry of a particular parameter. Any characters to the right of the cursor are truncated when the <Enter> key is pressed.

<Backspace> This key is used to delete one character to the left of the cursor. If the cursor is at the beginning of the entry, nothing is deleted.

<Delete> This key is used to delete the character at the present cursor location.

3. File Names: File names may be any legal MS-DOS filename. File extensions may be used to facilitate organization of files.

4. Unknown Parameters: When entering parameters into the editor, the user may signify that a value is unknown by entering only a period or decimal point. Entering a period for an input parameter defining the land treatment site will result in further prompting for the entry. In many cases, the additional prompt will provide additional information about the required parameter. It may also provide a method of estimating the parameter from other parameters which may be known.

5. Specifying No Data: When tables or graphs of concentration as functions of time or depth are selected as outputs, the user has opportunity to specify 15 times or depths of interest. If fewer times or depths are desired, 'no data' can be specified for the remaining entries. No data is specified by entering a period or decimal point instead of a number.

6. Copy Graphics On Printer: When graphs are displayed on the screen, they can be printed on an IBM graphics printer or a compatible machine by pressing the <P> key or the <Shift> and <PrtScr> keys. The <P> key results in smaller copies of the screen. The GRAPHICS.COM must be executed before RITZ if copies of graphs will be made.

GETTING STARTED

Making a Working Copy: The software is distributed on a single diskette. The first step is to make a working copy of the software. The original copy should then be placed in a safe place. The following steps can be followed to make a working copy.

Fixed Disk Systems

1. Make a new directory for the RITZ model using the MKDIR command of DOS. For example:
   MKDIR \RITZ <Enter>

2. Copy the contents of the distribution diskette to the new directory using the COPY command of DOS. If the distribution diskette is in disk drive A, enter the following command:
   COPY A:*.* \RITZ /V <Enter>

Floppy Disk Systems

1. FORMAT a new floppy diskette with the /S option. To do this place your DOS diskette in drive A and a new diskette in drive B. Then enter
   FORMAT B:/S <Enter>

2. If you have a color/graphics card, copy the GRAPHICS.COM program from the DOS diskette to the working diskette using the COPY command. To do this enter
   COPY A:GRAPHICS.COM B: /V <Enter>

3. Copy the contents of the distribution diskette to the new diskette using the COPY command. This can be done by removing the DOS diskette in drive A and replacing it with the distribution diskette and entering the command
   COPY A:*.* B: /V <Enter>

Details on the use of the COPY, FORMAT, and MKDIR commands are given in your DOS manual.

The software is distributed to run on a system with a color graphics card. If your computer has this card, your working copy is now complete. If your computer does not have this card, you will need to execute the configuration program included on the diskette. To configure the software for a monochrome system

1. In a floppy disk system, place the working diskette in the default disk drive. In a fixed disk system, use the CD command to make the directory containing the RITZ software the default directory.

2. Execute program CONFIG by entering

   CONFIG <Enter>

   The program will ask you to specify the type of monitor. Specify the monitor matching that in your system. The program will modify the RITZ software for your system. The software on the working diskette should then be ready for use.

Executing the Program: To execute the program,

1. Place the floppy diskette in the default disk drive (or define the directory containing the software to be the default directory).

2. Enter GRAPHICS <Enter> to install the memory resident software for printing graphics screens.

3. Enter RITZ <Enter> to execute the model.

You may find it more convenient to make a batch file to execute steps 2 and 3 as one command. This file would contain the following lines:

```
GRAPHICS
RITZ
```

EXAMPLE OF SOFTWARE USE

RITZ

REGULATORY AND INVESTIGATIVE TREATMENT ZONE MODEL

This software is designed to estimate the movement and fate of chemicals applied as oily wastes in land treatment sites. The user is required to enter the properties of the chemicals and oil in the waste material, the soil properties of the treatment site, the management practices used, and the relevant parameters describing the environment at the site. Outputs of the model include the quantity of the pollutant degraded, leached, and volatilized, the concentration of pollutant in the different phases at different times and depths, and the quantity of pollutant volatilized and leached as a function of time. Outputs may be displayed in graphical and tabular forms.

This software was developed by D.L. Nofziger and J.R. Williams, Oklahoma State University, Stillwater, Oklahoma. The software is based on a mathematical model of the treatment zone developed by Thomas E. Short, R.S. Kerr Environmental Research Laboratory, Ada, Oklahoma.

Press any key to continue:

Screen 1. Purpose of the program.

Introduction: The first screen which appears when the software is run is displayed in Screen 1. This gives the user the purpose of the software and the individuals responsible for it.

Parameter Entry: This part of the software enables the user to define the properties of the treatment site and chemicals. The data entry editor is used for this purpose. (See OPERATING CONVENTIONS for details on the use of the editor.) Three screens are used for these inputs. The <PgUp> and <PgDn> keys can be used to move from one screen to another. Values shown in this manual are for illustration only.

Soil Properties	
Identification code	: Site #1
Soil name	: Tipton Sandy Loam
Fraction organic carbon	: 0.0050
Bulk density, kg/m3	: 1500
Saturated water content, m3/m3	: 0.410
Sat. hydraulic conductivity, m/day	: 5.0000E-001
Clapp and Hornberger constant	: 4.9000

<F1> : Display help for entries
<F2> : Average across depths
<F7> : Input parameters from data file
<F8> : Save parameters in output data file
<F10> : Proceed - all entries made
<Esc> : Abort program
<PgUp>, <PgDn> : Edit other entry screens

Screen 2. Data entry screen for soil properties.

Screen 2 is the screen used for defining the soil properties of the treatment site. Since the model assumes the soil at the treatment site is uniform with depth, only one value is entered for each property. If the soil is not uniform with depth, the user may obtain an average from known values at different depths by pressing the <F2> key. The averaging scheme used is described in the Appendix. If the site is not uniform from one position to another, the user may obtain a spatial average for use in this model or the model may be run several times for different smaller sites. The parameters to be entered on this screen are

1. Identification code: This is simply a string of characters which serve to identify this set of data for the user's reference. It is displayed with outputs from the program.

2. Soil name: This again serves to identify the soil at the treatment site.

3. Fraction organic carbon (f_{OC}): This is the ratio of the mass of organic carbon in the soil to the mass of soil solids.

4. Bulk density (ρ): This is the ratio of the mass of soil solids to the total volume of the soil. That is, it is the ratio of the mass of solids to the volume of solids, liquids, and gases in the soil.

5. Saturated water content (θ_s): This is the ratio of the volume of water in the soil to the total volume of the soil when the soil pores are filled with water.

6. Saturated hydraulic conductivity (k_s): This is the hydraulic conductivity of the soil when all of the soil pores are filled with water. It is the constant of proportionality between the flux density and the gradient in potential in Darcy's law.

7. Clapp and Hornberger constant (b): This is the constant in the equation of Clapp and Hornberger (1978) relating the relative saturation of the soil to the relative conductivity of the soil. That is

$$\frac{\theta}{\theta_s} = \left(\frac{k}{k_s}\right)^{2b+3}$$

where k is the hydraulic conductivity of the soil at a volumetric water content θ and k_s is the saturated hydraulic conductivity at the saturated water content, θ_s.

Oil and Pollutant Properties	
Name of pollutant in sludge	: Pollutant#1
CAS number	: 123-4567
Concentration of pollutant in sludge, g/kg	: 1.0000E+000
Organic carbon partition coefficient, m3/kg	: 2.2000E-002
Oil-water partition coefficient	: 5.0000E+001
Henry's law constant	: 5.5000E-005
Diffusion coef. of pollutant in air, m2/day	: 4.3000E-001
Half-life of pollutant, days	: 3.0000E+001
Concentration of oil in sludge, g/kg	: 2.5000E+002
Density of oil, kg/m3	: 1.0000E+003
Half-life of oil, days	: 4.5000E+001

<F1> : Display help for entries
<F7> : Input parameters from data file
<F8> : Save parameters in output data file
<F10> : Proceed - all entries made
<Esc> : Abort program
<PgUp>, <PgDn> : Edit other entry screens

Screen 3. Data entry screen for pollutant and oil properties.

Screen 3 is used to enter the properties of the pollutant and the oil in the waste material. These entries are described below.

1. Name of the pollutant in sludge: This is the name of the pollutant whose properties are entered below. This name is for identifying output tables and graphs.

2. CAS number: This unique Chemical Abstracts Number may be entered to provide positive identification for the pollutant being modeled. This number is also displayed with the outputs.

3. Concentration of pollutant in sludge (S_p): This is the concentration of the pollutant in the sludge when it was applied to the soil.

4. Organic carbon-water partition coefficient (K_{OC}): This is the partition coefficient between the pollutant in soil and water normalized to the soil's organic carbon content. That is

$$C_s = K_{oc} f_{oc} C_w$$

where C_S and C_W are the concentrations of pollutant in the soil and water, respectively, and f_{OC} is the fraction organic carbon in the soil.

5. Oil-water partition coefficient (K_o): This is the partition coefficient for the pollutant between the oil and water phases.
   That is

$$C_O = K_o C_W$$

   where C_O and C_W are the concentrations of the pollutant in the oil and water phases, respectively, and K_o is the oil-water partition coefficient.

6. Henry's law constant (K_H): This is the constant for partitioning the pollutant between the vapor and water phases. That is

$$C_V = K_H C_W$$

   where C_V and C_W are the concentrations of the pollutant in the vapor and water phases, respectively.

7. Diffusion coef. of pollutant in air (D_A): The diffusion coefficient of the pollutant in air is used to determine pollutant losses in the vapor phase.

8. Half-life of the pollutant ($t_{½P}$): This is the time required for one-half of the original amount of pollutant to be transformed to some other product. It is based on the assumption that the transformation follows first-order or pseudo first-order kinetics.

9. Concentration of oil in the sludge (S_o): This is the concentration of oil in the sludge at the time of application.

10. Density of oil (ρ_o): This is the density of the oil in the sludge. That is, it is the mass of oil per unit volume of oil.

11. Half-life of oil ($t_{½o}$): This is the time required for one-half of the original amount of oil in the sludge to be biologically degraded. It is based on the assumption that the transformation of the oil in the sludge will follow first-order kinetics.

Operational and Environmental Factors

Sludge application rate, kg/ha	: 1.5000E+005
Plow zone depth, m	: 0.150
Treatment zone depth, m	: 1.500
Recharge rate, m/day	: 0.0060
Evaporation rate, m/day	: 0.0025
Temperature, degrees C	: 25.0
Relative humidity	: 0.500
Diffusion coef. of water vapor in air, m2/day	: 2.0000E+000

<F1> : Display help for entries
<F7> : Input parameters from data file
<F8> : Save parameters in output data file
<F10> : Proceed - all entries made
<Esc> : Abort program
<PgUp>, <PgDn> : Edit other entry screens

Screen 4. Data entry screen for operational and environmental factors.

Screen 4 is used to enter or edit data relating to the operation of the treatment site and the environment at the site. The parameters needed include the following:

1. Sludge application rate (SAR): This is the mass of sludge or waste material applied per hectare of land area.

2. Plow zone depth (pzd): This is the depth to which the sludge or waste material is incorporated. See Figure 1 for more information.

3. Treatment zone depth (tzd): This is the depth of the bottom of the soil considered to be part of the treatment zone. Chemical movement below this depth is lost from the system and is considered as leached.

4. Recharge rate (V_d): This is the average downward flux density of water through the treatment zone.

5. Evaporation rate (E): This is the average flux density of water evaporating from the soil.

6. Air temperature (T): This is the average air temperature at the site.

7. Relative humidity (RH): This is the average relative humidity at the site expressed as a fraction (rather than a percent).

8. Diffusion coef. of water vapor in air (D_W): This diffusion coefficient of water vapor in air is used to estimate the vapor losses of the pollutant.

The keyboard will be the primary method of entering parameters into the model. However, the software enables the user to save manually entered values in data files for use at a later time. This is done from within the data entry editor by meansof the <F7> and <F8> function keys as explained in the section on OPERATING CONVENTIONS. When saving data, the system will request the name of the output file from the user. It will then write the current values of the input parameters in that file. When reading parameters from a file, the system will prompt the user for the name of the input file. The data will then be read and the editing screens updated to those values. When naming input and output files, the user is advised to develop a system of names and extensions which will facilitate identification of the file contents. When a file name is requested, the user may press the <F1> key to view a directory of files.

Output Options	
Graphs:	
Mass balance	: Y
Pollutant volatilized vs. time	: Y
Pollutant leached vs. time	: Y
Position of pollutant vs. time	: Y
Concentration vs. time at selected depths	: Y
Concentration vs. depth at selected times	: Y
Concentration bar graphs	: Y
Tables:	
Input parameters	: Y
Calculated parameters	: Y
Mass balance	: Y
Pollutant volatilized vs. time	: Y
Pollutant leached vs. time	: Y
Position of pollutant vs. time	: Y
Concentration vs. time at selected depths	: Y
Concentration vs. depth at selected times	: Y
Output device for tables	: SCREEN

<F1> : Display help for entries
<F10> : Proceed - all entries made
<Esc> : Abort option and return to parameter entry screen

Screen 5. Screen for selection of desired outputs from model.

Output Selection: This portion of the software enables the user to select the types of outputs desired and the desired output device. This selection process begins with Screen 5. If any concentration outputs are selected, one or two additional screens are required to select the depths and times of interest. The use of the three screens are illustrated in this section.

Screen 5 illustrates the selection of outputs from the model. For each option, the user enters Y if that option is desired or N if it is not desired. In this example, all the entries are Y to generate all the possible types of output. The entries on Screen 5 are as follows:

1. Graphs:
   a. Mass balance: This option displays a pie chart of the relative amount of the pollutant degraded, leached, and volatilized.

   b. Pollutant volatilized vs. time: This option displays a graph of the flux density of pollutant removed from the treatment site in the vapor phase as a function of time.

c. Pollutant leached vs. time: This option displays a graph of the flux density of pollutant leached from the treatment zone as a function of time.

d. Position of pollutant vs. time: This option displays a graph of the location of the top and bottom of the pollutant as a function of time.

e. Concentration vs. time at selected depths: This option displays a graph of the concentration of pollutant as a function of time at one or more depths selected by the user using Screen 6. Graphs of the total concentration of pollutant and concentrations in water, soil, vapor, and oil phases are displayed sequentially. For each phase, the software displays a depth and draws the line for that depth. It then waits for the user to press a key. If that key is not <N>, <P>, or <Esc> the system will display the line for the next depth selected. If <N> is pressed, the remaining depths for this phase are not drawn and the system proceeds to draw the graph for the next phase. If <P> is pressed, the screen is printed on the printer. If <Esc> is pressed, the system returns to Screen 5.

f. Concentration vs. depth at selected times: This option displays a graph of the concentration of pollutant as a function of depth for one or more times selected by the user using Screen 7. This option operates in the same manner as the concentration vs. time graphs described above.

g. Concentration bar graphs: This option presents a series of bars representing the treatment zone. Within each bar the concentration of pollutant in one phase at a particular time is displayed qualitatively using one of six patterns. The bars are redrawn for different times selected by the user (Screen 7). In this way the user can see the change in depth and concentration of the pollutant with changes in time. Different bars on the screen represent the total concentration of pollutant, pollutant concentration in water, soil, vapor, and oil, and the oil content.

2. Tables:

a. Input parameters: This table displays the parameters entered by the user to define the current scenario.

b. Calculated parameters: This table contains selected chemical and physical parameters calculated from the input parameters.

c. Mass balance: This table lists the absolute and relative amounts of pollutant degraded, volatilized, and leached along with the mass balance error.

d. Pollutant volatilized vs. time: This is a table of the flux density of pollutant leaving the treatment site in the vapor phase as a function of time.

e. Pollutant leached vs. time: This is a table of the flux density of pollutant leached from the treatment zone as a function of time.

f. Position of pollutant vs. time: This table displays the location of the top and bottom of the pollutant slug at different times.

g. Concentration vs. time at selected depths: This table contains the total pollutant concentration, the concentration of pollutant in water, soil, vapor, and oil, and the oil content at user selected times and depths. These tables are structured so that concentrations for all times at one depth occur on one page.

h. Concentration vs. depth at selected times: This table is similar to that described above. It differs in that the output is organized so that concentrations for all depths and one time occur on one page.

i. Output device for tables: Tabular output can be displayed on the screen or printer. It may also be saved in disk files for later use. This line enable the user to specify the desired device. Entries in this line may be <u>SCREEN</u>, <u>PRINTER</u>, or a legal file name.

If one or more of the concentration options is desired the depths or times desired are entered using Screens 6 and 7, respectively. In each case the user enters the depths or times of interest. A period indicates 'no data' or no value.

<u>Outputs of Model</u>: The following pages illustrate the outputs from the RITZ model for the inputs shown in screens 2, 3, and 4 and the outputs selected in screens 5, 6, and 7. Graphical outputs were generated by pressing the <P> key.

```
Depths of Interest
          Depth  1 (meters) : 0.00
          Depth  2 (meters) : 0.05
          Depth  3 (meters) : 0.10
          Depth  4 (meters) : 0.15
          Depth  5 (meters) : 0.25
          Depth  6 (meters) : 0.50
          Depth  7 (meters) : 0.75
          Depth  8 (meters) : 1.00
          Depth  9 (meters) : 1.25
          Depth 10 (meters) : 1.50
          Depth 11 (meters) : .
          Depth 12 (meters) : .
          Depth 13 (meters) : .
          Depth 14 (meters) : .
          Depth 15 (meters) : .


       <F1> : Display help for entries
      <F10> : Proceed - all entries made
      <Esc> : Abort option and return to output option screen
```

Screen 6. Selection of depths of interest for concentration tables and graphs.

```
Times of  Interest
          Time  1 (days) : 0.00
          Time  2 (days) : 10.00
          Time  3 (days) : 20.00
          Time  4 (days) : 30.00
          Time  5 (days) : 40.00
          Time  6 (days) : 50.00
          Time  7 (days) : 75.00
          Time  8 (days) : 100.00
          Time  9 (days) : .
          Time 10 (days) : .
          Time 11 (days) : .
          Time 12 (days) : .
          Time 13 (days) : .
          Time 14 (days) : .
          Time 15 (days) : .


       <F1> : Display help for entries
      <F10> : Proceed - all entries made
      <Esc> : Abort option and return to output option screen
```

Screen 7. Selection of times of interest for concentration table and graphs

Table 1. Table of input parameters describing land treatment site.

INPUT DATA - SOIL PROPERTIES

Fraction organic carbon	: 0.0050
Bulk density (kg/m3)	: 1500.0
Saturated water content (m3/m3)	: 0.4100
Saturated hydraulic conductivity (m/day)	: 5.0000E-001
Clapp and Hornberger constant	: 4.9000

INPUT DATA - OIL AND POLLUTANT PROPERTIES

Concentration of pollutant in the sludge (g/kg)	: 1.0000E+000
Organic carbon partition constant (m3/kg)	: 2.2000E-002
Oil-water partition coefficient	: 5.0000E+001
Henry's law constant	: 5.5000E-005
Diffusion coefficient of pollutant in air (m2/day)	: 4.3000E-001
Half-life of the pollutant (day)	: 3.0000E+001
Concentration of oil in the sludge (g/kg)	: 2.5000E+002
Density of the oil (kg/m3)	: 1.0000E+003
Half-life of the oil (day)	: 4.5000E+001
Diffusion coefficient of water vapor in air (m2/day)	: 2.0000E+000

INPUT DATA - OPERATIONAL AND ENVIRONMENTAL FACTORS

Sludge application rate (kg/ha)	: 1.5000E+005
Plow zone depth (m)	: 0.150
Treatment zone depth (m)	: 1.500
Recharge rate (m/day)	: 0.0060
Evaporation Rate (m/day)	: 0.0025
Air Temperature (deg C)	: 25.0
Relative humidity	: 0.500

Identification Code: Site #1
Soil Name: Tipton Sandy Loam
Compound Name: Pollutant#1
CAS Number: 123-4567 RITZ

Table 2. Table of calculated parameters for site described in Table 1.

CALCULATED PARAMETERS

Ratio of the density of water vapor to liquid	: 2.3E-005
Boundary layer thickness (m)	: 4.6E-003
Soil-water partition coefficient (m3/kg)	: 1.1E-004
Degradation rate constant of pollutant (1/day)	: 2.3E-002
Degradation rate constant of oil (1/day)	: 1.5E-002
Water content of soil (m3/m3)	: 2.9E-001
Soil pore water velocity (m/day)	: 2.1E-002
Initial oil content in the plow zone (m3/m3)	: 2.5E-002
Initial pollutant content in the plow zone (g/m3)	: 1.0E+002
Air content of the soil (m3/m3)	: 9.5E-002
Effective diffusion coefficient of pollutant vapor in soil (m2/day)	: 9.9E-004
Initial pollutant loading (g/m2)	: 1.5E+001

BASIC INFORMATION ABOUT THE SYSTEM

Maximum residence of the pollutant in the plow zone (days)	: 35
Maximum residence of the pollutant in the treatment zone (days)	: 138
Treatment zone breakthrough time (days)	: 102
Retardation factor in the lower treatment zone	: 1.6E+000
Velocity of the pollutant in the lower treatment zone (m/day)	: 1.3E-002

Identification Code: Site #1
Soil Name: Tipton Sandy Loam
Compound Name: Pollutant#1
CAS Number: 123-4567 RITZ

Table 3. Mass balance table summarizing the amount of pollutant degraded, volatilized, and leached as well as the computational error.

MASS BALANCE

	Mass of Pollutant g/m2	Relative Amount %
Amount loaded	1.5E+001	1.0E+002
Amount degraded	1.4E+001	9.4E+001
Amount volatilized	7.7E-003	5.1E-002
Amount leached	9.4E-001	6.3E+000
Computational error	4.8E-009	3.2E-008

Identification Code: Site #1
Soil Name: Tipton Sandy Loam
Compound Name: Pollutant#1
CAS Number: 123-4567 RITZ

Figure 2. Mass balance graph summarizing information in Table 3.

Table 4. The flux density of pollutant lost to the atmosphere as a function of time.

VAPOR FLUX VERSUS TIME

Time days	Flux g/m2-day	Time days	Flux g/m2-day	Time days	Flux g/m2-day
0.00	3.0E-001	19.78	3.2E-005	42.42	7.0E-006
1.55	5.7E-004	21.04	3.0E-005	49.74	4.3E-006
3.09	2.8E-004	22.29	2.7E-005	57.05	2.8E-006
4.60	1.8E-004	23.53	2.5E-005	64.37	1.9E-006
6.09	1.3E-004	24.75	2.4E-005	71.69	1.4E-006
7.55	1.1E-004	25.95	2.2E-005	79.00	1.0E-006
8.99	8.6E-005	27.14	2.1E-005	86.32	7.6E-007
10.41	7.3E-005	28.32	1.9E-005	93.63	5.8E-007
11.80	6.2E-005	29.48	1.8E-005	100.95	4.4E-007
13.18	5.5E-005	30.63	1.7E-005	108.27	3.4E-007
14.54	4.8E-005	31.77	1.6E-005	115.58	2.6E-007
15.87	4.3E-005	32.89	1.5E-005	122.90	2.1E-007
17.19	3.9E-005	34.01	1.4E-005	130.21	1.6E-007
18.49	3.5E-005	35.11	1.4E-005	137.53	1.3E-007

Identification Code: Site #1
Soil Name: Tipton Sandy Loam
Compound Name: Pollutant#1
CAS Number: 123-4567 RITZ

Figure 3. Graph of flux density of pollutant in vapor phase as a function of time.

Table 5. The flux density of pollutant leached below the treatment zone as a function of time.

LEACHATE FLUX VERSUS TIME

Time days	Flux g/m2-day	Time days	Flux g/m2-day	Time days	Flux g/m2-day
102.42	3.3E-002	114.41	2.9E-002	126.40	2.5E-002
103.28	3.3E-002	115.27	2.8E-002	127.26	2.4E-002
104.14	3.2E-002	116.12	2.8E-002	128.11	2.4E-002
104.99	3.2E-002	116.98	2.8E-002	128.97	2.4E-002
105.85	3.2E-002	117.84	2.7E-002	129.82	2.3E-002
106.71	3.1E-002	118.69	2.7E-002	130.68	2.3E-002
107.56	3.1E-002	119.55	2.7E-002	131.54	2.3E-002
108.42	3.1E-002	120.41	2.6E-002	132.39	2.3E-002
109.27	3.0E-002	121.26	2.6E-002	133.25	2.2E-002
110.13	3.0E-002	122.12	2.6E-002	134.11	2.2E-002
110.99	3.0E-002	122.97	2.6E-002	134.96	2.2E-002
111.84	2.9E-002	123.83	2.5E-002	135.82	2.2E-002
112.70	2.9E-002	124.69	2.5E-002	136.67	2.1E-002
113.56	2.9E-002	125.54	2.5E-002	137.53	2.1E-002

Identification Code: Site #1
Soil Name: Tipton Sandy Loam
Compound Name: Pollutant#1
CAS Number: 123-4567 RITZ

Figure 4. Graph of flux density of pollutant leached below the treatment zone as a function of time.

Table 6. The location of the top and bottom of the pollutant as a function of time.

DEPTH OF BOTTOM AND TOP OF POLLUTANT VERSUS TIME

Time days	Top m	Bottom m	Time days	Top m	Bottom m
0.00	0.00	0.15	35.11	0.15	0.61
4.15	0.01	0.20	45.35	0.29	0.75
8.13	0.03	0.26	55.59	0.42	0.88
11.94	0.04	0.31	65.83	0.56	1.02
15.61	0.06	0.36	76.08	0.69	1.15
19.14	0.07	0.40	86.32	0.83	1.29
22.54	0.09	0.45	96.56	0.96	1.42
25.83	0.10	0.49	106.80	1.09	> 1.50
29.02	0.12	0.53	117.05	1.23	> 1.50
32.11	0.14	0.57	127.29	1.36	> 1.50
35.11	0.15	0.61	137.53	1.50	> 1.50

Identification Code: Site #1
Soil Name: Tipton Sandy Loam
Compound Name: Pollutant#1
CAS Number: 123-4567 RITZ

Figure 5. Location of the top and bottom of the pollutant as a function of time.

Table 7. Concentration of pollutant in different phases and oil content as a function of time at selected depths.

CONCENTRATION PROFILE

Depth = 0.000 meters

Time days	Total Pollutant g/m3	Pollutant in Water g/m3	Pollutant in Soil g/kg	Pollutant in Vapor g/m3	Pollutant in Oil g/m3	Oil Content m3/m3
0.00	1.0E+002	5.9E+001	6.5E-003	3.2E-003	2.9E+003	2.5E-002
10.00	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	2.1E-002
20.00	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	1.8E-002
30.00	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	1.6E-002
40.00	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	1.4E-002
50.00	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	1.2E-002
75.00	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	7.9E-003
100.00	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	5.4E-003

Identification Code: Site #1
Soil Name: Tipton Sandy Loam
Compound Name: Pollutant#1
CAS Number: 123-4567 RITZ

CONCENTRATION PROFILE

Depth = 0.050 meters

Time days	Total Pollutant g/m3	Pollutant in Water g/m3	Pollutant in Soil g/kg	Pollutant in Vapor g/m3	Pollutant in Oil g/m3	Oil Content m3/m3
0.00	1.0E+002	5.9E+001	6.5E-003	3.2E-003	2.9E+003	2.5E-002
10.00	7.9E+001	5.2E+001	5.7E-003	2.9E-003	2.6E+003	2.1E-002
20.00	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	1.8E-002
30.00	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	1.6E-002
40.00	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	1.4E-002
50.00	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	1.2E-002
75.00	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	7.9E-003
100.00	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	5.4E-003

Identification Code: Site #1
Soil Name: Tipton Sandy Loam
Compound Name: Pollutant#1
CAS Number: 123-4567 RITZ

Table 7. Continued.

CONCENTRATION PROFILE

Depth = 0.100 meters

Time days	Total Pollutant g/m3	Pollutant in Water g/m3	Pollutant in Soil g/kg	Pollutant in Vapor g/m3	Pollutant in Oil g/m3	Oil Content m3/m3
0.00	1.0E+002	5.9E+001	6.5E-003	3.2E-003	2.9E+003	2.5E-002
10.00	7.9E+001	5.2E+001	5.7E-003	2.9E-003	2.6E+003	2.1E-002
20.00	6.3E+001	4.6E+001	5.0E-003	2.5E-003	2.3E+003	1.8E-002
30.00	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	1.6E-002
40.00	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	1.4E-002
50.00	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	1.2E-002
75.00	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	7.9E-003
100.00	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	5.4E-003

Identification Code: Site #1
Soil Name: Tipton Sandy Loam
Compound Name: Pollutant#1
CAS Number: 123-4567 RITZ

CONCENTRATION PROFILE

Depth = 0.150 meters

Time days	Total Pollutant g/m3	Pollutant in Water g/m3	Pollutant in Soil g/kg	Pollutant in Vapor g/m3	Pollutant in Oil g/m3	Oil Content m3/m3
0.00	1.0E+002	5.9E+001	6.5E-003	3.2E-003	2.9E+003	2.5E-002
10.00	7.9E+001	5.2E+001	5.7E-003	2.9E-003	2.6E+003	2.1E-002
20.00	6.3E+001	4.6E+001	5.0E-003	2.5E-003	2.3E+003	1.8E-002
30.00	5.0E+001	4.0E+001	4.4E-003	2.2E-003	2.0E+003	1.6E-002
40.00	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	1.4E-002
50.00	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	1.2E-002
75.00	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	7.9E-003
100.00	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	5.4E-003

Identification Code: Site #1
Soil Name: Tipton Sandy Loam
Compound Name: Pollutant#1
CAS Number: 123-4567 RITZ

Table 7. Continued.

CONCENTRATION PROFILE

Depth = 0.250 meters

Time days	Total Pollutant g/m3	Pollutant in Water g/m3	Pollutant in Soil g/kg	Pollutant in Vapor g/m3	Pollutant in Oil g/m3	Oil Content m3/m3
0.00	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000
10.00	2.2E+001	4.8E+001	5.3E-003	2.6E-003	0.0E+000	0.0E+000
20.00	1.9E+001	4.2E+001	4.7E-003	2.3E-003	0.0E+000	0.0E+000
30.00	1.7E+001	3.7E+001	4.1E-003	2.1E-003	0.0E+000	0.0E+000
40.00	1.5E+001	3.3E+001	3.6E-003	1.8E-003	0.0E+000	0.0E+000
50.00	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000
75.00	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000
100.00	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000

Identification Code: Site #1
Soil Name: Tipton Sandy Loam
Compound Name: Pollutant#1
CAS Number: 123-4567 RITZ

CONCENTRATION PROFILE

Depth = 0.500 meters

Time days	Total Pollutant g/m3	Pollutant in Water g/m3	Pollutant in Soil g/kg	Pollutant in Vapor g/m3	Pollutant in Oil g/m3	Oil Content m3/m3
0.00	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000
10.00	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000
20.00	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000
30.00	1.4E+001	3.0E+001	3.4E-003	1.7E-003	0.0E+000	0.0E+000
40.00	1.2E+001	2.7E+001	3.0E-003	1.5E-003	0.0E+000	0.0E+000
50.00	1.1E+001	2.4E+001	2.6E-003	1.3E-003	0.0E+000	0.0E+000
75.00	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000
100.00	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000

Identification Code: Site #1
Soil Name: Tipton Sandy Loam
Compound Name: Pollutant#1
CAS Number: 123-4567 RITZ

Table 7. Continued.

CONCENTRATION PROFILE

Depth = 0.750 meters

Time days	Total Pollutant g/m3	Pollutant in Water g/m3	Pollutant in Soil g/kg	Pollutant in Vapor g/m3	Pollutant in Oil g/m3	Oil Content m3/m3
0.00	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000
10.00	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000
20.00	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000
30.00	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000
40.00	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000
50.00	8.8E+000	1.9E+001	2.1E-003	1.1E-003	0.0E+000	0.0E+000
75.00	6.4E+000	1.4E+001	1.6E-003	7.8E-004	0.0E+000	0.0E+000
100.00	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000

Identification Code: Site #1
Soil Name: Tipton Sandy Loam
Compound Name: Pollutant#1
CAS Number: 123-4567 RITZ

CONCENTRATION PROFILE

Depth = 1.000 meters

Time days	Total Pollutant g/m3	Pollutant in Water g/m3	Pollutant in Soil g/kg	Pollutant in Vapor g/m3	Pollutant in Oil g/m3	Oil Content m3/m3
0.00	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000
10.00	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000
20.00	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000
30.00	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000
40.00	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000
50.00	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000
75.00	5.3E+000	1.2E+001	1.3E-003	6.4E-004	0.0E+000	0.0E+000
100.00	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000

Identification Code: Site #1
Soil Name: Tipton Sandy Loam
Compound Name: Pollutant#1
CAS Number: 123-4567 RITZ

Table 7. Continued.

CONCENTRATION PROFILE

Depth = 1.250 meters

Time days	Total Pollutant g/m3	Pollutant in Water g/m3	Pollutant in Soil g/kg	Pollutant in Vapor g/m3	Pollutant in Oil g/m3	Oil Content m3/m3
0.00	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000
10.00	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000
20.00	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000
30.00	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000
40.00	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000
50.00	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000
75.00	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000
100.00	3.2E+000	7.0E+000	7.7E-004	3.8E-004	0.0E+000	0.0E+000

Identification Code: Site #1
Soil Name: Tipton Sandy Loam
Compound Name: Pollutant#1
CAS Number: 123-4567 RITZ

CONCENTRATION PROFILE

Depth = 1.500 meters

Time days	Total Pollutant g/m3	Pollutant in Water g/m3	Pollutant in Soil g/kg	Pollutant in Vapor g/m3	Pollutant in Oil g/m3	Oil Content m3/m3
0.00	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000
10.00	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000
20.00	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000
30.00	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000
40.00	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000
50.00	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000
75.00	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000
100.00	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000

Identification Code: Site #1
Soil Name: Tipton Sandy Loam
Compound Name: Pollutant#1
CAS Number: 123-4567 RITZ

Figure 6. Concentration of total pollutant as a function of time for depths of 0.1, 0.5, 1.0, and 1.5 meters.

Figure 7. Concentration of pollutant in water as a function of time for depths of 0.1, 0.5, 1.0, and 1.5 meters.

Figure 8. Concentration of pollutant in soil as a function of time for depths of 0.1, 0.5, 1.0, and 1.5 meters.

Figure 9. Concentration of pollutant in vapor as a function of time for depths of 0.1, 0.5, 1.0, and 1.5 meters.

Figure 10. Concentration of pollutant in oil as a function of time for depth of 0.1 meters. Curves for 0.5, 1.0, and 1.5 meter depths are not visible since the concentration at these depths is zero.

Figure 11. Oil content as a function of time for depths of 0.1 meters. Oil content curves for 0.5, 1.0, and 1.5 meter depths are not shown since the oil content is zero below the plow zone.

Table 8. Concentration of pollutant in various phases and oil content as a function of depth at selected times.

CONCENTRATION PROFILE

Time = 0.00 days

Depth m	Total Pollutant g/m3	Pollutant in Water g/m3	Pollutant in Soil g/kg	Pollutant in Vapor g/m3	Pollutant in Oil g/m3	Oil Content m3/m3
0.000	1.0E+002	5.9E+001	6.5E-003	3.2E-003	2.9E+003	2.5E-002
0.050	1.0E+002	5.9E+001	6.5E-003	3.2E-003	2.9E+003	2.5E-002
0.100	1.0E+002	5.9E+001	6.5E-003	3.2E-003	2.9E+003	2.5E-002
0.150	1.0E+002	5.9E+001	6.5E-003	3.2E-003	2.9E+003	2.5E-002
0.250	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000
0.500	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000
0.750	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000
1.000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000
1.250	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000
1.500	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000

Identification Code: Site #1
Soil Name: Tipton Sandy Loam
Compound Name: Pollutant#1
CAS Number: 123-4567 RITZ

CONCENTRATION PROFILE

Time = 10.00 days

Depth m	Total Pollutant g/m3	Pollutant in Water g/m3	Pollutant in Soil g/kg	Pollutant in Vapor g/m3	Pollutant in Oil g/m3	Oil Content m3/m3
0.000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	2.1E-002
0.050	7.9E+001	5.2E+001	5.7E-003	2.9E-003	2.6E+003	2.1E-002
0.100	7.9E+001	5.2E+001	5.7E-003	2.9E-003	2.6E+003	2.1E-002
0.150	7.9E+001	5.2E+001	5.7E-003	2.9E-003	2.6E+003	2.1E-002
0.250	2.2E+001	4.8E+001	5.3E-003	2.6E-003	0.0E+000	0.0E+000
0.500	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000
0.750	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000
1.000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000
1.250	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000
1.500	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000

Identification Code: Site #1
Soil Name: Tipton Sandy Loam
Compound Name: Pollutant#1
CAS Number: 123-4567 RITZ

Table 8. Continued.

CONCENTRATION PROFILE

Time = 20.00 days

Depth m	Total Pollutant g/m3	Pollutant in Water g/m3	Pollutant in Soil g/kg	Pollutant in Vapor g/m3	Pollutant in Oil g/m3	Oil Content m3/m3
0.000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	1.8E-002
0.050	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	1.8E-002
0.100	6.3E+001	4.6E+001	5.0E-003	2.5E-003	2.3E+003	1.8E-002
0.150	6.3E+001	4.6E+001	5.0E-003	2.5E-003	2.3E+003	1.8E-002
0.250	1.9E+001	4.2E+001	4.7E-003	2.3E-003	0.0E+000	0.0E+000
0.500	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000
0.750	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000
1.000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000
1.250	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000
1.500	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000

Identification Code: Site #1

Soil Name: Tipton Sandy Loam

Compound Name: Pollutant#1

CAS Number: 123-4567 RITZ

CONCENTRATION PROFILE

Time = 30.00 days

Depth m	Total Pollutant g/m3	Pollutant in Water g/m3	Pollutant in Soil g/kg	Pollutant in Vapor g/m3	Pollutant in Oil g/m3	Oil Content m3/m3
0.000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	1.6E-002
0.050	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	1.6E-002
0.100	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	1.6E-002
0.150	5.0E+001	4.0E+001	4.4E-003	2.2E-003	2.0E+003	1.6E-002
0.250	1.7E+001	3.7E+001	4.1E-003	2.1E-003	0.0E+000	0.0E+000
0.500	1.4E+001	3.0E+001	3.4E-003	1.7E-003	0.0E+000	0.0E+000
0.750	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000
1.000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000
1.250	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000
1.500	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000

Identification Code: Site #1

Soil Name: Tipton Sandy Loam

Compound Name: Pollutant#1

CAS Number: 123-4567 RITZ

Table 8. Continued.

CONCENTRATION PROFILE

Time = 40.00 days

Depth m	Total Pollutant g/m3	Pollutant in Water g/m3	Pollutant in Soil g/kg	Pollutant in Vapor g/m3	Pollutant in Oil g/m3	Oil Content m3/m3
0.000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	1.4E-002
0.050	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	1.4E-002
0.100	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	1.4E-002
0.150	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	1.4E-002
0.250	1.5E+001	3.3E+001	3.6E-003	1.8E-003	0.0E+000	0.0E+000
0.500	1.2E+001	2.7E+001	3.0E-003	1.5E-003	0.0E+000	0.0E+000
0.750	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000
1.000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000
1.250	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000
1.500	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000

Identification Code: Site #1

Soil Name: Tipton Sandy Loam

Compound Name: Pollutant#1

CAS Number: 123-4567 RITZ

CONCENTRATION PROFILE

Time = 50.00 days

Depth m	Total Pollutant g/m3	Pollutant in Water g/m3	Pollutant in Soil g/kg	Pollutant in Vapor g/m3	Pollutant in Oil g/m3	Oil Content m3/m3
0.000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	1.2E-002
0.050	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	1.2E-002
0.100	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	1.2E-002
0.150	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	1.2E-002
0.250	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000
0.500	1.1E+001	2.4E+001	2.6E-003	1.3E-003	0.0E+000	0.0E+000
0.750	8.8E+000	1.9E+001	2.1E-003	1.1E-003	0.0E+000	0.0E+000
1.000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000
1.250	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000
1.500	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000

Identification Code: Site #1

Soil Name: Tipton Sandy Loam

Compound Name: Pollutant#1

CAS Number: 123-4567 RITZ

Table 8. Continued.

CONCENTRATION PROFILE

Time = 75.00 days

Depth m	Total Pollutant g/m3	Pollutant in Water g/m3	Pollutant in Soil g/kg	Pollutant in Vapor g/m3	Pollutant in Oil g/m3	Oil Content m3/m3
0.000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	7.9E-003
0.050	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	7.9E-003
0.100	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	7.9E-003
0.150	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	7.9E-003
0.250	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000
0.500	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000
0.750	6.4E+000	1.4E+001	1.6E-003	7.8E-004	0.0E+000	0.0E+000
1.000	5.3E+000	1.2E+001	1.3E-003	6.4E-004	0.0E+000	0.0E+000
1.250	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000
1.500	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000

Identification Code: Site #1
Soil Name: Tipton Sandy Loam
Compound Name: Pollutant#1
CAS Number: 123-4567 RITZ

CONCENTRATION PROFILE

Time = 100.00 days

Depth m	Total Pollutant g/m3	Pollutant in Water g/m3	Pollutant in Soil g/kg	Pollutant in Vapor g/m3	Pollutant in Oil g/m3	Oil Content m3/m3
0.000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	5.4E-003
0.050	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	5.4E-003
0.100	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	5.4E-003
0.150	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	5.4E-003
0.250	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000
0.500	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000
0.750	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000
1.000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000
1.250	3.2E+000	7.0E+000	7.7E-004	3.8E-004	0.0E+000	0.0E+000
1.500	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000	0.0E+000

Identification Code: Site #1
Soil Name: Tipton Sandy Loam
Compound Name: Pollutant#1
CAS Number: 123-4567 RITZ

Figure 12. Concentration of total pollutant as a function of depth for times of 10, 50, and 100 days.

Figure 13. Concentration of pollutant in water as a function of depth for times of 10, 50, and 100 days.

Figure 14. Concentration of pollutant in soil as a function of depth for times of 10, 50, and 100 days.

Figure 15. Concentration of pollutant in vapor as a function of depth for times of 10, 50, and 100 days.

Figure 16. Concentration of pollutant in oil as a function of depth for 10 days after application. Note the concentration decreases to zero at the plow zone depth. The concentration was zero at 50, and 100 days.

Figure 17. Oil content as a function of depth for times of 10, 50, and 100 days. The oil does not move downward but the oil content decreases due to degradation.

Figure 18. Concentration bar graphs representing the pollutant and oil in the treatment zone at a time of 10 days. The concentrations represented by the patterns in each phase can be displayed by pressing the <F1> key.

Figure 19. Concentration bar graphs for 30 days.

Figure 20. Concentration bar graphs for 50 days.

Figure 21. Concentration bar graphs for 100 days.

FILE STRUCTURE

Disk files are used in this software for two purposes. The first is to store input parameters entered at one time for use at another time. The second is for storing output tables for later printing or display or for use in other documents.

The input parameter files are made up of a single record of binary information. The record is composed of parameters in the sequence listed in screens 2, 3, and 4. All numeric entries are stored as floating point values. All alphanumeric entries are stored as strings.

Tabular data stored in files are written as text in ASCII characters.

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APPENDIX

MATHEMATICAL BASIS OF RITZ

This section summarizes the mathematical equations used in this version of the RITZ software. They are presented for your information only. No attempt is made here to explain the mathematical derivations of these equations. See Short(1985) for those derivations.

Total Pollutant Concentration: The total concentration of the pollutant $C_T(x,t)$ at position x and time t is given by

$C_T(x,t) = 0$ for x < top of pollutant slug

$C_T(x,t) = C_{To}\exp(-\mu_p t)$ for top of pollutant slug $\leq$ x $\leq$ pzd

$C_T(x,t) = C_{To}R\exp(-\mu_p t)/(R + R_T\exp(-\mu_o(t-(x-pzd)/V_p)))$

for pzd < x $\leq$ bottom of pollutant slug

$C_T(x,t) = 0$ for x > bottom of pollutant slug

where
- C_{To} is the initial pollutant concentration,
- μ_p is the degradation constant for the pollutant ($\mu_p = \ln(2)/t_{½P}$),
- μ_o is the degradation constant for the oil ($\mu_o = \ln(2)/t_{½o}$),
- R is the retardation factor for the pollutant in the treatment zone,
- R_T is the contribution of oil to the retardation,
- V_p is the velocity of the pollutant in the lower treatment zone, and
- pzd is the depth of the plow zone.

$C_T(x,t)$ is the mass of pollutant per unit volume of soil. In this software these units are grams of pollutant per cubic meterof soil. The initial pollutant concentration is given by

$C_{To} = SAR \cdot S_P / (10^4 pzd)$

where
- SAR is the sludge application rate and
- S_P is the concentration of pollutant in the sludge.

The retardation factor, R, is given by

$R = 1 + (\rho K_D + (\theta_s - \theta)K_H) / \theta$

where

- ρ is the bulk density of the soil,
- θ is the water content of the soil on a volume basis,
- θ_s is the saturated water content of the soil on a volume basis,
- K_D is the partition coefficient for pollutant in the soil, and
- K_H is the dimensionless value of Henry's Law constant, (C_v/C_w).

The partition coefficient is given by $K_D = K_{OC} f_{OC}$ where K_{OC} is the organic carbon partition coefficient and f_{OC} is the fractional organic carbon content of the soil.

The parameter R_T is given by

$$R_T = \Phi_o(K_o - K_H) / \theta$$

where

- Φ_o is the initial oil content or the volume fraction occupied by oil, and
- K_o is the partition coefficient for oil.

The volumetric water content of the soil, θ, is given by

$$\theta = \theta_s[V_d/k_s]^{1/(2b+3)}$$

where

- V_d is the recharge rate,
- k_s is the saturated conductivity of the soil, and
- b is the Clapp and Hornberger constant for the soil.

The velocity of the pollutant in the lower treatment zone, V_p, is given by

$$V_p = V_a / R$$

where $V_a = V_d/\theta$ is the aqueous or pore water velocity.

Pollutant Concentration in Water: The concentration of pollutant in water, $C_W(x,t)$ at position x and time t is given by

$C_W(x,t) = 0$ for x < top of pollutant slug

$C_W(x,t) = C_T(x,t) / \theta(R + R_T\exp(-\mu_o t))$ for top of pollutant slug $\leq$ x $\leq$ pzd

$C_W(x,t) = C_T(x,t) / R\theta$ for pzd < x $\leq$ bottom of pollutant slug

$C_W(x,t) = 0$ for x > bottom of pollutant slug where all the symbols are those defined for the total pollutant concentration. $C_W(x,t)$ is the mass of pollutant in water per unit volume of water. In this software these units are grams of pollutant per cubic meter of water.

Concentration of Pollutant in Soil: The concentration of the pollutant in the soil phase $C_S(x,t)$ at position x and time t is given by

$$C_S(x,t) = K_D C_W(x,t)$$

where

K_D is the soil:water partition coefficient for the pollutant and
$C_W(x,t)$ is the concentration of pollutant in water.

$C_S(x,t)$ is the mass of pollutant in water per unit mass of soil solids. In this software these units are grams of pollutant per kilogram of soil.

Concentration of Pollutant in Vapor: The concentration of the pollutant in the vapor phase $C_V(x,t)$ at position x and time t is given by

$$C_V(x,t) = K_H C_W(x,t)$$

where

K_H is the dimensionless (Henry's Law) vapor: water partition coefficientand
$C_W(x,t)$ is the concentration of pollutant in water.

$C_V(x,t)$ is the mass of pollutant per unit volume of vapor. In this software these units are grams of pollutant per cubic meter of vapor.

Concentration of Pollutant in Oil: The concentration of pollutant in the oil phase $C_O(x,t)$ at position x and time t is given by

$$C_O(x,t) = K_o C_w(x,t) \qquad \text{for } x \leq pzd$$

$$C_O(x,t) = 0 \qquad \text{for } x > pzd$$

where

K_o is the dimensionless oil:water partition coefficient for the pollutant,
pzd is the depth of the plow zone, and
$C_W(x,t)$ is the concentration of the pollutant in water.

$C_O(x,t)$ is the mass of pollutant per unit volume of oil. In this software these units are grams of pollutant per cubic meter of oil.

Oil Content: The oil content $\Phi(t)$ in the plow zone at time t is the volume of oil per unit volume of soil and is given by

$$\Phi(t) = \Phi_o \exp(-\mu_o t)$$

where
Φ_o is the initial oil content in the plow zone and
μ_o is the degradation constant for oil.

The oil content is uniform throughout the plow zone at each instant of time. The oil content is zero below the plow zone at all times. The initial oil content Φ_o is given by

$$\Phi_o = SAR \cdot S_O/(10^7 \rho_O pzd)$$

where
SAR is the sludge application rate,
S_O is the concentration of oil in the sludge,
and ρ_O is the density of oil.

Time at Which the Top of the Pollutant Slug Reaches a Specified Depth: In this model, the pollutant is contained within a specific soil volume called a pollutant slug. Above and below this slug, the concentration of pollutant is zero. The location of the top and bottom of the slug changes with time. The equation describing the location of the top of the slug cannot be solved explicitly as a function of time. However, the time t_{top} at which the top of the slug reaches a position x_{top} can be solved explicitly. This equation is

$$t_{top}(x_{top}) = \mu_o^{-1} \ln\{(1 + R_T/R)\exp[\mu_o x_{top}/V_p - F(x_{top})] - R_T/R\}$$

for $0 \leq x_{top} \leq pzd$

$$t_{top}(x_{top}) = t_{top}(pzd) + (x_{top} - pzd)/V_p - G(x_{top})$$

for $pzd < x_{top} \leq tzd$

where
$F(x_{top}) = \mu_o a V_p^{-1} \ln(1 + x_{top}/g)$,
$G(x_{top}) = a V_p^{-1} \ln[(g + x_{top})/(g + pzd)]$,
$g = D_S\, \delta/D_A + a$,
$a = K_H D_S/V_a\, \theta$,
D_A is the diffusion coefficient of the pollutant vapor in air,

D_S is the diffusion coefficient of the pollutant vapor in the soil,
δ is the thickness of the stagnant boundary layer above the soil, and
tzd is the depth of the treatment zone.

Although the equations above hold for all depths, numerical overflow occurs in the first equation when $\mu_o x_{top}/V_p$ is very large. In this case, an approximate form of the equation is used which is

$$t_{top}(x_{top}) = \mu_o^{-1}\{\mu_o x_{top}/V_p - F(x_{top}) + \ln(1 + R_T/R)\}$$
$$\text{for } 0 \le x_{top} \le \text{pzd.}\}$$

The diffusion coefficient of the pollutant in the soil, D_S is given by

$$D_S = D_A \eta^{10/3}/\theta_s^2$$

where η is the initial air content of the soil (Millington and Quirk,1961).

The thickness of the stagnant boundary layer (Jury et al., 1983) is given by

$$\delta = D_W \rho_{WV}(1 - RH)/2E\rho_{WL}$$

where
D_W is the diffusion coefficient of water vapor in air,
RH is the relative humidity of the air,
E is the evaporation rate,
ρ_{WV} is the density of water vapor, and
ρ_{WL} is the density of liquid water.

The ratio of the density of water vapor to the density of liquid water is given by (Short, 1985)

$$\rho_{WV}/\rho_{WL} = \alpha_0 + \alpha_1 T + \alpha_2 T^2 + \alpha_3 T^3$$

where
T is the temperature in degrees Celsius,
α_0= 4.60843696E-06,
α_1 = 4.0710817E-07,
α_2 = 3.02943E-09, and
α_3 = 3.9405E-10.

Time at Which the Bottom of the Pollutant Slug Reaches a Specified Depth: The bottom of the pollutant slug is located at the plow zone depth at time zero. It moves downward through the treatment zone as time increases. The time at which the bottom of the slug reaches a position x_{bottom} is given by

$t_{bottom}(x_{bottom}) = 0$ for $x_{bottom} \leq pzd$

$t_{bottom}(x_{bottom}) = (x_{bottom} - pzd)/V_p$ for $x_{bottom} > pzd$

where
pzd is the depth of the bottom of the plow zone and
V_p is the velocity of the pollutant in the lower treatment zone.

Flux of Pollutant Vapor for a Specified Position of the Top of the Pollutant Slug and the Corresponding Time: The flux of pollutant vapor, $J(t(x_{top}))$, moving upward out of the treatment zone at the time t is given by

$$J(t) = aV_pC_{To}\exp(-\mu_p t)/\{(g - a + x_{top})[1 + (R_T/R)\exp(-\mu_o t)]\} \quad \text{for } 0 \leq x_{top} \leq pzd$$

$$J(t) = aV_pC_{To}\exp(-\mu_p t)/\{(g - a + x_{top})[1 + (R_T/R)\exp(-\mu_o \Delta t)]\} \quad \text{for } pzd < x_{top} \leq tzd$$

where
$t = t_{top}(x_{top})$ as defined previously and
$\Delta t = t_{top}(x_{top}) - (x_{top} - pzd)/V_p$.

Total Amount of Pollutant Lost as Vapor: The amount of pollutant lost in the vapor form can be obtained by integrating the vapor flux over the time in which the pollutant is in the plow zone and the treatment zone. That is

$$M_V = \int_0^t J(t)\,dt$$

where t is the time at which the top of the pollutant slug reaches the bottom of the treatment zone. It is computationally more efficient to change variable of integration and integrate over distance. This integral then becomes

$$M_{funcV} = \int_0^{pzd} J(t(x))\left(\frac{dt}{dx}\right)dx + \int_{pzd}^{tzd} J(t(x))\left(\frac{dt}{dx}\right)dx$$

The integrands in the above equation are

$I_1 = aC_{To}\exp(-\mu_p t_{top}(x)/(g + x)$ for $0 \leq x \leq pzd$ (term 1)

$I_2 = aC_{To}\exp(-\mu_p t_{top}(x)/\{(g + x)(1 + (R_T/R)\exp(-\mu_o]\Delta t))\}$
for $pzd \leq x \leq tzd$ (term 2)}

where $\Delta t = t_{top}(x) - (x - pzd)/V_p$. The integration is carried out numerically using Romberg integration. Convergence is assumed when the difference between consecutive approximations to the integral is less than 1.0E-06 percent of the pollutant applied.

Total Amount of Pollutant Leached Below the Treatment Zone: The amount of pollutant leached below the treatment zone, M_L, is obtained by integrating the product of the recharge rate and the pollutant concentration in water at the treatment zone depth. That is

$$M_L = \int_0^t V_a \theta C_W(tzd, t)\,dt$$

where
$V_a\theta$ = the recharge rate and
$C_W(tzd,t)$ is the concentration of pollutant in water defined previously.

This integration is also performed numerically using Romberg integration (Ralston, 1965). Convergence is assumed when the difference between consecutive approximations to the integral is less than 1.0E-06 percent of the pollutant applied..

Total Amount of Pollutant Degraded in the Treatment Zone: The amount of the pollutant degraded, M_D, within the entire treatment zone is equal to the sum of the amounts degraded in the plow zone and in the treatment zone.That is

$$M_D = \int_0^{pzd} \mu_p (pzd - x)\, C_T(x, t_{top}(x)) \left(\frac{dt}{dx}\right) dx + \int_0^{tb} \mu_p \,\mathrm{Acc}(t)\,dt + \int_{pzd}^{tzd} \mu_p \,\mathrm{Acc}(t) \left(\frac{dt}{dx}\right) dx$$

where tb = t_{top}(pzd) is the time at which the top of the slug reaches the depth of the plow zone and Acc(t) is the mass of pollutant accumulated in the lower treatment zone. The first integral represents the degradation within the plow zone. The second integral represents the degradation in the lower treatment zone before the top of the slug reaches the lower treatment zone. The third integral represents the degradation in the lower treatment zone after the slug is entirely in that zone. These integrals are evaluated by the Romberg integration with the same convergence criteria as for volatilization and leaching.

The accumulation of pollutant in the lower treatment zone, Acc(t), is given by

$$Acc(t) = C_{To}\exp(-\mu_p t)\{(x_{bottom} - x_{top}) - V_p \mu_o^{-1} \ln(H(x_{bottom})/H(x_{top}))\}$$

where

$$H(x) = 1 + (R_T/R)\exp(-\mu_o(xb - x)/V_p)$$

and

$$xb = pzd + V_p t.\}$$

Mass Balance Error: Pollutant applied to the soil must be volatilized, leached, or degraded by the time the top the slug reaches the treatment zone depth. Each of these three components are evaluated above. If the computational techniques are accurate, the sum of these should be equal to the amount of pollutant applied. The mass balance computational error is given by

$$Error = M_T - M_V - M_L - M_D$$

where M_T is the mass of pollutant applied to the plow zone. The other symbols were defined previously.

Table 9. List of symbols with meaning and units as used in this section.

b	Clapp and Hornberger constant, dimensionless
C_T	total concentration of pollutant in all phases, g/m^3
C_W	concentration of pollutant in water, g/m^3
C_S	concentration of pollutant in soil, g/kg
C_V	concentration of pollutant in vapor, g/m^3
C_O	concentration of pollutant in oil, g/m^3
C_{To}	total concentration of pollutant at time zero, g/m^3
D_A	diffusion coefficient of pollutant in air, m^2/day
D_S	diffusion coefficient of pollutant vapor in soil, m^2/day
D_W	diffusion coefficient of water vapor in air, m^2/day
E	evaporation rate, m/day
f_{OC}	fractional organic carbon content of soil
J	flux of pollutant vapor, $g/m^2 \bullet day$
k	unsaturated hydraulic conductivity, m/day
k_s	saturated hydraulic conductivity of soil, m/day
K_D	soil:water partition coefficient of pollutant, m^3/kg
K_H	vapor:water partition coefficient of pollutant or the dimensionless Henry's law constant, dimensionless
K_o	oil:water partition coefficient of pollutant, dimensionless
K_{OC}	organic-carbon:water partition coefficient, m^3/kg
M_D	total amount of pollutant degraded, g/m^2
M_L	total amount of pollutant leached below treatment zone, g/m^2
M_V	total amount of pollutant lost in vapor form, g/m^2
pzd	plow zone depth, m
R	retardation factor for pollutant (ignoring oil), dimensionless
R_T	contribution of oil to retardation of pollutant, dimensionless
RH	relative humidity, dimensionless
SAR	sludge application rate, kg/ha
S_o	initial concentration of oil in the sludge, g/kg
S_P	initial concentration of pollutant in the sludge, g/kg
T	temperature, °C
t	time, days
$t_{½P}$	degradation half-life of the pollutant, days
$t_{½o}$	degradation half-life of the oil, days
tzd	treatment zone depth, m
V_d	recharge rate, m/day
V_a	pore water velocity, m/day
V_p	velocity of the pollutant in the lower treatment zone, m/day
x	distance from the soil surface, m
ρ	bulk density of soil, kg/m^3
ρ_o	density of oil, kg/m^3

Table 9. Continued.

ρ_{WV}	density of water vapor, kg/m^3
ρ_{WL}	density of liquid water, $kg/^3$
θ	water content on a volume basis, m^3/m^3
θ_s	saturated water content on a volume basis, m^3/m^3
$\Phi(t)$	oil content (volume fraction of oil) at time t, m^3/m^3
Φ_o	initial oil content (volume fraction of oil), m^3/m^3
μ_p	degradation constant of pollutant, $days^{-1}$
μ_o	degradation constant of oil, $days^{-1}$
δ	thickness of stagnant boundary layer, m
η	initial air content of soil, m^3/m^3

INPUT PARAMETER ESTIMATION

The user of this software must provide soil, chemical, and environmental parameters to define the land treatment site. The parameters may be obtained experimentally for the site, based on published values such as those inVerschuren (1983), or estimated from related parameters. The software includes a few built in estimators for certain required parameters. These are intended for use in situations in which the required parameter is unknown. They should be used with caution. In this section, the approximations available for each parameter are described briefly. Table 10 contains a list of the numerical parameters with their units and symbols used in the previous section.

Fractional organic carbon content

If this is not known but the organic matter content of the soil is known, this is approximately equal to the product of 0.4 and the fractional organic matter content.

Saturated water content

This can be estimated from the bulk density, ρ,and particle density, ρ_s, of the soil using the equation $\theta_s = 1 - \rho/\rho_s$. The particle density for most mineral soils is between 2600 and 2700 kg/m^3. If the particle density is not known a value of 2650 kg/m^3 is usually a good estimate.

Clapp and Hornberger constant

If this parameter is not known, it can be estimated using the values presented by Clapp and Hornberger for different soil textures. This table will be displayed on the screen if the help key is pressed.

Organic carbon partition coefficient

If this parameter is not known, it can be estimated (Karickhoff, 1981) from the water solubility, S (g/m^3), the molecular weight, MW (g/mole), and the melting point, MP (°C) of the pollutant. If $x = -0.92\log(S/(55556 \cdot MW) - 4.404)$, then the organic carbon partition coefficient, K_{OC}, is approximately

$$K_{OC} \approx 10^{x} \qquad \text{if melting point} \leq 25°C$$

$$K_{OC} \approx 10^{x - 0.01(MP - 25)} \qquad \text{if melting point} > 25°C.$$

If these pollutant properties are not known, K_{OC} can be estimated from the octonal-water partition coefficient, K_{OW}, using the relation of Karickhoff et al. (1979)

$$K_{OC} \approx 10^{-3.21 + \log(K_{OW})}$$

Table 10. Input parameters required by the RITZ model.

Input Parameter	Units	Symbol
Fractional organic carbon content	--	f_{OC}
Bulk density	kg/m^3	ρ
Saturated water content of soil	m^3/m^3	θ_s
Saturated hydraulic conductivity	m/day	k_s
Clapp and Hornberger constant	--	b
Concentration of pollutant in sludge	g/kg	S_P
Organic carbon partition coefficient	m^3/kg	K_{OC}
Oil-water partition coefficient	--	K_o
Henry's law constant	--	K_H
Diffusion coefficient of pollutant in air	m^2/day	D_A
Half-life of pollutant	days	$t_{½P}$
Concentration of oil in sludge	g/kg	S_O
Density of oil	kg/m^3	ρ_O
Half-life of oil	days	$t_{½o}$
Sludge application rate	kg/ha	SAR
Plow zone depth	m	pzd
Treatment zone depth	m	tzd
Recharge rate	m/day	V_d
Evaporation rate	m/day	E
Air temperature	degrees C	T
Relative humidity	--	RH
Diffusion coefficient of water vapor in air	m^2/day	D_W

Oil-water partition coefficient

If this is not known, it can be approximated by the octonal water partition coefficient for the pollutant.

Henry's law constant

If the dimensionless Henry's law constant is not known, it can be determined from the value of the constant in units of atm-m^3/mole by dividing the dimensioned value by 0.024.

If the dimensioned constant is not known, the dimensionless value of K_H can be estimated according to Laskowski et al. (1982) from the water solubility, molecular weight, and vapor pressure of the pollutant using the relation

$$K_H \approx VP \cdot MW / (760 \cdot S)$$

where S is the solubility of the pollutant (g/m_3), MW is the molecular weight (g/mole), and VP is the vapor pressure (mm of Hg).

PARAMETER AVERAGING

The soil parameters in this model are assumed to be uniform throughout the treatment site. This will not be true in general. The software includes an option to calculate a weighted average value for soil properties known for different layers in the soil. This section outlines the averaging schemes employed. The software enables the user to enter values of d_i and V_i for each layer. It then calculates the average and places it in the data entry screen.

Depth Weighted Average: The average value calculated for all parameters except the saturated hydraulic conductivity is the depth weighted average of the values for each layer. Consider a site in which the depth of the soil layer i is d_i for i = 1, 2, 3, ..., N and $d_0 = 0$ and d_N is equal to the treatment zone depth. If the parameter of interest has a value V_i for i = 1, 2, 3, ..., N, then the depth-weighted average V is given by

$$V = \sum_{i=1}^{N} w_i V_i$$

where

$$w_i = (d_i - d_{i-1})/d_N \qquad \text{for } i = 1, 2, 3, ..., N.$$

Average Saturated Hydraulic Conductivity: If d_i contains the depths of each layer of soil as explained above for depth weighted averages and if k_i contains the corresponding saturated hydraulic conductivities for each layer, the equivalent conductivity, k_s, for the layered soil (Swartzendruber, 1960) is given by

$$k_s = \frac{d_N}{\sum_{i=1}^{N} \frac{(d_i - d_{i-1})}{k_i}}$$

Screen 8 illustrates the use of the averaging feature built in to the software. In this case, the <F2> key was pressed when the user was being prompted for the fraction organic carbon content. The treatment zone was made up of 5 layers so the user chose to use this averaging scheme to compute the average value for the site. In this case, each line includes an entry for the depth of the layer and the fraction organic carbon content for the layer. The two numbers must be separated by a comma or a blank space. When the <F10> key is pressed, the average value is calculated and placed in the appropriate line on Screen 2. The user can then continue entering data there.

<u>NOTE: THE AVERAGE IS CALCULATED TO THE MAXIMUM DEPTH ENTERED. THIS MAXIMUM DEPTH SHOULD CORRESPOND TO THE DEPTH OF THE TREATMENT ZONE.</u>

```
   Averaging Screen
  1. Depth, m, and fraction organic carbon : 0.10 0.02
  2. Depth, m, and fraction organic carbon : 0.15 0.007
  3. Depth, m, and fraction organic carbon : 0.30 0.005
  4. Depth, m, and fraction organic carbon : 1.05 0.002
  5. Depth, m, and fraction organic carbon : 1.50 0.001
  6. Depth, m, and fraction organic carbon :
  7. Depth, m, and fraction organic carbon :
  8. Depth, m, and fraction organic carbon :
  9. Depth, m, and fraction organic carbon :
 10. Depth, m, and fraction organic carbon :
 11. Depth, m, and fraction organic carbon :
 12. Depth, m, and fraction organic carbon :
 13. Depth, m, and fraction organic carbon :
 14. Depth, m, and fraction organic carbon :
 15. Depth, m, and fraction organic carbon :



     <F1> : Display help for entries
    <F10> : Proceed - all entries made
    <Esc> : Abort option and return to parameter entry screen
```

Screen 8. Screen for depth weighted average of fraction organic carbon.

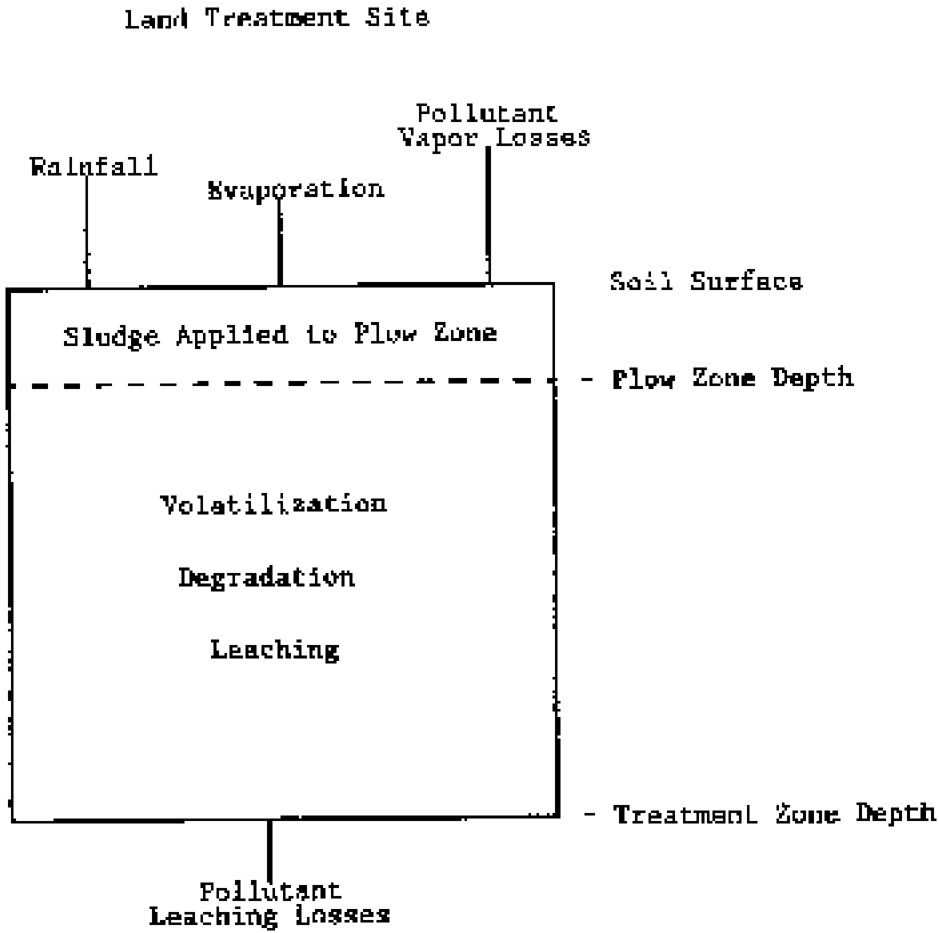

Figure 1. Diagram of land treatment site.

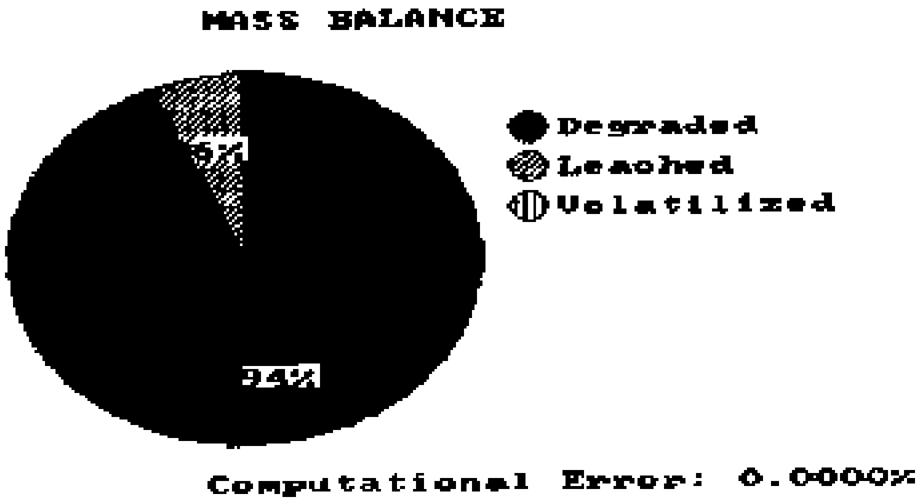

Figure 2. Mass balance graph summarizing information in Table 3.

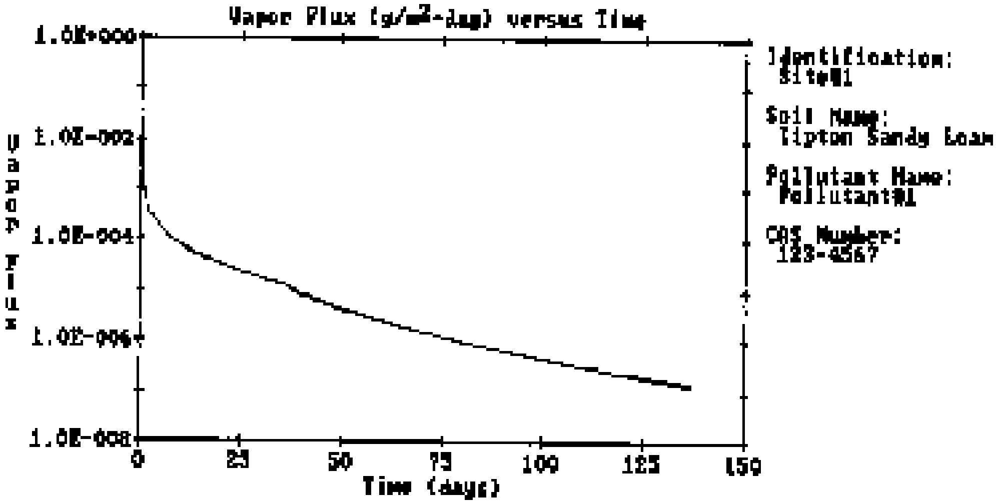

Figure 3. Graph of flux density of pollutant in vapor phase as a function of time.

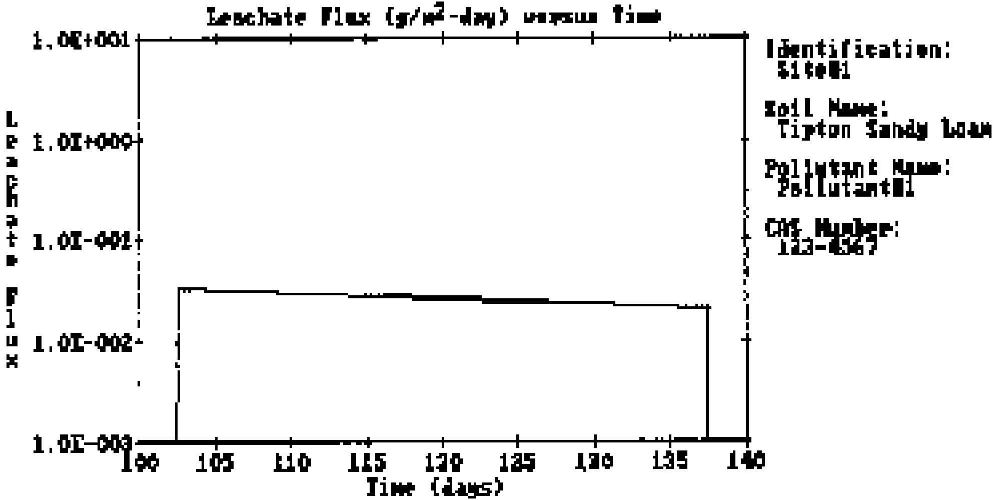

Figure 4. Graph of flux density of pollutant leached below the treatment zone as a function of time.

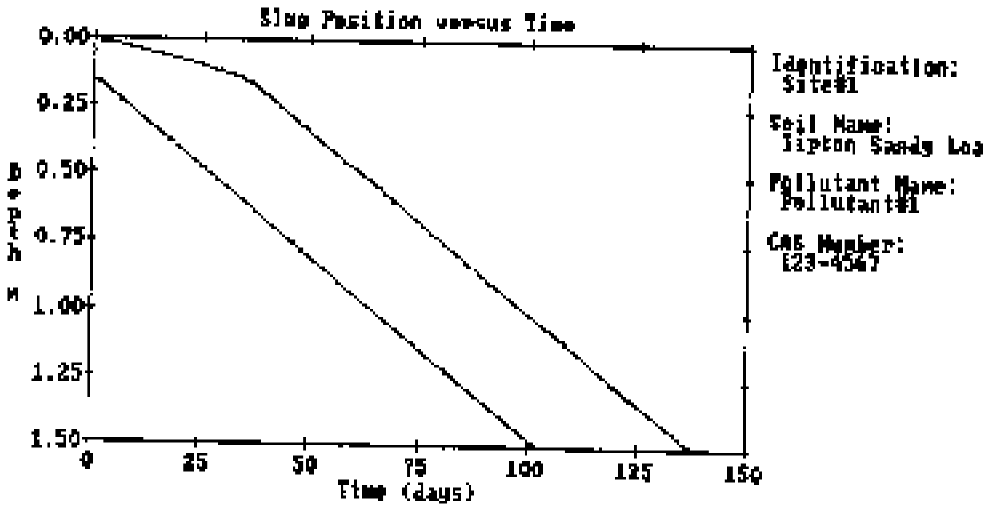

Figure 5. Location of the top and bottom of the pollutant as a function of time.

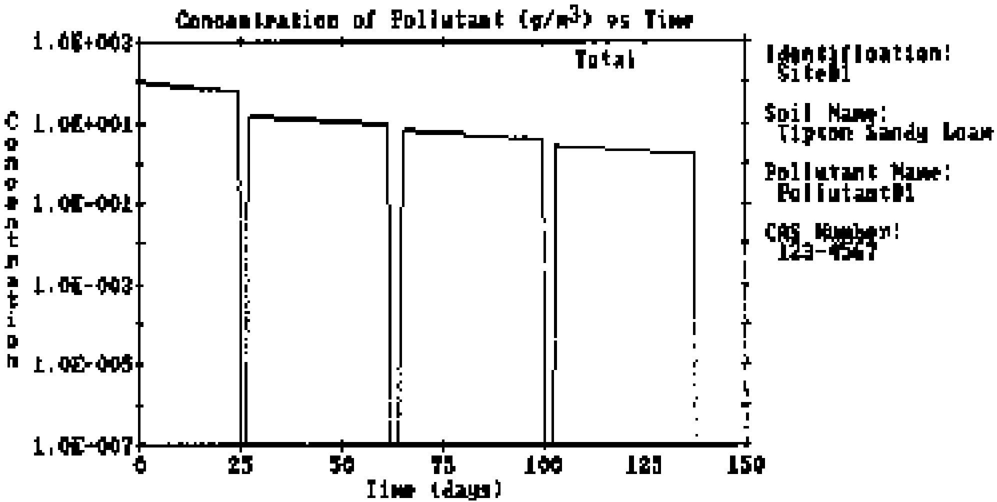

Figure 6. Concentration of total pollutant as a function of time for depths of 0.1, 0.5, 1.0, and 1.5 meters.

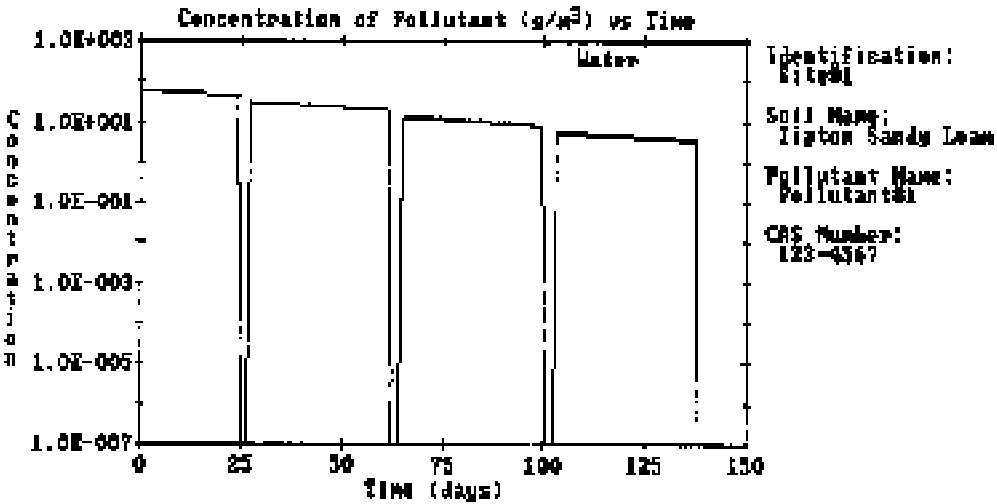

Figure 7. Concentration of pollutant in water as a function of time for depths of 0.1, 0.5, 1.0, and 1.5 meters.

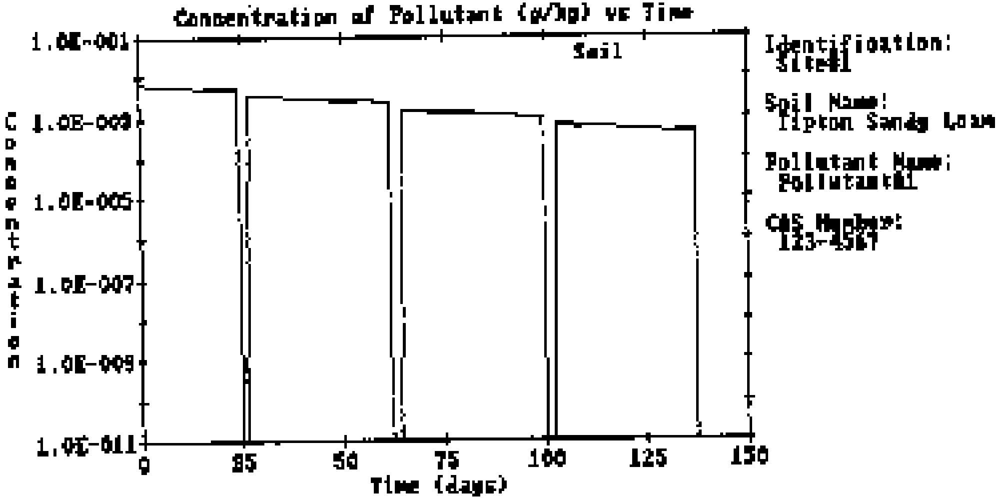

Figure 8. Concentration of pollutant in soil as a function of time for depths of 0.1, 0.5, 1.0, and 1.5 meters.

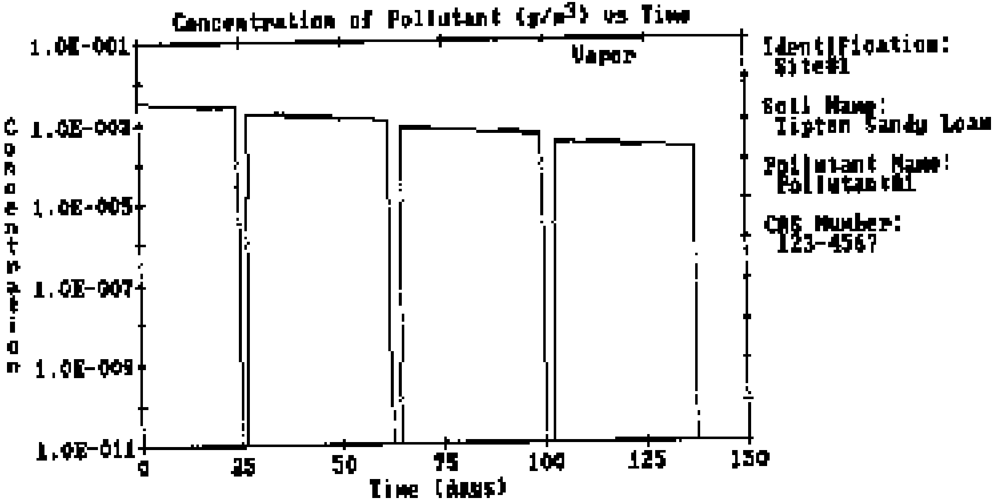

Figure 9. Concentration of pollutant in vapor as a function of time for depths of 0.1, 0.5, 1.0, and 1.5 meters.

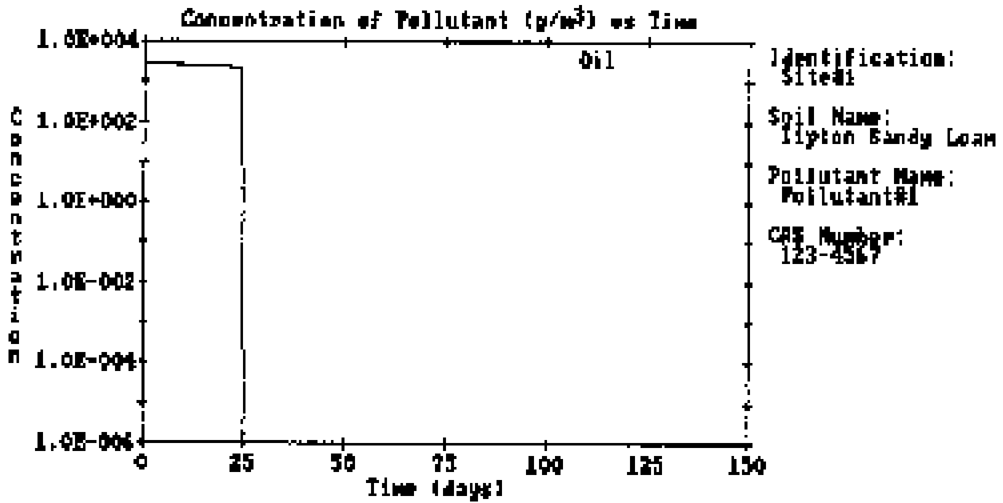

Figure 10. Concentration of pollutant in oil as a function of time for depth of 0.1 meters. Curves for 0.5, 1.0, and 1.5 meter depths are not visible since the concentration at these depths is zero.

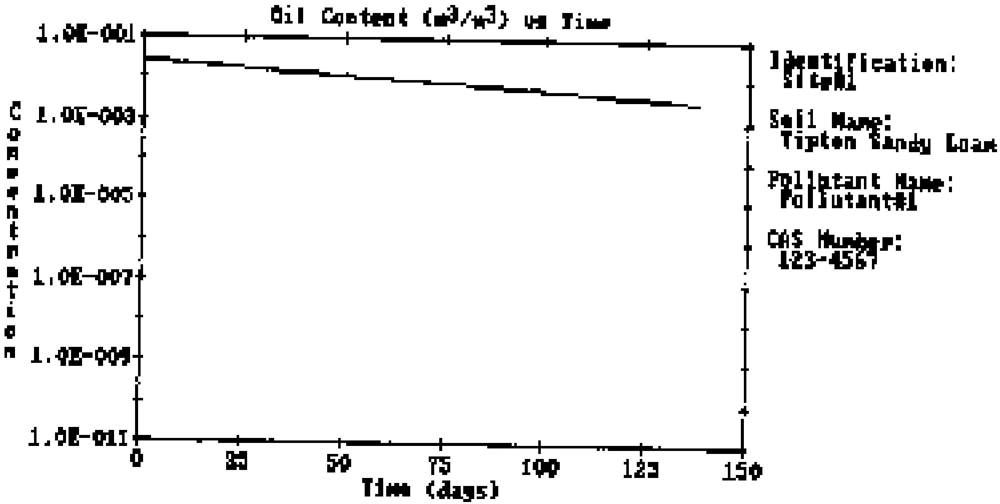

Figure 11. Oil content as a function of time for depths of 0.1 meters. Oil content curves for 0.5, 1.0, and 1.5 meter depths are not shown since the oil content is zero below the plow zone.

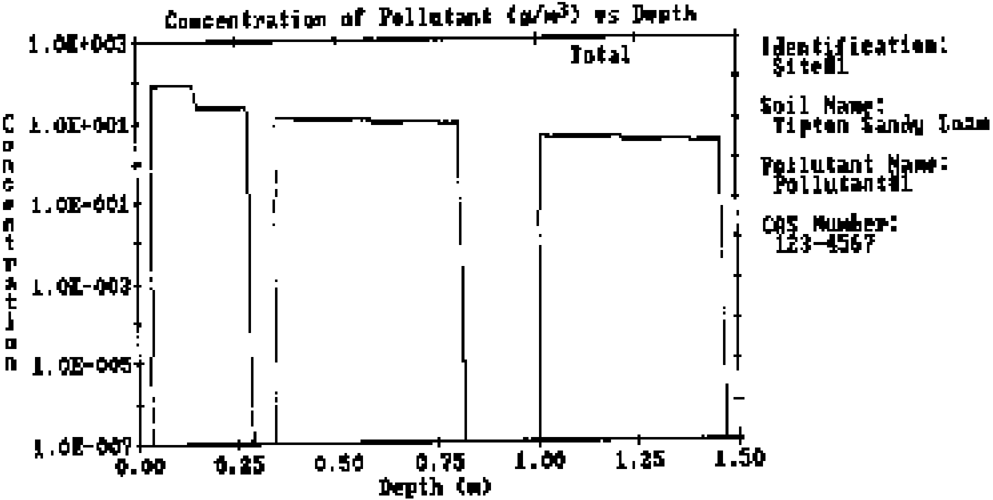

Figure 12. Concentration of total pollutant as a function of depth for times of 10, 50, and 100 days.

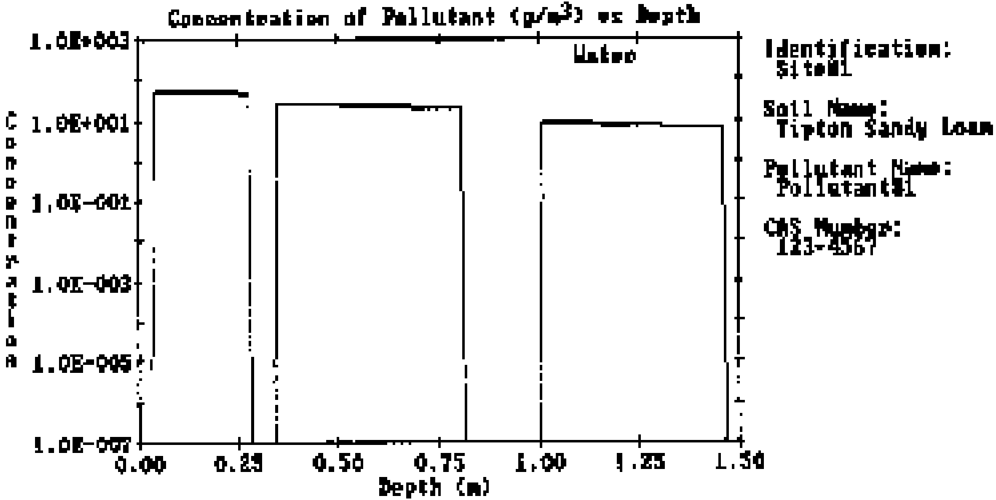

Figure 13. Concentration of pollutant in water as a function of depth for times of 10, 50, and 100 days.

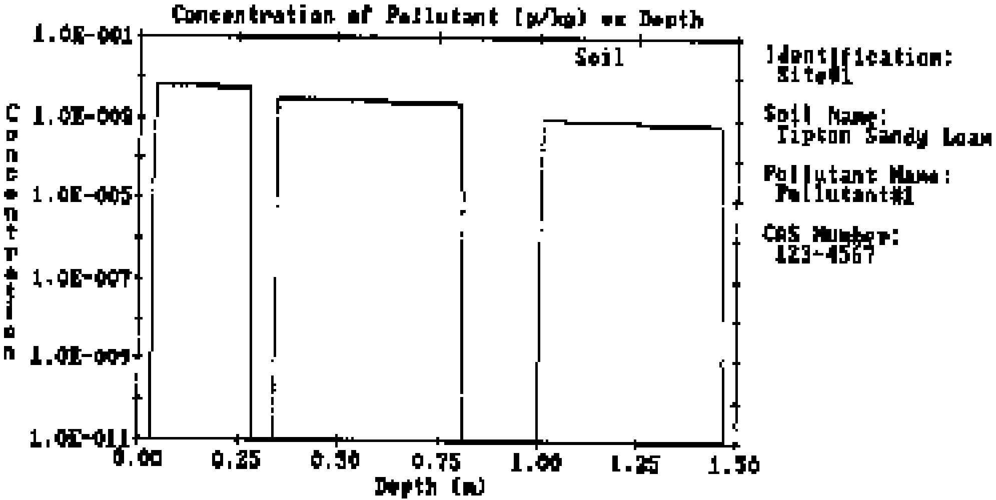

Figure 14. Concentration of pollutant in soil as a function of depth for times of 10, 50, and 100 days.

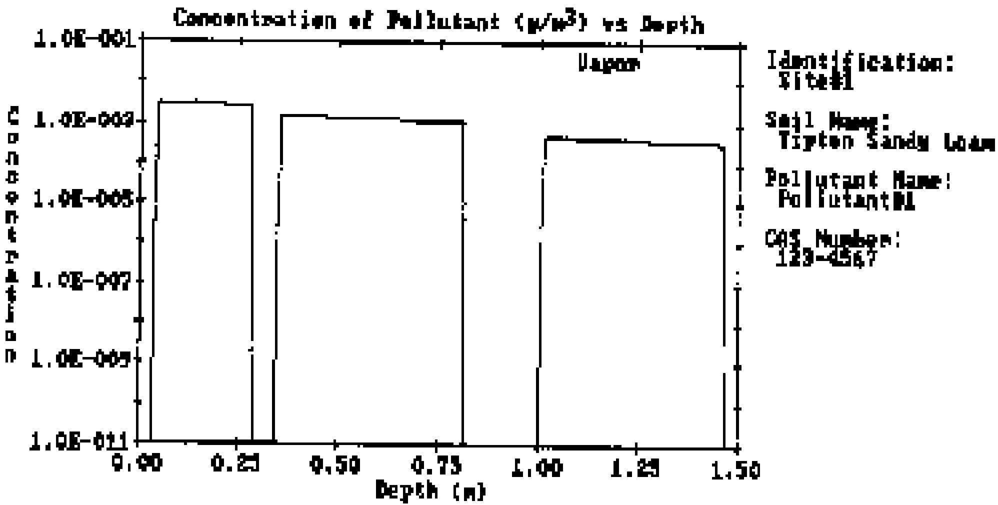

Figure 15. Concentration of pollutant in vapor as a function of depth for times of 10, 50, and 100 days.

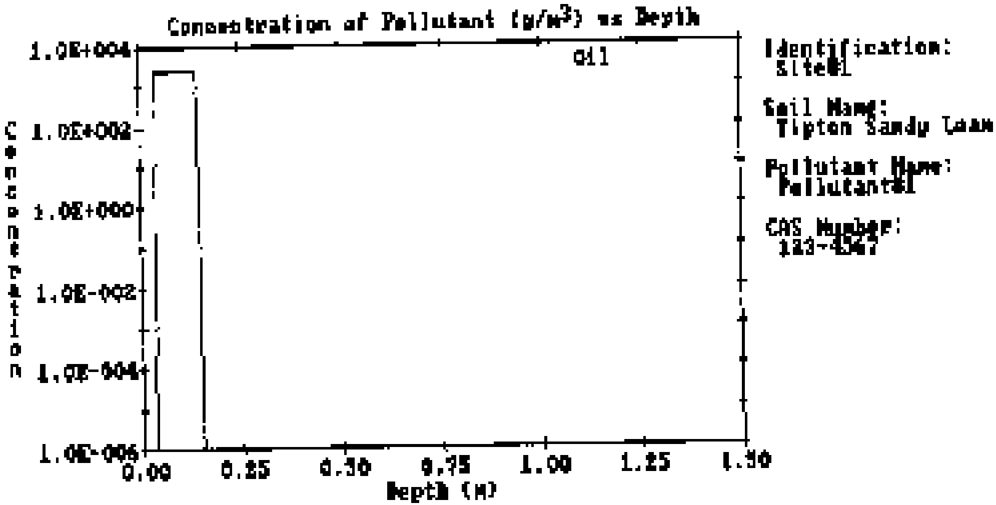

Figure 16. Concentration of pollutant in oil as a function of depth for 10 days after application. Note the concentration decreases to zero at the plow zone depth. The concentration was zero at 50, and 100 days.

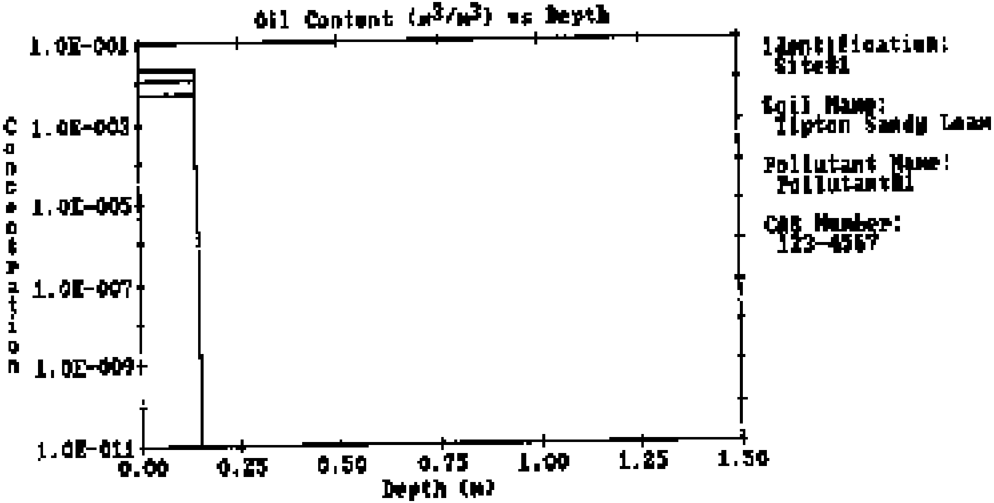

Figure 17. Oil content as a function of depth for times of 10, 50, and 100 days. The oil does not move downward but the oil content decreases due to degradation.

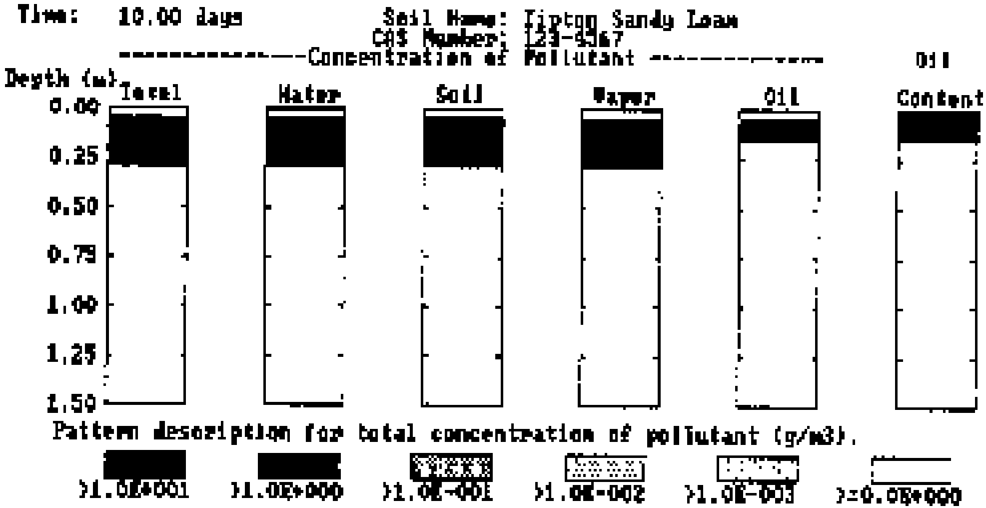

Figure 18. Concentration bar graphs representing the pollutant and oil in the treatment zone at a time of 10 days. The concentrations represented by the patterns in each phase can be displayed by pressing the <F1> key.

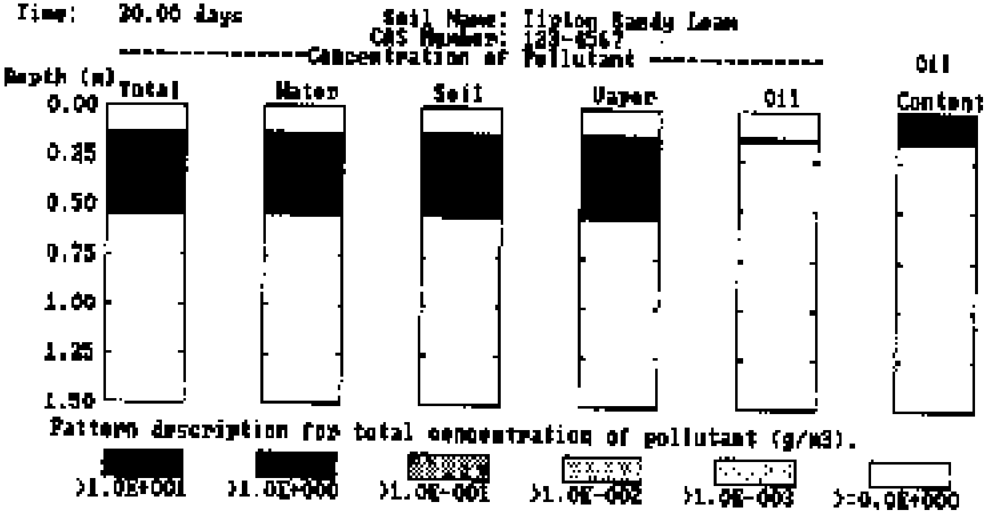

Figure 19. Concentration bar graphs for 30 days.