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PESTAN

Pesticide Analytical Model

Version 4.0

Developed for:

The United States Environmental Protection Agency
Office of Research and Development
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1. INTRODUCTION

The PESTAN (Pesticide Analytical) model is a computer code for estimating the transport of organic solutes through soil to groundwater. The model is based on a closed-form analytical solution of the advective-dispersive-reactive transport equation. The model was developed by Enfield, et al. in 1982 and has since been used by the EPA Office of Pesticides Program (OPP) for initial screening assessments to evaluate the potential for groundwater contamination of currently registered pesticides and those submitted for registration (Donigian and Rao 1986). The model has also been tested under field and laboratory conditions (Enfield et al., 1982; Jones and Back, 1984; Melancon et al., 1986). Although the model is based on a simple analytical solution, it may be useful in making preliminary assessments as long as the user is fully aware of its assumptions and limitations. Therefore, it is the principal objective of this User's Guide to provide essential information on the aspects such as model conceptualization, model theory, assumptions and limitations, determination of input parameters, analysis of results and sensitivity analysis (parameter studies). With the information presented, it is hoped that this manual will help the user in making the best possible use of the model.

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2. MODEL CONCEPTUALIZATION, ASSUMPTIONS, AND LIMITATIONS

The vertical transport of dissolved pollutants through the vadose zone is simulated in PESTAN as a "slug" of contaminated water that migrates into a homogeneous soil (see Figure 2.1). The concentration of the chemical slug equals the solubility of the pollutant in water, and the thickness of the slug is conceptualized principally as the volume of pore water required to dissolve the total available pollutant mass at the solubility of the pollutant. The total available mass is defined as that mass existing at the time of recharge. When no lapse of time occurs between the application and recharge, the total mass available will equal the applied mass (see Figure 2.2a). However, when a significant time lapse occurs between the application and recharge events there will be a loss of mass due to solid-phase decay, which begins at the time of application, and the total available mass will be less than the applied mass (see Figure 2.2b).

The slug begins to enter the soil at the first precipitation/irrigation event at a rate equal to the pore water velocity. PESTAN assumes steady flow conditions through the soil domain. Once the slug enters the soil, the pollutant transport is influenced by sorption and dispersion. Mass of the pollutant can be lost via liquid-phase decay or via migration out of the soil domain.

When developing a model simulation, it is important to fully understand the implications of the PESTAN conceptualization. The following assumptions are made in the development of PESTAN and are based primarily on those made by Enfield et al. (1982).

1. The PESTAN conceptualization assumes the leachate concentration equals the maximum possible concentration, i.e. solubility. This assumption results in maximum (conservative) concentration values and a minimum slug thickness. Therefore, the pollutant concentration profile in the soil will be thinner and at concentrations greater than those actually occurring in the soil.

2. The slug enters the soil at the velocity of the pore water, which is the ratio of the recharge rate to the pore water content. If the recharge rate incorporates losses due to evapotranspiration or is averaged over long time periods, then this value will be significantly less than the recharge rate experienced during an actual rainfall event. Hence, the calculated pore water velocity will be considerably less than that under true conditions and will result in the simulated slug migrating at a slower rate than under true conditions.

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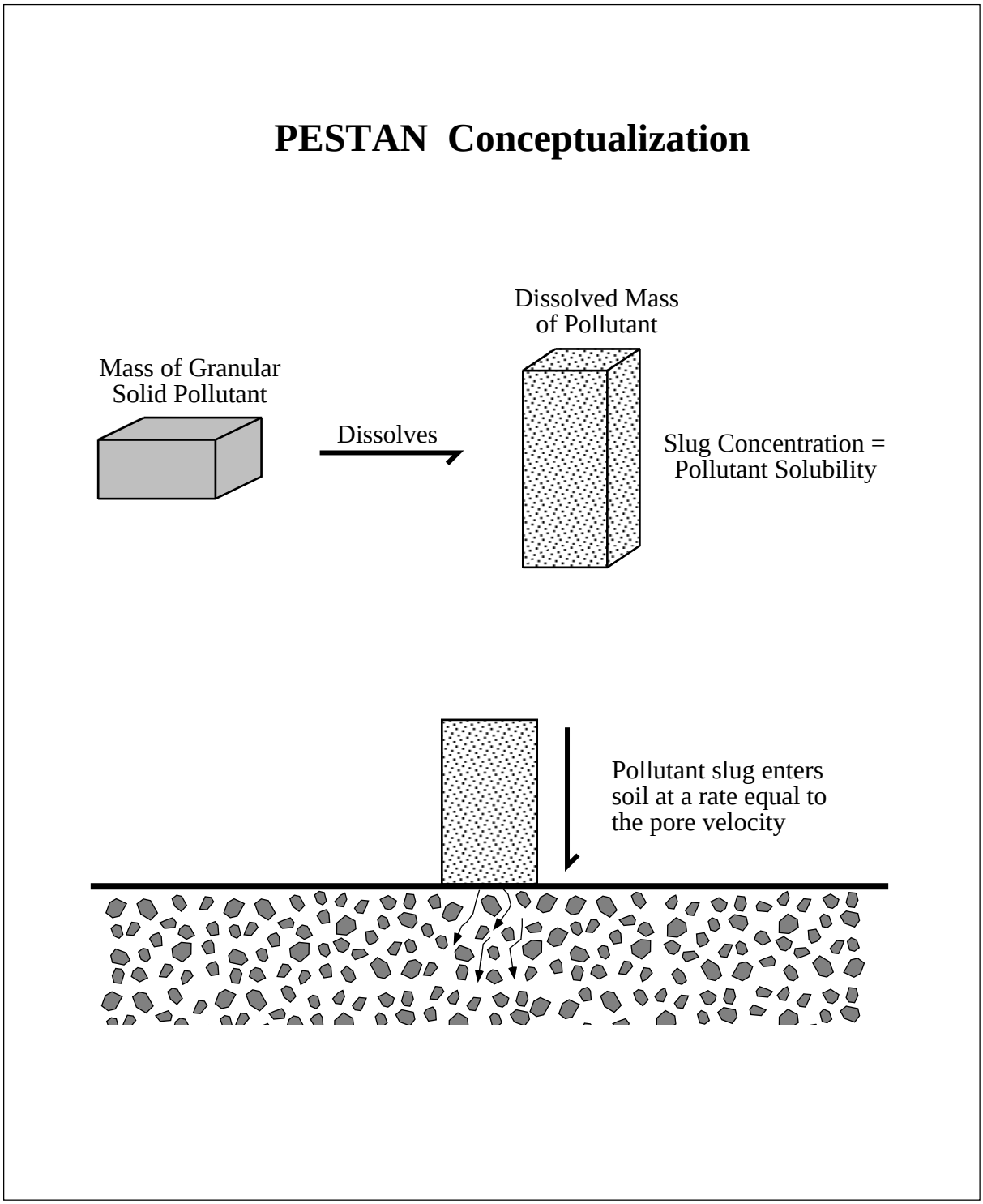

Figure 2.1. PESTAN conceptualization of pollutant migration with the soil system.

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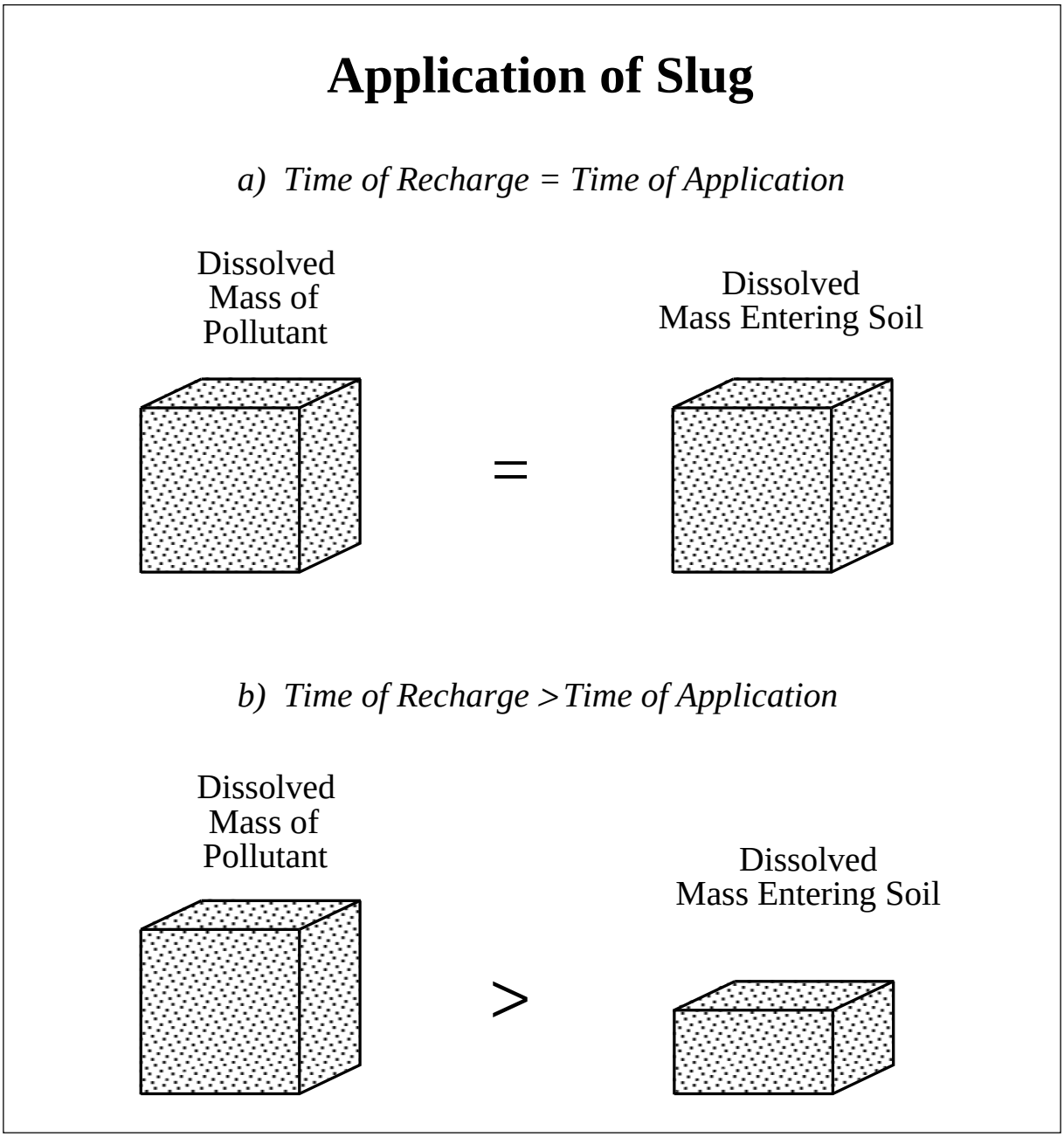

Figure 2.2. PESTAN Conceptualization of pollutant application.

Granular pollutant is dissolved in slug at concentration equal to the pollutant solubility. When time of recharge is the same as the time of application all the pollutant mass enters the soil. When time of recharge occurs after the time of application pollutant mass will be lost due to decay, hence the dissolved mass entering the soil will be less than original mass of pollutant.

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3. Steady-state flow conditions are assumed in the code. The time required for flow to establish steady conditions during a rainfall event is determined as being approximately equal to $5S^2/2K^2$, based on Philip's (1969) work, where S is sorptivity (LT^{-2}) and K is saturated hydraulic conductivity. Steady-state conditions in clay-rich soils develop in about 48 hours and in sandy soils develop in less than 1 hour (see Table 2.1). Therefore, results for simulations made prior to reaching steady-state conditions could be in error.

4. Homogeneous soil conditions are assumed in the model. This assumption will rarely occur in the field. The user can estimate the impact of non-uniform soils by comparing results from several simulations covering the range of soil properties present at the site.

5. Linear isotherms describe the partitioning of the pollutant between the liquid and soil phases. Local or instantaneous equilibrium between these phases is assumed.

6. First order degradation of the pollutant is assumed. Solid-phase degradation occurs at the surface between the time of application and time of recharge. Liquid-phase degradation occurs within the soil system. The rate of liquid-phase degradation does not change with soil depth or time. This assumption ignores potential changes in biological activity with soil depth.

7. The water content of the soil is related to the hydraulic conductivity as described by Campbell (1974).

$$\frac{K}{K_{sat}} = \left(\frac{\theta}{\theta_{sat}}\right)^{2b+3} \qquad (1)$$

where K is the hydraulic conductivity at a volumetric water content of θ; K_s is the hydraulic conductivity of the soil at the saturated water content, θ_{sat} ; and b is the characteristic curve coefficient for the soil. This relationship assumes steady-state conditions for the flow.

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TABLE 2.1. ESTIMATED TIME TO ESTABLISH STEADY FLOW CONDITIONS*

Soil Texture	Time (minutes)
Sand	5
Loamy Sand	30
Sandy Loam	60
Silt Loam	2130
Loam	690
Sandy Clay Loam	416
Silty Clay Loam	2310
Clay Loam	3330
Sandy Clay	735
Silty Clay	3810
Clay	3030

* *Table is based on the work of Philip (1969). It is obtained by multiplying* $\frac{S^2}{4K_s^2}$ *by a factor of 10, where* S = *sorptivity and* K_S = *saturated hydraulic conductivity.*

8. The model does not account for non-aqueous phase liquids or any flow conditions derived from variable density.

The model presents results for the specific input values without accounting for any parameter uncertainty. The user is encouraged to compare results for a series of simulations using a range of values to obtain an estimate of potential uncertainty. For example, if three different recharge values are likely, three simulations should be run rather than averaging the three values to obtain only one value.

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3. MATHEMATICAL MODEL

A brief discussion of the mathematical development and important aspects of the model theory with a few modifications from the formulation of Enfield et al. (1982) is presented below. A detailed description of the model theory is presented in the original paper by Enfield et al. (1982).

The vertical transport of a pollutant dissolved in water through the soil can be described by the following equation:

$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2} - v\frac{\partial C}{\partial x} - \frac{\rho_b}{\theta}\frac{\partial S}{\partial t} - k_l C \qquad (2)$$

where:

- C = liquid-phase pollutant concentration (mass of pollutant in water / volume of water) (M/L^3)
- t = time (T)
- x = distance along the flow path (L)
- D = dispersion coefficient (L^2/T)
- v = interstitial or pore-water velocity (L/T)
- ρ_b = bulk density (M/L^3)
- θ = volumetric water content (volume of pore water/total volume) (L^3/L^3)
- S = solid-phase concentration (mass of pollutant in soil/mass of soil) (M/M)
- k_l = first-order decay coefficient in liquid phase (/T)

The term $\partial S/\partial t$ is the rate of loss of solute from liquid phase to solid phase due to sorption. Under the assumption of linear, instantaneous sorption, $\partial S/\partial t$ can be evaluated as:

$$\frac{\partial S}{\partial t} = K_d\frac{\partial C}{\partial t} \qquad (3)$$

where K_d = linear Freundlich sorption coefficient.

Substituting for $\partial S/\partial t$ from (2) into (1), one obtains

$$R\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2} - v\frac{\partial C}{\partial x} - k_l C \qquad (4)$$

where

$$R = 1 + \frac{K_d\,\rho_b}{\theta} \text{ (unitless)} \qquad (5)$$

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The partial differential equation (4) can be solved for C(x,t) along with the following initial and boundary conditions:

$$C(x,t=0) = \begin{cases} 0, & -\infty < x < -x_o \\ C_0, & -x_o \le x < 0 \\ 0, & 0 \le x < \infty \end{cases} \tag{6}$$

$$\lim_{|x| \to \infty} \frac{\partial C}{\partial x} = 0 \tag{7}$$

The solution is given as follows :

$$C(x,t) = \frac{C_0}{2} \exp(-k_l t) \left\{ \mathrm{erf}\left[\frac{x + x_o - \frac{vt}{R}}{2\sqrt{Dt/R}} \right] - \mathrm{erf}\left[\frac{x - \frac{vt}{R}}{2\sqrt{Dt/R}} \right] \right\} \tag{8}$$

where erf(z) is the error function which is defined as,

$$\mathrm{erf}\,(z) = \frac{2}{\sqrt{\pi}} \int_0^z \exp(-y^2)\, dy \tag{9}$$

Boundary condition (1) is obtained based on the reasoning that the dissolved pollutant, which is applied at the soil surface, can be represented as a "slug" of thickness x_o that enters the soil at time zero. x_o is calculated using water solubility when the chemical is applied in a granular form by determining the equivalent depth of water from the soil water content required to dissolve all of the available mass of pollutant. The slug thickness is calculated as

$$x_o = \frac{M_a \exp(-k_s t_r)}{S\,(\theta + K_d \rho_b)} \tag{10}$$

where:

x_o	=	slug thickness in (L)
M_a	=	total pollutant mass applied per unit area (M/L^2)
k_s	=	solid-phase decay coefficient (/T)
t_r	=	time lapse between application and recharge (T)
S	=	solubility of pollutant in water (M/L^3)

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4. HARDWARE AND SOFTWARE REQUIREMENTS

The minimum hardware and software requirements for PESTAN are:

- IBM-PC or compatible computer with INTEL 8086, 80286, 80386, or 80486 CPU based system
- 256K RAM
- Color Graphic Adapter (CGA) board
- One floppy disk drive
- (MS/PC) DOS 2.0 or higher

Additional recommended hardware and software include:

- A math coprocessor
- A hard disk
- A FORTRAN Compiler for modifications of the source code
- A commercial graphics software such as Grapher by Golden Software, Inc.

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5.0 GETTING STARTED

PESTAN is distributed by the EPA's Center for Subsurface Modeling Support (CSMoS) on a single IBM-formatted 5.25 or 3.5 inch diskette. PESTAN version 4.0 includes the following files.

PESTAN.FOR	PESTAN.INP
PESTAN.EXE	ALDCB1.INP
SHOW.EXE	PESTAN.OUT
WHAT.EXE	ALDCB1.OUT
PMENU.BAT	LEACHBTC.DAT
FORMENU1.TXT	LEACHFLX.DAT
FORMENU2.TXT	SOILCON.DAT
CHGNAME.TXT	

Prior to installing or implementing the program make a back-up copy of PESTAN using the DISKCOPY command of MS-DOS or PC-DOS. Once completed, copy the PESTAN files to the hard disk in a selected directory. Because the program requires ample storage for the output files, approximately 700KB, the program should be run from the hard disk. In addition, a text editor will have to be defined in the AUTOEXEC.BAT file. The text editor could be DOS edlin, DOS edit, Norton Classic editor, WordPerfect, or any other commercial editor. Define the text editor in AUTOEXEC.BAT (including its path) . For example,

SET EDITOR=C:\WP51\WP

Finally, the ANSI.SYS driver (see your MS-DOS manual) must be installed in the CONFIG.SYS file. This is done by adding a statement such as

DEVICE=C:\DOS\ANSI.SYS

It is important that the correct path for ANSI.SYS is given.

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5.1 Program execution

PESTAN is executed by typing <**PMENU**> at the appropriate directory prompt.

C:\PMENU

This will initiate the model execution, and a menu of options will be displayed on the screen.

```
                    PESTAN  PREPROCESSOR

            <<<< Welcome  to  PESTAN  Version  4.0  >>>>

                 Current  Working  File:  NONE.INP
                 1  – List of input files
                 2  – Select an input file
                 3  – View the input file
                 4   – Edit/Create  input  file
                 5  – Run the PESTAN program
                 6  – View the output file
                 7  – Print input data ( .INP ) file
                 8  – Print output ( .OUT ) file
                 0  – Quit and return to DOS

        Please  enter  your  selection  :
```

Select an option by typing the appropriate number of the selection. **Do not** hit ENTER, the code will automatically continue.

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6. INPUT PARAMETERS

The following describes the input parameters for PESTAN. It is important that this information be fully understood for proper application of the code.

1. **Water Solubility (S)**. Values defining the water solubility of the pollutant must have units of milligrams per liter (mg/l). Appendix A provides water solubility information on over 50 different chemicals. If data regarding the pollutant being modeled is not presented, refer to the standard reference manuals that are documented in Appendix C or consult the chemical manufacturer.

2. **Recharge**. This parameter describes the infiltration rate of water entering the soil. This rate is dependent upon the nature of the precipitation (or irrigation), the character of the soil, and the duration of the precipitation event. The rate of infiltration will be equal to the rain or irrigation intensity when this precipitation rate is less than the saturated hydraulic conductivity (K_s) of the soil. For the special case when the rainfall intensity is greater than the saturated hydraulic conductivity, the recharge value may be greater than K_s. In particular, infiltration can significantly exceed K_s when the rainfall event is relatively short. When simulating large time periods, the recharge parameter can be viewed in terms of net groundwater recharge, which incorporates losses due to evapotranspiration.

3. **Sorption Constant (K_d)**. The sorption constant is the linear partition coefficient, K_d, which describes the relative distribution of the pollutant between that which is sorbed to the solid phase and that which is dissolved in water. The higher the value of the partition coefficient the greater the tendency for sorption to the solid phase; in contrast, low partition values indicate most of pollutant distribution is retained in the water. The partition coefficient is a constant for a given set of conditions. As a result, it is a site specific value. In particular, it is a function of the fraction organic content of the soil (f_{oc}) and can be estimated as the product of the fraction organic content and the organic carbon partition coefficient (K_{oc}) of the pollutant.

$$K_d = K_{oc} \; f_{oc} \qquad (11)$$

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Appendix A lists the organic carbon partition coefficient for numerous pollutants. The fraction organic content of the soil (f_{oc}) can be determined from laboratory analyses or is commonly documented in soil descriptions by the U.S. Soil Conservation Service. Generic values for organic content for soils of different texture are listed in Appendix B.

4. **Solid-phase degradation rate constant (k_s)**. This parameter describes the decay of the pollutant at the surface prior to infiltration into the soil. The decay is defined as rate of loss per hour. It should be noted that in PESTAN degradation begins at the time of application. Values for solid-phase decay could involve processes such as photodecomposition and volatilization. Rates for solid-phase decay may be obtained from pollutant reference texts (see Appendix C).

5. **Liquid-phase degradation rate constant (k_l)**. Liquid-phase decay describes those processes where mass is lost within the soil system. In general, degradation occurs primarily by soil microorganisms and may vary depending upon soil temperature and moisture. Appendix C lists pollutant reference texts that document values for the liquid-phase degradation rate constant.

6. **Bulk Density (ρ_b)**. This parameter defines the mass of dry soil relative to the bulk volume of soil. It is described in units of grams per square centimeters. Ranges for bulk density with respect to different soil types are given in Appendix B.

7. **Saturated Water Content (θ_{sat})**. The saturated water content of the soil is the volume of water at saturation relative to the bulk volume density. Typical values for saturated water content for different soil textures are given in Appendix B.

8. **Characteristic Curve Coefficient (b)**. This parameter is defined by equation (1), which relates the relative saturation of the soil to the relative conductivity of the soil under steady-state conditions. If this constant cannot be determined, it can be obtained from the table presented by Clapp and Hornberger (1978) for different soil textures. These values are presented in Appendix B.

9. **Saturated Hydraulic Conductivity (K_{sat})**. This parameter is a coefficient of proportionality that describes the rate at which water can move through a soil at saturation. The units of conductivity are centimeters per hour (cm/hr). It should be noted that the density and kinematic viscosity of the water are considered in the measurement. The standard value of hydraulic conductivity is defined for pure water at a temperature of 15.6°C.

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Appendix B provides average values for saturated hydraulic conductivity for different soil textures.

10. **Dispersion Coefficient (D)**. Dispersion is a difficult parameter to define as it is not fully understood despite considerable efforts by the researchers in the field. This parameter may be best evaluated through calibration of the model. However, it should be noted that empirical relationships have been developed based on numerous experiments. Biggar and Nielsen (1976) proposed the relationship

$$D = D_p + 2.93\ v^{1.11} \qquad (12)$$

where D_p = diffusion coefficient of the chemical in soil (cm^2/day), and v = the interstitial pore velocity (cm/day). The parameter D_p can be estimated at 0.72 cm^2/day (Biggar and Nielsen, 1976).

11. **Minimum x-value**. The minimum x-value refers to the upper depth of the model domain. In most cases, this location will be the surface, which defines the minimum x-value at 0. The unit is centimeters.

12. **Maximum x-value**. The maximum x-value defines the lower depth of the model domain. This depth in many cases will be water table. The maximum x-value is defined in centimeters.

13. **Minimum time value**. The minimum time value defines the initial time boundary in days.

14. **Maximum time value**. This is the time in days when simulation ends. It is the final time of interest.

15. **Number of time intervals for printing out results**. Enter the number of time intervals at which the output will be documented.

16. **Time values**. This parameter defines the time values in days at which the output will be documented.

17. **Number of applications of waste**. Number of applications prior to recharge in the simulation.

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18. **Waste application rate and starting time**. This is the mass of pollutant applied per hectare of land area. One hectare equals 10,000 square meters. The starting time is the time interval between the application and the initiation of recharge. The code will simulate degradation during the time interval between the application and recharge event. Conservative conditions would define the starting time as zero. In creating or editing the input file, separate the waste application rate value and the starting time value by a comma.

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7. OUTPUT

7.1 Options

Several output options can be defined by the user to convert the output from PESTAN into files which can be plotted using GRAPHER (Golden Software, 1987) or other compatible commercial graphics packages. Three graphs can be constructed: a breakthrough curve, a pollutant flux curve, and a soil-depth pollutant concentration profile. These can be selected by defining the following options.

1. **Option for creating a breakthrough curve dataset**. This output constructs two datasets; one for the breakthrough curve and one for the pollutant flux graph. The breakthrough curve dataset consists of values of pollutant concentration versus time, and the pollutant flux dataset consists of values of pollutant flux versus time. To construct the breakthrough dataset and the pollutant flux dataset, type either "Y" or "y". If this is not desired, type "N" or "n".

2. **Location at which breakthrough curve is desired**. If a breakthrough curve and pollutant flux graphs are desired then input the depth in centimeters at which the dataset will define. If these curves are not desired, delete this line.

3. **Option for creating a soil-depth profile graph**. This output option constructs a dataset with values of depth and concentration that can be used with a commercial graphics package to depict the concentration/soil depth profile. To construct a soil-depth dataset, type "Y" or "y"; if this is not desired, type "N" or "n".

4. **Time at which soil-depth profile is desired**. If a soil-depth profile is desired input the time in days at which the dataset will be defined. If this graph is not desired, delete this line.

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7.2 Output results

PESTAN output file (with the extension .OUT) provides information regarding the input parameters, the physical nature of the water/pollutant conditions within the soil, the concentration profile within the soil, and the pollutant mass balance. The code allows the user to view the output as well as to print the output. These options can be selected from the main menu screen.

The initial section of the output is a summary of the model scenario. The information presented includes the title of the scenario and the input parameter values. In particular, the input summary should be closely reviewed to ensure that the appropriate values were utilized. An example of the input summary is given below.

TITLE: STUDY OF ALDICARB RESIDUES IN FLORIDA SOIL AND WATER (JONES AND BACK, 1984)

Solubility (mg/l)	:	0.78000E+04
Recharge rate (cm/hr)	:	0.35000E–02
Sorption constant (cc/g)	:	0.73000E–01
Saturated water content	:	0.39500E+00
Solid-phase decay (/hr)	:	0.22200E–03
Liquid-phase decay (/hr)	:	0.22200E–03
Curve coefficient	:	0.40500E+01
Bulk density (g/cc)	:	0.15000E+01
Dispersion coefficient (cm^2/hr)	:	0.60000E–03
Saturated hydrualic conductivity	:	0.10000E+01
Minimum depth (cm)	:	0.00000E+00
Maximum depth (cm)	:	0.20000E+03
Minimum time (day)	:	0.00000E+00
Maximum time (day)	:	0.50000E+03

For application 1 the active ingredient (ai) applied is 0.112E+02 kg ai/ha, and has been applied 0.000E+00 days prior to recharge.

After the summary of the model scenario, the output lists the calculated values that define the water and pollutant conditions within the soil. These parameters are (1) the projected water content, (2) the pore water velocity, (3) the pollutant velocity, and (4) the length of pollutant slug. An example of the output defining the water and pollutant conditions within the soil is shown below.

Project water content	:	0.237E+00
Pore water velocity (cm/hr)	:	0.147E–01
Pollutant velocity (cm/hr)	:	0.101E–01
Length of pollutant slug (cm)	:	0.414E–01
Mass decayed prior to recharge (kg)	:	0.000E+00

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1. The projected water content (q) is calculated from the following relationship

$$\theta = \theta_s \left(\frac{r}{K_s}\right)^{\frac{1}{2b+3}}, \quad r \le K_s$$
$$\theta = \theta_s, \quad r > K_s \tag{13}$$

where r is the rate of infiltration.

2. The pore water velocity (v) describes the rate of movement of the interstitial water in the soil. It is calculated as

$$v = r / q \tag{14}$$

3. The pollutant velocity describes the rate of pollutant movement within the soil. Under most conditions due to sorption of the pollutant from the liquid to the solid phase, the pollutant velocity will be less than the pore water velocity. This is determined from the relation

$$v_p = v/R \tag{15}$$

4. As was described in section 3, the length of the pollutant slug is determined by equation (10).

The output describing the pollutant concentration profile is presented as a series of tables for each time value defined in the model input. The defined time value is shown above each tabulation. The output tabulation lists four columns: (1) Depth (cm); (2) Pollutant Concentration in Water, C_w, (mg/l) (3) Pollutant Concentration in Soil, C_s, (mg/kg) and (4) Total Pollutant Concentration, C_{tot}, (mg/l). The concentration is given at eleven equally spaced depths between the previously defined minimum and maximum depths. An example of the concentration profile tabulation is shown below.

Time = 0.50E+02 (days)

Depth (cm)	**Cw (mg/l)**	**Cs (mg/kg)**	**Ctot (mg/l)**
2.000	0.65E+01	0.47E+00	0.22E+01
20.000	0.79E+01	0.57E+00	0.27E+01
40.000	0.21E+00	0.15E–01	0.72E–01
60.000	0.19E–03	0.14E–04	0.67E–04
80.000	0.00E+00	0.00E+00	0.00E+00
100.000	0.00E+00	0.00E+00	0.00E+00
120.000	0.00E+00	0.00E+00	0.00E+00
140.000	0.00E+00	0.00E+00	0.00E+00
160.000	0.00E+00	0.00E+00	0.00E+00
180.000	0.00E+00	0.00E+00	0.00E+00
200.000	0.00E+00	0.00E+00	0.00E+00

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Mass balance results for the total pollutant within the soil is given for each defined time value. The mass balance output describes the mass of pollutant in the liquid-phase, the solid-phase, the total mass of pollutant remaining, and the loss of pollutant due to decay. An example of the mass balance output is shown below.

Mass Balance Results

Pollutant remaining in liquid-phase (kg)	=	0.590E+01
Pollutant remaining in solid-phase (kg)	=	0.272E+01
Total mass of pollutant remaining (kg)	=	0.862E+01
Liquid-phase decay of pollutant (kg)	=	0.172E+01

The total mass of pollutant remaining is the sum of the mass of pollutant in the liquid-phase and solid-phase. It should be noted that the loss of pollutant due to decay can occur prior to the pollutant leaching into the soil. Therefore, if the rate of decay is rapid and the time prior to recharge is sufficiently long, it is possible for significant losses of mass to result prior to leaching. Likewise, since leaching is a function of the water velocity a quantity of mass may remain outside the soil system, especially at times in the beginning of the simulation. Thus, the sum of the total mass of pollutant remaining and the loss of pollutant due to decay may not equal the total applied. In addition, losses due to leaching the pollutant from the defined depth interval will result in differences between the sum of the total mass of pollutant remaining and the loss of pollutant due to decay, and the total mass applied.

7.3. Graphical output displays

Using commercial graphics packages three graphs can be plotted using the output from the model simulation. PESTAN automatically writes output data to three files named LEACHBTC.DAT, LEACHFLX.DAT, and SOILCON.DAT. The file LEACHBTC.DAT contains the pollutant concentration versus time array for the specified depth. LEACHFLX.DAT consists of the pollutant flux versus time array for the specified depth. The file SOILCON.DAT contains the values for pollutant concentration versus depth array for the specified time.

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8. SENSITIVITY ANALYSIS

A sensitivity analysis was performed to evaluate the effects of various model inputs on the model response (concentration profiles). This was accomplished by plotting the model simulations for three different values for each parameter. These correspond to low, typical, and high values for each parameter. The results are shown in Figures 8.1 through 8.9. It is seen that the model is most sensitive to changes in recharge values. It is also quite sensitive to the changes in sorption coefficient, dispersion coefficient, and decay values. The model is relatively insensitive to solubility, saturated hydraulic conductivity, and characteristic curve coefficient, (Figures 8.1, 8.4 and 8.7), as evidenced by the overlapping of the curves corresponding to three different parameter values.

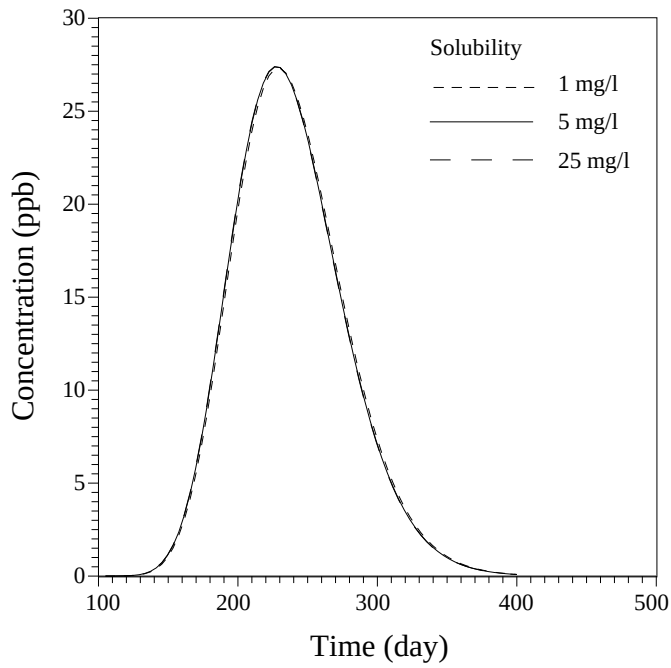

Figure 8.1. The effect of solubility on the leachate breakthrough.

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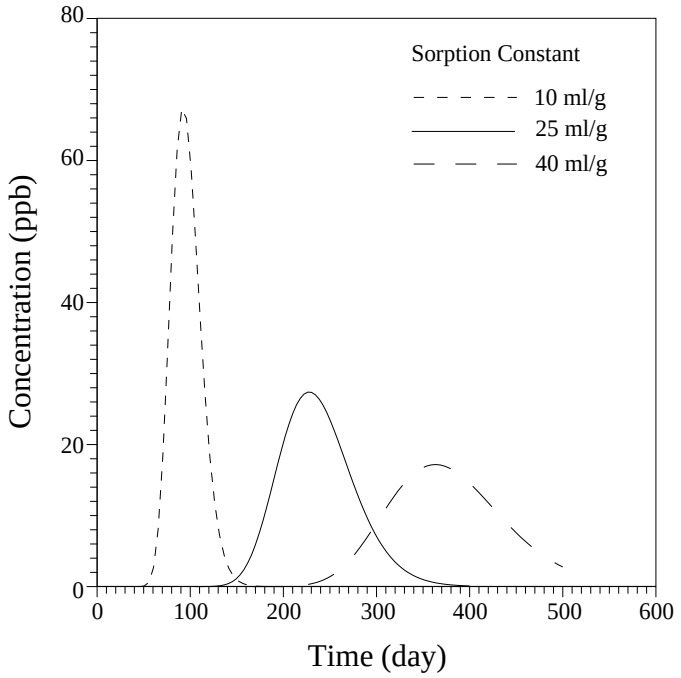

Figure 8.2. The effect of sorption constant on the leachate breakthrough.

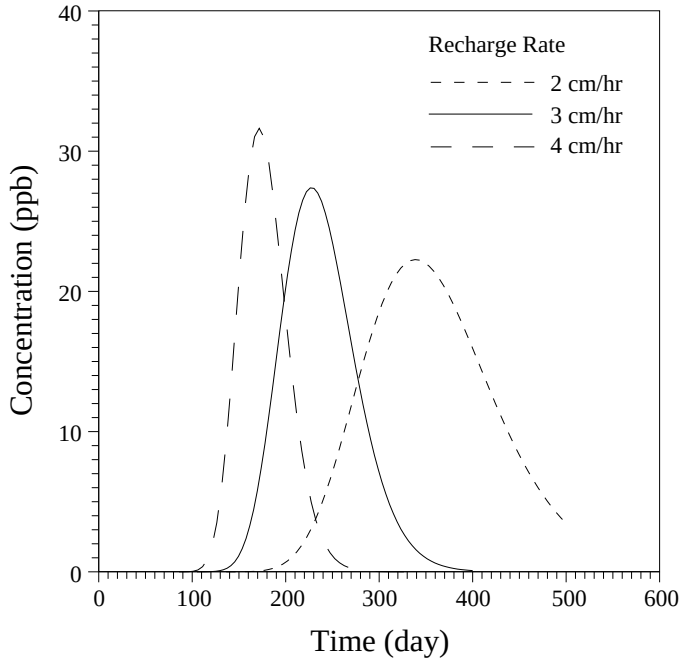

Figure 8.3 The effect of recharge rate on the leachate breakthrough.

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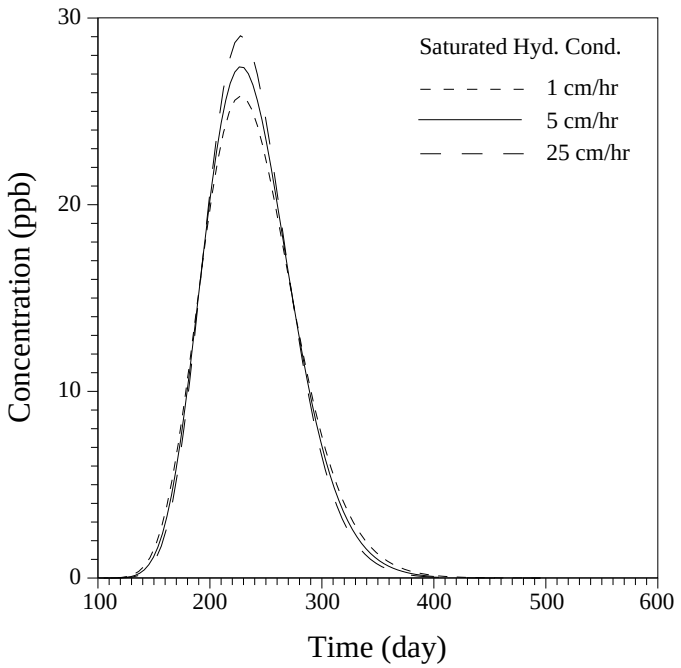

Figure 8.4. The effect of saturated hydraulic conductivity on the leachate breakthrough.

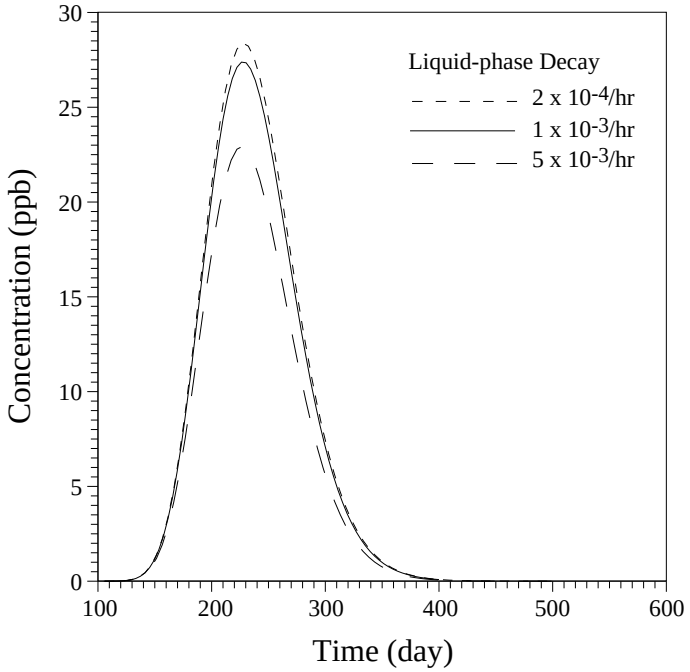

Figure 8.5. The effect of liquid-phase decay constant on the leachate breakthrough.

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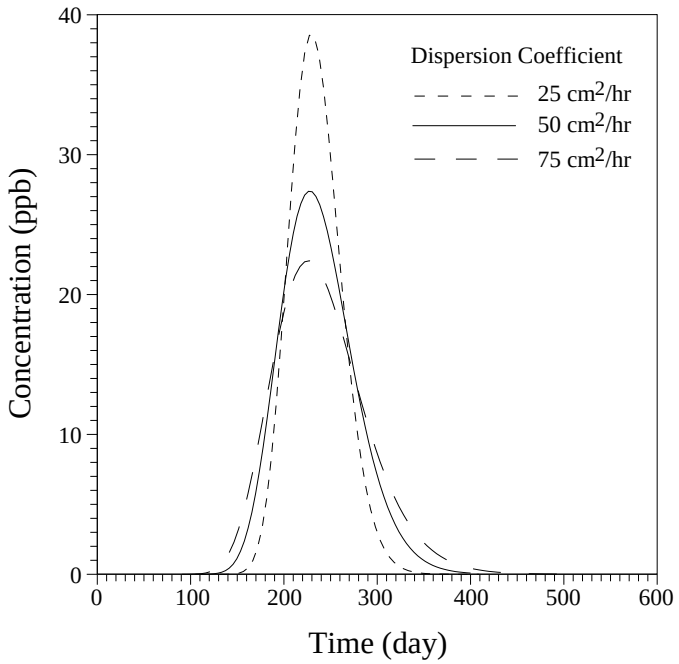

Figure 8.6. The effect of dispersion coefficient on the leachate breakthrough.

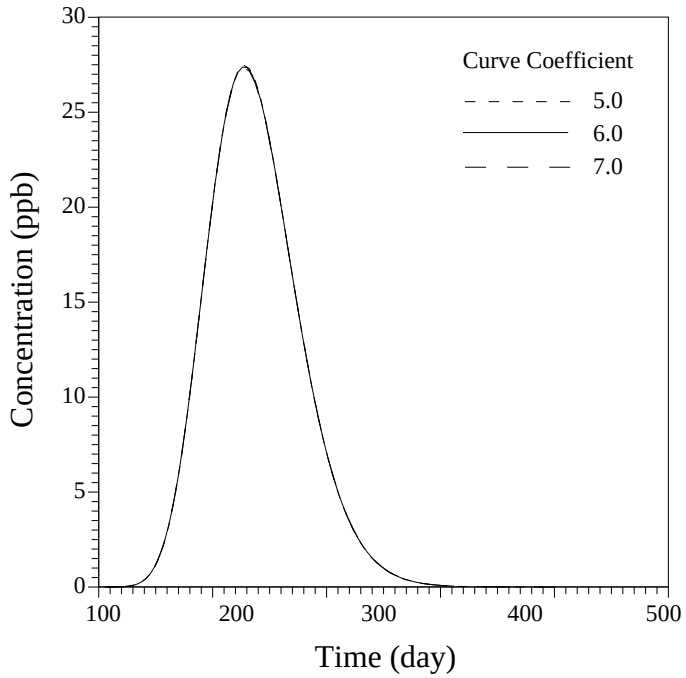

Figure 8.7. The effect of characteristic curve coefficient on the leachate breakthrough.

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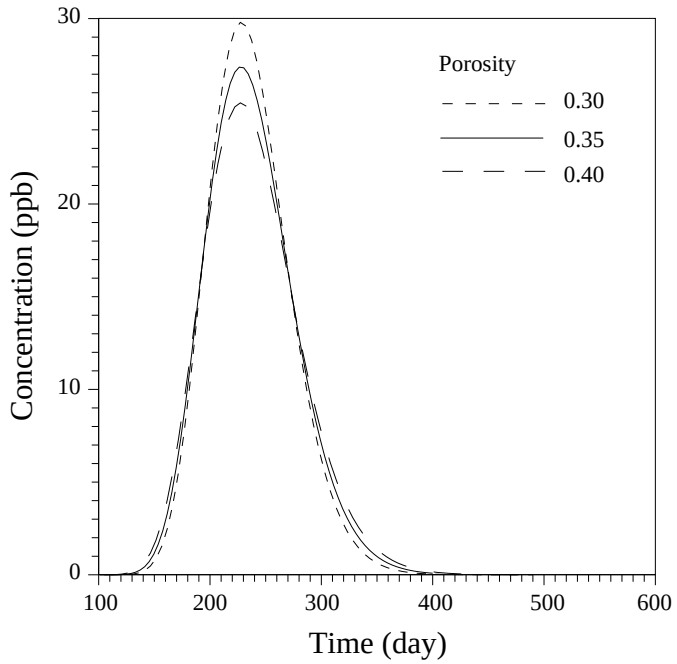

Figure 8.8. The effect of porosity on the leachate breakthrough.

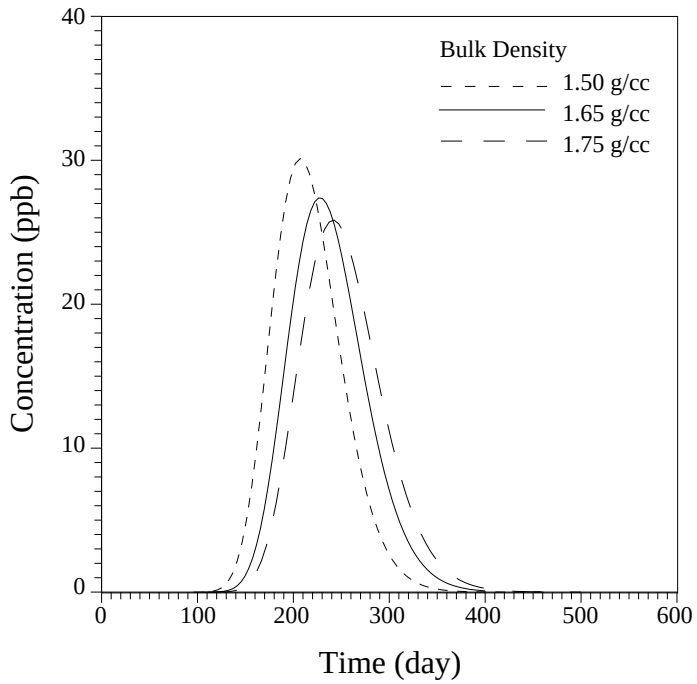

Figure 8.9. The effect of soil bulk density on the leachate breakthrough.

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9. SAMPLE PROBLEM

The following application of PESTAN is based on the study of Jones and Back (1984). Soil and water monitoring studies were conducted to characterize the movement of aldicarb (trade mark TEMIK) residues in Florida citrus groves. TEMIK is primarily used for the control of nematodes, aphids, and mites in citrus groves. Jones and Back (1984) compared the monitoring results with the simulations of PESTAN. They used PESTAN to demonstrate that the use of TEMIK in Florida citrus groves would not result in the persistence of aldicarb residues in groundwater.

The input parameters as used by Jones and Back (1984) are summarized in Table 9.1. It should be noted that the first-order degradation rates of the pollutant in both the liquid and the solid phases are provided. The liquid-phase decay was calculated based on a half-life of 30 days,

$$k_l = 0.693/(30 \times 24) = 9.63 \times 10^{-4} \text{ per hour}$$

The solid phase decay was assumed to be equal to the liquid phase decay, although, in general, these two values could be significantly different. The value of recharge used, 0.0035 cm/hr, corresponds to that of 30 cm/year. The value, 4.05, for the characteristic curve coefficient corresponds to that of a sandy soil.

The model input and output are presented in Tables 9.1 and 9.2. Figures 9.1 and 9.2 illustrate, respectively, graphs of pollutant concentration in water as a function of time at three different depths, and pollutant concentrations in water as a function of depth at three different times.

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TABLE 9.1 INPUT FILE FOR THE SAMPLE PROBLEM

STUDY OF ALDICARB RESIDUES IN FLORIDA SOIL AND WATER (JONES AND BACK, 1984)

```
7.8e03          /*  Water solubility (mg/l)
0.0035          /*  Recharge (cm/hr)
7.3e-02         /*  Sorption constant (cc/g)
2.22e-04        /*  Solid-phase decay rate constant (/hr)
2.22e-04        /*  Liquid-phase decay rate constant (/hr)
1.50            /*  Bulk density (g/cc)
0.395           /*  Porosity (cc/cc)
4.05            /*  Characteristic curve coefficient
1.0             /*  Saturated hydraulic conductivity (cm/hr)
0.06            /*  Dispersion coefficient (cm**2/hr)
0.0             /*  Minimum X-value (cm)
200.0           /*  Maximum X-value (cm)
0.0             /*  Minimum time value (day)
500.0           /*  Maximum time value (day)
3               /*  Number of time intervals for printing out the results
50.             /*  Time values at which output is desired
150.
300.
1               /*  Number of applications of waste
11.2, 0.0       /*  Application rate (kg/ha), Starting time of appl. (day)
y               /*  Option for creating a breakthrough curve data (Yes/No)
100.            /*  Location at which breakthrough curve is desired (cm)
y               /*  Option for creating a soil-depth profile data (Yes/No)
50.             /*  Time at which soil-depth profile is desired (day)
```

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TABLE 9.2 RESULTS OF PESTAN SIMULATION FOR THE SAMPLE PROBLEM.

PESTAN
Version 4.0, 1992

Developed by :
Varadhan Ravi and Jeffrey A. Johnson (Dynamac)
Center for Subsurface Modeling Support
Robert S. Kerr Environmental Research Laboratory
U.S. Environmental Protection Agency
P.O. Box 1198
Ada, OK 74820

TITLE: STUDY OF ALDICARB RESIDUES IN FLORIDA SOIL AND WATER (JONES AND BACK, 1984)

Solubility (mg/l)	:	0.78000E+04
Recharge rate (cm/hr)	:	0.35000E-02
Sorption constant (cc/g)	:	0.73000E-01
Saturated water content	:	0.39500E+00
Solid-phase decay (/hr)	:	0.22200E-03
Liquid-phase decay (/hr)	:	0.22200E-03
Curve coefficient	:	0.40500E+01
Bulk density (g/cc)	:	0.15000E+01
Dispersion coefficient (cm^2/hr)	:	0.60000E-01
Saturated hydraulic conductivity	:	0.10000E+01
Minimum depth (cm)	:	0.00000E+00
Maximum depth (cm)	:	0.20000E+03
Minimum time (day)	:	0.00000E+00
Maximum time (day)	:	0.50000E+03

For application 1 the active ingredient (ai) applied is 0.112E+02 kg ai/ha, and has been applied 0.000E+00 days prior to recharge

Results

Projected water content	:	0.237E+00
Pore water velocity [cm/hr]	:	0.147E-01
Pollutant velocity [cm/hr]	:	0.101E-01
Length of pollutant slug [cm]	:	0.414E-01
Mass decayed prior to recharge [kg]	:	0.000E+00

Time . 0.50E+02 (days)

Depth [cm]	Cw [mg/l]	Cs [mg/kg]	Ctot [mg/l]
2.000	0.65E+01	0.47E+00	0.22E+01
20.000	0.79E+01	0.57E+00	0.27E+01
40.000	0.21E+00	0.15E-01	0.72E-01
60.000	0.19E-03	0.14E-04	0.67E-04
80.000	0.00E+00	0.00E+00	0.00E+00
100.000	0.00E+00	0.00E+00	0.00E+00
120.000	0.00E+00	0.00E+00	0.00E+00
140.000	0.00E+00	0.00E+00	0.00E+00
160.000	0.00E+00	0.00E+00	0.00E+00
180.000	0.00E+00	0.00E+00	0.00E+00
200.000	0.00E+00	0.00E+00	0.00E+00

Mass Balance Results

Pollutant remaining in liquid-phase (kg)	=	0.590E+01
Pollutant remaining in solid-phase (kg)	=	0.272E+01
Total mass of pollutant remaining (kg)	=	0.862E+01
Liquid-phase decay of pollutant (kg)	=	0.172E+01

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Time = 0.15E+03 (days)

Depth [cm]	Cw [mg/l]	Cs [mg/kg]	Ctot [mg/l]
2.000	0.59E+00	0.43E-01	0.21E+00
20.000	0.28E+01	0.20E+00	0.96E+00
40.000	0.42E+01	0.31E+00	0.15E+01
60.000	0.17E+01	0.12E+00	0.58E+00
80.000	0.17E+00	0.13E-01	0.60E-01
100.000	0.46E-02	0.33E-03	0.16E-02
120.000	0.00E+00	0.00E+00	0.00E+00
140.000	0.00E+00	0.00E+00	0.00E+00
160.000	0.00E+00	0.00E+00	0.00E+00
180.000	0.00E+00	0.00E+00	0.00E+00
200.000	0.00E+00	0.00E+00	0.00E+00

Mass Balance Results

Pollutant remaining in liquid-phase (kg)	=	0.438E+01
Pollutant remaining in solid-phase (kg)	=	0.202E+01
Total mass of pollutant remaining (kg)	=	0.640E+01
Liquid-phase decay of pollutant (kg)	=	0.466E+01

Time = 0.30E+03 (days)

Depth [cm]	Cw [mg/l]	Cs [mg/kg]	Ctot [mg/l]
2.000	0.26E-01	0.19E-01	0.90E-01
20.000	0.17E+00	0.12E-01	0.59E-01
40.000	0.72E+00	0.53E-01	0.25E+00
60.000	0.16E+01	0.11E-00	0.54E+00
80.000	0.17E+01	0.12E+00	0.59E+00
100.000	0.94E+00	0.69E-01	0.33E+00
120.000	0.27E+00	0.19E-01	0.92E-01
140.000	0.38E-01	0.28E-02	0.13E-01
160.000	0.27E-02	0.20E-03	0.95E-03
180.000	0.78E-04	0.57E-05	0.27E-04
200.000	0.00E+00	0.00E+00	0.00E+00

Mass Balance Results

Pollutant remaining in liquid-phase (kg)	=	0.256E+01
Pollutant remaining in solid-phase (kg)	=	0.118E+01
Total mass of pollutant remaining (kg)	=	0.375E+01
Liquid-phase decay of pollutant (kg)	=	0.744E+01

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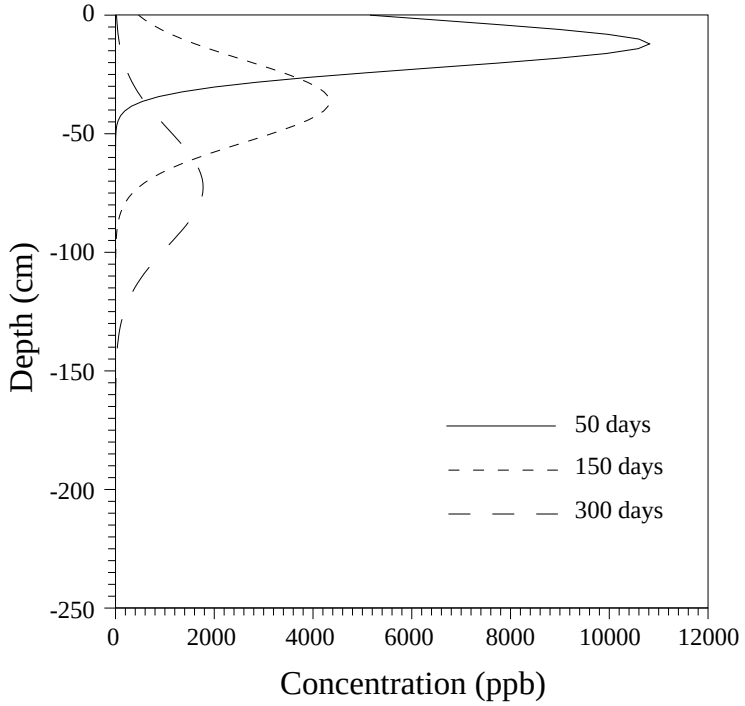

Figure 9.1. Leachate concentration profiles across depth at 3 different times.

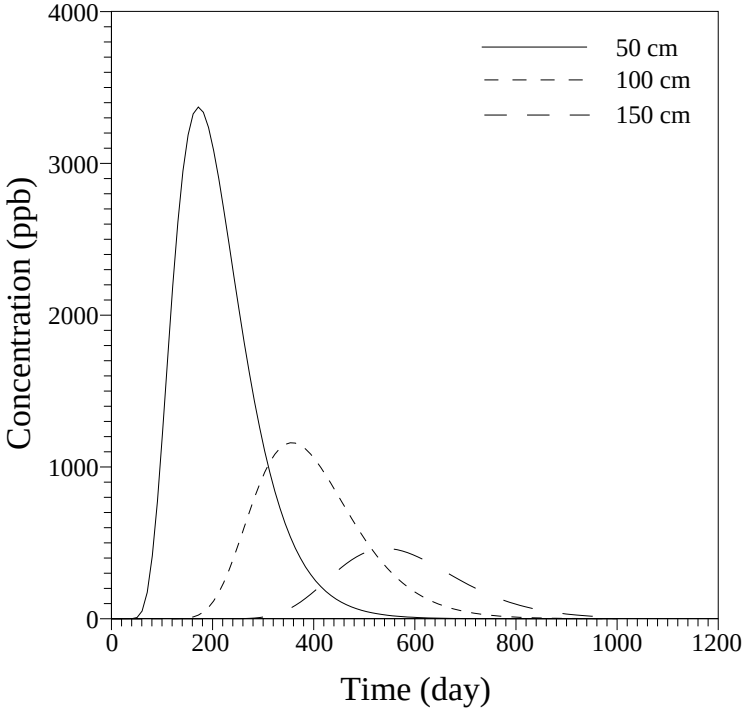

Figure 9.2. Leachate breakthrough curves at 3 different depths.

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10. REFERENCES

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Appendices

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PROPERTIES OF SELECTED PESTICIDES

CAS No	Pesticide	Solubility (water, mg/l)	Koc(L/kg)
542-75-6	1,3-D	2.8 E+09@20	2.51E+01
93-76-5	2,4,5-T	268.3@25	7.94E+01
94-75-7	2,4-D	677@25	1.10E+02
94-82-6	2,4-DB	53@25	5.25E+02
51-36-5	3,5-dichlorobenzoic acid		
100-02-7	4-Nitrophenol	11570@20	2.14E+02
62476-59-9	Acifluorfen-sodium	>250,000@25	
15972-60-8	Alachlor	242@25	1.91E+02
116-06-3	Aldicarb	6,030@25	1.58E+01
1646-88-4	Aldicarb Sulfone	10,000,000@25	9.99E+02
1646-87-3	Aldicarb Sulfoxide		
309-00-2	Aldrin	0.017@25	4.06E+02
834-12-8	Ametryn	185@20	3.89E+02
1327-53-3	Arsenic (III)	17,000@25	
1303-28-2	Arsenic (v)	2,300,000@20	
1610-17-9	Atraton	1,800@20	
1912-24-9	Atrazine	22-30@20	3.89E+01
86-50-0	Azinphos-methyl	20.9@20	
101-27-9	Barban	11@25	
17804-35-2	Benomyl	2@25	
25057-89-0	Bentazon	500@20	
319-84-6	BHC (alpha)	2.00@25	1.99E+03
319-85-7	BHC(beta)	0.24@25	4.26E+03
319-86-8	BHC(gamma)	31.4@25	4.26E+03
314-40-9	Bromacil	815@25	2.00E+01
23184-66-9	Butachlor	20@20	
2008-41-5	Butylate	45@22	
133-06-2	Captan	3.3@25	1.99E+02
63-25-2	Carbaryl	104@25	1.02E+02
1563-66-2	Carbofuran	320@20	9.55E+01
1563-38-8	Carbofuran, phenol		
5234-68-4	Carboxin	170@25	
133-90-4	Chloramben	700@25	2.00E+01
57-74-9	Chlordane	0.056@25	1.23E+03
5103-74-2	Chlordane (cis)	0.051@20	2.51E+05
5103-71-9	Chlordane (trans)	nd	5.89E+04
510-15-6	Chlorobenzilate	13@20	1.06E+03
2675-77-6	Chloroneb	8@25	
1897-45-6	Chlorothalonil	0.60@25	5.76E+03
101-21-3	Chlorpropham	80@25	2.51E+01
2921-88-2	Chlorpyrifos	2@25	
1861-32-1	Chlorthal dimethyl (DCPA)	0.500@25	6.46E+03
15096-52-3	Cryolite		
21725-46-2	Cyanazine	171@25	1.82E+02
1134-23-2	Cycloate	75@20	3.47E+02
75-99-0	Dalapon	9.0 E+11@nd	2.29E+00

PROPERTIES OF SELECTED PESTICIDES

96-12-8	DBCP	1,230@20	1.02E+02
CAS No	**Pesticide**	**Solubility (water, mg/l)**	**Koc(L/kg)**
8003-19-8	DD (1,2-D +1,3-D)	2,000,000@20	
72-54-8	DDD (p, p')	0.090@25	1.62E+04
72-55-9	DDE (p,p')	0.12@25	5.01E+04
50-29-3	DDT (p,p')	0.025@25	1.51E+05
333-41-5	Diazinon	40@25	2.29E+02
1918-00-9	Dicamba	6,500@25	1.00E+01
120-36-5	Dichlorprop	350@20	
62-73-7	Dichlorvos	1 E+10@2O	1.59E+02
60-57-1	Dieldrin	0.195@25	8.32E+03
60-51-5	Dimethoate	25000@21	2.51E+01
88-85-7	Dinoseb	52@25	1.23E+02
957-51-7	Diphenamid	260@27	
298-04-4	Disulfoton	16.3@20	4.01E+01
2497-06-5	Disulfoton sulfone		
2497-07-6	Disulfoton sulfoxide		
330-54-1	Diuron	40@20	1.62E+02
106-93-4	EDB	4,040@20	6.61E+01
959-98-8	Endosulfan (alpha)	0.510@20	6.31E+03
33213-65-9	Endosulfan (beta)	0.45@20	6.76E+03
115-29-7	Endosulfan I	0.45@20	6.31E+03
1031-07-8	Endosulfan sulfate	16.1@25	2.34E+03
72-20-8	Endrin	0.25@25	1.15E+04
7421-93-4	Endrin aldehyde	0.26@25	2.69E+04
759-94-4	EPTC	365@20	1.10E+02
13194-48-4	Ethoprop	700@20	
2593-15-9	Etridiazole	50@20	
96-45-7	ETU	62,000@nd	1.00E+01
22224-92-6	Fenamiphos	700@20	1.99E+02
60168-88-9	Fenarimol	13.7@25	
2164-17-2	Fluometuron	85@24	1.74E+02
59756-60-4	Fluridone	12@nd	8.51E+02
944-22-9	Fonofos	13@nd	
1071-83-6	Glyphosate	12,000@25	2.63E+03
76-44-8	Heptachlor	0.18@25	3.47E+03
1024-57-3	Heptachlor epoxide	0.200@25	1.06E+01
118-74-1	Heptachlorobenzene	0.0062@25	1.42E+04
51235-04-2	Hexazinone	33,000@25	
122-42-9	IPC (Propham)	32@25	
25311-71-1	Isofenfphos	23.8@20	
58-89-9	Lindane	7.3@25	1.07E+03
330-55-2	Linuron	75@25	8.70E+02
121-75-5	Malathion	143@20	1.80E+03
8018-01-7	Mancozeb		
12427-38-2	Maneb		5.01E+02
94-74-6	MCPA	1,174@25	1.10E+02
150-50-5	Merphos		
57837-19-1	Metalaxyl	7,100@20	
10265-92-6	Methamidophos	>2,000,000@20	
2032-65-7	Methiocarb	30@20	2.09E+02

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PROPERTIES OF SELECTED PESTICIDES

16752-77-5	Methomyl	57,900@25	2.00E+01
CAS No	**Pesticide**	**Solubility (water, mg/l)**	**Koc(L/kg)**
72-43-5	Methoxychlor	0.10@25	7.94E+04
51218-45-2	Metolachlor	530@20	
21087-64-9	Metribuzin	1,200@20	9.98E+01
35045-02-4	Metribuzin DA		
7786-34-7	Mevinphos	Completely miscible	1.99E+02
113-48-4	MGK 264		
2212-67-1	Molinate	880@20	7.94E+01
300-76-5	Naled	nd	
15299-99-7	Napropamide	73@20	3.09E+02
555-37-3	Neburon	5@25	2.29E+03
27314-13-2	Norfluazon	28@20	1.90E+03
23135-22-0	Oxamyl	280,000@25	5.00E+00
950-35-6	Paraoxon (methyl)		
1910-42-5	Paraquat	700,000@20	
56-38-2	Prathion	6.54@25	1.06E+04
298-00-0	Prathion (methyl)	55-60@25	5.01E+03
82-68-8	PCNB	0.55@25	2.63E+04
1114-71-2	Pebulate	60@20	6.31E+02
40487-42-1	Pendimethalin	0.300@20	
87-86-5	Pentachorohenol	1,950@25	3.80E+03
61949-76-6	Permethrin (cis)		
52645-53-1	Permethrin (cis+trans)	0.2@20	6.31E+04
61949-77-7	Permethrin (trans)		
298-02-2	Phorate	20@25	5.01E+02
732-11-6	Phosmet	25@25	
6.61E+03	Picloram	430@25	1.58E+01
1610-18-0	Prometon	750@20	
7287-19-6	Prometryn	48@20	3.26E+03
23950-58-5	Pronamide	32.8@25	1.99E+02
1918-16-7	Propachlor	613@25	2.63E+02
709-98-8	Propanil	500,000@25	
139-40-2	Propazine	8.6@20	
114-26-1	Propoxur (Baygon)	2,000,000@20	
78-87-5	Propylene dichloride)	2,800@25	2.69E+01
93-72-1	Silvex (2,4,5-TP)	176@25	5.02E+01
122-34-9	Simazine	3.5@20	5.02E+01
1014-70-6	Simetryn	450@rm temp	
22248-79-9	Stirofos	11@20	
35400-43-2	Sulprofos	<5@29	
1918-18-9	Swep		5.50E+02
27355-22-2	TCP	2.49@25	1.99E+03
34014-18-1	Tebuthiuron	2,300@25	6.17E+02
5902-51-2	Terbacil	710@25	3.98E+01
13071-79-9	Terbufos	5.07@25	6.61E+02
886-50-0	Terbutryn	0.0012@25	7.09E+02
8001-35-2	Toxaphene	0.74@25	2.00E+05
43121-43-3	Triadimenfon	260@20	
2303-17-5	Triallate	4@25	2.24E+03
41814-78-2	Tricyclazole	1,600@25	

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1582-09-8	Trifluralin	8.11@20	1.10E+04
1929-77-7	Vernolate		

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Appendix B

Soil Parameter Information

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PHYSICAL PROPERTIES OF SOIL

Soil Texture	Bulk Density (g/cc)	Saturated Water Content		Percent Organic Matter
	(Jury, 1986)	(Li et al., 1976)	(Brakensiek, et al., 1981)	(Rawls, 1983)
		mean (std. deviation)	mean (std. deviation)	mean (std. deviation)
Sand	1.59 — 1.65	0.359 (0.056)	0.349 (0.107)	0.71 (1.06)
Loamy Sand		0.410 (0.068)	0.410 (0.065)	0.61 (1.16)
Sandy Loam	1.20 — 1.47	0.435 (0.086)	0.423 (0.076)	0.71 (1.29)
Silt Loam	1.47	0.485 (0.059)	0.484 (0.057)	0.58 (1.29)
Loam		0.451 (0.078	0.452 (0.069)	0.52 (0.99)
Sandy Clay Loam		0.420 (0.059)	0.406 (0.049)	0.19 (0.34)
Silty Clay Loam		0.477 (0.057)	0.473 (0.046)	0.13 (0.42)
Clay Loam	1.20 — 1.36	0.476 (0.053)	0.476 (0.054)	0.10 (0.42)
Sandy Clay		0.426 (0.057)		0.38 (1.20)
Silty Clay	1.26	0.492 (0.064)		
Clay		0.482 (0.050)	0.475 (0.048)	0.38 (0.83)

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SOIL HYDRAULIC PROPERTIES

Soil Texture	Saturated Hydraulic Conductivity (cm/hr)		Characteristic Curve Constant
	(Li et al., 1976)	(McCuen et al., 1981)	(Li et al. , 1976)
Sand	63.36	24.6	4.05 (1.78)
Loamy Sand	56.28	78.84	4.38 (1.47)
Sandy Loam	12.48	17.93	4.90 (1.75)
Silt Loam	2.59	1.62	5.30 (1.96)
Loam	2.5	5.98	5.39 (1.87)
Sandy Clay Loam	2.27	4.72	7.12 (2.43)
Silty Clay Loam	0.61	1.07	7.75 (2.77)
Clay Loam	0.88	3.64	8.52 (3.44)
Sandy Clay	0.78	1.25	10.4 (1.64)
Silty Clay	0.37	1.8	10.4 (4.45)
Clay	0.46	1.07	11.4 (3.70)

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Appendix C

Reference Information

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Appendix C

Reference Information

1. Howard, P.H., R.S. Boethling, W.F. Jarvis, W.M. Meylan, and E.M. Michalenko (1991). Handbook of Environmental Degradation Rates, Lewis Publishers, Chelsea, MI.

2. Montgomery, J.H., and L.M. Welkom (1990). Groundwater Chemicals Desk Reference, Lewis Publishers, Chelsea, MI.

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4. Sims, R.C., J.L. Sims, and S.G. Hansen (1991). Soil Transport and Fate Database 2.0 and Model Management System, Robert S. Kerr Environmental Research Laboratory, Ada, OK.

5. Verschueren, K. (1983). Handbook of Environmental Data on Organic Chemicals, 2nd Ed., Van Nostrand Reinhold Company, New York.

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Appendix D

Model Data Sheet

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PESTAN MODEL DATA SHEET

Simulation Title: _____
Date: _____
Chemical Name: _____
Soil Texture: _____

Required Data	Input Value		Source
Chemical Parameters			
Water Solubility	_____	mg/l	_____
Sorption Constant	_____	cc/g	_____
Solid-Phase Decay Rate	_____	/hr	_____
Liquid-Phase Decay Rate	_____	/hr	_____
Soil Properties			
Bulk Density	_____	g/cc	_____
Saturated Water Content	_____		_____
Curve Coefficient	_____		_____
Saturated Hydraulic Conductivity	_____	cm/hr	_____
Dispersion Coefficient	_____	cm^2/hr	_____
Environmental Characteristics			
Recharge	_____	cm/r	_____
Number of Applications	_____		_____
Application Rate	_____	kg/ha	_____
	_____	kg/ha	_____
	_____	kg/ha	_____
	_____	kg/ha	_____

Model Descritization

Minimum X-value	_____	cm	Maximum X-value	_____	cm
Minimum Time Value	_____	day	Maximum Time Value	_____	day