

THE DEVELOPMENT OF AN EXPERT SYSTEM AS  
A SCREENING TOOL TO MINIMIZE  
GROUNDWATER CONTAMINATION  
FROM PESTICIDES

BY

PANKAJ ARORA

Master of Technology

Indian Institute of Technology

Kanpur, India

1987

Submitted to the Faculty of the  
Graduate College of the  
Oklahoma State University  
in partial fulfillment of  
the requirements for  
the Degree of  
MASTER OF SCIENCE  
December, 1991

THE DEVELOPMENT OF AN EXPERT SYSTEM AS  
A SCREENING TOOL TO MINIMIZE  
GROUNDWATER CONTAMINATION  
FROM PESTICIDES

Thesis Approved:

*William F. McKinnon*

Thesis Adviser

*John M. [unclear]*

*Ann Clark*

*Thomas C. Collins*

Dean of the Graduate College

## ACKNOWLEDGMENTS

I wish to express my deep sense of gratitude to Prof. W.F. McTernan for supervising the work. I am deeply indebted to him for building my interest in this field, his inspiring guidance, meticulous attention, and untiring devotion throughout the tenure of this work. I am also thankful to Dr. W.W. Clarkson and Dr. J.N. Veenstra for all their support and help for serving on my graduate committee.

I am very grateful for the financial support from the University Center for Water Research and School of Civil Engineering at Oklahoma State University without which this work would not have been possible.

I would like to express my deepest appreciation to my parents, my sister and her husband, Taruna and Baldev, their children Umang and Ishita, and my wonderful younger brother Mickey for their support, encouragement, and understanding.

Finally, I wish to thank Wadhwas from Milwaukee, and Tom Mordecai for their love and constant support during my stay away from home, that kept me going.

## TABLE OF CONTENTS

Chapter	Page
I. EXECUTIVE SUMMARY .....	1
II. THE DEVELOPMENT AND APPLICATION OF A PROBABILISTIC EXPERT SYSTEM TO DETERMINE THE PROBABILITY OF PESTICIDE LEACHING .....	5
Introduction .....	5
The Development of Expert System .....	8
The Code Structure .....	12
Development of Option 1 for Preliminary Analysis .....	17
Option 1 Example .....	23
Development of Option 2 for Site Specific Analysis .....	33
Option 2 Example .....	34
Conclusions .....	55
SELECTED BIBLIOGRAPHY .....	60
APPENDIXES .....	65
APPENDIX A - LOG NORMAL PLOTS .....	66
APPENDIX B - COMPLETE SERIES OF GUIDANCE SCREENS FOR OPTION 1 .....	87
APPENDIX C - COMPLETE SERIES OF GUIDANCE SCREENS FOR OPTION 2 .....	114
APPENDIX D - EXAMPLE CALCULATION: LOG NORMAL INTERPOLATION OF PESTICIDE LEACHING .....	149

## LIST OF TABLES

Table	Page
I. The Files Present in EXSYS with a Brief Introduction to their Contents .....	15

## LIST OF FIGURES

Figure	Page
1. Pesticide Root Zone Model Schematic .....	10
2. Flow Diagram Presenting An Overall View of EXSYS .....	13
3. Flow Diagram For Option 1 .....	16
4. Flow Diagram For Option 2 .....	18
5. Region of Simulation Selected For Option 2 ...	19
6. Example Screen Containing Input Parameters Information For Option 1 Simulation .....	24
7. Guidance Screen Providing General Information About Curve Number (CN) .....	25
8. Guidance Screen Describing Hydrologic Soil Groups .....	26
9. Guidance Screen Displaying Predominant Soil Distribution Map of Oklahoma .....	27
10. Guidance Screen Defining Hydrologic Group of the Soil Selected .....	28
11. Screen Outlining the Procedure to Select Curve Number (CN) .....	29
12. Guidance Screen Displaying A Partial Listing of Crops and Land Use Practices For Curve Number (CN) Selection .....	30
13. Screen Giving An Opportunity to Change Selected Parameters For Option 1 Simulation .....	31
14. Example Final Output For Option 1 Simulation .....	32
15. Screen Displaying Comparisons Between Example output and the Log normal Approximation ....	35
16. Example Screen Providing general Information About the Pan Evaporation Factor .....	37

Figure	Page
17. Example Screen providing General Information About the Snowmelt Factor .....	38
18. Example Screen Providing General Information About the Pan Evaporation Flag .....	39
19. Example Screen For Determining the Minimum Depth For Evaporative Water Extraction .....	40
20. Example Screen For Input of Surface Condition of Land After Harvest .....	41
21. Example Screen Giving General Information About the Plant Maximum Interception Storage .....	42
22. Example Screen Displaying Typical Values of Maximum Interception Storage For Some Crops .....	43
23. Example Screen Presenting General Information About the Maximum Plant Rooting Depth .....	44
24. Example Screen Displaying Values of Rooting Depth For some Crops and Location .....	45
25. Example Screen Requesting Input of the Depth of Pesticide Incorporation In the Soil .....	46
26. Example Screen giving General Information About Maximum Areal Coverage of the Crop ...	47
27. Example Screen Giving General Information About Plant Uptake Efficiency Factor .....	48
28. Example Screen Displaying Organic Carbon Contents of the Major Soils Shown In Soil Distribution Map For the Region Selected For Simulation .....	49
29. Example Screen Displaying Typical Bulk Densities of the Major Soils Encountered In the Region of Simulation .....	50
30. Example screen Displaying Typical Field Capacity of Major Soils Encountered In the Region of Simulation .....	51
31. Example Screen Displaying Typical Wilting Points of Major Soils Encountered In the Region of Simulation .....	52
32. Example Screen to Input Value for Hydrodynamic Dispersion .....	53

Figure		Page
33.	Example Screen For Input of the Initial Water Contents of the Soil .....	54
34.	Screen Displaying Location of Type 1 Weather Stations In Oklahoma User May Pick by Number and Input Appropriate Data Set .....	56
35.	Screen Presenting Plot Between Mean, Standard Deviation and Number of Simulations Completed .....	57



## CHAPTER I

### EXECUTIVE SUMMARY

This study addresses the problem of providing sophisticated analytical tools for the analysis of groundwater pollution problems to audiences with training in areas other than computer science and hydraulic engineering. Due to the "non-point" nature of pesticide contamination of shallow groundwaters, the best management approach often is the development of strategies for proper chemical selection and usage as well as the utilization of appropriate land use controls. Due to an overall lack of monitoring data this often involves the application of simulation models which may prove too complex for those who would benefit most from the analysis. In the present work a probabilistic expert system has been developed to assist in the quantification of risk to groundwater resources from pesticide applications and to evaluate alternative management approaches. The Pesticide Root Zone Model (PRZM) developed by the United States Environmental Protection Agency (USEPA) was incorporated within a Monte Carlo simulation approach to form the base for the expert system [5]. PRZM was developed to predict the leaching of pesticides from field size areas [3] and requires a relatively large number of input parameters, the availability of which can be a problem for some users.

The main objective for the subject expert system was to make simulation simple and provide results in a more useful and easy to interpret manner within a small amount of time. The expert system developed allowed the user the options of using existing databases or the development of a separate, independent simulation set. The recommended procedure is to complete a preliminary evaluation using the existing databases to identify the range of possible consequences at a location, then do a rigorous analysis with a simulation series focused upon more site specific concerns to allow for proper site selection. For Option 1 of this expert system, previously completed simulation results were used [8]. The Monte Carlo technique was applied for select input parameters to address inherent uncertainties associated with them. Three main parameters were fixed as constants creating a cause and effect simulation approach. Also, these parameters provided the user a greater degree of freedom to address the chemical properties of pesticides and different land management alternatives. The parameters fixed were: Soil Conservation Service curve number (CN), for infiltration characteristics of soils; decay coefficient (Ks), for decay of pesticides by physical and chemical processes and organic-carbon distribution coefficient (Koc), which described the retardation potential of a compound. The 540 Monte Carlo simulations completed in this initial effort were then pooled according to management practices, plotted on log-normal probability paper, and converted into equations describing these distributions.

While using Option 1 the user is asked to provide the values of CN, Ks, and Koc. A number of user friendly help screens are provided accompanied by brief introductions to the parameters and their values. For conditions intermediate to those used to develop the original Monte Carlo simulations upon which Option 1 was based, the means and standard deviations from the pooled data sets are accessed. A linear double interpolation between distributions is completed for a series of probabilities. Graphic and tabular outputs in terms of probability of pesticide leaching past 30 cm of soil depth are presented almost immediately.

For the second option, a user friendly pre-processor for PRZM was developed. This pre-processor creates input files for PRZM. Guidance is provided in selecting the values of the parameters needed to create input files for PRZM. The Monte Carlo technique is then applied to randomize meteorological data for different years. PRZM and the meteorological files are called until the user specified number of simulations has been completed. As with Option 1, the results are presented in the form of percent of the applied pesticide leached versus probability of this amount being leached in tabular and graphical manner. This makes the interpretation of results easy and more effective. In addition, Option 2 plots the moving average and standard deviation versus the number of simulations completed to determine if sufficient data have

been collected. The present work was developed for the state of Oklahoma and in particular for winter wheat crop.

CHAPTER II

THE DEVELOPMENT AND APPLICATION OF A  
PROBABILISTIC EXPERT SYSTEM TO  
DETERMINE THE PROBABILITY  
OF PESTICIDE LEACHING \*

Introduction

In recent years there has been a general increase in awareness of the importance of groundwater pollution [23]. This has led managers and researchers to develop strategies for protection of groundwater from toxic and hazardous materials [15]. These strategies have often developed as a function of the nature of pollution sources. In general, groundwater pollution can be classified as either point or non-point in origin [1,15].

The discrete nature of point sources such as landfills, hazardous waste sites and others has made it easier to remediate contamination while the management of non-point sources is more problematic. The absence of discrete sources and the presence of pollutants over large areas,

---

\* Authored by Pankaj Arora and William F. McTernan, Graduate Student and Professor, respectively, School of Civil Engineering, Oklahoma State University, Stillwater, Oklahoma 74078

sources and the presence of pollutants over large areas, in usually small quantities, has produced control strategies based upon best management policies where pollution minimization and/or elimination replace after the fact remediation.

Groundwater pollution from pesticides and other agricultural chemicals is a classic example of non-point contamination [24]. Dispersed over large areas at relatively small concentrations, these chemicals could place large water supplies at significant risk of contamination. The presence of 46 different pesticides in groundwater had been reported in 26 states [6,11]. In other studies conducted by U.S. Environmental Protection Agency (USEPA), 10.4% of U.S. community wells and 4.2% of U.S. rural domestic water supply wells have been reported to contain detectable levels of pesticides [30]. Limited monitoring data suggest that the problem could be even more widespread.

This lack of monitoring data has resulted in an increasing reliance upon computer simulation to assess risks and evaluate alternative management practices [25]. Frequently these computer models are misunderstood or difficult to use for practicing professionals trained in areas not dependent upon computer literacy. One way that this problem can be addressed is by developing expert systems where the user configures the model in response to a series of questions presented by the system. The advent of larger personal computers has allowed the development

of these systems which can be large and memory intensive. These systems, when developed, should be easy to use while requiring minimal computer training, thereby allowing individuals with specific, highly valued skills to participate in the simulation process. There are many examples of previously developed expert systems including, among others, First Response Expert System (FRES), GEOTOX, DEMOTOX, and SEPIC [13]. The FRES provides information on the acute and chronic toxicity of chemicals as well as assists local fire fighters in responding to emergency chemical spills [14]. GEOTOX was developed to rank hazardous waste site remediation technologies for use at a specific waste site [28]. Expert system DEMOTOX addresses the potential of groundwater contamination from hazardous waste sites [17]. For transportation of chemicals into the soil and groundwater DEMOTOX considers factors such as sorption, biodegradation and transformation rates, as well as recharge through the soil. SEPIC was developed to provide more consistent regulatory decisions to issue permits for onsite private sewage disposal systems [12].

In the present work an attempt was made to develop a prototype probabilistic expert system, EXSYS, for those professionals with strong agricultural management skills who also had computer deficiencies. The final output from the combined programs was designed to produce probability estimates of the amount of pesticide leaching to approximately the base of the rooting zone of winter wheat in Oklahoma. Pesticide passing this depth no longer yields

economic benefit to the farmer while representing a potential for groundwater contamination. EXSYS is intended to assist those individuals involved in site evaluation, the identification of appropriate farm practices, and final pesticide selections in configuring a best management approach to minimize the risk of pesticide contamination of shallow groundwaters. It is assumed that the intended audience for EXSYS is the professional highly skilled in one or more areas of agricultural management who may either lack adequate training in computer simulation or may have insufficient time to assemble the necessary data sets to properly apply current leaching models. EXSYS is intended to be a screening tool to evaluate leaching probabilities of potential pesticides which can be used on a particular crop. A range of pesticides, farm practices or site locations can be evaluated for the probability of leaching.

#### THE DEVELOPMENT OF AN EXPERT SYSTEM

EXSYS was developed to provide results in an easy to interpret manner and was structured to be interactive and user friendly in a menu driven format. All of these features attempt to make this program easy to learn for those with little computer training.

The Pesticide Root Zone Model (PRZM) developed by United States Environmental Protection Agency (USEPA) was selected as the public domain code to determine the amount



of pesticide leached into the root zone [3]. PRZM, in addition to being available to all potential users, is widely used and supported by the USEPA [5]. Also, PRZM has been validated against field data and found very effective in predicting the leaching of chemicals into the root zone [2,4,16, and 18]. The model includes hydrology and chemical transport components that simulate runoff, erosion, plant uptake, decay, leaching, and foliar washoff of a single pesticide [5]. Figure 1, taken from the PRZM user manual presents an idealized cross-section of a farm field illustrating the critical physical, microbial, and chemical mechanisms involved in pesticide leaching. Even with a model as generally easy to use as PRZM with its relatively simplified input requirements, the untrained user can become intimidated when attempting to configure and interpret a simulation.

PRZM divides the soil profile into compartments corresponding approximately with horizons. Infiltration and leaching are simulated in one dimension into and through underlying unsaturated zones. Mass balance equations for water and chemicals are developed for surface and subsurface layers. The surface zone mass balance equations used in PRZM are :

$$\frac{A \Delta X \partial(C_W \theta)}{\partial t} = -J_D - J_V - J_{DW} - J_U - J_{QR} - J_{ADS} + J_{DES} + J_{APP} + J_{FOF} \quad (1)$$

$$\frac{A \Delta X \partial(C_S \rho_S)}{\partial t} = -J_{DS} - J_{ER} - J_{DES} + J_{ADS} \quad (2)$$

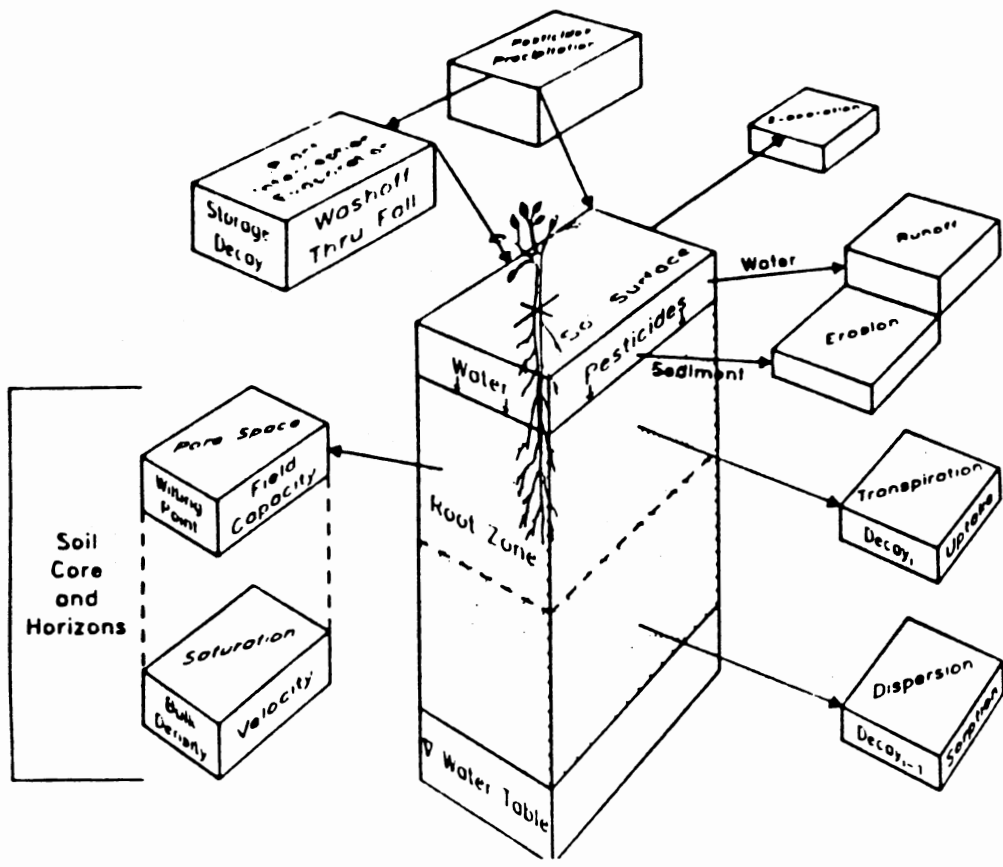


Figure 1. Pesticide Root Zone Model Schematic  
 (Source: PRZM User Manual [ 5 ] )

where  $A$  = cross-sectional area of soil column,  $L^2$   
 $\Delta X$  = depth dimension of compartment,  $L$   
 $C_W$  = dissolved concentration of pesticide,  $ML^{-3}$   
 $C_S$  = sorbed concentration of pesticide,  $MM^{-1}$   
 $\theta$  = volumetric water content of soil,  $L^3L^{-3}$   
 $\rho_S$  = soil bulk density,  $ML^{-3}$   
 $t$  = time,  $T$   
 $J_D$  = mass rate of change by dispersion,  $MT^{-1}$   
 $J_V$  = mass rate of change by advection,  $MT^{-1}$   
 $J_{DW}$  = mass rate of change by transformation of dissolved phase,  $MT^{-1}$   
 $J_U$  = mass rate of change by plant uptake of dissolved phase,  $MT^{-1}$   
 $J_{QR}$  = mass rate of change by removal in runoff,  $MT^{-1}$   
 $J_{APP}$  = mass rate of change by pesticide application,  $MT^{-1}$   
 $J_{FOF}$  = mass rate of change by washoff from plants to soil,  $MT^{-1}$   
 $J_{DS}$  = mass rate of change by transformation of sorbed phase,  $MT^{-1}$   
 $J_{ER}$  = mass rate of change by removal on eroded reclaims,  $MT^{-1}$   
 $J_{ADS}$  = mass rate of change by adsorption,  $MT^{-1}$   
 $J_{DES}$  = mass rate of change by desorption,  $MT^{-1}$

( source: U.S. Environmental Protection Agency PRZM user manual [5] )

The subsurface equivalent is similar lacking only the  $J_{QR}$ ,  $J_{FOF}$ , and  $J_{ER}$  terms. Also,  $J_{APP}$  is only used when pesticide is soil incorporated. PRZM uses these mass balance equations to develop an overall chemical transport

equation, which is subsequently solved using a finite difference method.

EXSYS uses the PRZM code unaltered. A shell of menu screens, questions, guidance tables, and base maps for Oklahoma conditions has been provided to assist the user in configuring PRZM input files. Two options are provided: the use of existing data or starting a new simulation independently. The recommended procedure is to perform a preliminary study assessing the probability of pesticide leaching using the existing data of Option 1 and then proceeding with an original simulation set in Option 2. This allows one to configure a simulation for site specific conditions rather than use the more generic state wide data base used to prepare Option 1.

### THE CODE STRUCTURE

The computer code for EXSYS was developed for IBM-PC and compatible microcomputers and was written in GW basic which allowed superior graphics capabilities in an easy to use shell. The coding was divided into twelve sub programs totalling approximately 786,000 bytes. All twelve sub programs were compiled using Microsoft DOS version 3.1. These sub programs are linked to the main program by user responses to questions regarding input data and simulation configuration and are called as needed. The flow diagram giving an overall view of the EXSYS is shown in Figure 2, while a list of all the files present in EXSYS with a

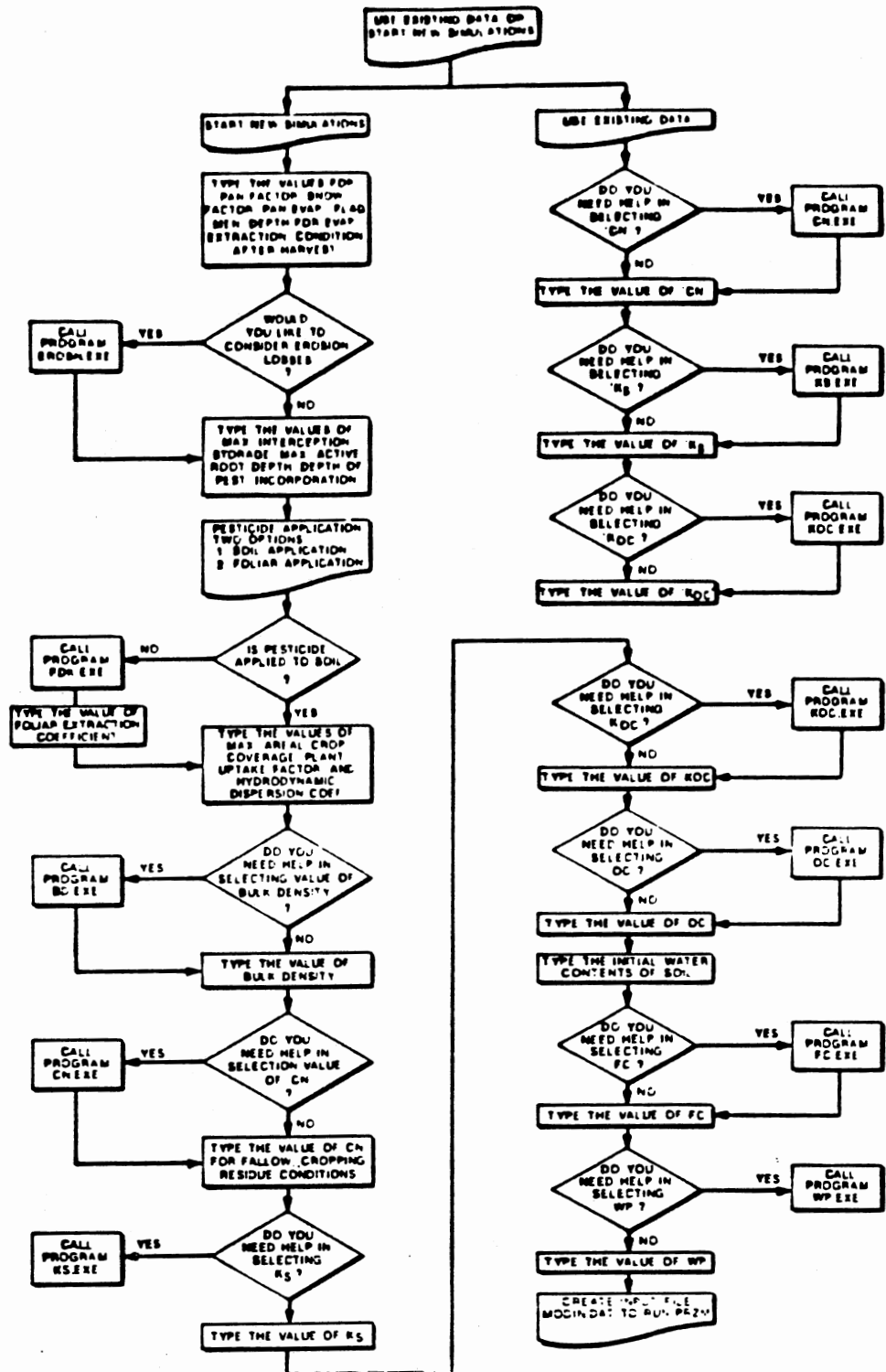


Figure 2. Flow Diagram Presenting An Overall View of EXSYS

brief description is provided in Table I. These subprograms are called by the main program EXSYS.EXE in response to answers given by the user.

The main program primarily handles Option 1 where existing data are used for evaluating the probability of leaching. During Option 1, a general introduction and assistance in selecting the values of three critical parameters [Soil Conservation Service Curve Number (CN), pesticide decay rate (Ks), and soil partition coefficient (Koc)] is provided by subroutines from the main program in response to answers provided by the user. The flow diagram for Option 1 is presented in Figure 3, where the sequence of operations performed in this option is shown.

For Option 2 a subprogram called OPTION2.EXE is called by the main program. This program functions as a preprocessor for creating input files to configure PRZM for individual, site specific simulations. Again, help in selecting critical parameters is provided by select sub programs in response to answers provided by the user. If the user wishes to simulate erosion losses, help is provided in selecting appropriate parameters for the Modified Universal Soil Loss Equation (MUSLE) [27,29]. The erodibility (K), length slope and steepness (LS), supporting practice (P), and cover management factors (C) are called program EROSN.EXE. Further, to assist in selecting the nearest Type 1 meteorological station, a location map is provided within the option. The user is required to provide the meteorologic data corresponding to

**TABLE 1. The files present in EXSYS with brief introduction to their contents**

file name	contents
EXSYS.EXE	main program, including option 1
OPTION2.EXE	preprocessor for PRZM, creates input file MODIN.DAT. Monte Carlo on rain fall data, runs program PRZM, abstracts amount of pesticide present in the last compartment and puts this value in file IND.DAT
BD.EXE	help program for values of bulk density for major soils of Oklahoma
CN.EXE	help program with brief introduction and values for curve number with soil distribution map of Oklahoma
KS.EXE	help program with brief introduction and values for decay coefficient for selected pesticides used in Oklahoma
KOC.EXE	help program with brief introduction and values for organic-carbon distribution coefficient for selected pesticides used in Oklahoma
OC.EXE	help program for values of organic carbon contents of major soils of Oklahoma
FC.EXE	help program for values of field capacity for major soils of Oklahoma
WP.EXE	help program for values of wilting point for major soils of Oklahoma
FDK.EXE	help program for values of foliar decay coefficient for major group of pesticides used
EROSN.EXE	help program for selecting the values of K, LS, P, and C to simulate erosion losses
WSTATN.EXE	Oklahoma map with location of weather stations, to assist in selecting rain fall data required to run PRZM

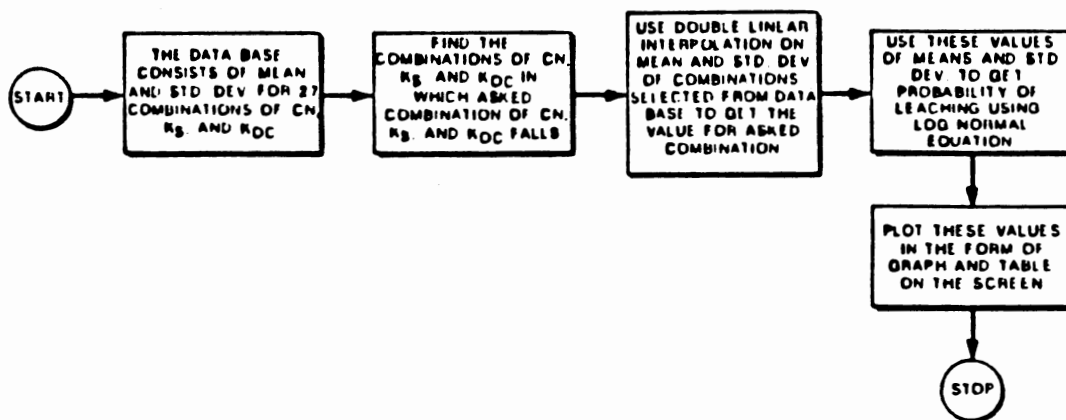


Figure 3. Flow Diagram For Option 1



the station selected in the PRZM compatible format. For convenience of the user fourteen diskettes containing meteorologic data corresponding to the Type 1 stations in Oklahoma are provided with the EXSYS. The flow diagram for Option 2 is shown in Figure 4, which presents the basic operating structure of this option.

### Development of Option 1 for Preliminary Analysis

The first option is relatively simple to use and the results are provided within seconds. The database needed for this option was developed using the results obtained by Daniels and McTernan [8]. The simulations in that study were performed using PRZM to determine an overall probability of leaching from Oklahoma's winter wheat areas (Figure 5 shows the study area) and involved Monte Carlo techniques to address the spatial variability of soil bulk density, field capacity, wilting point, and soil organic matter. Other parameters were fixed at three incremental values to isolate pesticide selection (pesticide decay rate,  $K_s$  and soil partition coefficient,  $K_{oc}$ ) as well as land use management alternatives (Soil Conservation Service Curve Number, CN) for additional analysis. Fixing these three parameters at predetermined levels allowed the user to incorporate various agronomic variables within the simulations for comparisons while still bracketing the majority of the situations found within the state.

The CN addresses the hydrologic soil group and such

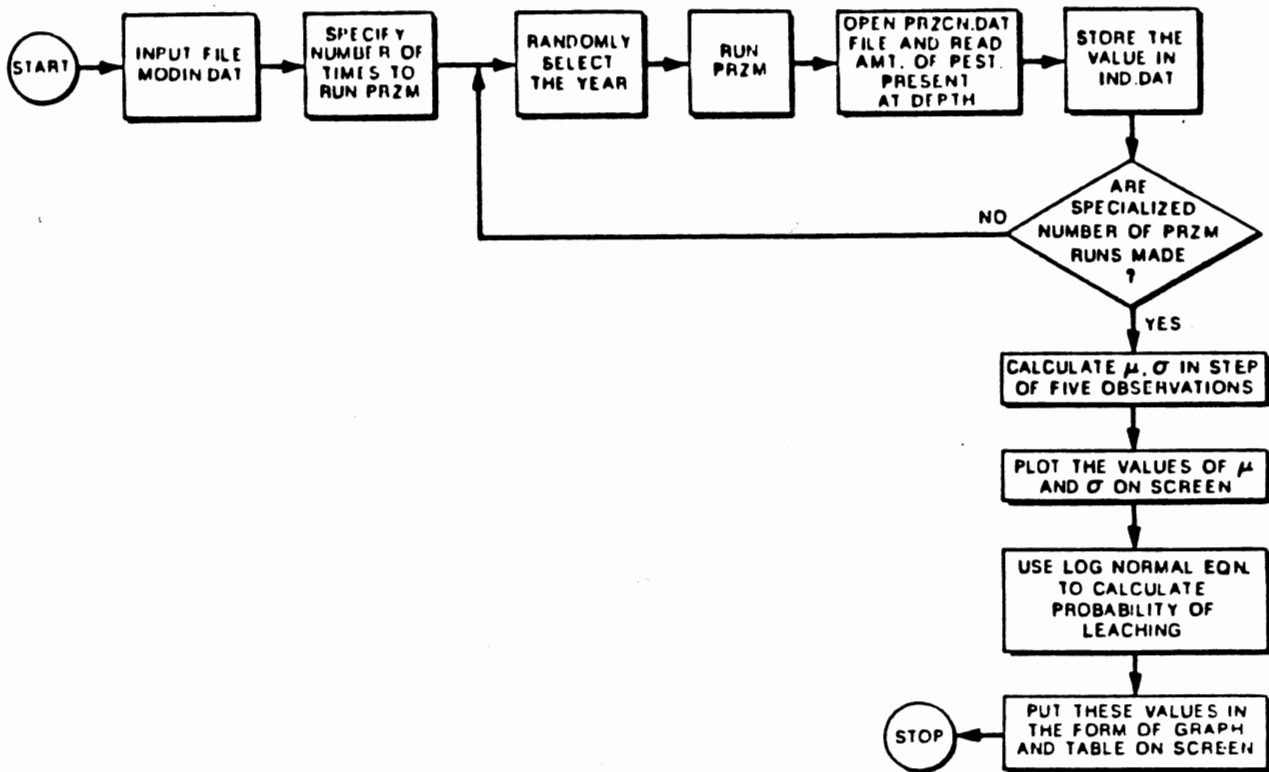


Figure 4. Flow Diagram For Option 2

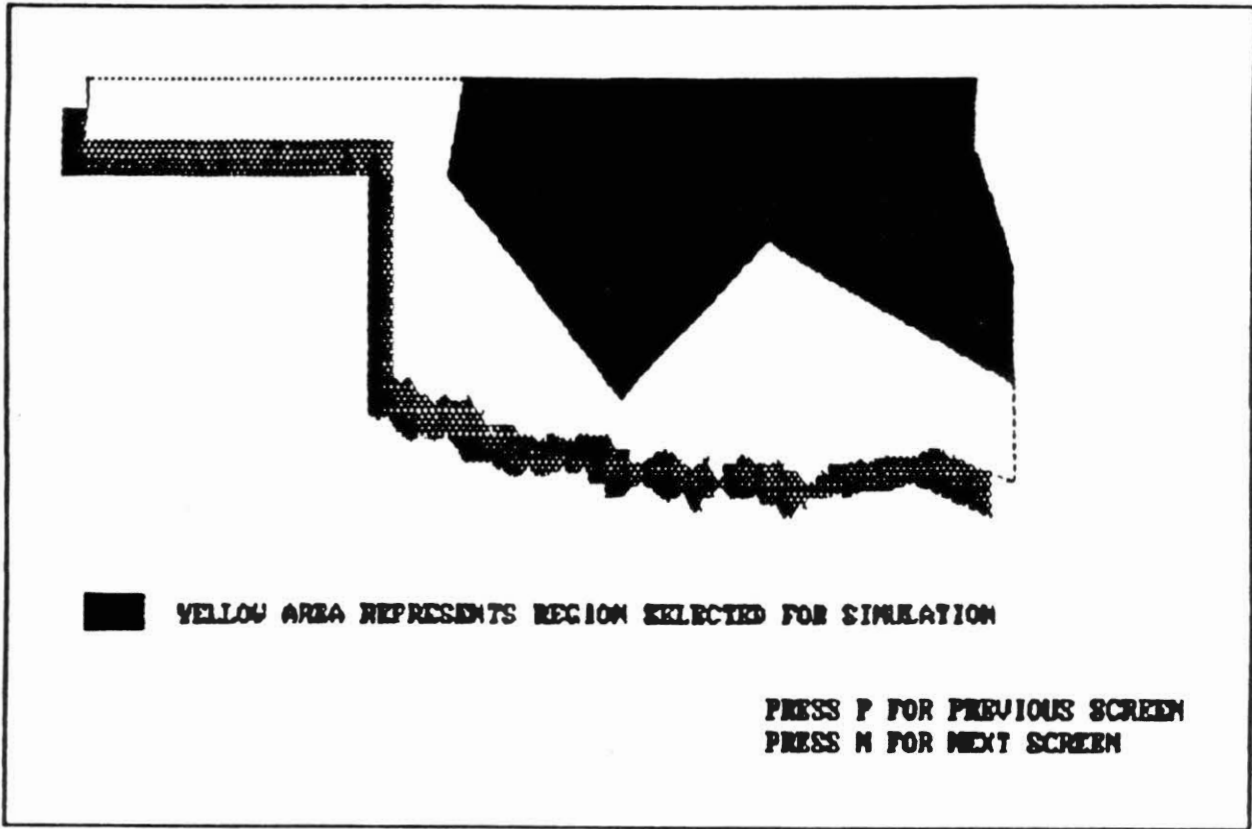


Figure 5. Region of Simulation Selected for Option 1.

land use practices as plowing in straight or contoured rows, or on contoured and terraced areas. The effects of fallow conditions, row crop, and small grain selection, among others, can be addressed by proper selection of CN. A comparison of different hydrologic soil groups can also be simulated by CN allowing the potential user to make site comparisons. The range fixed for Soil Conservation Services Curve Number (CN) was from 59 to 88, while the pesticide decay coefficient (Ks) varied from 0.001 to 0.1, and the soil partition coefficient (Koc) varied from 2 to 1200. A total of 540 simulations were completed combining the random selection of soil properties and rainfall year together with the incremental parameters describing land use and pesticide selection.

To simulate Oklahoma's principal cash crop, winter wheat, the planting date was fixed as February 1st and corresponded to that time when the wheat emerges from winter dormancy [7]. This eliminated the need to simulate across two hydrologic years. Similarly, the wheat maturation and harvest dates were taken as April 20th and June 15th respectively, while the pesticide application date was established as February 1st. These dates approximated those cited in the available literature [5,9].

Data from two zones approximating soil horizons were described in the available literature [10]; the top with relatively high organic carbon contents was typically 30 cm thick while the second extended from 30 cm to 183 cm.

The depth to groundwater was not given in these records, but other data indicate groundwater levels from near land surface to over several hundred feet [20,26]. For the present work, which was concerned with shallow aquifers, only the top horizon was considered. That is, only leaching probabilities at 30 cm were determined. As suggested by Daniels and McTernan [8], the number of compartments in the soil horizon needed to run PRZM was also set at 6. To facilitate interpretation of results (which were shown as percentage of applied pesticide leached), the amount of pesticide applied was fixed at 1 Kg/Ha. This was appropriate due to the use of linear equilibrium adsorption within PRZM which assumed that the amount of pesticide leached was always a constant ratio to that applied. This is consistent with other works in the area [21,22].

For the development of database for Option 1, additional statistical analysis was done on the outputs from the original 540 simulations. It was observed that for a fixed combination of CN, Ks, and Koc the probability distributions for the pesticide leaching outputs very closely followed log normal type distributions. The probability density function for log normal distribution can be expressed as follows:

$$f(x) = \frac{1}{\sqrt{2\pi}\sigma x} \exp\left\{ -\frac{1}{2\sigma^2} [\ln(x) - \mu]^2 \right\} \quad (3)$$

where,

x = non negative random variable

$\mu$  = mean of the log values of x

$\sigma$  = standard deviation of the log values of x

Log normal plots of original 540 simulations are shown in Appendix A.

Equations of these distributions were developed and the mean and standard deviation for each calculated. In accordance with the user defined values of CN, Ks, and Koc means and standard deviations of appropriate distributions are retrieved from the database and substituted into the standardized log normal equation, which has the form:

$$z = \frac{\ln X - \mu}{\sigma} \quad (4)$$

where,

z = standard normal random variable

X = continuous random variable

$\mu$  = mean of the log values of X

$\sigma$  = standard deviation of the log values of X

The equation is then solved for a series of incremental probabilities. Double interpolation between existing distributions allows the user to determine the probability of pesticide leaching at CN, Ks, and/or Koc values intermediate to those employed on the original effort. The probability of pesticide leaching for a wide range of generic conditions then can be obtained by solving these equations. An example calculation is shown in Appendix D.

### Option 1 Example

Several of the guidance screens encountered by the user during an interactive session using Option 1 of EXSYS are shown in this section. Figure 6 describes the type of input parameters required to run Option 1, while Figures 7 to 11 illustrate information needed to select a value of curve number. Figures 7 and 8 give a brief introduction to CN and the types of hydrologic soil groups respectively. The user can select the soil type from the general soil distribution map of Oklahoma (Figure 9) and subsequently obtain hydrologic information from Figures 10 and 11. The final selection of a CN is further facilitated with information contained in Figure 12. A curve number of 71 was selected for this example. Similar guidance for the selection of the pesticide decay and soil partition coefficients is available within EXSYS. Appendix B contains the complete set of guidance screens encountered in Option 1.

The screen shown in Figure 13 provides the user a final opportunity to change any parameter value. Figure 14 presents example output from Option 1 simulation. A plot and corresponding table compare the percent of pesticide leached to 30 cm with the percent of time exceeded. This defines a probability of occurrence. For example, 30, 50, and 70% of the applied pesticide could be expected to leach 0, 50, and 5% of the time respectively, given the results provided in Figure 14.

IN OPTION ONE, THE USER WILL BE ASKED TO PROVIDE :

- a. SCS CURVE NUMBER ( CN )
- b. FIRST ORDER PESTICIDE DECAY COEFF. (  $K_d$  )
- c. SOIL-ORGANIC CARBON DIST. COEFF. (  $K_{oc}$  )

THIS PORTION OF THE EFFORT LIMITS THE CN SELECTION RANGE TO 59-98,  $K_d$  TO 0.001 TO 0.1, AND  $K_{oc}$  TO 2 TO 1298. GUIDANCE FOR THE SELECTION OF THESE PARAMETERS IS PROVIDED WITH IN THE CODE.

PRESS P FOR PREVIOUS SCREEN  
PRESS N FOR NEXT SCREEN

Figure 6. Example Screen Containing Input Parameters Information for Option 1 Simulation.



**NEXT FIVE SCREENS ARE DEVELOPED TO HELP SELECT THE VALUE  
OF PARAMETER CURVE NUMBER (CN)**

**THE CURVE NUMBERS (CN) DEVELOPED BY SOIL CONSERVATION SERVICES  
CHARACTERIZE SOILS ON THE BASIS OF INFILTRATION PROPERTIES.  
THERE ARE FOUR DIFFERENT HYDROLOGIC SOIL GROUPS (A,B,C, and D)  
AND ARE IN ORDER OF DECREASING PERCOLATION POTENTIAL.**

**PRESS P FOR PREVIOUS SCREEN  
PRESS N FOR NEXT SCREEN**

Figure 7. Guidance Screen Providing General Information About Curve Number (CN).

**SOIL CHARACTERISTICS ASSOCIATED WITH EACH HYDROLOGIC GROUPS ARE  
AS FOLLOWS :**

**GROUP A : DEEP SAND, DEEP LOESS, AGGREGATED SILTS. MINIMUM  
INFILTRATION OF 0.76 - 1.14 cm/hr .**

**GROUP B : SHALLOW LOESS, SANDY LOAM, MINIMUM INFILTRATION  
0.38 - 0.76 cm/hr .**

**GROUP C : CLAY LOAMS, SHALLOW SANDY LOAM, SOILS LOW IN ORGANIC  
CONTENTS, AND SOILS USUALLY HIGH IN CLAY, MINIMUM  
INFILTRATION 0.13 - 0.38 cm/hr .**

**GROUP D : SOILS THAT SWELL SIGNIFICANTLY WHEN WET, HEAVY PLASTIC  
CLAYS, AND CERTAIN SALINE SOILS. MINIMUM INFILTRATION  
0.03 - 0.13 cm/hr .**

**PRESS P FOR PREVIOUS SCREEN  
PRESS N FOR NEXT SCREEN**

Figure 8. Guidance Screen Describing Hydrologic Soil Groups.

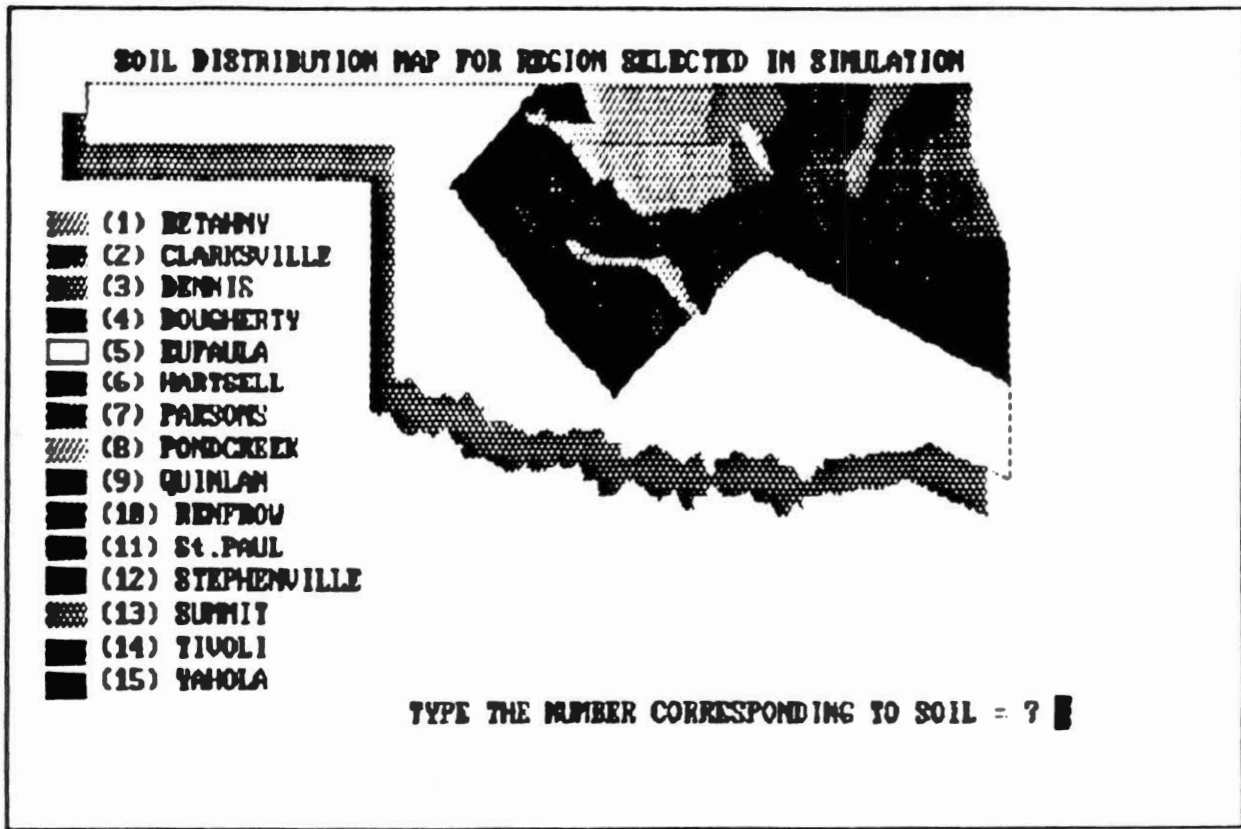


Figure 9. Guidance Screen Displaying Predominant Soil Distribution Map of Oklahoma.

**THE SOIL TYPE FOR CURRENT SIMULATION IS = CLARKSVILLE**

**THE HYDROLOGIC GROUP OF THIS SOIL IS = B**

**DO YOU WANT TO CHANGE THE SOIL SELECTED ? (Y/N) ? █**

Figure 10. Guidance Screen Defining Hydrologic Group of the Soil Selected.

TO MAKE FINAL SELECTION OF 'CN' SOME ADDITIONAL INFORMATION IS NEEDED. A TABLE HAS BEEN PROVIDED ON NEXT SCREEN TO ASSIST IN PROVIDING THIS INFORMATION. PLEASE, FOLLOW THE PROCEDURE MENTIONED BELOW :

1. FROM TABLE FIND THE LAND USE AND TREATMENT OR PRACTICES THAT IS TO BE SIMULATED (e.g. ROW CROPS, STRAIGHT ROW) .
2. FROM TABLE FIND THE HYDROLOGIC CONDITION OF THE SOIL THAT IS TO BE SIMULATED (e.g. GOOD) .
3. FROM THE TABLE FIND THE ' CN ' FOR ABOVE SELECTED CONDITIONS

EXAMPLE : HYDROLOGIC GROUP = A  
TREATMENT PRACTICE IS STRAIGHT ROW  
LAND USE IS ROW CROPS  
HYDROLOGIC CONDITION IS GOOD

THE CURVE NUMBER IS 67

PRESS P FOR PREVIOUS SCREEN  
PRESS N FOR NEXT SCREEN

Figure 11. Screen Outlining Procedure To Select Curve Number (CN) .

COVER			HYDROLOGIC GROUP			
LAND USE	TREATMENT/PRACTICE	HYDROLOGIC CONDITION	A	B	C	D
FALLOW	STRAIGHT ROW	-----	77	86	91	94
ROW CROPS	STRAIGHT ROW	POOR	72	78	85	91
	STRAIGHT ROW	GOOD	67	78	85	89
	CONTOURED	POOR	78	79	84	88
	CONTOURED	GOOD	65	75	82	86
	CONTOURED & TERRACED	POOR	66	74	80	82
	CONTOURED & TERRACED	GOOD	62	71	78	81
TYPE THE VALUE BY CN = 7 71						

Figure 12. Guidance Screen Displaying A Partial Listing of Crop and Land Use Practices For Curve Number Selection.

THE VALUES SELECTED FOR DIFFERENT PARAMETERS ARE :

THE CURVE NUMBER (CN) FOR CURRENT SIMULATION IS = 71

THE DECAY COEFFICIENT (K<sub>d</sub>) FOR CURRENT SIMULATION IS = .0063

THE ORG. CARBON DIST. COEFF. (K<sub>oc</sub>) FOR CURRENT SIMULATION IS = 173.70

DO YOU WANT TO CHANGE THE VALUES ? (Y/N) ?

Figure 13. Screen Giving An Opportunity To Change Selected Parameters For Option 1 Simulation.

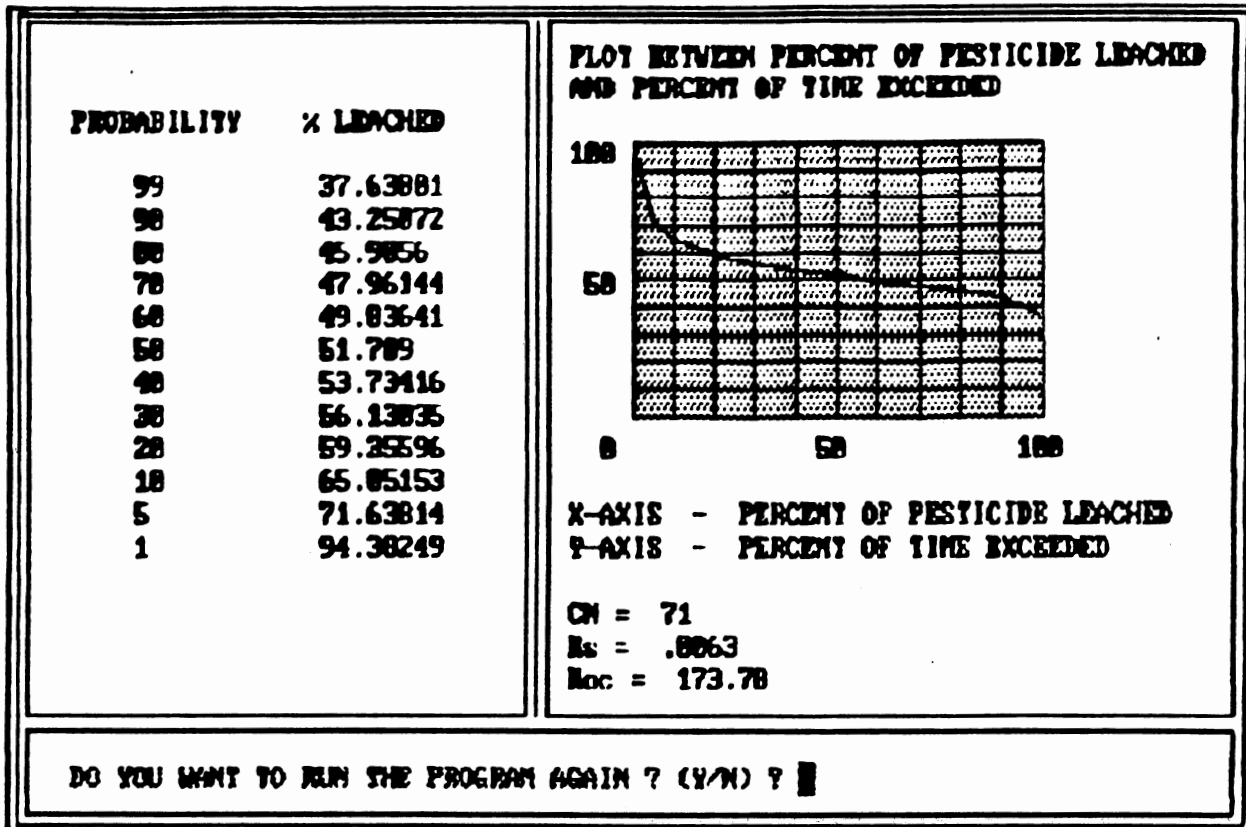


Figure 14. Example Final Output For Option 1 Simulation.



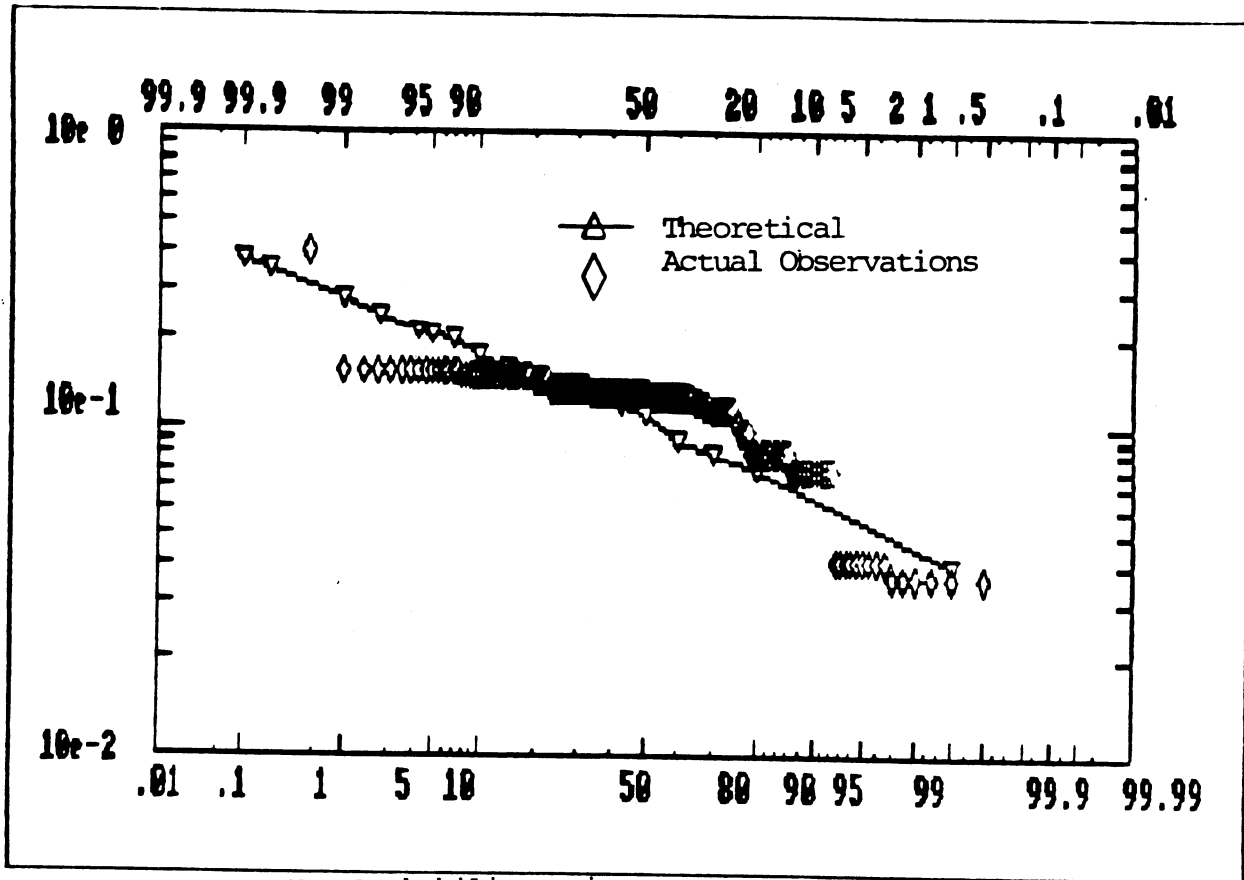
## Development of Option 2 for Site Specific Analysis

The second option available within EXSYS allows the user to configure and complete Monte Carlo simulations for a specific farm site of 1-2 Ha in size. For this option, a user friendly pre-processor was developed to create the input files needed to run PRZM. Crop planting, maturation, harvesting and pesticide application dates were fixed, however, as in Option 1. Similarly horizon depth and the amount of pesticide applied was also maintained at similar levels. Other inputs such as pan evaporation and snow melt factors, depth of pesticide incorporation, curve number, decay rate, soil partition coefficient, hydrodynamic dispersion etc. needed to complete a PRZM simulation are requested by EXSYS through a series of questions and menus. Guidance in the form of tables, equations and instructions accompanies these questions. As the user defines site conditions the soil properties become fixed to that site. Similarly, the chemical properties of the pesticides used are also constants for a particular pesticide. Monte Carlo randomization was applied only to meteorological data where a 25 year period of record at the 12 type 1 meteorological stations located throughout Oklahoma was available. The data from these individual stations were provided in PRZM format by the Oklahoma Climatological Survey in Norman, Oklahoma. A period of record from 1954 through 1978 was selected as it was the only record consistent to all of the available stations [19].

Following configuration of the site specific parameters, the user determines the number of simulations to be employed and the location of the nearest type 1 weather station. EXSYS randomly accesses a single year of meteorological data from a 25 year record at the location specified and calls the PRZM module for simulation. The process is repeated until the specified number of simulations has been completed. The amount of pesticide leached past the 30 cm depth is retrieved from an output file, the mean and standard deviation calculated and probability of leaching obtained using a log-normal distribution equation. Figure 15 presents comparisons between example output and these log normal approximations. The use of the distribution seemed justified when compared to a simpler plotting position approach as it reduced demands upon available memory.

### Option 2 Example

In this section a brief description of the guidance screens appearing in Option 2 is provided. For the example problem, erosion losses were not considered as pesticide was incorporated into the soil at 10 cm depth. Atrazine was selected as pesticide with decay and soil partition coefficients ( $K_s$  and  $K_{oc}$ ) of 0.0063 and 173.82 respectively. The soil selected was a Clarksville series on a field of row crop of good hydrologic condition with CN values 66, 71, and 66 for fallow, cropping, and residue conditions respectively. The number of simulations for the



X - Probability axis  
 Y - Log of pesticide leached past 30 cm (Kg/Ha)

Figure 15. Plot Showing Comparisons between Example Output and the Log normal Approximation

Monte Carlo was established at 100 for illustrative purposes. In cases, where the user does not have apriori knowledge about the number of Monte Carlo simulations to run, suggested number is 50. Afterwards the user can increase or decrease this number by selecting the value after which mean and standard deviation do not change appreciably. The screens presented in Figures 16 to 20 give the user general information about the pan and snowmelt factors, pan evaporation flag, the minimum depth for evaporative extraction and the condition of the land surface. Assistance in defining acceptable ranges for these parameters is included with the information given on these.

In similar manner, Figures 21 to 27 present information and request inputs for maximum interception storage, plant rooting depth, and depth of pesticide incorporation as well as for the maximum areal coverage achieved by the crop and its uptake efficiency factor for the pesticide. Where appropriate these are crop and/or region specific. If the user requests help in selecting soil organic carbon, soil bulk density, field capacity, and/or wilting points of their soils, Figures 28 through 31 present representative values.

Hydrodynamic dispersion and initial water contents are input as shown in the screens presented in Figures 32 and 33. If the user does not want to simulate hydrodynamic dispersion, its value can be taken as 0 and the value of initial water contents can range from wilting point to

PAN FACTOR IS A DIMENSIONLESS NUMBER. THIS FACTOR IS MULTIPLIED BY DAILY PAN EVAPORATION TO ESTIMATE DAILY EVAPOTRANSPIRATION (ET). IF DAILY AIR TEMPERATURES ARE USED FOR 'ET', ANY DUMMY NUMBER CAN BE INPUT (e.g. 0.75) .

THE SELECTION RANGE FOR PAN FACTOR IS FROM 0.6 TO 1.0 .

THE RANGE FOR OKLAHOMA IS FROM 0.69 TO 0.72.

TYPE THE VALUE OF PAN FACTOR ? 0.71

PRESS P FOR PREVIOUS SCREEN  
PRESS N FOR NEXT SCREEN

Figure 16. Example Screen Providing General Information About the Pan Evaporation Factor.

SNOW FACTOR, cm snowmelt/deg. c above freezing. VALUES OF  
SNOW FACTOR ARE IN THE ORDER OF 0.45 . IF SNOWMELT IS NOT  
CALCULATED, ENTER 0.88 .

WHEN THE MEAN AIR TEMPERATURE FALLS BELOW 0.0 deg. C,  
ANY PRECIPITATION THAT FALLS IS CONSIDERED TO BE IN THE FORM  
OF SNOW. WHEN THE MEAN AIR TEMPERATURE IS ABOVE 0.0 deg. C .  
HOWEVER , THE SNOW ACCUMULATION IS DECREASED BY A SNOWMELT FACTOR.  
THE SELECTION RANGE FOR SNOW FACTOR IS FROM 0.0 TO 1.0 .  
TYPE THE VALUE OF SNOW FACTOR ? 0.1

PRESS P FOR PREVIOUS SCREEN  
PRESS N FOR NEXT SCREEN

Figure 17. Example Screen Providing General Information About the Snow Melt Factor.

PAN EVAPORATION FLAG. IF THIS FLAG IS SET TO BE 0, PAN  
EVAPORATION DATA ARE READ. IF SET EQUAL TO 1, TEMPERATURE DATA  
ARE READ AND USED TO CALCULATE POTENTIAL 'ET'. IF SET EQUAL TO 2,  
THEN PAN EVAPORATION , IF AVAILABLE, IS USED IN THE METEOROLOGIC  
FILE; IF NOT, TEMPERATURE IS USED TO COMPUTE POTENTIAL 'ET'.

SUGGESTED VALUE FOR THIS FLAG IS 2.

TYPE THE VALUE OF PAN EVAPORATION FLAG ? 2

PRESS P FOR PREVIOUS SCREEN  
PRESS N FOR NEXT SCREEN

Figure 18. Example Screen Providing General Information About the Pan Evaporation Flag.

THE MINIMUM DEPTH, cm , IN WHICH EVAPORATION IS EXTRACTED  
YEARLY ( e.g. 20.0 ) .

	cm
MINIMUM	10.000
MAXIMUM	35.000

TYPE THE MINIMUM DEPTH ? 10

PRESS P FOR PREVIOUS SCREEN  
PRESS N FOR NEXT SCREEN

Figure 19. Example Screen For Determining the Minimum Depth For Evaporative Water Extraction.



**THE CONDITION OF SURFACE AFTER HARVEST :**

<b>FALLOW</b>	<b>1</b>
<b>CROPPING</b>	<b>2</b>
<b>RESIDUE</b>	<b>3</b>

**TYPE THE NUMBER CORRESPONDING TO CONDITION AFTER HARVEST ? 1**

**PRESS P FOR PREVIOUS SCREEN  
PRESS N FOR NEXT SCREEN**

Figure 20. Example Screen For Input of Surface Condition of Land After Harvest.

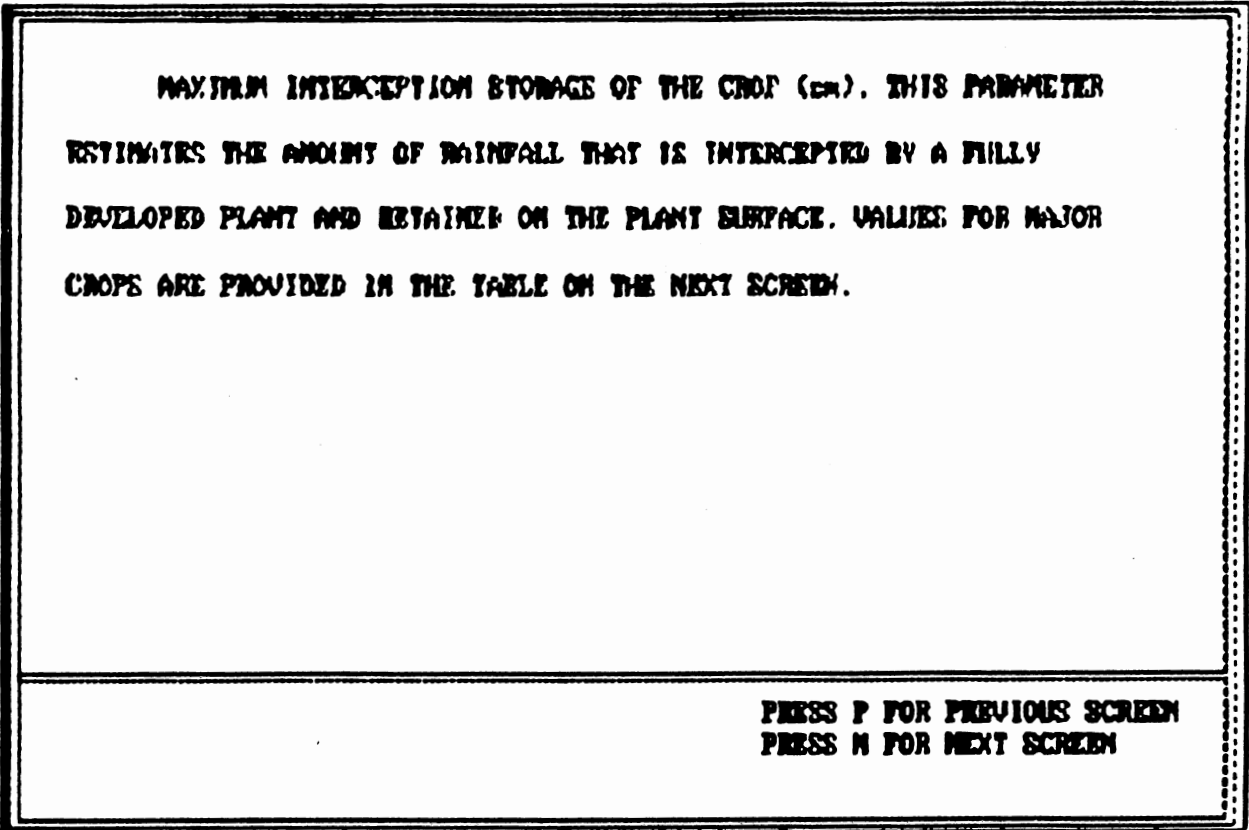


Figure 21. Example Screen Giving General Information About the Plant Maximum Interception Storage.

CROP	DENSITY	INTERCEPTION (cm)
CORN SOYBEAN WHEAT OATS BARLEY POTATOES PEANUTS COTTON TOBACCO	HEAVY MODERATE LIGHT LIGHT LIGHT LIGHT LIGHT MODERATE MODERATE	0.25-0.30 0.20-0.25 0.0-0.15 0.0-0.15 0.0-0.15 0.0-0.15 0.0-0.15 0.20-0.25 0.20-0.25
TYPE THE VALUE FOR MAX. INTERCEPTION = Y 0.15		
PRESS P FOR PREVIOUS SCREEN PRESS N FOR NEXT SCREEN		

Figure 22. Example Screen Displaying Typical Values of Maximum Interception Storage For Some Crops.

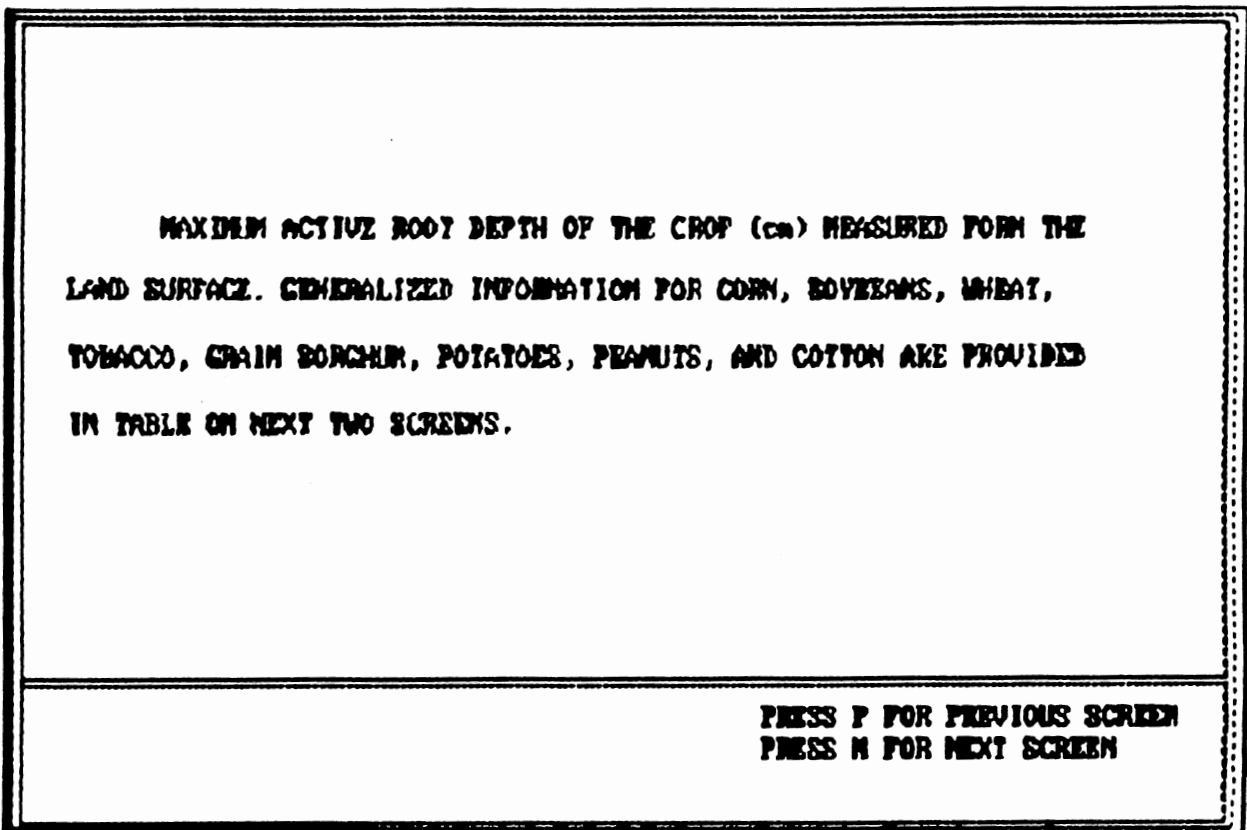


Figure 23. Example Screen Presenting General Information About the Maximum Plant Rooting Depth.

CROP	MAJOR STATES PRODUCTION	RANGE OF ROOT DEPTH (cm)
CORN	IA, IL, IN, MI, OH	60-120
SOYBEANS	IA, IL, IN, MI, OH	30-60
COTTON	TX, MS, AR, AZ, AL	30-90
WHEAT	NE, DE, CA, ND, MT WA, OR, ID	15-30

TYPE THE MAX. ACTIVE ROOTING DEPTH = ? 15

DO YOU WANT TO GO TO PREVIOUS OR NEXT SCREEN (P/N) ?

Figure 24. Example Screen Displaying Values of Rooting Depth For Some Crops and Locations.

**TYPE THE DEPTH OF PEST. INCORPORATION IN cm. (IF BROADCAST THEN S) = 7 18**

**PRESS P FOR PREVIOUS SCREEN  
PRESS N FOR NEXT SCREEN**

Figure 25. Example Screen Requesting Input of the Depth of Pesticide Incorporation In the Soil.

THE PARAMETER MAX. AREAL COVERAGE OF THE CROP AT FULL CANOPY  
ESTIMATES THE GROUND COVER AS THE CROP GROWS TO SOME MAXIMUM VALUE.  
IT DETERMINES THE FRACTION OF GROUND COVER AFFORDED BY THE CROP AND  
THIS INFLUENCES THE MASS OF PESTICIDE THAT REACHES THE GROUND.

TYPE THE VALUE OF MAX. AREAL COVERAGE (x) = ? 0

PRESS P FOR PREVIOUS SCREEN  
PRESS N FOR NEXT SCREEN

Figure 26. Example Screen Giving General Information About Maximum Areal Coverage of the Crop.

THE PLANT UPTAKE EFFICIENCY FACTOR PROVIDES FOR REMOVAL OF PESTICIDES BY PLANT AND IS A FUNCTION OF CROP ROOT ZONE AND THE INTERACTION OF WATER AND CHEMICAL PROPERTIES OF THE PESTICIDES. FOR FURTHER REMOVAL OF PESTICIDE BY PLANT UPTAKE IS BASED ON THE ASSUMPTION THAT UPTAKE OF PESTICIDE IS RELATED TO THE TRANSPIRATION RATE. SENSITIVITY TESTS INDICATE AN INCREASE IN THE UPTAKE BY PLANTS AS THE ROOT DEPTH INCREASES, AND A DECREASE AS THE PARTITION COEFFICIENT INCREASES. VALUES CAN BE FROM 0.0 TO 1.0 (e.g. 0.10) INDICATES UPTAKE IS A FRACTION OF CROP TRANSPIRATION RATE.

TYPE THE PLANT UPTAKE EFFICIENCY FACTOR = 7 0.1

PRESS P FOR PREVIOUS SCREEN  
PRESS N FOR NEXT SCREEN

Figure 27. Example Screen Giving General Information About Plant Uptake Efficiency Factor.



SOIL	ORGANIC CARBON (%)
BEYBAY	8.98
CLARKVILLE	8.51
DENNIS	1.58
DUGHERTY	8.38
ELPALLA	8.72
HARTSELL	8.85
PARDONS	8.96
PONDCREEK	1.21
QUINLAN	8.53
REYFORD	1.54
ST. PAUL	8.85
STEPHENVILLE	8.46
SUPPIT	2.98
TIVOLI	8.22
YANOLA	8.53

TYPE THE VALUE = 7 8.51

WOULD YOU LIKE TO CHANGE THE VALUE (Y/N) ?

Figure 28. Example Screen Displaying Organic Carbon Contents of the Major Soils Shown In Soil Distribution Map For the Region Selected For Simulation.

SOIL	BULK DENSITY (g/cm <sup>3</sup> )
BETHANY	1.14
CLARKSVILLE	1.37
DENNIS	1.13
DOUGHERTY	1.45
ELFALA	1.47
HARTSELL	1.25
PARSONS	1.26
PONDREEK	1.17
QUINLAN	1.49
RENFROW	1.15
St. PAUL	1.26
STEPHENVILLE	1.48
SUMMIT	1.89
TIVOLI	1.51
YANOLA	1.41

TYPE THE VALUE = Y 1.37

WOULD YOU LIKE TO CHANGE THE VALUE (Y/N) ?

Figure 29. Example Screen Displaying Typical Bulk Densities of the Major Soils Encountered In the Region of Simulation.

SOIL	FIELD CAPACITY (cm <sup>3</sup> /cm <sup>3</sup> )
BETHANY	0.32
CLARKSVILLE	0.30
DENNIS	0.36
DOUGHERTY	0.12
BIFALVA	0.20
HARTSELL	0.25
PRECONS	0.31
PONDCREEN	0.37
QUINLAN	0.15
KENTON	0.37
St. PAUL	0.29
STEPHENVILLE	0.12
SUNNY	0.48
TIVOLI	0.09
YANOLA	0.18

TYPE THE VALUE = Y 0.30

WOULD YOU LIKE TO CHANGE THE VALUE (Y/N) ? █

Figure 30. Example Screen Displaying Typical Field Capacity of Major Soils Encountered In the Region of Simulation.

SOIL	WILTING POINT (cm <sup>3</sup> /cm <sup>3</sup> )
BETHANY	0.14
CLARKSVILLE	0.12
DENNIS	0.17
DOUGHERTY	0.04
HYPOLIA	0.11
HARTSELL	0.12
PARSONS	0.13
POND CREEK	0.18
QUINLAN	0.07
KENTON	0.19
ST. PAUL	0.14
STEPHENVILLE	0.05
SARIT	0.26
TIVOLI	0.04
YANOLA	0.08

TYPE THE VALUE = 7 0.12

WOULD YOU LIKE TO CHANGE THE VALUE (Y/N) ?

Figure 31. Example Screen Displaying Typical Wilting Point of Major Soils Encountered In the Region of Simulation.

IF YOU WOULD LIKE TO SIGNATE DISPERSION, THEN ENTER THE VALUE  
FOR HYDRODYNAMIC DISPERSION (cm<sup>2</sup>/day) OTHERWISE ENTER 0.

TYPE THE VALUE FOR HYDRODYNAMIC DISPERSION (cm<sup>2</sup>/day) = 7 0

PRESS P FOR PREVIOUS SCREEN  
PRESS N FOR NEXT SCREEN

Figure 32. Example Screen to Input Values For Hydrodynamic Dispersion.

**THE SELECTION RANGE FOR INITIAL WATER CONTENTS IS FROM  
WILTING POINT TO POROSITY.**

**TYPE INITIAL WATER CONTENTS IN SOIL (cm<sup>3</sup>/cm<sup>3</sup>) = ? 0.165**

**PRESS P FOR PREVIOUS SCREEN  
PRESS N FOR NEXT SCREEN**

Figure 33. Example Screen For Input of the Initial Water Contents of the Soil.

soil porosity. Figure 34 displays the location of type 1 weather stations in Oklahoma to assist the user in selecting the nearest station. With all of these guidance screens, the user can either use the parameters directly or can input a separate entry should another source provide a more appropriate value.

To maintain consistency with Option 1, the final results for Option 2 simulation are shown as plots of percent of pesticide leached versus the percent of time exceeded or probability. An additional screen is provided, however, for Option 2 which plots the mean and standard deviation of sequential, incremental simulations against the number of simulations completed. These are calculated for first 5,10,15,20... values and are intended to assist in determining the number of simulations required to achieve an acceptable level of precision. That is, as the curves resulting from these determinations asymptote to a constant level, there is additional certainty that a sufficiently large sample of simulations was determined. Figure 35 presents an example of these comparisons. In Appendix C, all the guidance screens displayed in Option 2 are presented.

### CONCLUSIONS

In the recent past simulation procedures were limited to those individuals with good computer skills, serving to reduce the contributions of those professionals with

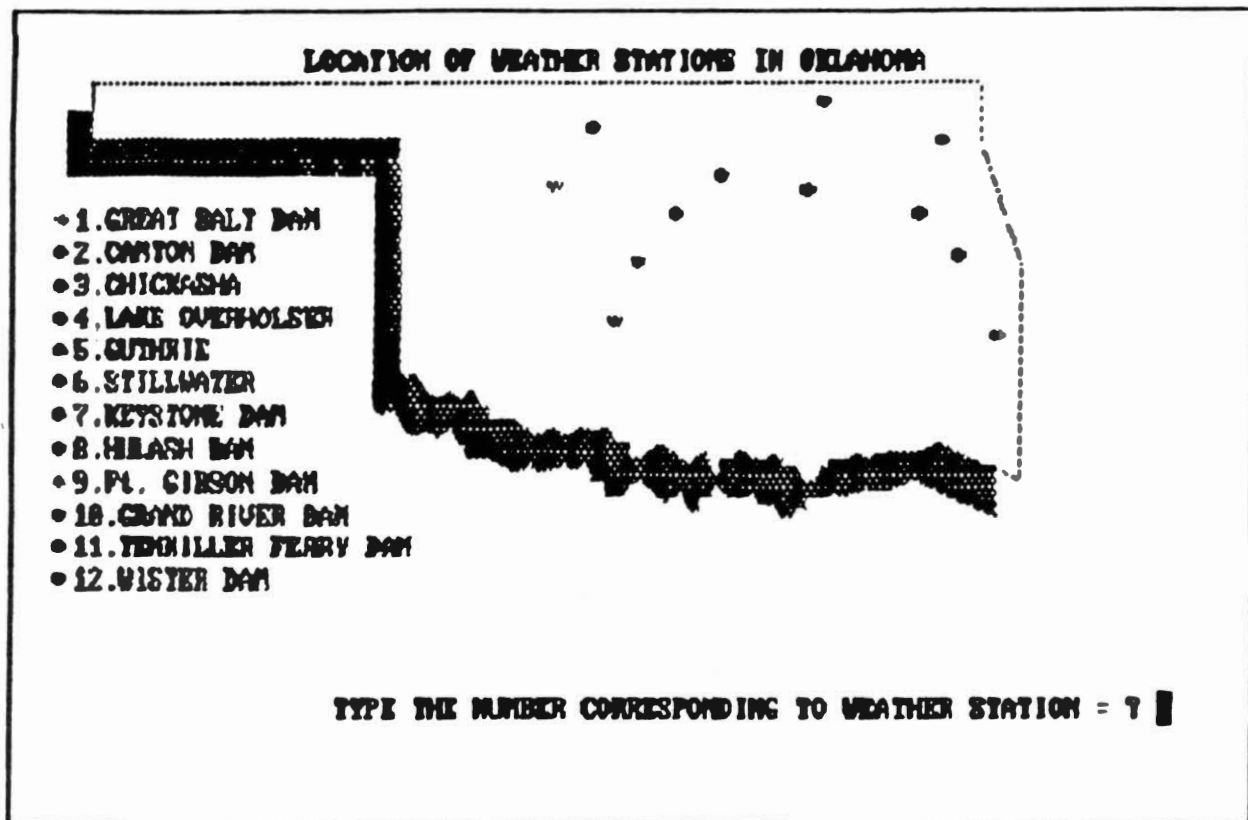


Figure 34. Screen Displaying Location of Type 1 Weather Stations In Oklahoma  
User May Pick by Number and Input Appropriate Data Set.



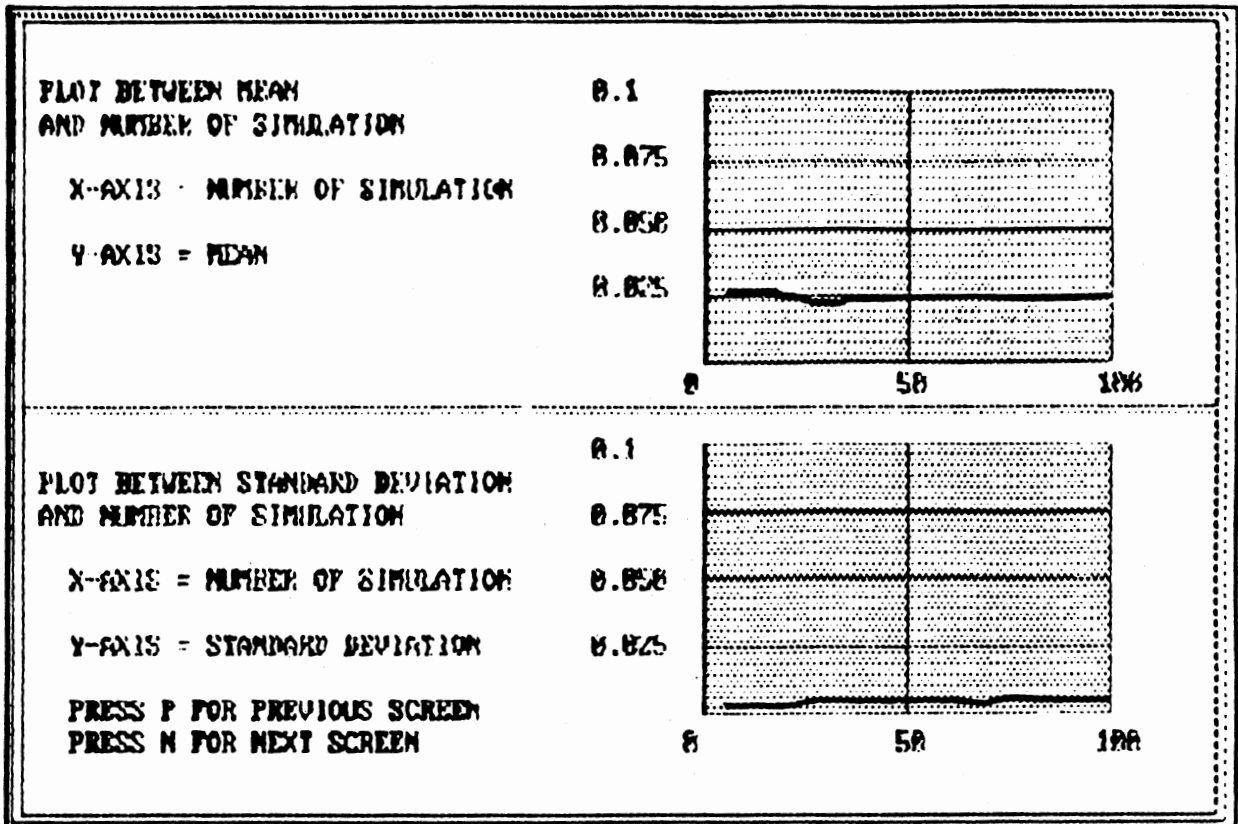


Figure 35. Screen Presenting Plot Between Mean, Standard Deviation and Number of Simulations Completed

useful skills, and knowledge in related fields. EXSYS was developed to help eliminate this deficiency by attempting to make modeling of pesticide leaching easier. EXSYS affords planners, county officials, and other land use managers access to current technologies available to define the risks of groundwater pollution from pesticides so that additional alternative management options can be evaluated. A public domain, widely accepted deterministic code (PRZM) developed by U.S. Environmental Protection Agency was chosen to complete the simulations. The expert system developed in this effort is a shell built around the unaltered EPA code.

The Option 1 of EXSYS was developed for a quick preliminary analysis of the probability of pesticide leaching past 30 cm and is based upon statistical distributions describing previous Monte Carlo simulation outputs. This option requires only three simulation parameters: curve number, pesticide decay and soil partition coefficients (CN, Ks, and Koc). By proper selection of these parameters the user can evaluate the effects of chemical properties associated with pesticide, land use and practices/treatment on leaching of the pesticide. This helps in making decisions about proper pesticide selection and farm practices so that the probability of pesticide leaching can be minimized. Assistance is provided in selecting the values of these simulation parameters.

Option 2 allows the user to configure and complete

simulations using Monte Carlo techniques for specific farm conditions. A user friendly preprocessor was developed to assist the user in creating input files for PRZM. The user can seek guidance in selecting values of the input parameters, and the preprocessor responds to these requests by calling subprograms which provide general information, values, and guidelines for proper selection of these parameters.

The simplistic nature of Option 1 and user friendly interactive menu driven preprocessor developed for Option 2 attempt to help professionals lacking adequate computer training. The overall ease in using EXSYS could make this expert system an effective screening tool.

This expert system was developed to address winter wheat areas in Oklahoma. This approach could very easily be applied to other crops and other areas.

## SELECTED BIBLIOGRAPHY

1. Alm, A.L., "Non point Sources of Water Pollution", *Environmental Science & Technology*, Vol. 24, p 967, July 1990.
2. Banton, O., and Villeneuve, J-P, "Evaluation of Groundwater Vulnerability to Pesticides: A Comparison Between the Pesticide Drastic Index and the PRZM Leaching Quantities", *Journal of Contaminant Hydrology*, 4, p 285-296, 1989.
3. Carsel, R.F., Lober, M.N., and Baskin, L.B., "The Pesticide Root Zone Model (PRZM): A Procedure for Evaluating Pesticide Leaching Threats to Groundwater", *Ecological Modelling*, 30 , p 49-69, 1985.
4. Carsel, R.F., Nixon, W.B., and Ballantine, L.G., "Comparison of Pesticide Root Zone Model Predictions with Observed Concentrations for the Tobacco Pesticide Metalaxyl in Unsaturated Zone Soils", *Environmental Toxicology and Chemistry*, Vol. 5, No. 4, p 345-353, April 1986.
5. Carsel, R.F., Smith, C.N., Mulkey, L.A., Dean, J.D., and Jowise, P.P., "User Manual for Pesticide Root Zone Model (PRZM)", Office of Research and Development, U.S. Environmental Agency, Athens, Georgia, 1984.

6. "EPA Reports Extent of Groundwater Pesticides", Civil Engineering, Vol. 59, March 1989.
7. Cuperus, G. et al., "Wheat Production Calendar", Extension Facts No. 2080, Oklahoma State University, Stillwater, Oklahoma, 1983.
8. Daniels, B.T., "An Evaluation of Methods for Defining the Variability in Pesticide Contamination of Groundwater in Oklahoma", M.S. Thesis Report, Oklahoma State University, Stillwater, Oklahoma, 1988.
9. "Usual Planting and Harvesting Dates", Agricultural Handbook No. 283, U.S. Department of Agriculture, Washington D.C., 1972.
10. Gray, F., and Roozttalab, M.H., "Benchmark and Key Soils of Oklahoma", Agricultural Experiment Station, Oklahoma State University, Stillwater, Oklahoma.
11. Groundwater Newsletter, The. Vol.27, No. 3, p 445, May/June 1989.
12. Hadden, W.J., Jr., and Hadden, S.G., "Expert Systems for Environmental Regulation", IEEE Computer Society, p 558-566, 1985.
13. Hushon, J.M., "Expert systems for Environmental Problems", Environmental Science & Technology, Vol. 21, p 838-841, September 1987.
14. Hushon, J.M., "Expert System for First Responders to Chemical Emergencies", American Chemical Society Annual Meeting, April 1986.
15. Jaffe, M., "Best Management for Point and Non-

- point Sources of Groundwater Contamination",  
School of Urban Planning and Policy, University of  
Illinois, Chicago.
16. Jones, R.L., Black, G.W., and Estes, T.L.,  
"Comparison of Computer Model Predictions with  
Unsaturated Zone Field Data for Aldicarb and  
Aldoxycarb", Environmental Toxicology and  
Chemistry, Vol. 5, No. 12, p 1027-1037, December  
1986.
  17. Ludvigsen, P.J., Simms, R.C., and Grenney, W.J.,  
"Development of a Prototype Expert System for  
Assessing Organic Chemical Mobility and  
Degradation to Determine Soil Treatment  
Requirements", ASCE Fourth Conference on Computing  
in Civil Engineering, ASCE, October 1986.
  18. Pennel, K.D., Hornsby, A.G., Jessup, R.E., and  
Rao, P.S.C., "Evaluation of Five Simulation Models  
for Predicting Aldicarb and Bromide Behavior Under  
Field Conditions", Water Resources Research, Vol.  
26, No. 11, p 2679-2693, November 1990.
  19. Personal Communication, Oklahoma Climatological  
Survey, Norman, Oklahoma, 1988.
  20. Pettyjohn, W.A., White, H., and Dunn, S., " Water  
Atlas of Oklahoma", University Center for Water  
Research, Oklahoma State University, Stillwater,  
Oklahoma, 1983.
  21. Rao, P.S.C., and Davidson, J.M., "Adsorption and  
Movement of Selected Pesticides at High  
Concentrations in Soils", Water Research, Vol. 13,

p 375-380,1979.

22. Sabatine, D.A., and Austin, T.A., "Sorption and Transportation of Pesticides in Ground Water: Critical Review", Journal of Irrigation and Drainage Engineering, Vol. 116, No. 1, February 1990.
23. Schiffman, A., "Groundwater Contamination - A Regulatory Framework", Groundwater, Vol. 26, No. 5, 1988.
24. Shields, D.A., "Agricultural Chemicals in Groundwater: Suggestions for the Environmental Protection Agency Strategy", Journal of Environmental Sciences, The, Vol 30, p 23-27, May/June 1987.
25. Shoemaker, L.L., Magette, W.L., and Shirmohammadi, A., "Modeling Management Practice Effects on Pesticide Movement to Groundwater", Ground Water Monitoring Review , Vol. 10, No. 1, p 109-115, Winter 1990.
26. Goemaat, R.L., Lionel D.M., Ambrose J.M., and Dannie, E.S., "Ground-water Levels in Observation Wells in Oklahoma Period of Records To March 1985", U.S. Geological Survey, Open File Report 86-314, 1986.
27. Williams, J.R., "Sediment Yield Prediction With Universal Equation Using Runoff Energy Factor", USDA-ARS-S-40, Oxford, Mississippi,1975.
28. Wilson, J.L., Mikroudis,G.K., and Fang, H.Y., "GEOTOX: A Knowledge-Based System for Hazardous

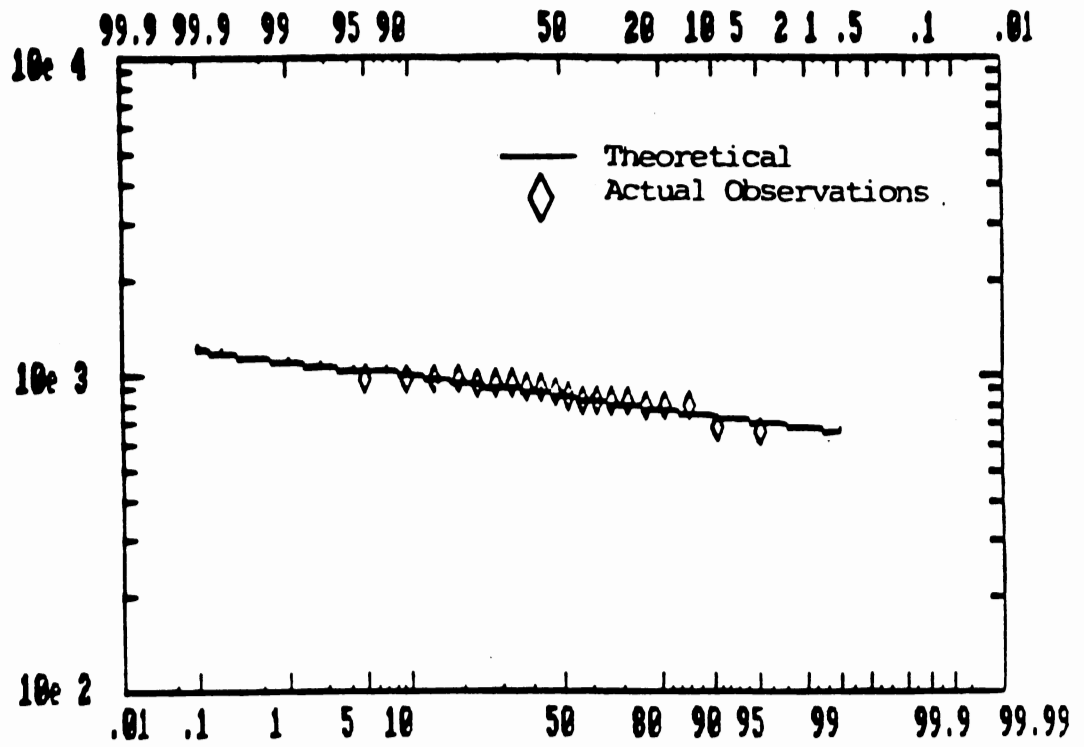
- Waste Site Evaluation", Application of Artificial Intelligence in Engineering Problems, D. Sriram and R. Adey (eds.), Springer-Verlag, April 1986.
29. Wischmeier, W.H. and Smith D.D., "Predicting Rainfall Erosion Losses. A Guide To Conservation Planning", USDA-SEA Agriculture Handbook 537, 1978.
  30. Worthy, W., "Pesticides, Nitrates Found in U.S. Wells", Chemical & Engineering News, Vol. 69, p 46-47, May 6 1991.



**APPENDIXES**

APPENDIX A

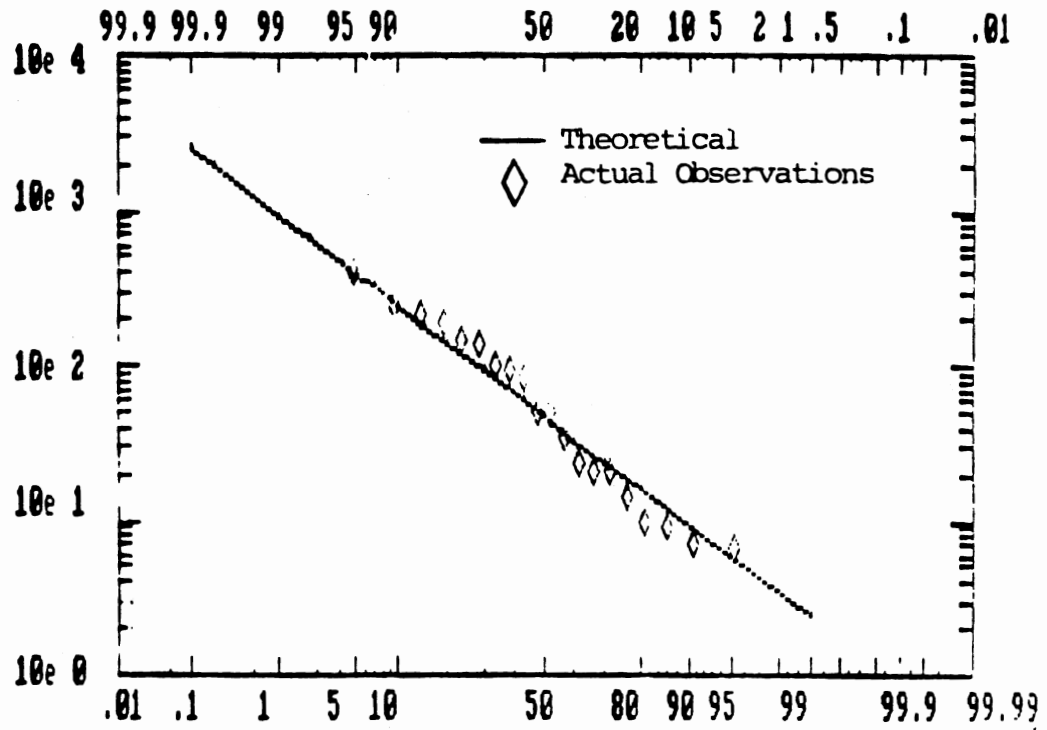
LOG NORMAL PLOTS



X - Probability axis

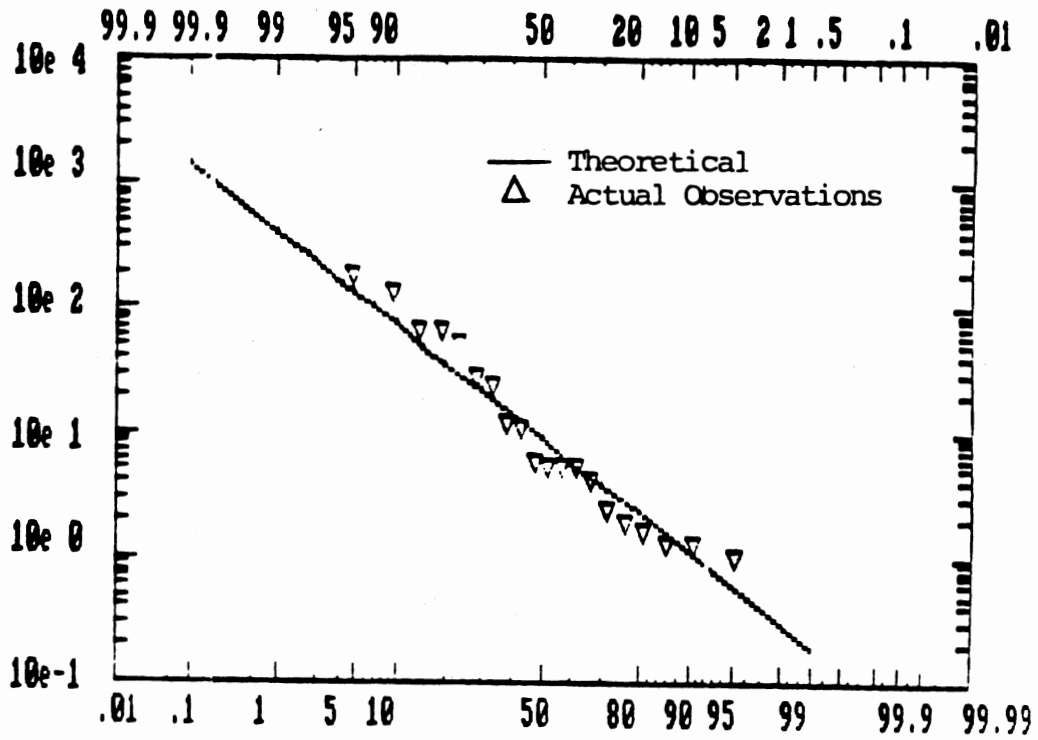
Y - Log of pesticide leached past 30 cm (Kg/Ha)

Log normal Plot for  $CN = 59$ ,  $Ks = 0.001$ , and  $Koc = 2$



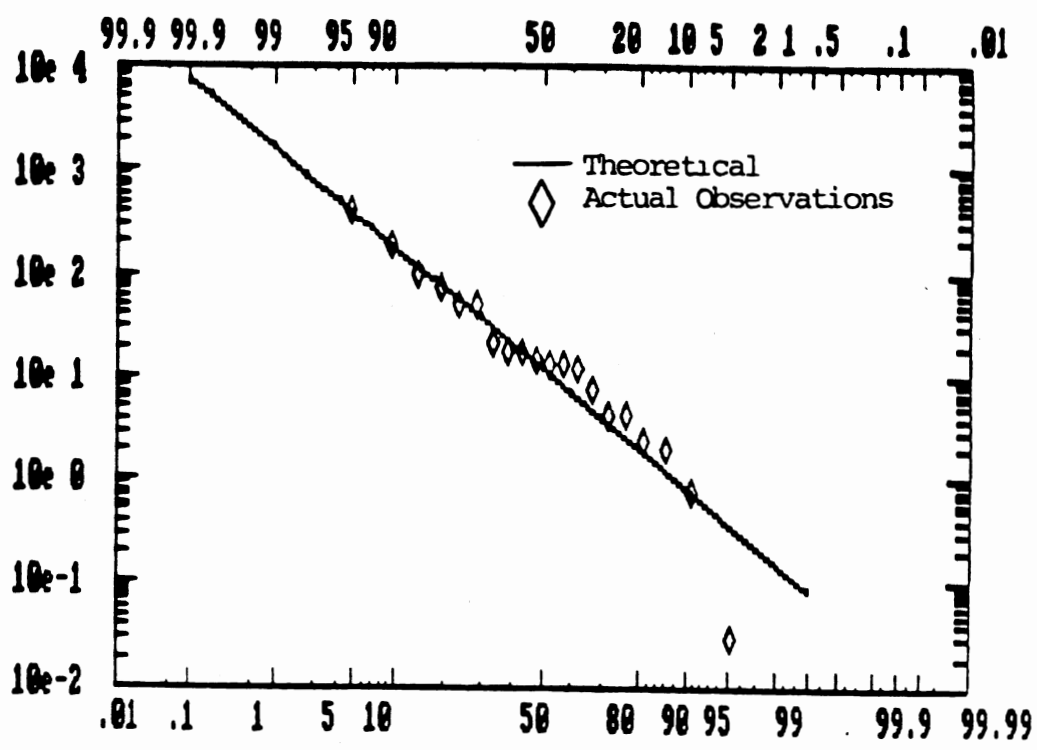
X - Probability axis  
 Y - Log of pesticide leached past 30 cm (Kg/Ha)

Log normal Plot for CN=59, Ks=0.05, and Koc=2

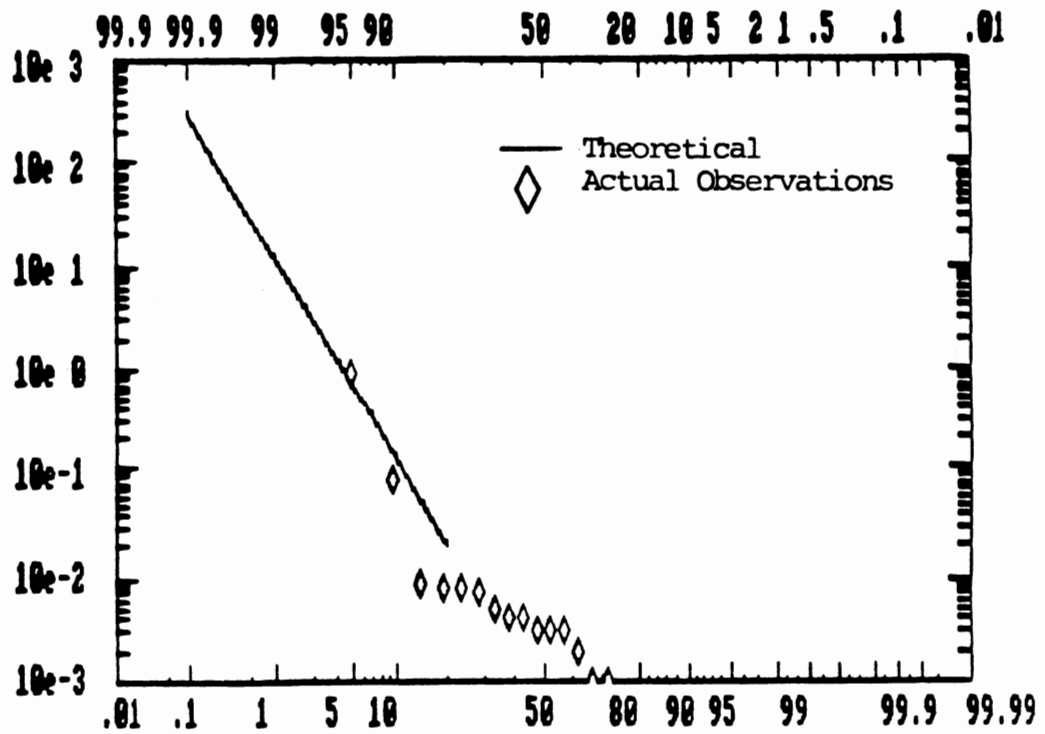


X - Probability axis  
 Y - Log of pesticide leached past 30 cm (Kg/Ha)

Log normal Plot for CN=59, Ks=0.1, and Koc=2



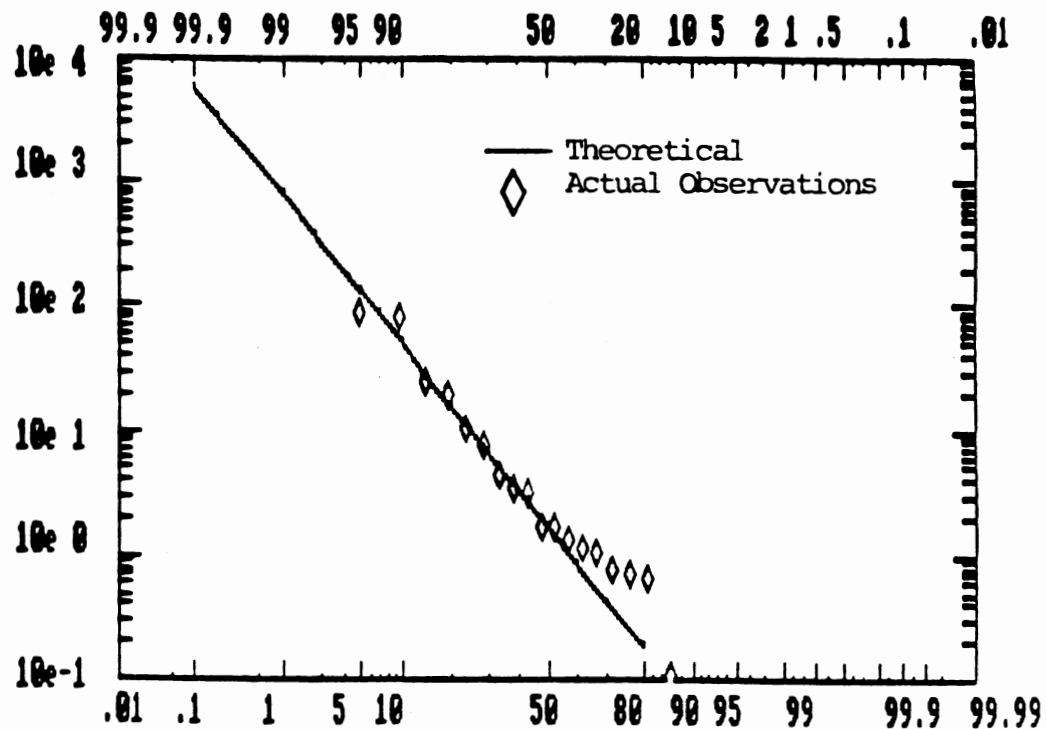
X - Probability axis  
 Y - Log of pesticide leached past 30 cm (Kg/Ha)  
 Log normal Plot for CN=59, Ks=0.001, and Koc=600



X - Probability axis

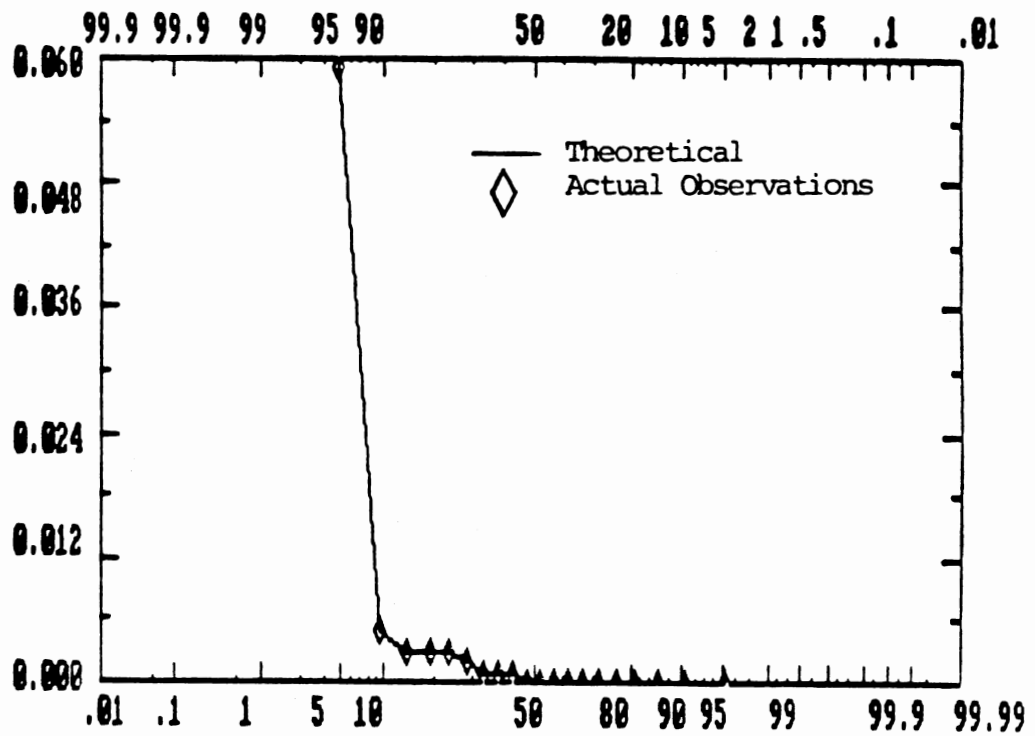
Y - Log of pesticide leached past 30 cm (Kg/Ha)

Log normal Plot for CN=59, Ks=0.05, and Koc=600



X - Probability axis  
 Y - Log of pesticide leached past 30 cm (Kq/Ha)  
 Log normal Plot for CN=59, Ks=0.001, and Koc=1200

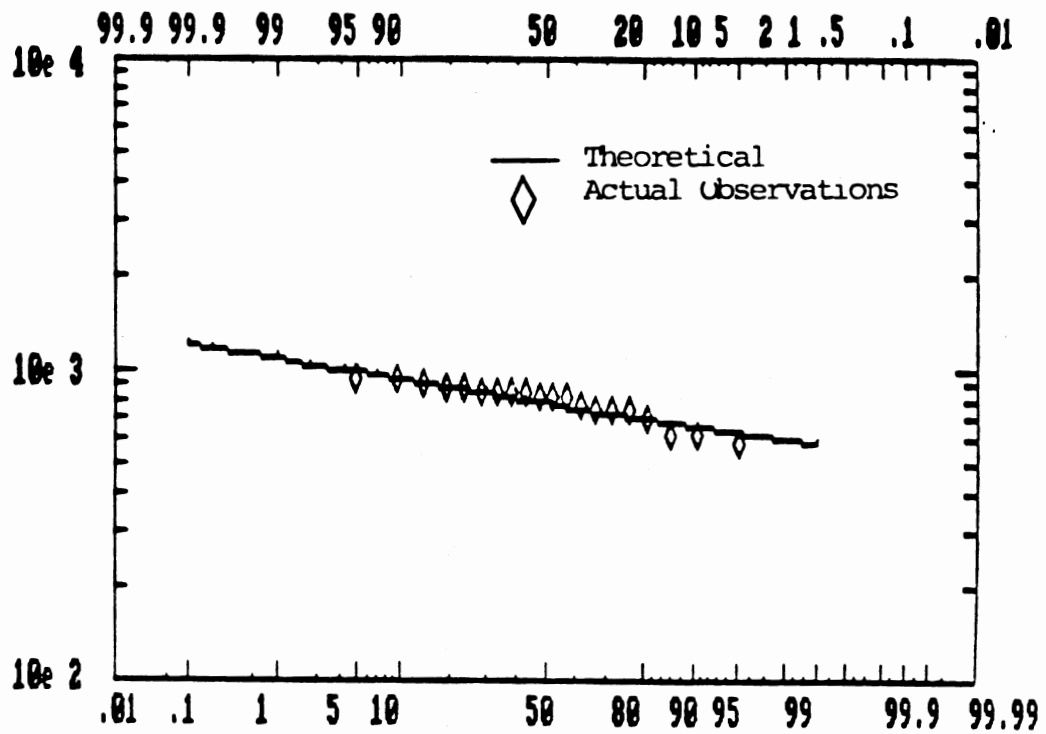




X - Probability axis

Y - Log of pesticide leached past 30 cm (Kg/Ha)

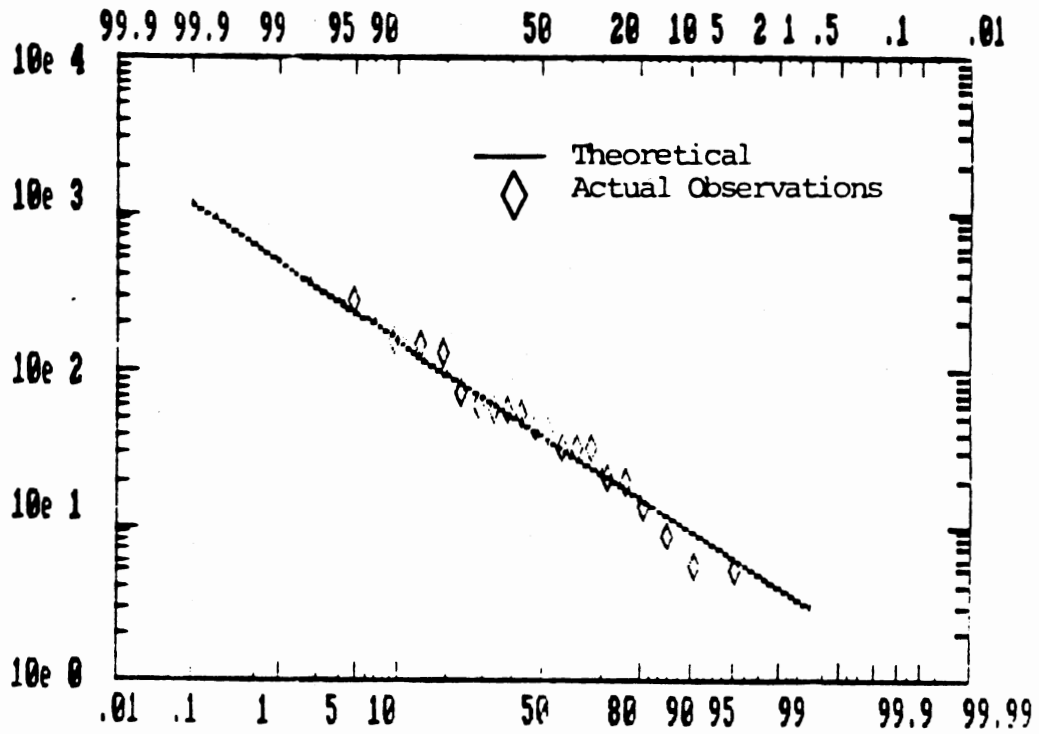
Log normal Plot for  $CN=59$ ,  $Ks=0.05$ , and  $Koc=1200$



X - Probability axis

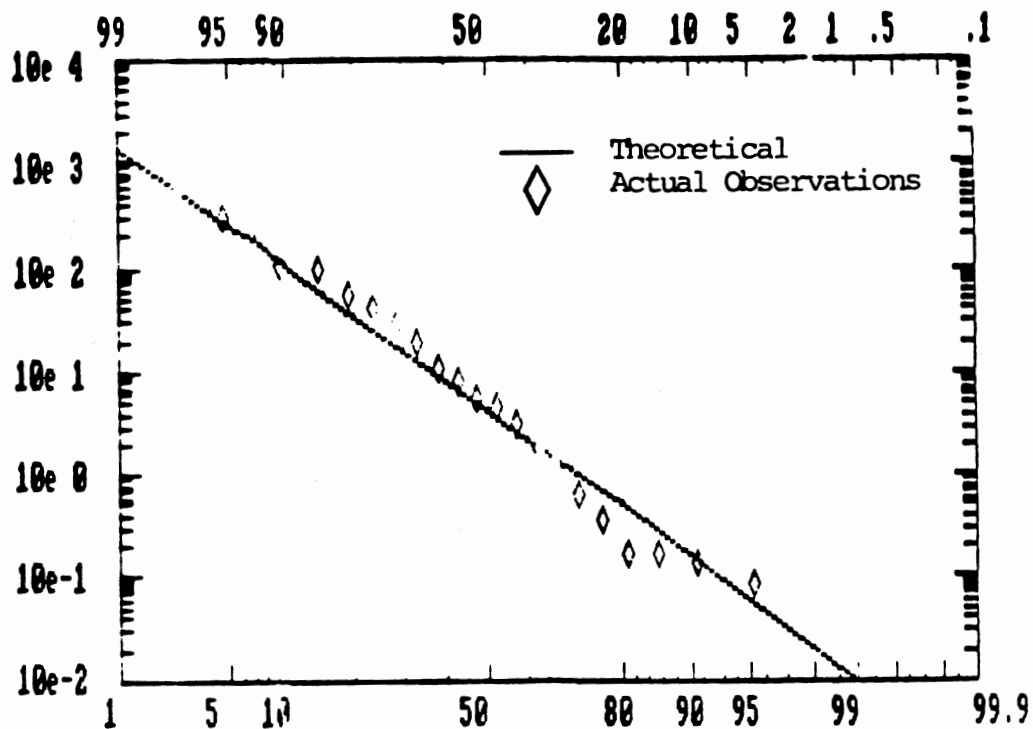
Y - Log of pesticide leached past 30 cm ( Kg/Ha)

Log normal Plot for CN=73, Ks=0.001, and Koc=2



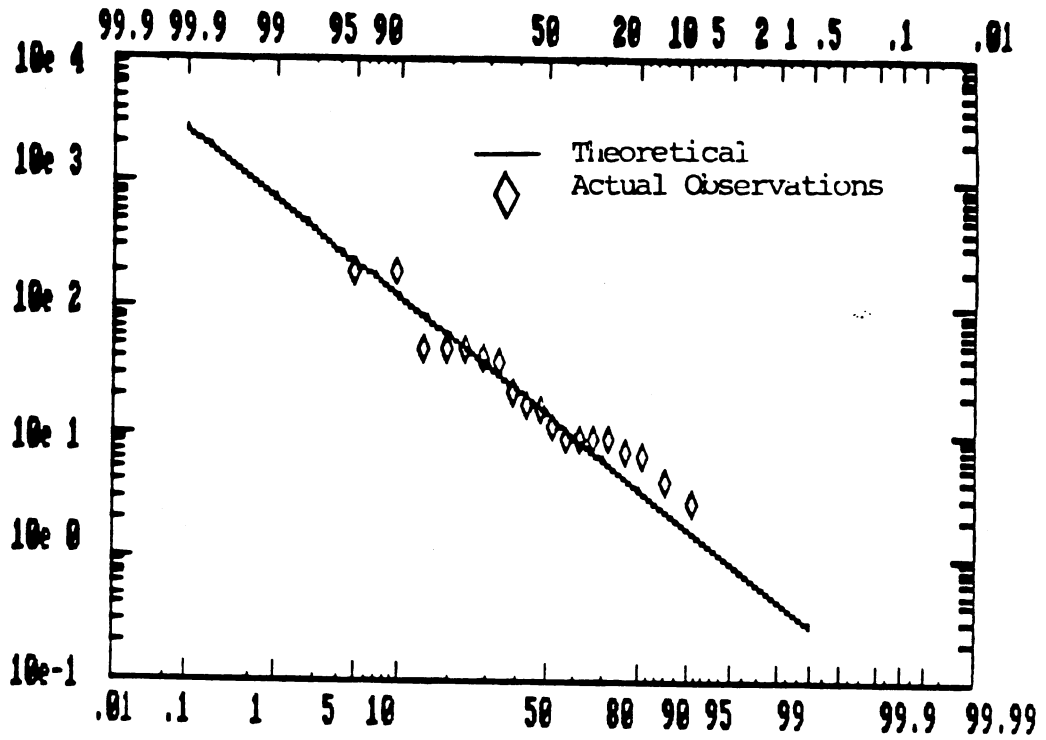
X - Probability axis  
 Y - Log of pesticide leached past 30 cm (Kg/Ha)

Log normal Plot for CN=73, Ks=0.05, and Koc=2



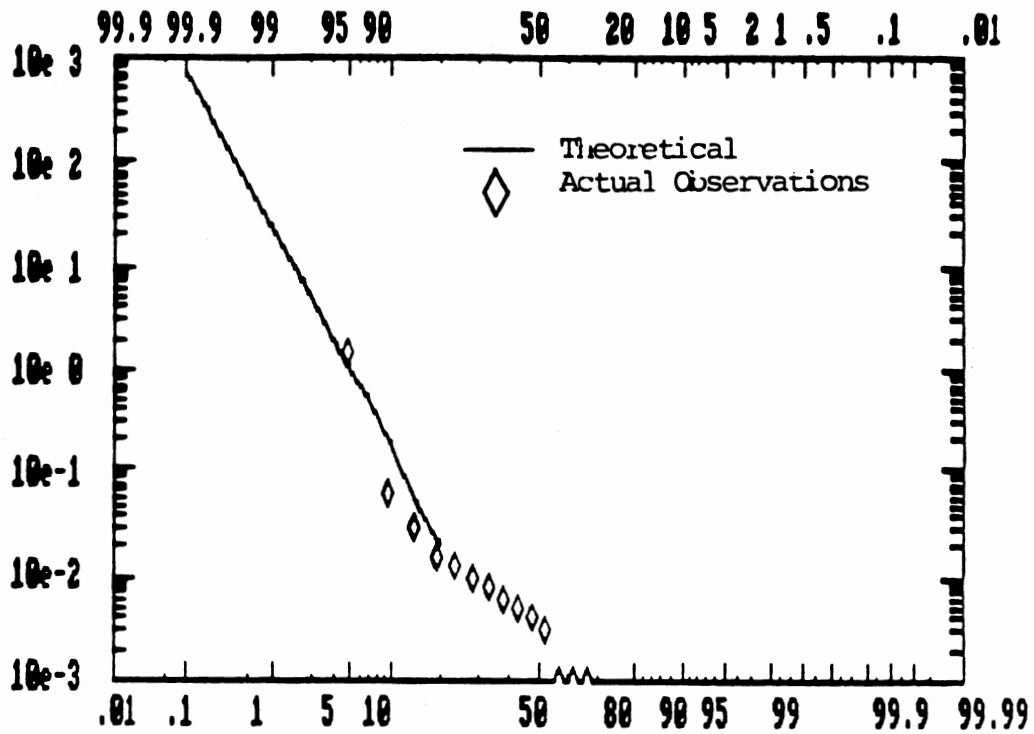
X - Probability axis  
 Y - Log of pesticide leached past 30 cm (Kg/Ha)

Log normal Plot for  $CN=73$ ,  $Ks=0.1$ , and  $Koc=2$



X - Probability axis  
 Y - Log of pesticide leached past 30 cm (Kg/Ha)

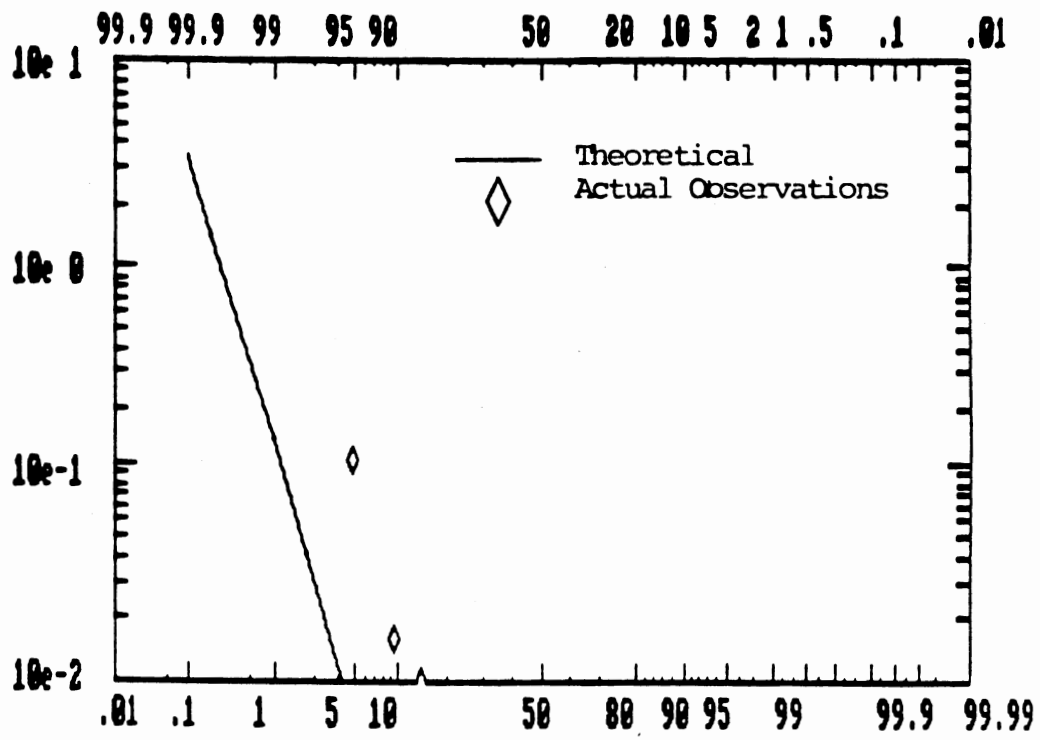
Log normal Plot for CN=73, Ks=0.001, and Koc=600



X - Probability axis

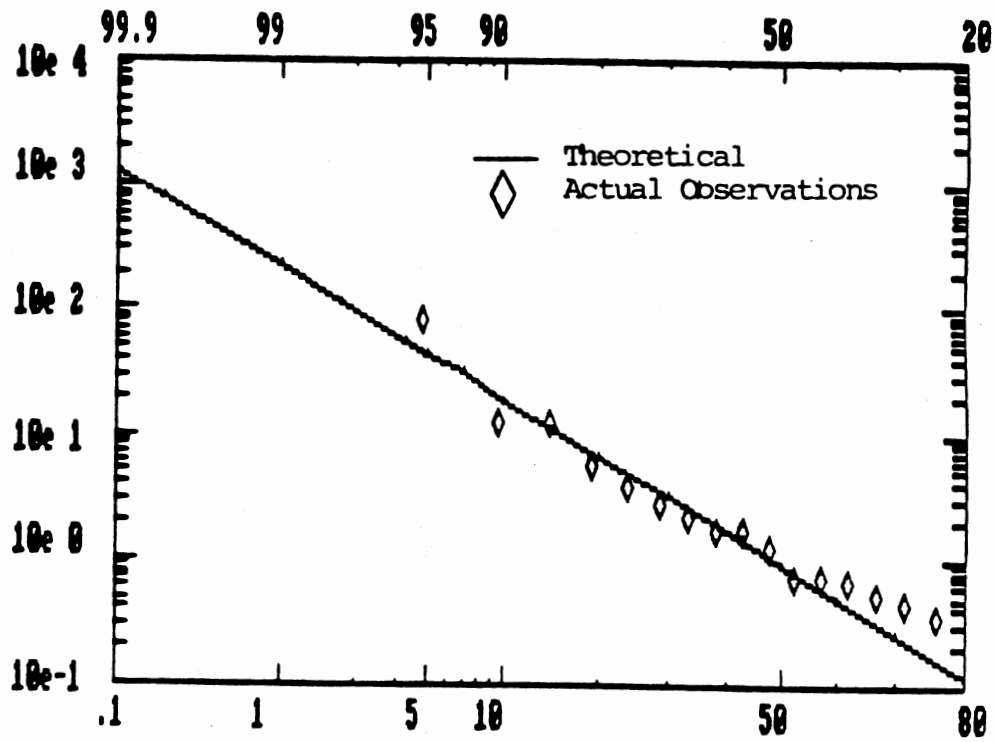
Y - Log of pesticide leached past 30 cm (Kg/Ha)

Log normal Plot for  $CN=73$ ,  $Ks=0.05$ , and  $Koc=600$



X - Probability axis  
 Y - Log of pesticide leached past 30 cm (kg/ha)

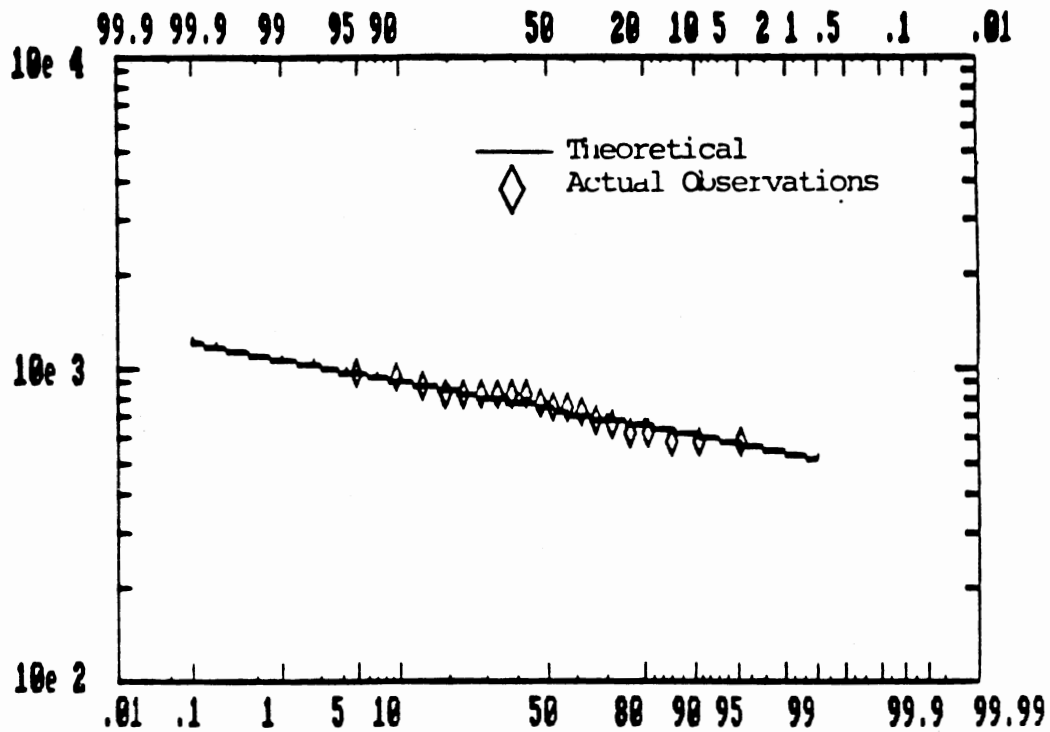
Log normal Plot for CN=73, Ks=0.1, and Koc=600



X - Probability axis  
 Y - Log of pesticide leached past 30 cm (Kg/Ha)

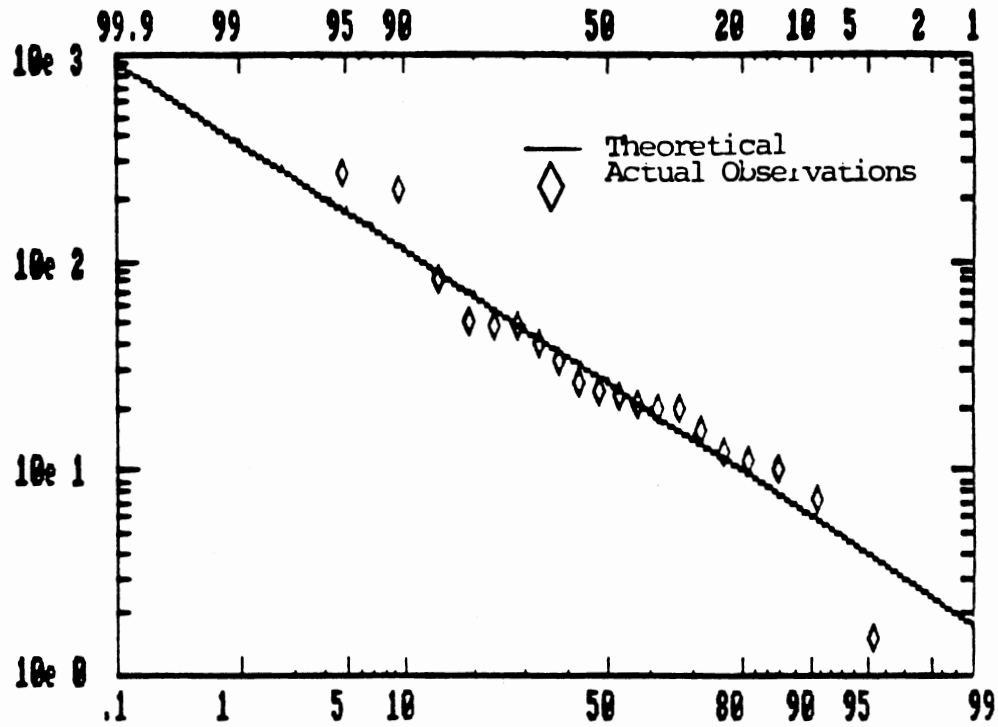
Log normal Plot for CN=73, Ks=0.001, and Koc=1200





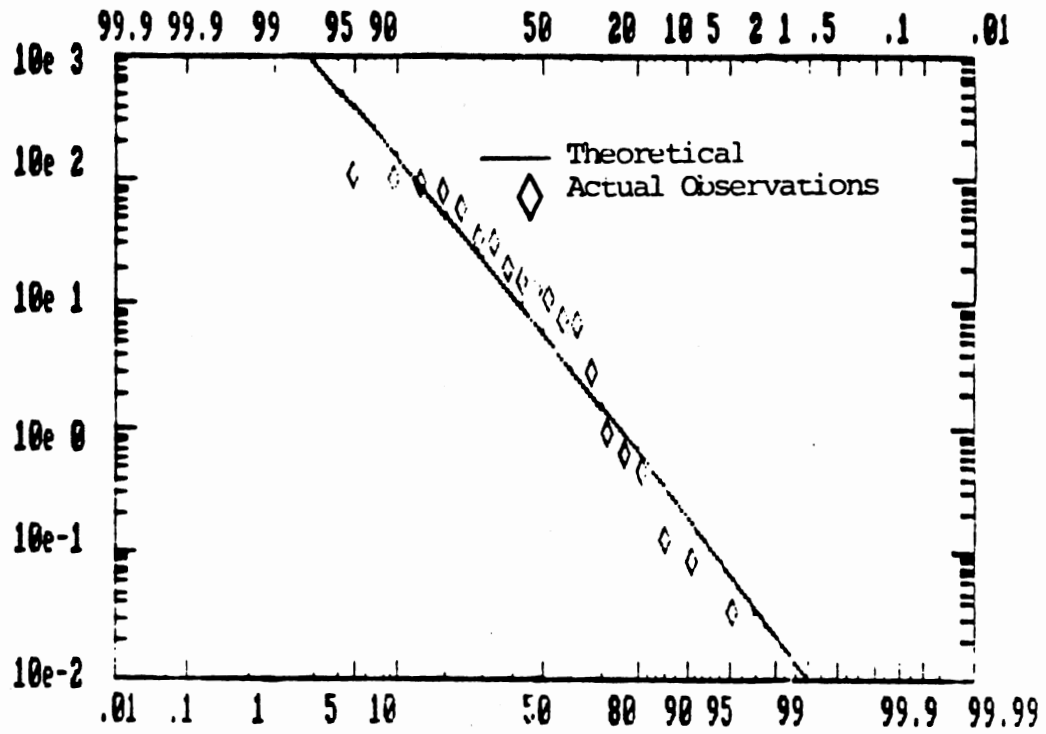
X - Probability axis  
 Y - Log of pesticide leached past 30 cm (Kg/Ha)

Log normal Plot for  $C_V=88$ ,  $K_s=0.001$ , and  $K_{oc}=2$



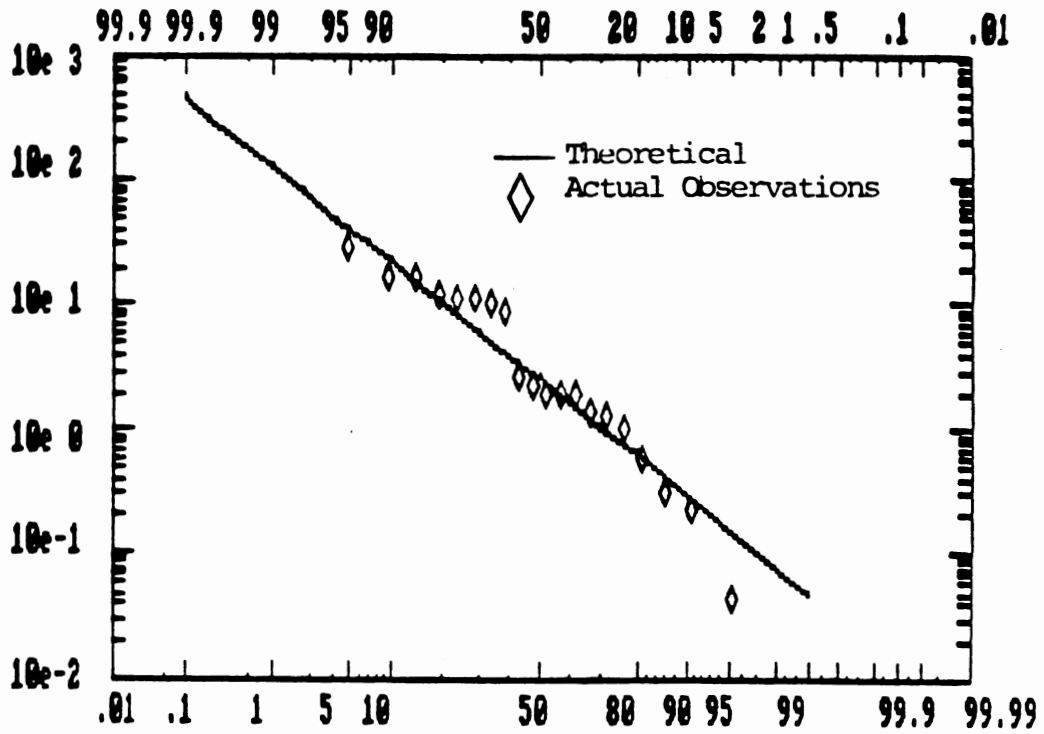
X - Probability axis  
 Y - Log of pesticide leached past 30 cm (Kg/Ha)

Log normal Plot for CN=88, Ks=0.05, and Koc=2



X - Probability axis  
 Y - Log of pesticide leached past 30 cm (Kg/Ha)

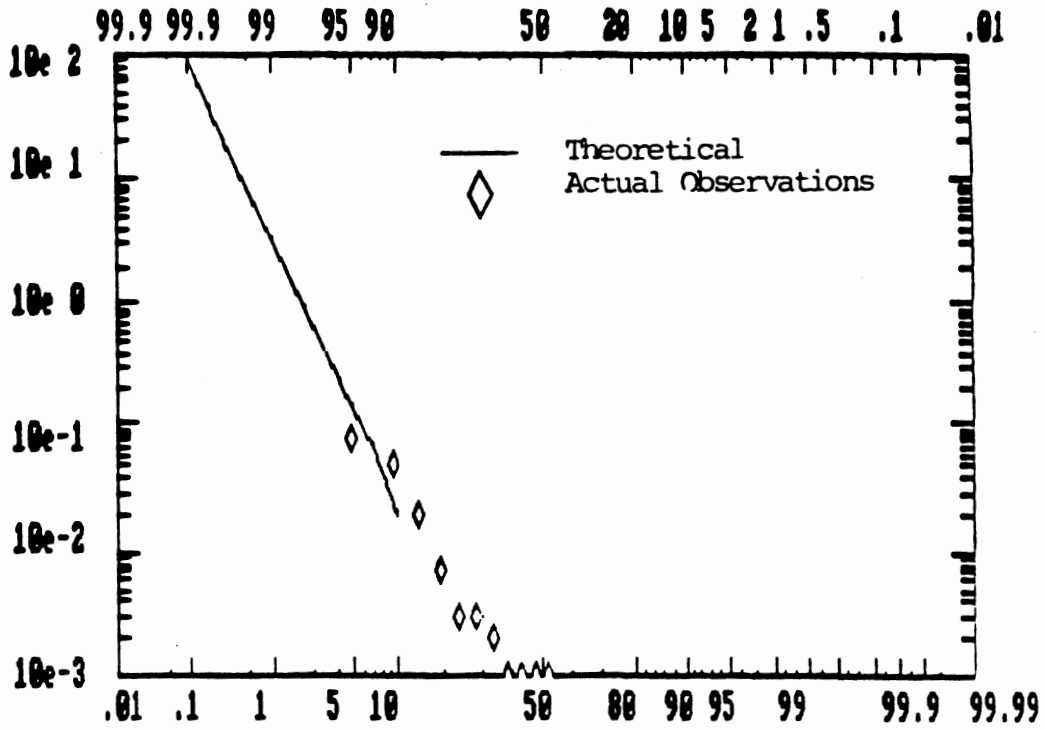
Log normal Plot for CN=88, Ks=0.1, and Koc=2



X - Probability axis

Y - Log of pesticide leached past 30 cm (Kg/Ha)

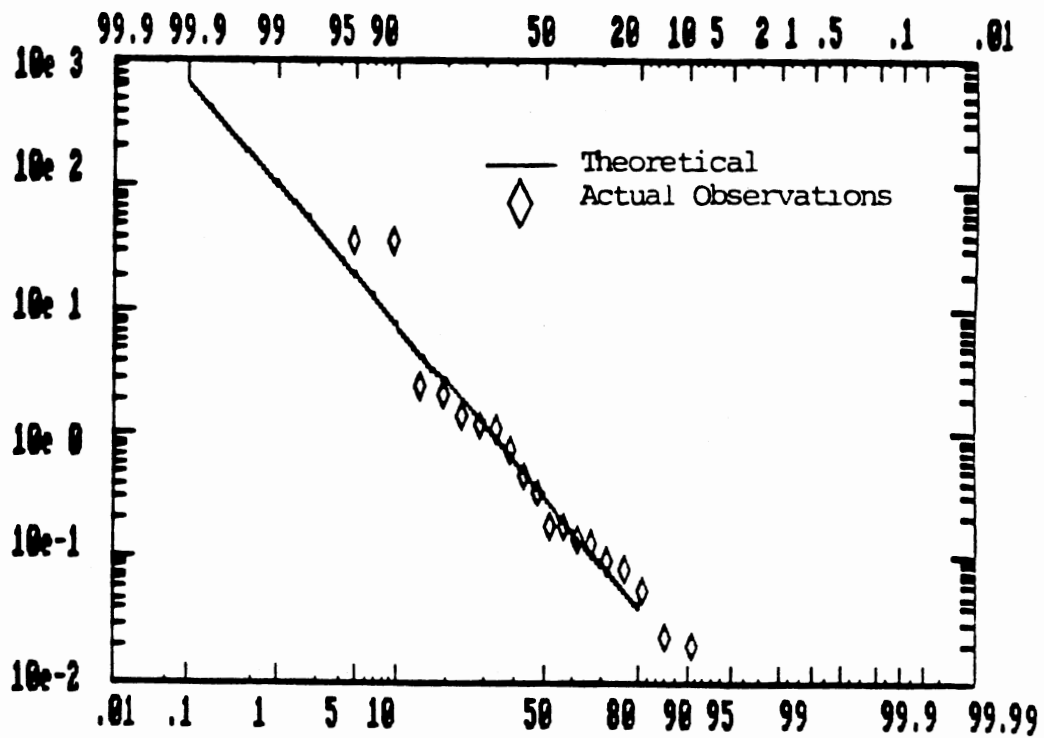
Log normal Plot for CN=88, Ks=0.001, and Koc=600



X - Probability axis

Y - Log of pesticide leached past 30 cm (Kg/Ha)

Log normal Plot for  $CN=88$ ,  $Ks=0.05$ , and  $Koc=600$



X - Probability axis  
 Y - Log of pesticide leached past 30 cm (Kg/Ha)

Log normal Plot for CN=88, Ks=0.001, and Koc=1200

APPENDIX B

COMPLETE SERIES OF GUIDANCE  
SCREENS FOR OPTION 1

**WELCOME TO THE OSU EXPERT SYSTEM  
FOR DETERMINING THE PROBABILITY OF  
PESTICIDE LEACHING IN OKLAHOMA WINTER WHEAT AREAS**

**PRESS ANY KEY TO CONTINUE**



**THIS PROGRAM HAS BEEN DEVELOPED AT  
OKLAHOMA STATE UNIVERSITY  
STILLWATER , OK 74078**

**BY**

**PANKAJ ABORA  
and  
WILLIAM P. McTERNAN**

**PRESS P FOR PREVIOUS SCREEN  
PRESS N FOR NEXT SCREEN**



OSU EXPERT SYSTEM

—ECSYS—

PANNAJ ABORA  
WILLIAM F. McTEMMAN

PRESS P FOR PREVIOUS SCREEN  
PRESS N FOR NEXT SCREEN

THIS EXPERT SYSTEM ACCESSES THE 'VZM1' PROGRAM WRITTEN,  
COMPILED AND RELEASED BY EPA ATHENS LABORATORY. NO MODIFICATIONS  
TO THE PROGRAM WERE MADE. ALL REFERENCES TO MICROSOFT COMPILER  
LICENCE NUMBER ARE TO THE ORIGINAL AGREEMENTS BETWEEN 'EPA' AND MICROSOFT.

PRESS P FOR PREVIOUS SCREEN  
PRESS N FOR NEXT SCREEN

THER ARE TWO OPTIONS FOR USER TO RUN THIS SOFTWARE :

1. USE EXISTING DATA
2. START NEW SIMULATIONS

THE RECOMMENDED PROCEDURE IS TO PERFORM AN INITIAL ANALYSIS WITH THE EXISTING DATA. SHOULD THE USER WISH TO PURSUE A MORE RIGOROUS SOLUTION THE SECOND OPTION IS RECOMMENDED.

PRESS P FOR PREVIOUS SCREEN  
PRESS N FOR NEXT SCREEN

FOR OPTION ONE, THE DATA REQUIRED ARE TAKEN FROM THE WORK OF B.T.DANIELS (M.S. THESIS, OKLAHOMA STATE UNIVERSITY) AND INVOLVES MONTE CARLO SIMULATIONS.

FOR THIS EFFORT EQUATIONS DESCRIBING THE  $c_{ij}$ 's OF THE OUTPUTS WERE DEVELOPED AND ARE ACCESSED TO PROVIDE CURRENT RESULTS. A LINEAR INTERPOLATION IS PROVIDED FOR THOSE CONDITIONS WHERE THE USER SPECIFIES INTERMEDIATE REQUIREMENTS.

PRESS P FOR PREVIOUS SCREEN  
PRESS N FOR NEXT SCREEN

THIS PROGRAM UTILIZES A 25 YEAR METEOROLOGICAL DATA SUPPLIED  
BY THE OKLAHOMA CLIMATOLOGICAL SURVEY LOCATED IN NORMAN, OKLAHOMA.  
THE YEARS 1954-1978 WERE SELECTED TO UTILIZE CONTINUOUS, OVERLAPPING  
RECORDS AVAILABLE AT ALL TYPE 1 STATIONS IN THE STATE. SOME PROBLEMS  
HAVE BEEN OBSERVED WHEN LONG PERIODS OF MISSING DATA ARE ENCOUNTERED  
BY THE CODE. SHOULD THE USER EXPERIENCE SUCH TROUBLES, PLEASE CONTACT  
THE 'OCS' TO DEVELOP THE MOST APPROPRIATE RESPONSE TO MISSING DATA.

PRESS P FOR PREVIOUS SCREEN  
PRESS N FOR NEXT SCREEN

**IN OPTION ONE, THE USER WILL BE ASKED TO PROVIDE :**

- a. SCS CURVE NUMBER ( CN )**
- b. FIRST ORDER PESTICIDE DECAY COEFF. (  $K_d$  )**
- c. SOIL-ORGANIC CARBON DIST. COEFF. (  $K_{oc}$  )**

**THIS PORTION OF THE EFFORT LIMITS THE CN SELECTION RANGE TO 59-86,  $K_d$  TO 0.001 TO 0.1, AND  $K_{oc}$  TO 2 TO 1200. GUIDANCE FOR THE SELECTION OF THESE PARAMETERS IS PROVIDED WITH IN THE CODE.**

**PRESS P FOR PREVIOUS SCREEN  
PRESS N FOR NEXT SCREEN**

**OPTION 1. EXISTING DATA**

**NOTE : INSTANTANEOUS RESULTS**

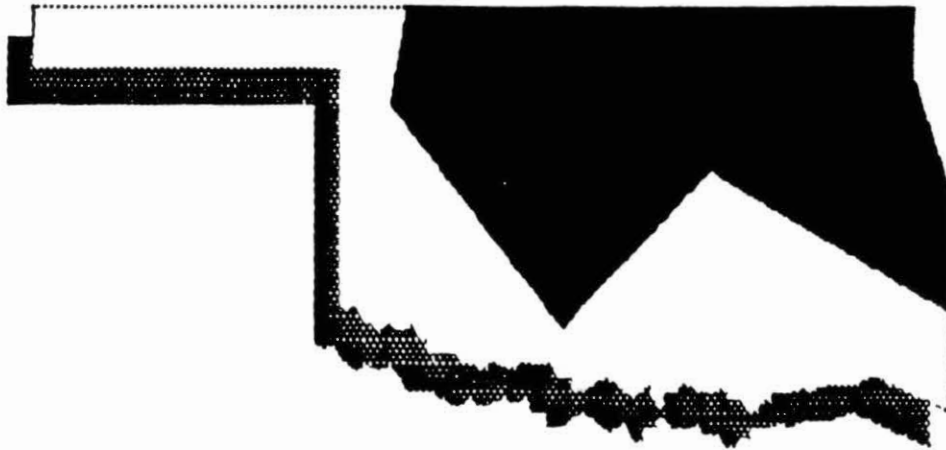
**OPTION 2. NEW SIMULATIONS**

**NOTE : WILL TAKE HOURS**

**SELECT THE OPTION (1/2) = ? 1**

**PRESS P FOR PREVIOUS SCREEN  
PRESS N FOR NEXT SCREEN**





 YELLOW AREA REPRESENTS REGION SELECTED FOR SIMULATION

PRESS P FOR PREVIOUS SCREEN  
PRESS N FOR NEXT SCREEN

THE SELECTION RANGE FOR RES CURVE NUMBER (CN) IS FROM 59 TO 88

DO YOU NEED HELP FOR SELECTING (CN) ? (Y/N)

**NEXT FIVE SCREENS ARE DEVELOPED TO HELP SELECT THE VALUE  
OF PARAMETER CURVE NUMBER (CN)**

**THE CURVE NUMBERS (CN) DEVELOPED BY SOIL CONSERVATION SERVICES  
CHARACTERIZE SOILS ON THE BASIS OF INFILTRATION PROPERTIES.  
THERE ARE FOUR DIFFERENT HYDROLOGIC SOIL GROUPS (A, B, C, and D)  
AND ARE IN ORDER OF DECREASING PERCOLATION POTENTIAL.**

**PRESS P FOR PREVIOUS SCREEN  
PRESS N FOR NEXT SCREEN**

**SOIL CHARACTERISTICS ASSOCIATED WITH EACH HYDROLOGIC GROUPS ARE  
AS FOLLOWS :**

**GROUP A : DEEP SAND, DEEP LOESS, AGGREGATED SILTS. MINIMUM  
INFILTRATION OF 0.76 - 1.14 cm/hr .**

**GROUP B : SHALLOW LOESS, SANDY LOAM, MINIMUM INFILTRATION  
0.38 - 0.76 cm/hr .**
















**GROUP C : CLAY LOAMS, SHALLOW SANDY LOAM, SOILS LOW IN ORGANIC  
CONTENTS, AND SOILS USUALLY HIGH IN CLAY, MINIMUM  
INFILTRATION 0.13 - 0.38 cm/hr .**

**GROUP D : SOILS THAT SWELL SIGNIFICANTLY WHEN WET, HEAVY PLASTIC  
CLAYS, AND CERTAIN SALINE SOILS. MINIMUM INFILTRATION  
0.03 - 0.13 cm/hr .**

**PRESS P FOR PREVIOUS SCREEN  
PRESS N FOR NEXT SCREEN**

DO YOU WANT TO SELECT SOIL TYPE FROM SOIL DISTRIBUTION MAP ? (Y/N) ?

**SOIL DISTRIBUTION MAP FOR REGION SELECTED IN SIMULATION**

-  (1) BETWYV
-  (2) CLARKSVILLE
-  (3) DENNIS
-  (4) DOUGHERTY
-  (5) EUPAULA
-  (6) HARTSELL
-  (7) PARSONS
-  (8) POND CREEK
-  (9) QUINLAN
-  (10) REMFROV
-  (11) St. PAUL
-  (12) STEPHENVILLE
-  (13) SUMMIT
-  (14) TIVOLI
-  (15) YAHOLA



TYPE THE NUMBER CORRESPONDING TO SOIL = ? 

**THE SOIL TYPE FOR CURRENT SIMULATION IS : CLARKSVILLE**

**THE HYDROLOGIC GROUP OF THIS SOIL IS - B**

**DO YOU WANT TO CHANGE THE SOIL SELECTED ? (Y/N) ?**

TO MAKE FINAL SELECTION OF 'CN' SOME ADDITIONAL INFORMATION IS NEEDED. A TABLE HAS BEEN PROVIDED ON NEXT SCREEN TO ASSIST IN PROVIDING THIS INFORMATION. PLEASE, FOLLOW THE PROCEDURE MENTIONED BELOW :

1. FROM TABLE FIND THE LAND USE AND TREATMENT OR PRACTICES THAT IS TO BE SIMULATED (e.g. ROW CROPS, STRAIGHT ROW) .
2. FROM TABLE FIND THE HYDROLOGIC CONDITION OF THE SOIL THAT IS TO BE SIMULATED (e.g. GOOD) .
3. FROM THE TABLE FIND THE ' CN ' FOR ABOVE SELECTED CONDITIONS

EXAMPLE : HYDROLOGIC GROUP = A  
TREATMENT PRACTICE IS STRAIGHT ROW  
LAND USE IS ROW CROPS  
HYDROLOGIC CONDITION IS GOOD

THE CURVE NUMBER IS 67

PRESS P FOR PREVIOUS SCREEN  
PRESS N FOR NEXT SCREEN



COVER			HYDROLOGIC GROUP			
LAND USE	TREATMENT/PRACTICE	HYDROLOGIC CONDITION	A	B	C	D
FALLOW	STRAIGHT ROW	-----	77	86	91	94
ROW CROPS	STRAIGHT ROW	POOR	72	78	85	91
	STRAIGHT ROW	GOOD	67	78	85	89
	CONTOURED	POOR	70	79	84	88
	CONTOURED	GOOD	65	75	82	86
	CONTOURED & TERRACED	POOR	66	74	80	82
	CONTOURED & TERRACED	GOOD	62	71	78	81
TYPE THE VALUE OF CN = ? ? ?						

THE SELECTION RANGE FOR DECAY COEFFICIENT ( $\lambda_n$ ) IS FROM 0.1 TO 0.001

DO YOU NEED HELP FOR SELECTING ( $\lambda_n$ ) ? (Y/N)

NEXT TWO SCREENS ARE DEVELOPED TO HELP SELECT THE VALUE  
OF PARAMETER DECAY COEFFICIENT ( $K_d$ ).

THE PROCESSES THAT CONTRIBUTE TO PESTICIDE DISAPPEARANCE IN SOILS  
ARE VARIED AND DEPEND ON ENVIRONMENTAL FACTORS AS WELL AS CHEMICAL  
PROPERTIES. TO BE ACCURATE,  $K_d$  SHOULD BE INDEPENDENT OF ALL SOIL  
AND CLIMATIC FACTORS. IN THE TABLE ON NEXT SCREEN,  $K_d$  VALUES ARE  
AT BEST ONLY ESTIMATES.  $K_d$  IS ASSUMED TO BE FIRST-ORDER RATE CONSTANT.

PRESS P FOR PREVIOUS SCREEN  
PRESS N FOR NEXT SCREEN

PESTICIDE	K <sub>s</sub>
ATRAZINE	0.0063
CARBOPHTHIN	0.0049
2,4- D	0.1036
DICAFEN	0.0151
DISULFOTON	0.1184
DIURON	0.0064
MALATHION	0.4152
METHYL PARATHION	0.0165
PRATHION	0.0046
PROPACINE	0.0056
TRIFLURALIN	0.0026

TYPE THE VALUE OF K<sub>s</sub> = 7 0.0063

PRESS P FOR PREVIOUS SCREEN  
PRESS N FOR NEXT SCREEN

THE SELECTION RANGE FOR ORGANIC-CARBON DISTRIBUTION COEFF. (K<sub>oc</sub>) IS FROM  
2 TO 1200

DO YOU NEED HELP FOR SELECTING (K<sub>oc</sub>) ? (Y/N)

NEXT TWO SCREENS ARE DEVELOPED TO HELP SELECT THE VALUE  
OF PARAMETER ORGANIC-CARBON DIST. COEFF.

THE FATE OF PESTICIDES IN SOIL AND WATER IS HIGHLY DEPENDENT ON THE  
SORPTIVE CHARACTERISTICS OF THE COMPOUND. THE SORPTIVE PROPERTIES  
OF PESTICIDES GENERALLY CORRELATE WELL WITH THE ORGANIC CONTENT OF  
SOILS. PARAMETER  $K_{oc}$  DESCRIBES THE AMOUNT OF PESTICIDES WHICH CAN  
BE ADSORBED IN THE SOIL ON ORGANIC MATTER.

PRESS P FOR PREVIOUS SCREEN  
PRESS N FOR NEXT SCREEN

PESTICIDE	Koc
ATRAZINE	173.78
CARBOFLUTHIN	169.82
2,4- D	398.11
DICAMBA	1.86
DISULFOTON	1687.88
DIFURON	392.11
MALATHION	478.63
METHYL PARATHION	1288.25
PARATHION	3981.87
PROPACINE	573.83
TRIFLURALIN	34,673.69

TYPE THE VALUE OF Koc = 7 173.78

PRESS P FOR PREVIOUS SCREEN  
PRESS N FOR NEXT SCREEN

THE VALUES SELECTED FOR DIFFERENT PARAMETERS ARE :

THE CURVE NUMBER (CN) FOR CURRENT SIMULATION IS = 71

THE DECAY COEFFICIENT ( $K_d$ ) FOR CURRENT SIMULATION IS = .0063

THE ORG. CARBON DISY. COEFF. ( $K_{oc}$ ) FOR CURRENT SIMULATION IS = 173.70

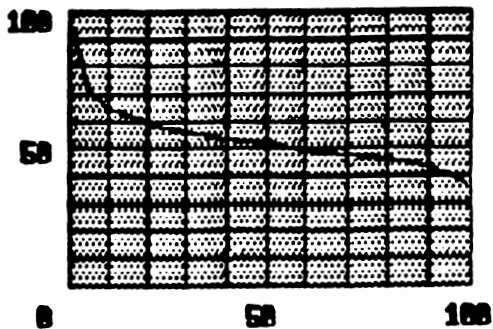
DO YOU WANT TO CHANGE THE VALUES ? (Y/N) ?



**PROBABILITY      % LEACHED**

99	37.63881
98	43.25872
88	45.9856
78	47.96144
68	49.83641
58	51.789
48	53.73416
38	56.13835
28	59.25596
18	65.85153
5	71.63814
1	94.38249

**PLOT BETWEEN PERCENT OF PESTICIDE LEACHED  
AND PERCENT OF TIME EXCEEDED**



**X-AXIS - PERCENT OF PESTICIDE LEACHED  
Y-AXIS - PERCENT OF TIME EXCEEDED**

CM = 71  
 Ks = .8863  
 Koc = 173.78

**DO YOU WANT TO RUN THE PROGRAM AGAIN ? (Y/N) ? █**

APPENDIX C

COMPLETE SERIES OF GUIDANCE  
SCREENS FOR OPTION 2

PESTICIDE ROOT ZONE MODEL (PRZM) IS BEING USED FOR THIS OPTION.  
USER IS GOING TO CREATE INPUT FILE TO RUN PRZM. GUIDANCE IS PROVIDED  
FOR SELECTION OF MOST OF THE PARAMETERS. THE INFORMATION ABOUT PARAMETERS  
IS TAKEN FROM PRZM USER MANUAL. USER IS REQUESTED TO LOOK AT USER MANUAL  
IF MORE INFORMATION IS DESIRED ABOUT SELECTION OF PARAMETERS.

PRESS P FOR PREVIOUS SCREEN  
PRESS N FOR NEXT SCREEN

PAN FACTOR IS A DIMENSIONLESS NUMBER. THIS FACTOR IS MULTIPLIED BY DAILY PAN EVAPORATION TO ESTIMATE DAILY EVAPOTRANSPIRATION (ET). IF DAILY AIR TEMPERATURES ARE USED FOR 'ET', ANY DUMMY NUMBER CAN BE INPUT (e.g. 0.75) .

THE SELECTION RANGE FOR PAN FACTOR IS FROM 0.6 TO 1.0 .

THE RANGE FOR OKLAHOMA IS FROM 0.69 TO 0.72.

TYPE THE VALUE OF PAN FACTOR ? 0.71

PRESS P FOR PREVIOUS SCREEN  
PRESS N FOR NEXT SCREEN

SNOW FACTOR,  $\text{cm snowmelt/deg. c}$  above freezing. VALUES OF  
SNOW FACTOR ARE IN THE ORDER OF 0.45 . IF SNOWMELT IS NOT  
CALCULATED, ENTER 0.88 .

WHEN THE MEAN AIR TEMPERATURE FALLS BELOW 0.0 deg. C,  
ANY PRECIPITATION THAT FALLS IS CONSIDERED TO BE IN THE FORM  
OF SNOW. WHEN THE MEAN AIR TEMPERATURE IS ABOVE 0.0 deg. C .  
HOWEVER , THE SNOW ACCUMULATION IS DECREASED BY A SNOWMELT FACTOR.  
THE SELECTION RANGE FOR SNOW FACTOR IS FROM 0.0 TO 1.0 .  
TYPE THE VALUE OF SNOW FACTOR ? 0.1

PRESS P FOR PREVIOUS SCREEN  
PRESS N FOR NEXT SCREEN

PAN EVAPORATION FLAG. IF THIS FLAG IS SET TO BE 0, PAN  
EVAPORATION DATA ARE READ. IF SET EQUAL TO 1, TEMPERATURE DATA  
ARE READ AND USED TO CALCULATE POTENTIAL 'ET'. IF SET EQUAL TO 2,  
THEN PAN EVAPORATION , IF AVAILABLE, IS USED IN THE METEOROLOGIC  
FILE; IF NOT, TEMPERATURE IS USED TO COMPUTE POTENTIAL 'ET'.

SUGGESTED VALUE FOR THIS FLAG IS 2.

TYPE THE VALUE OF PAN EVAPORATION FLAG ? 2

PRESS P FOR PREVIOUS SCREEN  
PRESS N FOR NEXT SCREEN

THE MINIMUM DEPTH, cm , IN WHICH EVAPORATION IS EXTRACTED  
YEARLY ( e.g. 20.0 ) .

	<small>cm</small>
MINIMUM	10.000
MAXIMUM	35.000

TYPE THE MINIMUM DEPTH ? 10

PRESS P FOR PREVIOUS SCREEN  
PRESS N FOR NEXT SCREEN

**THE CONDITION OF SURFACE AFTER HARVEST :**

<b>FALLOW</b>	<b>1</b>
<b>CROPPING</b>	<b>2</b>
<b>RESIDUE</b>	<b>3</b>

**TYPE THE NUMBER CORRESPONDING TO CONDITION AFTER HARVEST ? 1**

**PRESS P FOR PREVIOUS SCREEN  
PRESS N FOR NEXT SCREEN**



WOULD YOU LIKE TO CONSIDER THE EROSION LOSSES (Y/N) ? ■

MAXIMUM INTERCEPTION STORAGE OF THE CROP (cm). THIS PARAMETER ESTIMATES THE AMOUNT OF RAINFALL THAT IS INTERCEPTED BY A FULLY DEVELOPED PLANT AND RETAINED ON THE PLANT SURFACE. VALUES FOR MAJOR CROPS ARE PROVIDED IN THE TABLE ON THE NEXT SCREEN.

PRESS P FOR PREVIOUS SCREEN  
PRESS N FOR NEXT SCREEN

CROP	DENSITY	INTERCEPTION (cm)
CORN SOYBEANS WHEAT OATS BARLEY POTATOES PEANUTS COTTON TOBACCO	HEAVY MODERATE LIGHT LIGHT LIGHT LIGHT LIGHT MODERATE MODERATE	0.25-0.30 0.20-0.25 0.0-0.15 0.0-0.15 0.0-0.15 0.0-0.15 0.0-0.15 0.20-0.25 0.20-0.25
TYPE THE VALUE FOR MAX. INTERCEPTION = ? 0.15		
PRESS P FOR PREVIOUS SCREEN PRESS N FOR NEXT SCREEN		

MAXIMUM ACTIVE ROOT DEPTH OF THE CROP (cm) MEASURED FROM THE  
LAND SURFACE. GENERALIZED INFORMATION FOR CORN, SOYBEANS, WHEAT,  
TOBACCO, GRAIN BORCHUM, POTATOES, PEANUTS, AND COTTON ARE PROVIDED  
IN TABLE ON NEXT TWO SCREENS.

PRESS P FOR PREVIOUS SCREEN  
PRESS N FOR NEXT SCREEN

CROP	MAJOR STATES PRODUCTION	RANGE OF ROOT DEPTH (in)
CORN	IA, IL, IN, MI, OH	60-120
SOYBEANS	IA, IL, IN, MS, OH	30-60
COTTON	TX, MS, CA, AZ, AR	30-90
WHEAT	KS, OK, CA, ND, MT WA, TN, ID	15-30
TYPE THE MAX. ACTIVE ROOTING DEPTH = ? 15		
DO YOU WANT TO GO TO PREVIOUS OR NEXT SCREEN (P/N) ? <input type="checkbox"/>		

THERE ARE TWO OPTIONS FOR THE APPLICATION OF PESTICIDE :

1. APPLICATION TO SOIL ONLY

2. FOLIAR APPLICATION USING LINEAR NOZZEL

TYPE THE OPTION FOR PESTICIDE APPLICATION (1/2) = 1 1

PRESS P FOR PREVIOUS SCREEN  
PRESS N FOR NEXT SCREEN

TYPE THE DEPTH OF TEST. INCORPORATION IN CR. (IF BROADCAST THEN 8) = ? 18

PRESS P FOR PREVIOUS SCREEN  
PRESS N FOR NEXT SCREEN

THE PARAMETER MAX. AREAL COVERAGE OF THE CROP AT FILL GANOPY  
ESTIMATES THE GROUND COVER AS THE CROP GROWS TO SOME MAXIMUM VALUE.  
IT DETERMINES THE FRACTION OF GROUND COVER AFFORDED BY THE CROP AND  
THIS INFLUENCES THE MASS OF PESTICIDE THAT REACHES THE GROUND.

TYPE THE VALUE OF MAX. AREAL COVERAGE (x) = ? 0

PRESS P FOR PREVIOUS SCREEN  
PRESS N FOR NEXT SCREEN



THE PLANT UPTAKE EFFICIENCY FACTOR PROVIDES FOR REMOVAL OF PESTICIDES BY PLANT AND IS A FUNCTION OF CROP ROOT ZONE AND THE INTERACTION OF WATER AND CHEMICAL PROPERTIES OF THE PESTICIDES. FOR PZM THE REMOVAL OF PESTICIDE BY PLANT UPTAKE IS BASED ON THE ASSUMPTION THAT UPTAKE OF PESTICIDE IS RELATED TO THE TRANSPIRATION RATE. SENSITIVITY TESTS INDICATE AN INCREASE IN THE UPTAKE BY PLANTS AS THE ROOT DEPTH INCREASES, AND A DECREASE AS THE PARTITION COEFFICIENT INCREASES. VALUES CAN BE FROM 0.0 TO 1.0 (e.g. 0.10) INDICATES UPTAKE IS A FRACTION OF CROP TRANSPIRATION RATE.

TYPE THE PLANT UPTAKE EFFICIENCY FACTOR = ? 0.1

PRESS P FOR PREVIOUS SCREEN  
PRESS N FOR NEXT SCREEN

DO YOU NEED HELP IN SELECTING MELN DENSITY (V/M) ?

SOIL	BULK DENSITY (g/cm <sup>3</sup> )
BETHANY	1.14
CLARKSVILLE	1.37
DENNIS	1.13
DOUGHERTY	1.45
EUFALA	1.47
HAYSELL	1.35
PARSONS	1.26
POND CREEK	1.17
QUINLAN	1.49
KEMPSON	1.15
St. PAUL	1.26
STEPHENVILLE	1.48
SUMMIT	1.89
TIVOLI	1.51
WYOLA	1.41
TYPE THE VALUE = $\gamma$ 1.37	
WOULD YOU LIKE TO CHANGE THE VALUE (Y/N) ? <input type="checkbox"/>	

IF YOU WOULD LIKE TO SIMULATE DISPERSION, THEN ENTER THE VALUE  
FOR HYDRODYNAMIC DISPERSION (cm<sup>2</sup>/day) OTHERWISE ENTER 0.

TYPE THE VALUE FOR HYDRODYNAMIC DISPERSION (cm<sup>2</sup>/day) = ? 0

PRESS P FOR PREVIOUS SCREEN  
PRESS N FOR NEXT SCREEN

DO YOU NEED HELP IN SELECTING CURVE NUMBER (CN) (Y/N) ? N

TYPE THE VALUE OF 'CN' FOR FALLOW CONDITION = ? 66

TYPE THE VALUE OF 'CN' FOR CROPPING CONDITION = ? 71

TYPE THE VALUE OF 'CN' FOR RESIDUE CONDITION = ? 66

PRESS P FOR PREVIOUS SCREEN  
PRESS N FOR NEXT SCREEN

DO YOU NEED HELP IN SELECTING DECAY COEFFICIENT (K<sub>s</sub>) (Y/N)? N

TYPE THE VALUE OF 'K<sub>s</sub>' = ? 5.8863

PRESS P FOR PREVIOUS SCREEN  
PRESS N FOR NEXT SCREEN

DISTRIBUTION COEFF. ( $K_d$ ), IS CALCULATED USING FORMULA :

$$K_d = K_{oc} \cdot (\text{PERCENT ORGANIC CARBON}/100)$$

THE VALUE OF  $K_d$  SHOULD BE MORE THAN 0.0001. USER IS REQUESTED TO SELECT THE VALUES OF  $K_{oc}$  AND %ORGANIC CARBON SUCH THAT  $K_d$  IS GREATER THAN 0.0001.

DO YOU NEED HELP IN SELECTING DIST. COEFFICIENT ( $K_d$ ) (Y/N)? N

TYPE THE VALUE OF  $K_{oc}$  = ? 173.78

PRESS P FOR PREVIOUS SCREEN  
PRESS N FOR NEXT SCREEN

DO YOU NEED HELP SELECTING ORGANIC CARBON CONTENTS OF SOIL (P/N) ? ■



SOIL	ORGANIC CARBON (%)
BETHANY	8.98
CLARKSVILLE	8.51
DENNIS	1.58
DOUGHERTY	8.38
EUPHRA	8.72
HARTSELL	8.85
PARSONS	8.96
PONDCREEK	1.21
QUINLAN	8.53
RENFROW	1.54
St. PAUL	8.85
STEPHENVILLE	8.46
SUNNIT	2.98
TIVOLI	8.22
YANOLA	8.53

TYPE THE VALUE = Y 8.51

WOULD YOU LIKE TO CHANGE THE VALUE (Y/N) ?

THE SELECTION RANGE FOR INITIAL WATER CONTENTS IS FROM  
WILTING POINT TO POROSITY.

TYPE INITIAL WATER CONTENTS IN SOIL (cm<sup>3</sup>/cm<sup>3</sup>) = ? 0.105

PRESS P FOR PREVIOUS SCREEN  
PRESS N FOR NEXT SCREEN

DO YOU NEED HELP SELECTING FIELD CAPACITY OF SOIL (Y/N) ?

SOIL	FIELD CAPACITY (cm <sup>3</sup> /cm <sup>3</sup> )
BETHANY	0.32
CLARKSVILLE	0.38
DENNIS	0.36
DOUGHERTY	0.12
BIFALVA	0.28
HARTSELL	0.25
PARSONS	0.31
PONDCHIEX	0.37
QUINLAN	0.15
KENTON	0.37
ST. PAUL	0.29
STEPHENVILLE	0.12
SUMMIT	0.48
TIVOLI	0.03
VANOLA	0.18
TYPE THE VALUE = 7 8.30	
WOULD YOU LIKE TO CHANGE THE VALUE (Y/N) ? <input type="checkbox"/>	

DO YOU NEED HELP SELECTING WILTING POINT OF SOIL (Y/N)?

SOIL	WILTING POINT (cm <sup>3</sup> /cm <sup>3</sup> )
BETHANY	0.14
CLARKSVILLE	0.12
DENNIS	0.17
DOUGHERTY	0.04
HYPALIA	0.11
HARTSELL	0.12
PARSONS	0.13
POND CREEK	0.18
QUINLAN	0.07
KENTON	0.19
ST. PAUL	0.14
STEPHENVILLE	0.05
SUNNIT	0.26
TIVOLI	0.04
WYOLA	0.08
TYPE THE VALUE = ? 0.12	
WOULD YOU LIKE TO CHANGE THE VALUE (Y/N) ? <input type="checkbox"/>	

**LOCATION OF WEATHER STATIONS IN OKLAHOMA**

- 1. GREAT SALT DAM
- 2. CANTON DAM
- 3. CHICKASHA
- 4. LAKE OVERHOLSER
- 5. GUTHRIE
- 6. STILLWATER
- 7. KEYSTONE DAM
- 8. HEALSH DAM
- 9. Pt. GIBSON DAM
- 10. GRAND RIVER DAM
- 11. TIDWILLER FERRY DAM
- 12. WISTER DAM

**TYPE THE NUMBER CORRESPONDING TO WEATHER STATION = ?**

THE WEATHER STATION SELECTED IS = 3 CHICAGO

DO YOU WANT TO CHANGE THE WEATHER STATION SELECTED (Y/N)? N

PLEASE, PUT THE DISKETTE CORRESPONDING TO THE NUMBER IN DRIVE A.

HAVE YOU PUT DISKETTE IN DRIVE A (Y/N) ? ■



TYPE THE NUMBER OF TIMES YOU WANT TO RUN FROM (EVEN MULTIPLE OF 10) = 7 100

PRESS P FOR PREVIOUS SCREEN  
PRESS N FOR NEXT SCREEN

**NOTE : AFTER COMPLETION OF SIMULATION FOR EACH YEAR THE FOLLOWING**

**STATEMENT WILL APPEAR:**

**STOP-PROGRAM TERMINATED**

**PLEASE, IGNORE THIS STATEMENT AND LET PROGRAM RUN.**

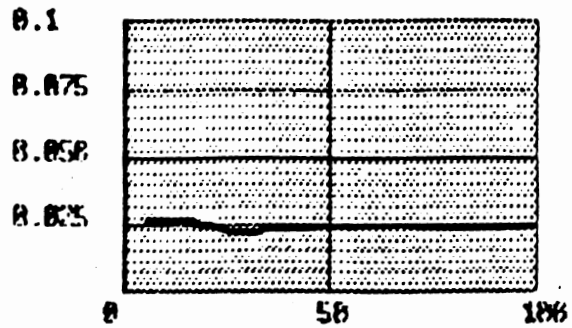
**WHEN NUMBER OF SIMULATIONS SPECIFIED BY USER ARE OVER A SCREEN  
WITH GRAPHS BETWEEN YEAR, STD. DEV. AND NUMBER OF SIMULATIONS WILL  
APPEAR.**

**PRESS P FOR PREVIOUS SCREEN  
PRESS N FOR NEXT SCREEN**

PLOT BETWEEN MEAN  
AND NUMBER OF SIMULATION

X-AXIS - NUMBER OF SIMULATION

Y-AXIS = MEAN

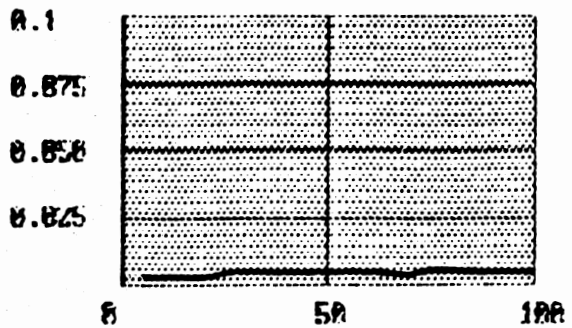


PLOT BETWEEN STANDARD DEVIATION  
AND NUMBER OF SIMULATION

X-AXIS = NUMBER OF SIMULATION

Y-AXIS = STANDARD DEVIATION

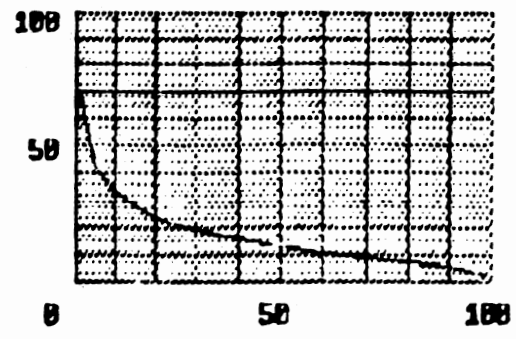
PRESS P FOR PREVIOUS SCREEN  
PRESS N FOR NEXT SCREEN



PROBABILITY      % LEACHED

99	2.484383
98	5.242621
88	7.179183
78	9.886463
68	18.93355
58	13.18242
48	15.78153
38	19.86114
28	23.91294
18	32.74574
5	42.45787
1	69.18329

PLOT BETWEEN PERCENT OF PESTICIDE LEACHED  
AND PERCENT OF TIME EXCEEDED



X - AXIS - PERCENT OF PESTICIDE LEACHED  
Y - AXIS - PERCENT OF TIME EXCEEDED

PRESS E TO EXIT

APPENDIX D

EXAMPLE CALULATION:LOG NORMAL INTERPOLATION  
OF PESTICIDE LEACHING

For the example problem, calculate the percent of pesticide (Atrazine) leached past 30 cm 30, 50, and 70% of the time. The  $K_s$ , and  $K_{oc}$  values for Atrazine are 0.0063 and 173.78 respectively and a CN value of 71. The first step in the calculations is to locate combinations of CN,  $K_s$ , and  $K_{oc}$  which bracket these coefficients. The combinations obtained are:

- combination 1. CN=59,  $K_s=0.001$ , and  $K_{oc}=2$
2. CN=73,  $K_s=0.001$ , and  $K_{oc}=2$
3. CN=59,  $K_s=0.05$ , and  $K_{oc}=2$
4. CN=73,  $K_s=0.05$ , and  $K_{oc}=2$
5. CN=59,  $K_s=0.001$ , and  $K_{oc}=600$
6. CN=73,  $K_s=0.001$ , and  $K_{oc}=600$
7. CN=59,  $K_s=0.05$ , and  $K_{oc}=600$
8. CN=73,  $K_s=0.05$ , and  $K_{oc}=600$

First linear interpolation is performed on the means and standard deviations (S.D.) to obtain their values for CN=71. By performing interpolation on mean and S.D. for combinations 1 and 2:

$$\begin{aligned} & \text{CN}=71, K_s=0.001, \text{ and } K_{oc}=2 \\ \text{Mean} &= [ ((6.76-6.68)/(59-73)) * (71-73) ] + 6.68 \\ &= 6.6885 \end{aligned}$$

Similarly the S.D. value of 0.1312 is obtained.

In the similar manner from combinations 3 and 4  
CN=71,  $K_s=0.05$ , and  $K_{oc}=2$

$$\text{Mean}=3.671$$

$$\text{S.D.}=1.1312$$

from combinations 5 and 6

$$\text{CN}=71, K_s=0.001, \text{ and } K_{oc}=600$$

Mean=2.6336

S.D.=1.7469

from combinations 7 and 8

CN=71, Ks=0.05, and Koc=600

Mean=-7.4299

S.D.=4.4997

The percent of Atrazine leached past 30 cm for 30, 50, and 70% of the time can be obtained by solving z-variable equation for log normal distribution. The equation can be written as follows:

$$z = \frac{\ln (\text{amount of pesticide leached}) - \text{mean}}{\text{S.D.}} \quad (1)$$

for CN=71, Ks=0.001, and Koc=2

for 30% probability  $z=0.524565$ , therefore,

$\ln (\text{amount of pesticide leached})=z*\text{S.D.}+\text{mean}$

or amount of pesticide leached= $\exp(z*\text{S.D.}+\text{mean})$

$$\begin{aligned} \text{amount of pesticide leached} &= \exp(0.524565*0.1312+6.688) \\ &= (860.33)*(100/1000) \\ &= 86.03\% \end{aligned}$$

During the initial calculations of means and S.D. for the development of database all the values were multiplied by 1000. Therefore, the value obtained above is divided by 1000.

Similarly for 50, and 70% probability, z values are 0, and -0.524565 respectively. By substituting these z values and corresponding mean and standard deviation in equation 1 the percent of pesticide leached 50, and 70% of the time is 80.31, and 74.97% respectively.

In the similar manner for  $CN=71$ ,  $Ks=0.05$ , and  $Koc=2$  amount of pesticide leached (%) for 30, 50, and 70% of the time can be obtained by using equation 1. In this case  $z$  values will be the same, only mean and standard deviation values will change corresponding to this combination. The amount of pesticide leached (%) for 30, 50, and 70% of the time calculated is 2.2, 3.9, and 7.12 respectively.

Similarly, for  $CN=71$ ,  $Ks=0.001$ , and  $Koc=600$  amount of pesticide leached (%) for 30, 50 and 70% of the time obtained is 0.55, 1.39, and 3.48 respectively.

for  $CN=71$ ,  $Ks=0.05$ , and  $Koc=600$  amount of pesticide leached (%) for 30, 50, and 70% of the time obtained is 0.

The linear interpolation on the percent of pesticide leached past 30 cm for the  $Ks$  value of 0.0063 on the above four combinations will provide the results as follows:

for  $CN=71$ ,  $Ks=0.0063$ , and  $Koc=2$  amount of pesticide leached (%) for 30, 50, and 70% of the time is 77.50, 72.05, and 67.1 respectively.

for  $CN=71$ ,  $Ks=0.0063$ , and  $Koc=600$  amount of pesticide leached (%) for 30, 50, and 70% of the time is 3.1, 1.25, and 0.5 respectively.

The final result is obtained by performing linear interpolation for  $Koc$  on the above two combinations.

$CN=71$ ,  $Ks=0.0063$ , and  $Koc=173.78$  amount of pesticide leached (%) for the 30, 50, and 7% of the time is 56.13, 51.7, and 47.96 respectively.

These results are consistent with the values obtained from Figure 14.



VITA

Pankaj Arora

Candidate for the Degree of

Master of Science

Thesis: THE DEVELOPMENT OF AN EXPERT SYSTEM AS A SCREENING TOOL TO MINIMIZE GROUNDWATER CONTAMINATION FROM PESTICIDES

Major Field: Environmental Engineering

Biographical:

Personal Data: Born in New Delhi, India, September 3, 1965, the son of Maqsudan Lal and Shiela Arora.

Education: Graduated from G.B.Sr.Sec. School, Ashok Vihar, India, in May 1980; received Bachelor of Science Degree in Chemistry from University of Delhi in India, in June, 1983; received Master of Science in Chemistry from University of Delhi in India, in June 1985; received Master of Technology in Nuclear Engineering from Indian Institute of Technology, Kanpur, India, in June 1987; completed requirements for the Master of Science Degree at Oklahoma State University in December 1991.

Professional Experience: Senior Research Assistant, Department of Nuclear Engineering, Indian Institute of Technology (IIT), Kanpur, India, June 1987, to June 1988; Teaching Assistant, School of Civil Engineering, Oklahoma State University, August, 1989, to December 1989; Teaching Assistant, School of Civil Engineering, Oklahoma State University, January 1990, to May 1990; Research Assistant, School of Civil Engineering, Oklahoma State University, June 1990, to May 1991.