APPLICATION OF MONTE CARLO TECHNIQUES TO THE DETERMINATION OF GROUND-WATER CONTAMINATION RISK IN SATURATED TWO-DIMENSIONAL AQUIFER SYSTEMS

By

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ABSTRACT

A Monte Carlo Simulation and uncertainty analysis was used to determine the risk of groundwater contamination in saturated two-dimensional aquifer systems. The effort was applied in two areas. The procedure for determination of groundwater contamination associated with the application of a pesticide is presented in Appendix A. The paper that follows details the analysis of uncertainty associated with the relatively new process, Underground Coal Gasification, for the production of synthetic fuels. Migration of organic contaminants was determined in terms of peak concentration and affected (contaminated) area. Natural controls of the groundwater quality , biological decay, retardance and dispersion, were included in the analysis. A generic analysis, applied to a wet site as well as a dry site, was completed. This was done to avoid limiting the applicability of the results, which would come from a site specific approach.

A DETERMINATION OF THE RISK OF GROUNDWATER CONTAMINATION FROM UNDERGROUND COAL GASIFICATION

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CHAPTER I

INTRODUCTION

There is uncertainty associated with the determination of risk regarding groundwater contamination. The uncertainty exists due to lack of information about the system and/or to the variable nature of properties and processes. This uncertainty can be found in the hydrologic properties, geologic properties, the source of the contamination or the combination of any of these.

There are two types of models available to evaluate groundwater contamination. A deterministic model produces a single output for a specific input while a stochastic model creates a probability distribution of output based on a randomized input. The Monte Carlo technique emulates the stochastic model using a deterministic model. The Monte Carlo simulation solution is obtained by repetitively solving a large number of deterministic simulations with a different set of input parameters for each simulation. The results are then analyzed statistically to define the probability distribution of each output parameter. The method is based on the assumption that each simulation is equally probable.

This method has been practiced and tested in several areas. The Monte Carlo simulation procedure has been utilized for evaluating the uncertainty of pesticide leaching in agricultural soils by Carsel, et al.(1988). Mercer, et al.(1983) applied the Monte Carlo simulation and uncertainty analysis to the contamination resulting at the Love Canal area near Niagara Falls, New York, to estimate contaminant travel times to the upper Niagara River. The procedure has yet to be utilized as a technique for handling uncertainty associated with In Situ Coal Gasification.

In Situ or Underground Coal Gasification (UCG) promises to provide economic access to an enormous deep-coal resource. The process involves the conversion of coal into combustible gases to be used as a source for synthetic fuels. Appendix B contains details of the process. The possibility of groundwater contamination arises because part of the gasification products and by-products remain underground within the coal seam, which is typically an aquifer. The process creates a cavern within the coal seam. The impact on the groundwater system can be separated into two stages. Stage one is the filling of the cavern with groundwater, altering the local flow patterns, while stage two is the point in time where the regional water level is met and export of contaminants into the aquifer system occurs. Being a relatively new process there is much uncertainty associated with the products and by-products (both organic and inorganic) that remain underground and their fate within the aquifer system.

The immediate and long term effects of this contamination need to be assessed to determine its impact. To guarantee that the UCG development is not unncessarily delayed, it is crucial that significant environmental effects be anticipated to determine the necessity for prevention and control.

This study utilizes Monte Carlo simulation techniques to evaluate the risk of contamination from UCG within the coal aquifer. The application of a numerical groundwater model, "Random-Walk" Solute Transport, is used to simulate groundwater contamination resulting from the organic compounds produced during gasification. The simulation considers natural controls of the groundwater quality including biological decay and retardance.

CHAPTER II

EXPERIMENTAL

Selection of Model

The numerical "Random-Walk" Solute Transport Model by Prickett, Naymik and Lonnquist for the microcomputer was acquired from the Holcomb Research Institute at Butler University (18). The model was selected primarily for the ability to generate a continuous, randomized source, representitive of the export of contaminants resulting from the UCG process. The model was applied in its two-dimensional form for steady flow conditions. Note that a two-dimensional model is the simulation of a three-dimensional process by integrating the thickness parameter in the output values.

The groundwater flow portion of this model is a finite difference code. In the flow calculations, the head distribution is solved by this numerical method from which a velocity can be calculated. The solute transport portion of the code is achieved by a particle-in-a-cell technique for the convective mechanisms and a random-walk technique for the dispersion effects. The model employs a normally distributed density function which calculates the dispersive properties for the simulation. A random number generator determines standard deviation locations to 6 plus and 6 minus units from a mean in each dimension of the dispersion. The mean pollutant location is then determined by the advective or velocity component solved by the code or input into the program.

For discretization, a finite difference grid is superposed over a map of the aquifer. The grid is defined by X and Y axes and the coordinates. This subdivides the aquifer into volumes having dimensions, $b\Delta X\Delta Y$, where b is the saturated thickness. The model is capable of handling varied grid lengths of ΔX and ΔY. Output values are given at each node, the intersection of X and Y coordinates, and encompasses the area half the distance to the surrounding nodes.

Modification of Model

For this simulation the computer code required some revisions. The code does not include the effects of biological decay. The program was revised to include varied values of the biological decay factor at both the source and in the system. A first order approximation was considered appropriate for this decay property. This was consistent with other modeling efforts (16). (For user manual of revised program see Appendix C) The reduction is accomplished through a first order exponential reduction of the quantity of the pollutant. In terms of the program variables, system decay is accomplished by equation 1.

$$PM = PM \exp^{(-BD1*DELP)} \tag{1}$$

where

PM is the particle mass, lb/particle
BD1 is the biological decay for the system, /day
DELP is the time increment, days

For the source decay the particle mass is replaced with the total pollutant load (PL) in pounds and BD2 is the biological decay at the source. A default value of 0 can be entered if biological decay effects are nonexistent.

Input Data

The degree of uncertainty associated with the process and the limited information and data available would make a site specific analysis less useful to the overall development of the process. There are two types of input data to be determined that are typical of the UCG process. Fixed parameters are constant values reflective of the characteristics of the coal seam and aquifer. The variable data has the most uncertainty associated with determining the values and are used as the Monte Carlo parameters.

The Department of Energy data collection programs at Hanna and Hoe Creek sites in Wyoming were used to establish basic geohydrologic parameters for the generic study sites. The data were accumulated from the open literature of various past studies performed at the sites.

Two types of coal seams, wet and dry, have been selected from previous UCG experiments. They differ by the amount and velocity of groundwater flow. For model input the dry velocity was defined as 100 ft/yr (0.27 ft/day) and the wet velocity was input as 1000 ft/yr (2.7 ft/day). These were selected to approximate the range of conditions available in a coal aquifer. To create a velocity or head distribution map, a ratio of 3:1 was used for the magnitude of velocity in the major direction, X axis, to the minor direction, Y axis. This ratio correlates to the ratio of major to minor values of dispersion found at the Hanna, Wyoming UCG sites (16,21).

Fixed or constant versus random parameters had to be determined for input. The geologic features which affect the UCG process include structure, permeability, porosity, water-bearing formations and rock strengths (1). It is the affect of these factors that presently restricts the coal seams used for the process to specific ranges of each parameter. Based on this information it was determined that the following data set of source area, transmissivity, thickness, permeability, porosity and storage coefficient would be fixed values for input (Table I).

The size of the cavity resulting from the UCG process is used as the source volume. The horizontal area of the cavern is the source input for the model. The cavern des-

TABLE I

FIXED INPUT VALUES

Parameter	Value
Thickness	30 feet
Transmissivity	58 gal/day/ft
Permeability	1.93 gal/day/ft^2
Porosity	0.15
Storage Coefficient	0.0001
Dispersion	
Longitudinal	33 feet
Transverse	10.5 feet
Source area	40,000 ft^2

cribed as Hanna I at the Hanna UCG site was considered typical. The horizontal area of 40,000 square feet was approximated by a square 200 feet by 200 feet (16). The values found for the thickness of the coal seam (confined aquifer) ranged from 22 to 34 feet (3,13,16,19). An average value of 30 feet was used as the saturated thickness for the aquifer. This value approximates the thickness of coal seams available for gasification. A storage coefficient of 0.0001 was used to describe the confined aquifer (13). Transmissivity values ranged from 0.14 to 150 gal/day/ft (9,13,16,19). Since the magnitude of the transmissivity is dependent on the thickness selected, an average value of 58 gal/day/ft was determined.

Permeability varied from 0.01 to 2.4 gal/day/ft^2 (9,11,13). An average value of 1.93 gal/day/ft^2 was determined which correlates with the transmissivity and thickness values previously ascertained. Porosity values were found to have a wide range from 0.2% to 15% with 15% being a fractured coal seam (11,13). Since coal is highly fractured with a fracture system normal to bedding and fractures are induced by the UCG process, the higher value of 15% was selected (13). The primary use of porosity by the model was in concentration determinations and velocity calculations.

Since a predetermined velocity was selected and the porosity and permeability are given, the variable will be the head distribution or hydraulic gradient needed to achieve this desired velocity. The head distribution was determined for both conditions, dry and wet, and used as input into the model. For this reason, the flow portion of the model that determines heads was not used. Velocities were calculated directly from the head distribution input.

Existing data indicated input of dispersion in the longitudinal direction of 33 feet and in the transverse direction of 10.5 feet (16,21). The actual dispersion coefficients utilized during simulations will be a fraction of the given values based on the random-walk technique used by the model.

The random data set should include the parameters with the most uncertainty associated with the values. There were three parameters, initial concentration, biological decay and retardance, in which values were difficult to obtain. Based on the minimal information available and the variable nature of the properties these parameters were used as the random input.

The desired organic constituent for simulation is phenol. Phenol has been found to be the largest fraction, at 90-98%, of the organics present in postburn samples (8). The exact quantity of this material is a function of the initial coal composition, combustion temperature, water temperature and groundwater composition (6).

Based on analytical difficulties in determining phenol concentrations, Total Organic Carbon (TOC) was used as a surrogate parameter. More and better TOC data were available for this investigation. As there is strong correlation between TOC and phenol in other UCG wastewaters it is assumed that TOC can be readily used as an indicator of phenolic contamination. The TOC values were determined from water quality well tests at the Hanna site (16). The TOC data ranged from 1 to 63 mg/l. A normal distribution was established with a mean of 30.13 mg/l and a standard deviation of 16.6 mg/l (Fig. 1).

Retardance values for phenols were calculated based on the distribution coeffecient (Kd) data for coal ascertained from the open literature (4,12,20). The values found in the literature were determined in the lab on ground or powdered media to determine its sorption characteristics. In the field, solid coal is the sorptive media and would be expected to exhibit lower sorptive properties. Therefore the input values used are probably optimistic rather than conservative. The unitless retardance factors were calculated using the Kd values, porosity and bulk density of 1.60 gm/cc (21). The values ranged from 1.209 to 1.995. These values indicate that the phenol moves at a velocity approximately the same as the groundwater (1.209) to half the velocity of the groundwater (1.995). The retardance values were found to be log normally distributed with a mean of 1.485 and a ln standard deviation of 0.522 (Fig. 2).

The biological decay values were determined from well

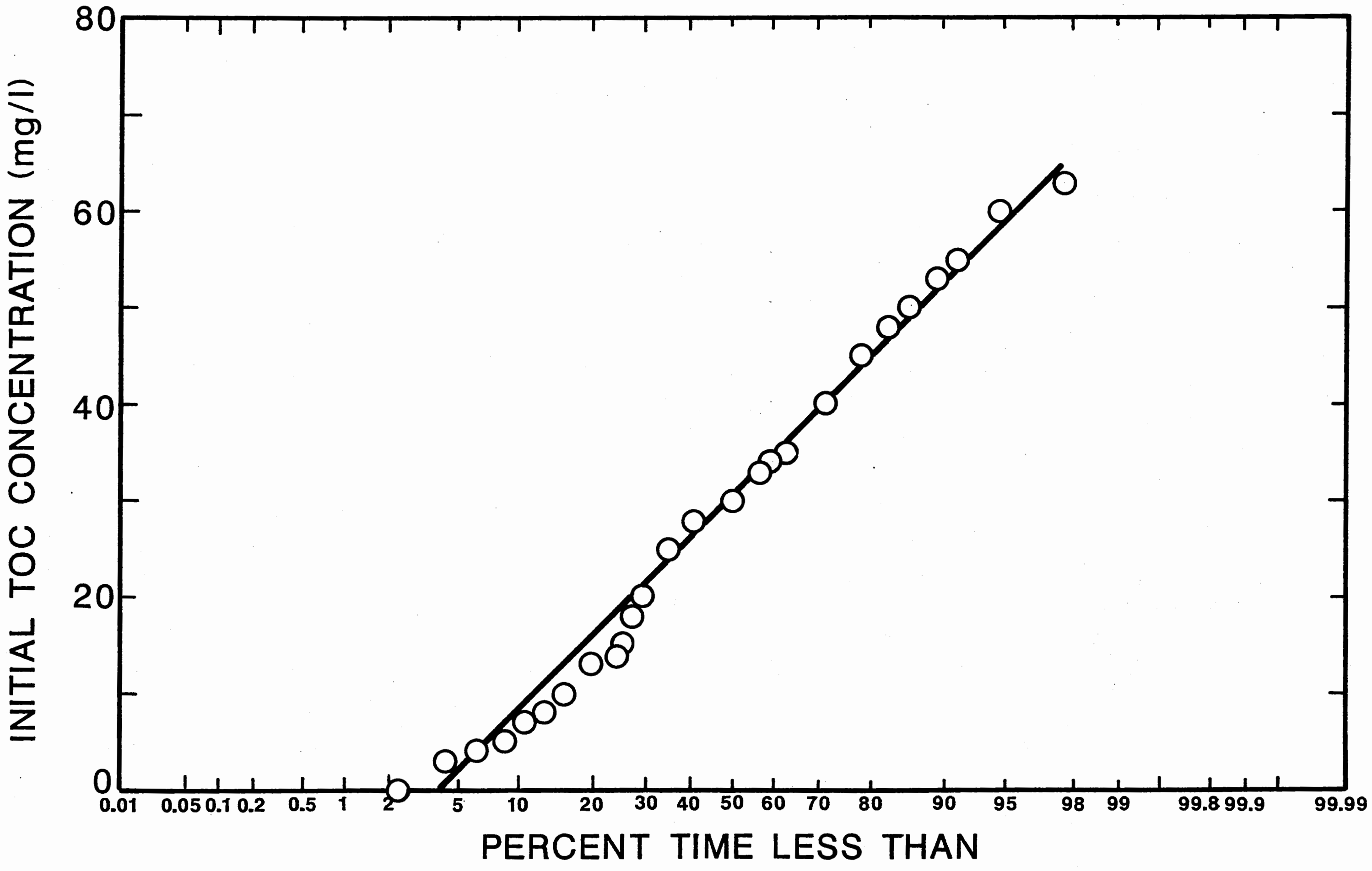

Figure 1. Total Organic Carbon Input Data Distribution

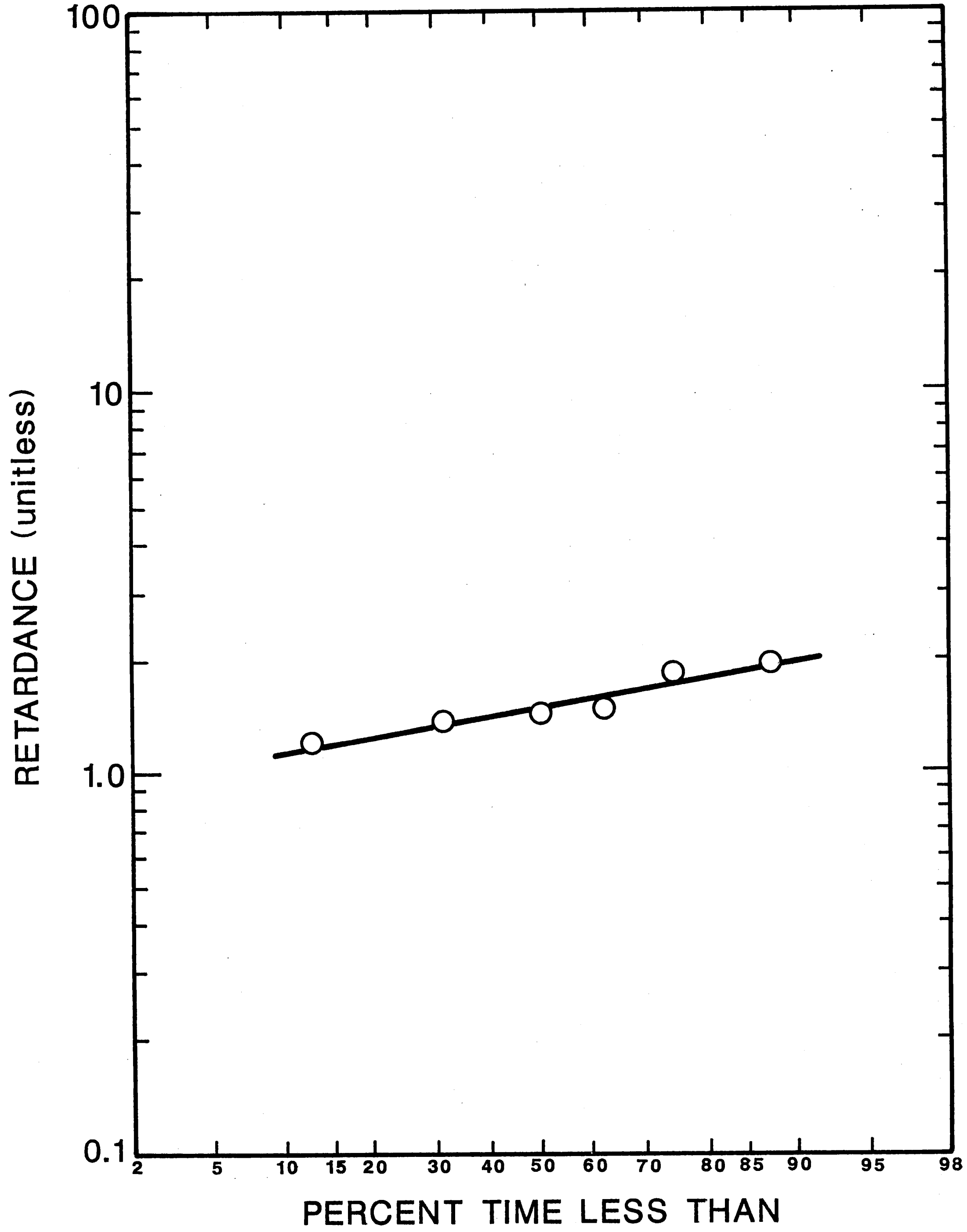

Figure 2. Retardance Input Data Distribution

tests at the Hanna site (16). For each well the reduction in TOC concentration and the time between samples was recorded. This reduction can be attributed to both retardance and biological decay. No studies were found to determine what fraction of the reduction is due to decay. Therefore it was arbitrarily determined that half of the concentration reduction was due to biological decay and half to the retardance values previously determined. The biological decay (kinetic rate) was then calculated by taking the difference of the natural logs of the concentrations divided by the time increment required for the reduction to occur. The resulting reduction factor is per day and the calculated values ranged from 0.0001 to 0.011 per day. A log normal distribution was determined with a mean of 0.0014 and a ln standard deviation of 1.081 (Fig. 3).

The biological decay should be applied both at the source, the cavity itself and in the system, locations within the coal aquifer. For this study, half of the biological decay factor calculated was applied at the source and half in the system. Spatial and temporal effects of the biological decay coefficient were neglected.

In accordance with the randomizing process of the model, a set of 13 values for each variable was developed based on the mean and standard deviation. Fractions of the standard deviation were added and subtracted from the mean to develop 6 values above the mean, the mean, and 6 values

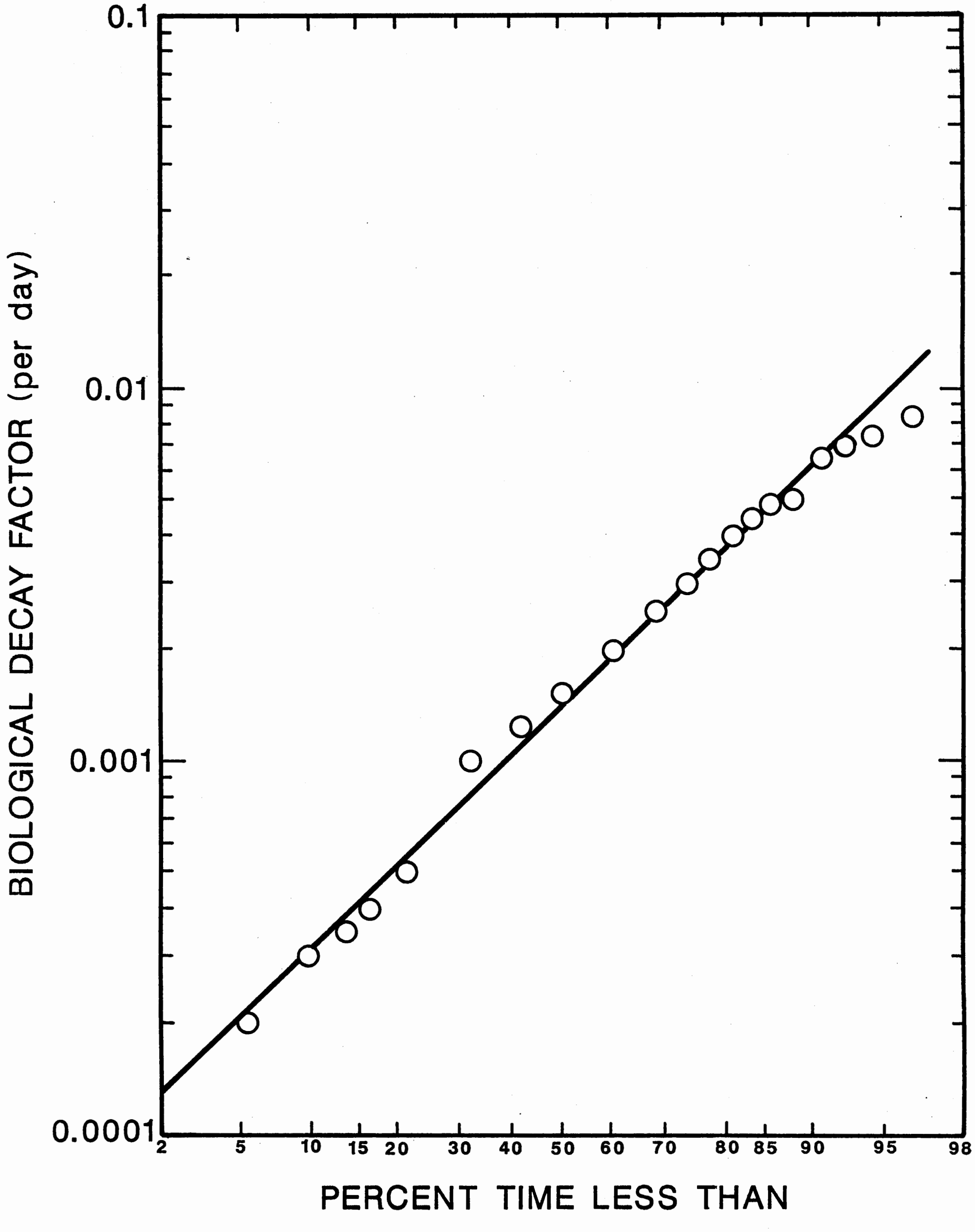

Figure 3. Biological Decay Input Data Distribution

below the mean. The values were kept within the range of original values found in the literature. The 13 values were then arbitrarily repeated 10 times to develop a total set of 130 values for each variable.

Using a publically available program each of the data sets were randomized (10). The resulting sequences of the data were used as input data for the model. Retardance, concentration and biological decay data sets were randomized separately to eliminate any interdependence or correlation between the variables. The data sets were randomly generated twice, once for the dry site input and once for the wet site input.

Simulation

Time zero for the simulation is the point where regional flow levels have been met in the UCG cavern and export of the contaminants to the aquifer has begun. Each simulation was arbitrarily terminated at 20 years. The source was allowed to generate in increments of 365 days from the generic 40,000 square feet area. The volume for the simulation can then be determined by using the thickness of 30 feet for the generic site.

For this investigation a finite difference grid 26 by 22 was created to cover the area of an aquifer (Fig.4). The area modeled was checked to assure it was large enough to contain the particles during all possible simulations.

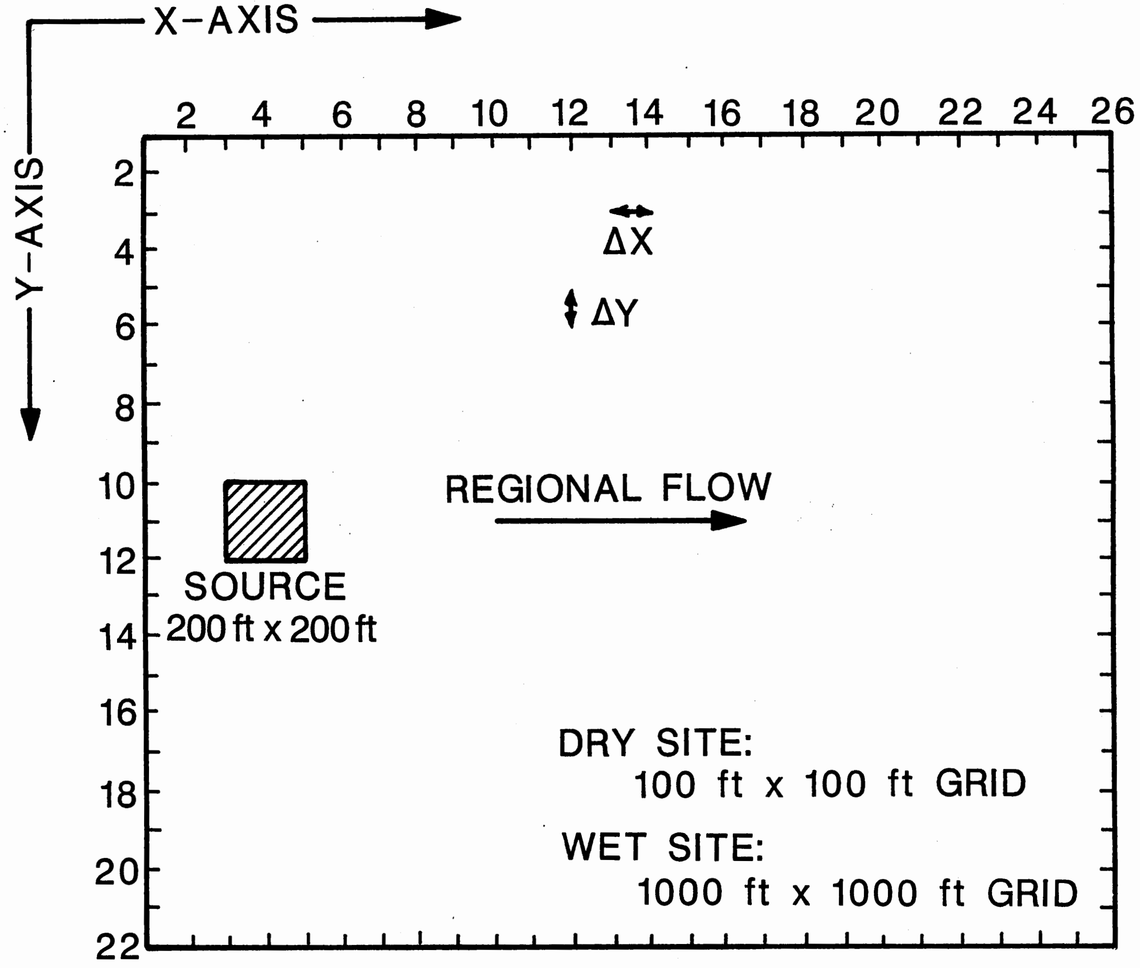

Figure 4. Plan View of Finite Difference Grid for Aquifer System

These sample simulations resulted in a 100 by 100 feet grid for the dry site while the wet site required a larger grid of 1000 by 1000 feet. The source was located to allow for any back flow from the cavern (Fig. 4).

For each condition, dry and wet, 20 years of flow and solute transport were simulated for the various random combinations of initial concentration, biological decay and retardance. Results of solute transport were produced at the end of each year. The 5, 10 and 20 year results were printed for evaluation.

CHAPTER III

RESULTS

Two conditions were selected for comparison that determine the extent and magnitude of groundwater contamination resulting from the UCG process. The affected (contaminated) area allows for prediction of the plume movement spatially and for a determination of the distance downgradient the contaminant has migrated. As a constant thickness was used for simulations the area term is equivalent to the aquifer volume contaminated when multiplied by the thickness. The peak concentration determines the magnitude of the groundwater contamination which can be used for comparison with given groundwater quality standards.

Model outputs were prepared at the 5, 10 and 20 year time periods. A quality assurance procedure was done to assure that enough events were simulated to determine repre-sentitive outputs of the system. This was accomplished by running the simulations in groups of 10. For each cumulative increment of 10, probability levels were determined at the 50, 70 and 90 percentiles for each 5, 10 and 20 years output. The probability levels were determined for both the dry and wet sites.

Simulations were continued until the value at each percentile reached a constant value. Once a constant value was reached, continued simulations could not produce a constant value of greater precision. This procedure was done to assure that the minimal number of simulations was made but also to avoid numerous unwarranted simulations. Examples of this asymptotic procedure/solution are illustrated in Figures 5 through 8. It was found that 100 simulations were adequate for both the dry and wet sites.

The output of the model is highly dependent on the grid size used. The discretization is decreased with increased grid dimensions. The grid size or cell dimensions are used to determine concentration values, making the concentration values dependent on an arithmetic factor as well as the input data. These factors should be considered when analyzing the output.

Within each time step (5, 10 and 20 years) all the data were used to assess the risk. Probability distributions were determined by plotting the accumulated simulation results. The lines shown on all graphs are not fit statistically but should be taken as an estimated fit. Figures 9 and 10 are the normal distribution of the affected area at 20 years for the dry and wet velocities, respectively. Interpretation of a plot would be, for the dry site, the simulated data showed that for 90% of the simulated scenarios, less than 1,460,000 square feet (30 feet thick) of the

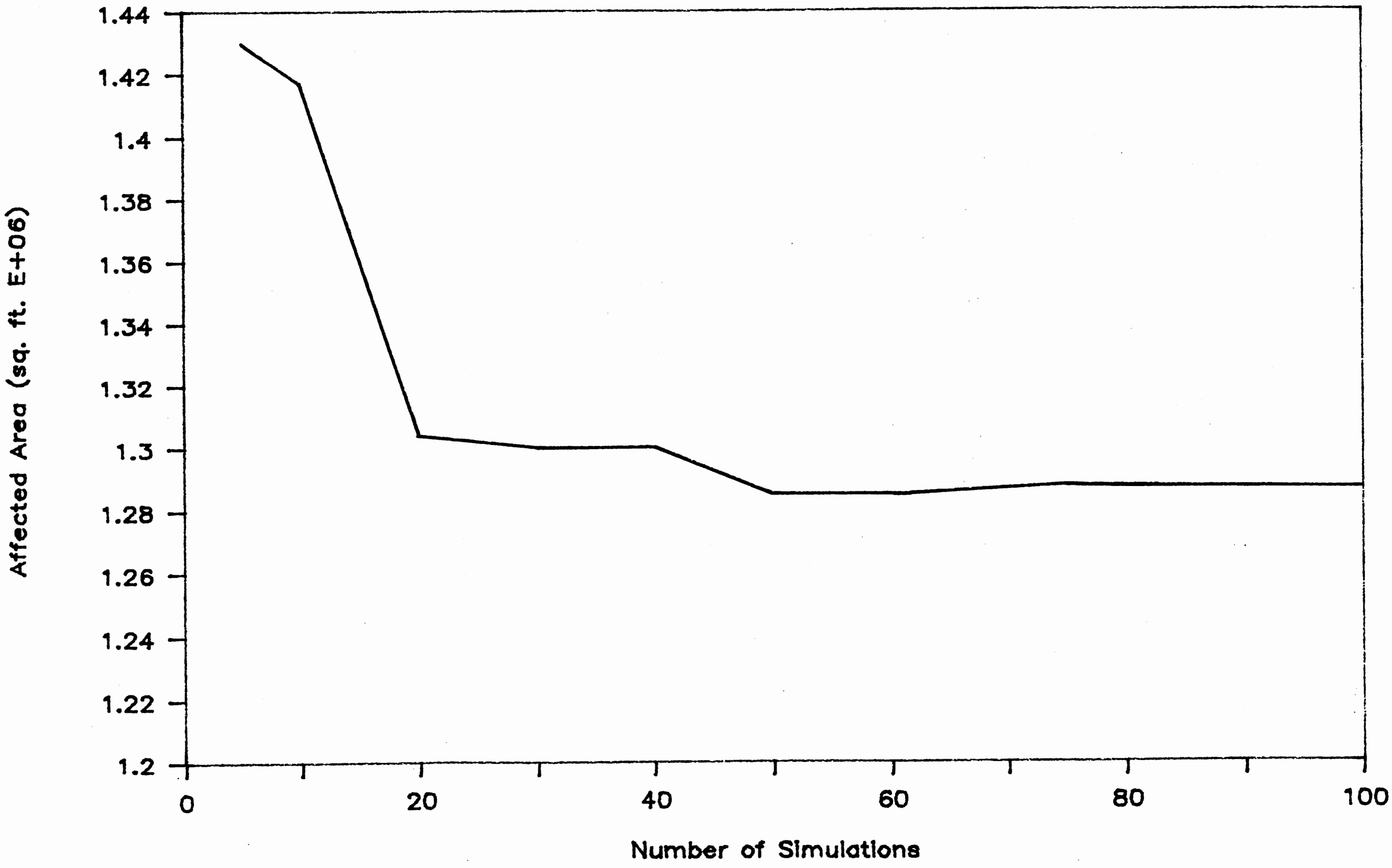

Figure 5. Dry Site-70 Percentile at 20 Years

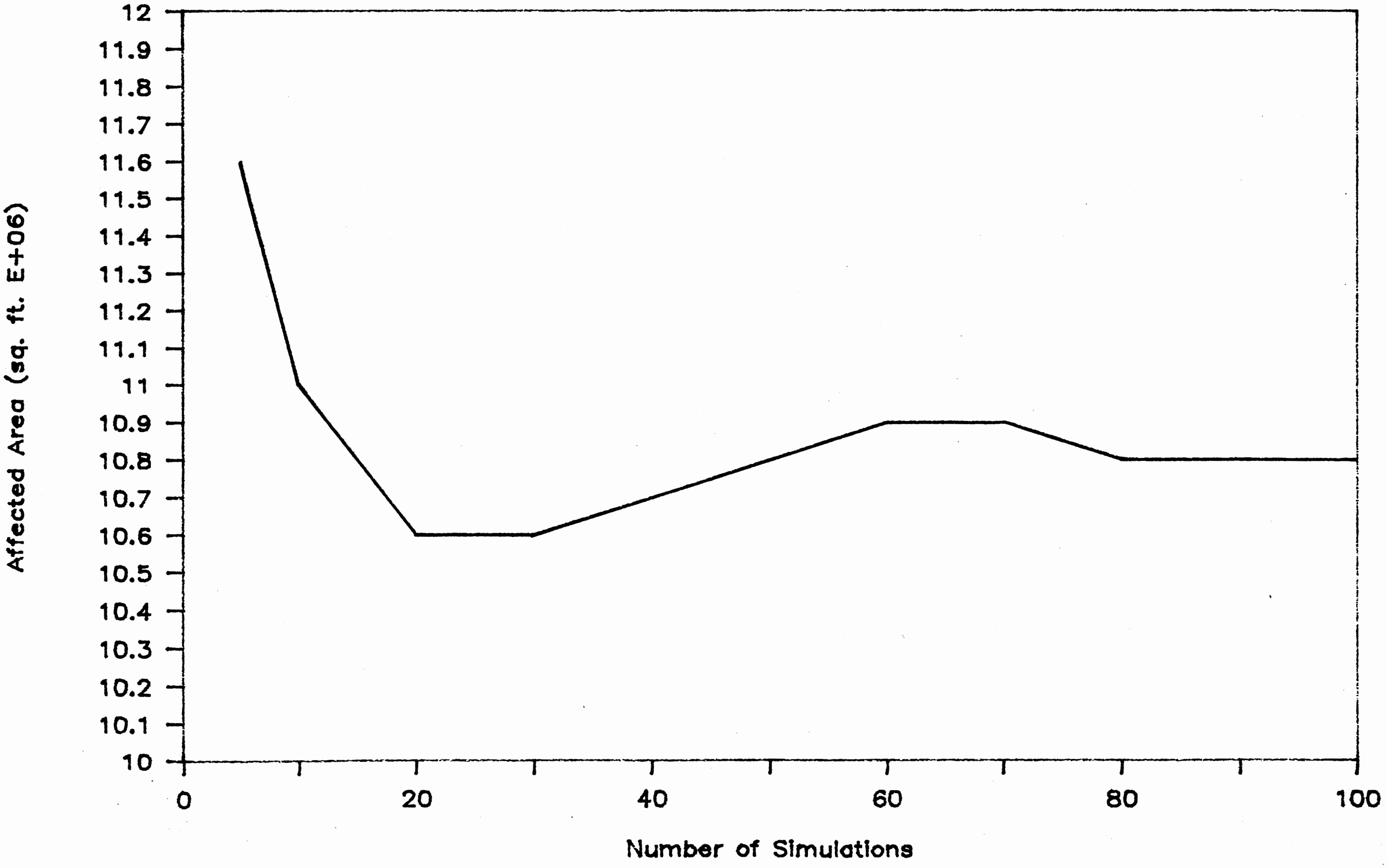

Figure 6. Wet Site-90 Percentile at 5 Years

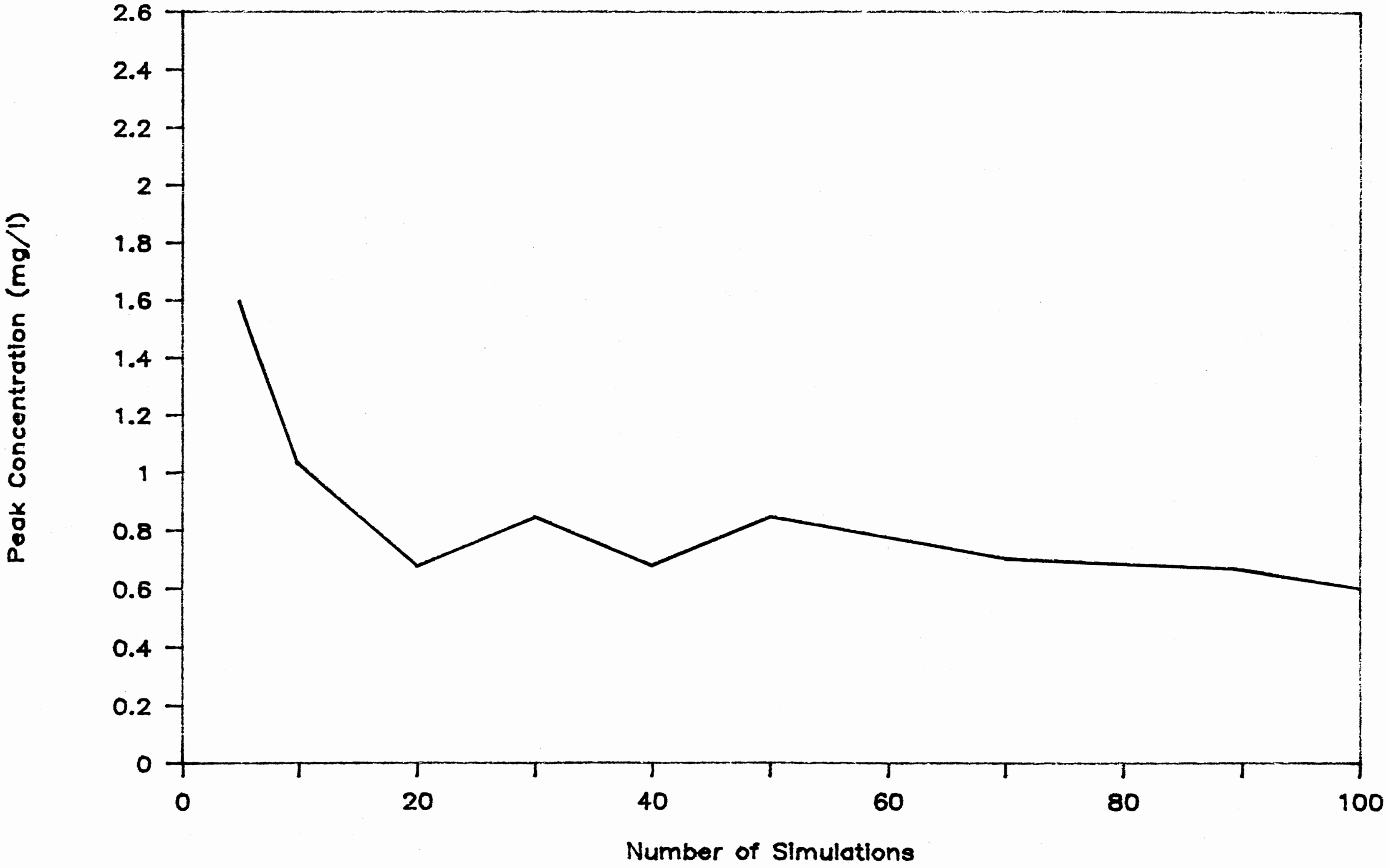

Figure 7. Wet Site-90 Percentile at 20 Years

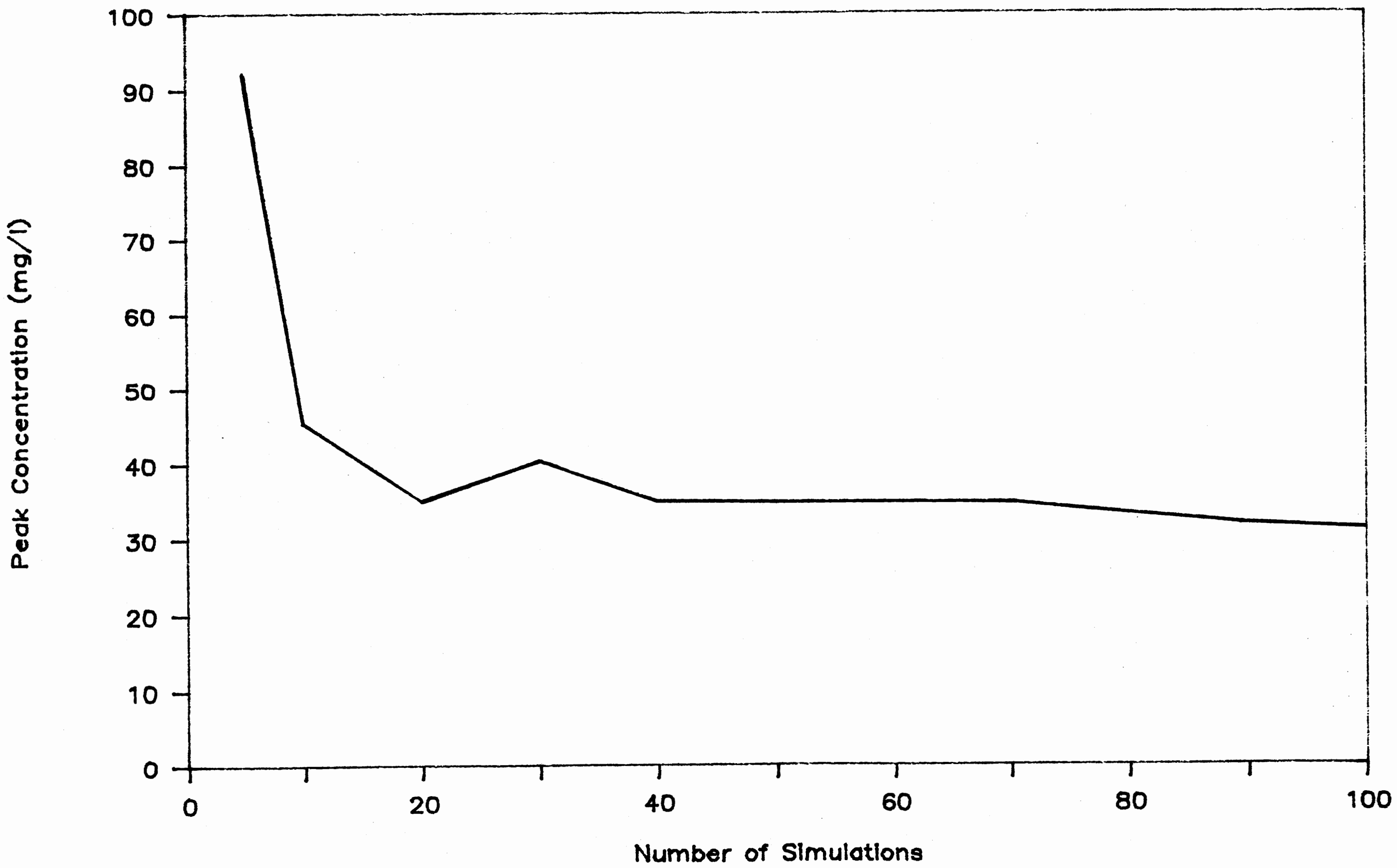

Figure 8. Dry Site-90 Percentile at 5 Years

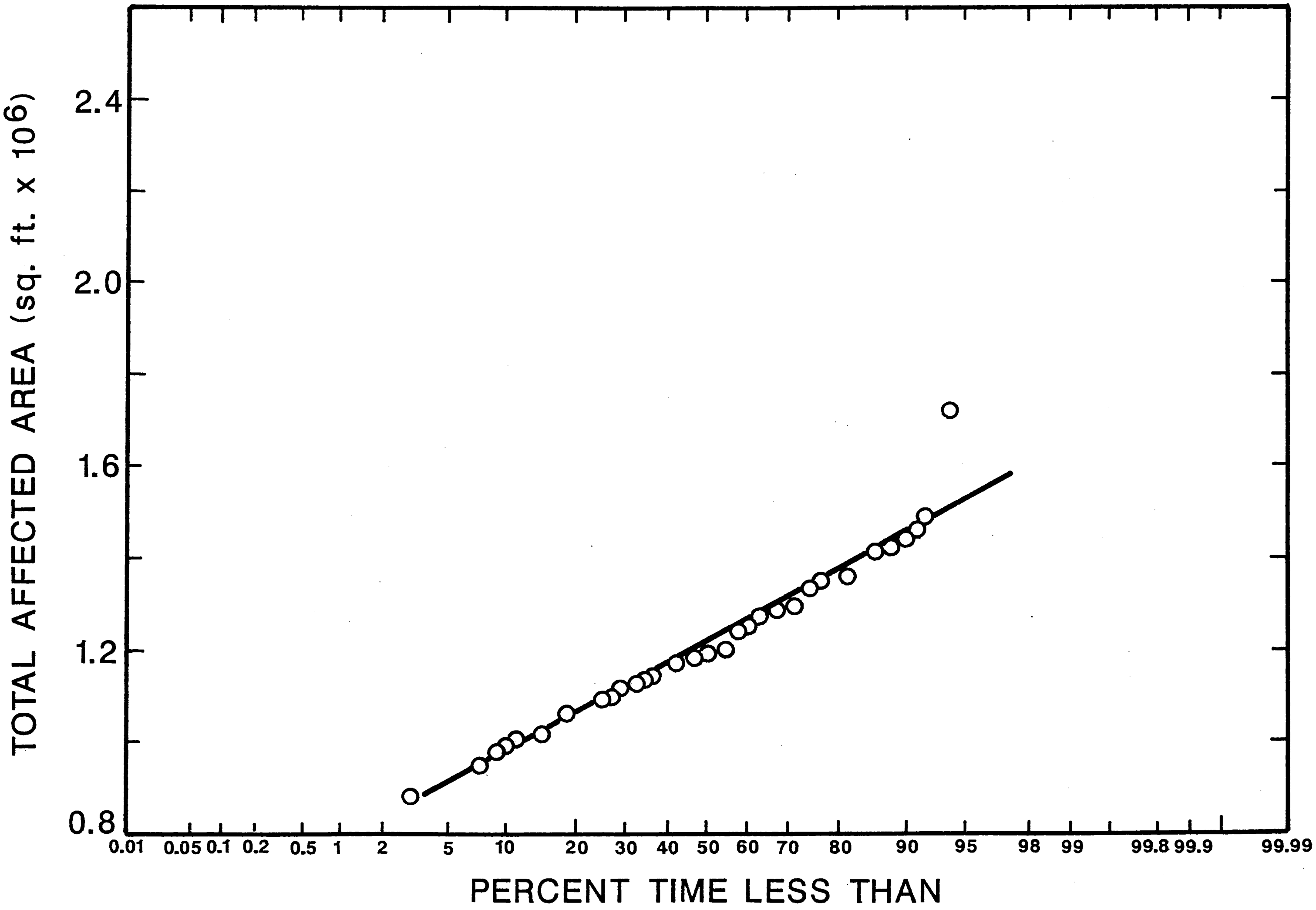

Figure 9. Distribution of Affected Area (Dry Site) at 20 Years

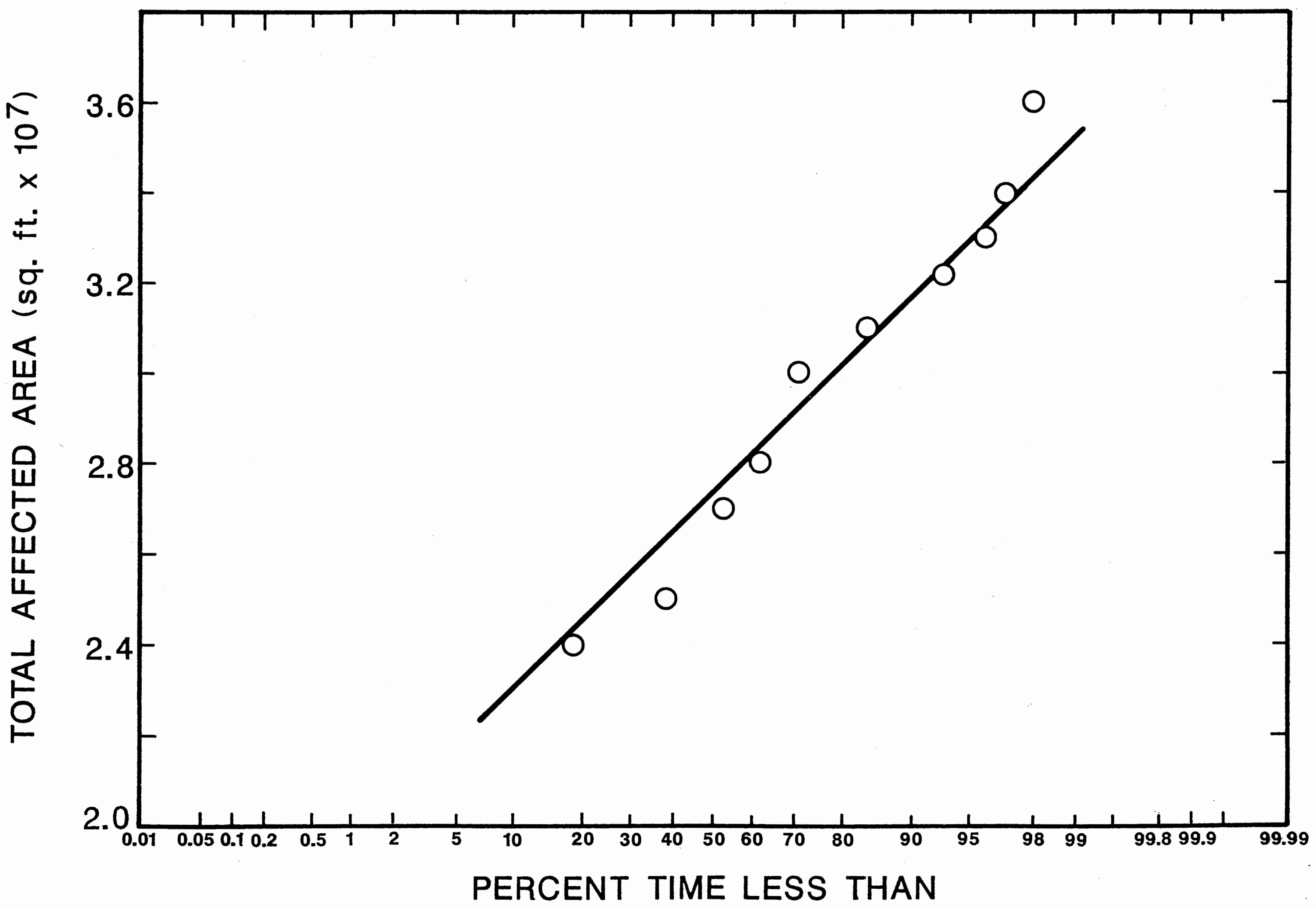

Figure 10. Distribution of Affected Area (Wet Site) at 20 Years

aquifer was affected by the contaminant. The simulated data also showed that 90% of the time, less than 31,600,000 square feet of the wet site aquifer was affected by the contaminant after 20 years.

The range of peak concentration values at each velocity was found to be log normally distributed (Figs. 11 & 12). Since all the data were used to determine the distribution, only a portion of the plot is depicted in the figures. After 20 years, the data from the wet site simulations revealed that 90% of the time, a supplementary peak concentration of 1.3 mg/l of TOC would be detected. At the dry site, 90% of the time the peak concentration of TOC is less than 50 mg/l. It should be noted that the model carries the accuracy of the concentration to a point greater than the detection limits of the analysis techniques. Tables II, III and IV are a summary of the area and concentration values for probability levels at 10% intervals at 5, 10 and 20 years.

To enhance the interpretation of the results, plume movement was examined. At both velocities the 90% value for the affected area was studied. One simulation from each velocity that best represented the 90% value of affected area was used to develop contours of concentration and the size of the plume at 5, 10 and 20 years. These contour maps can be found in figures 13 through 18.

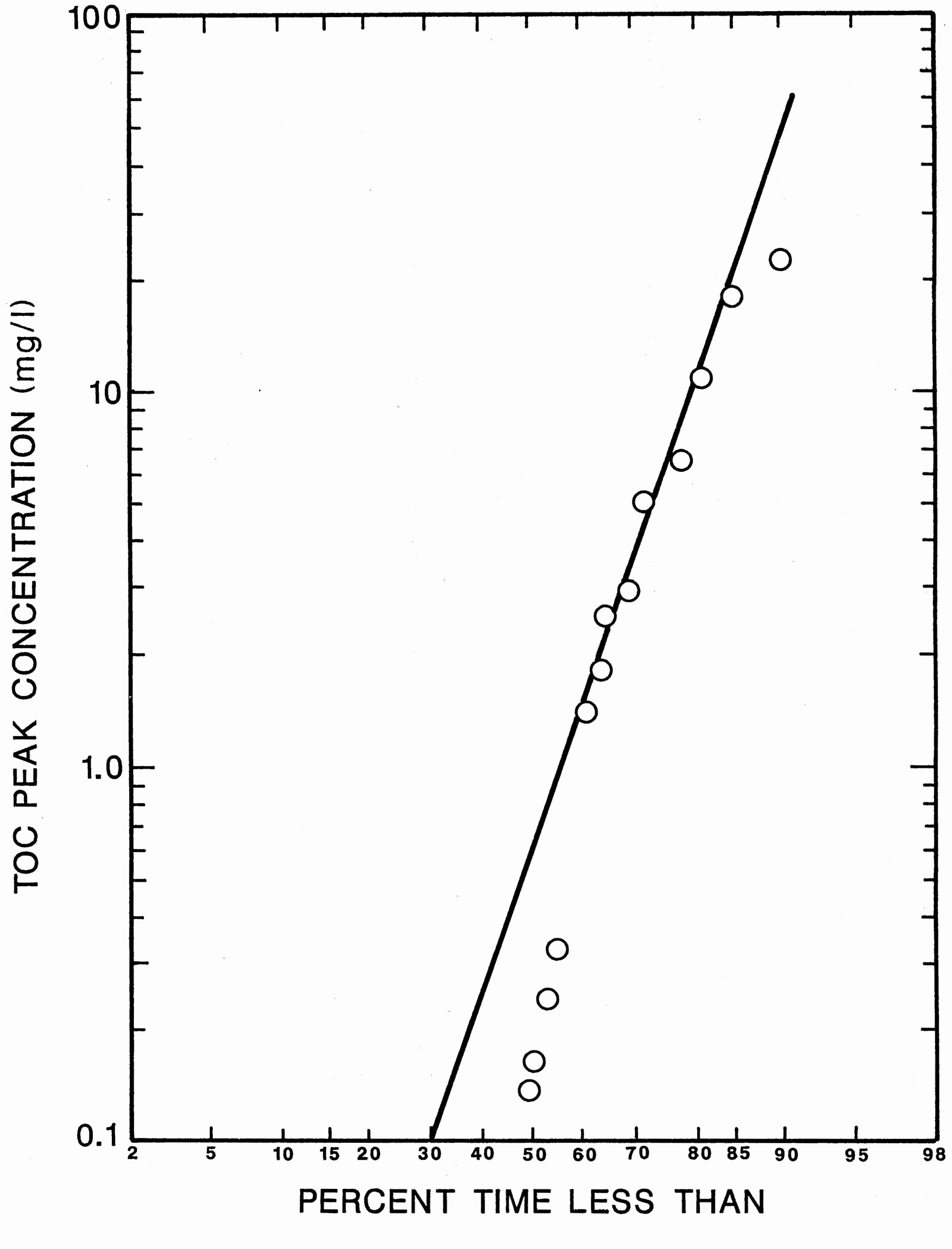

Figure 11. Distribution of TOC Peak Concentration (Dry Site) at 20 Years

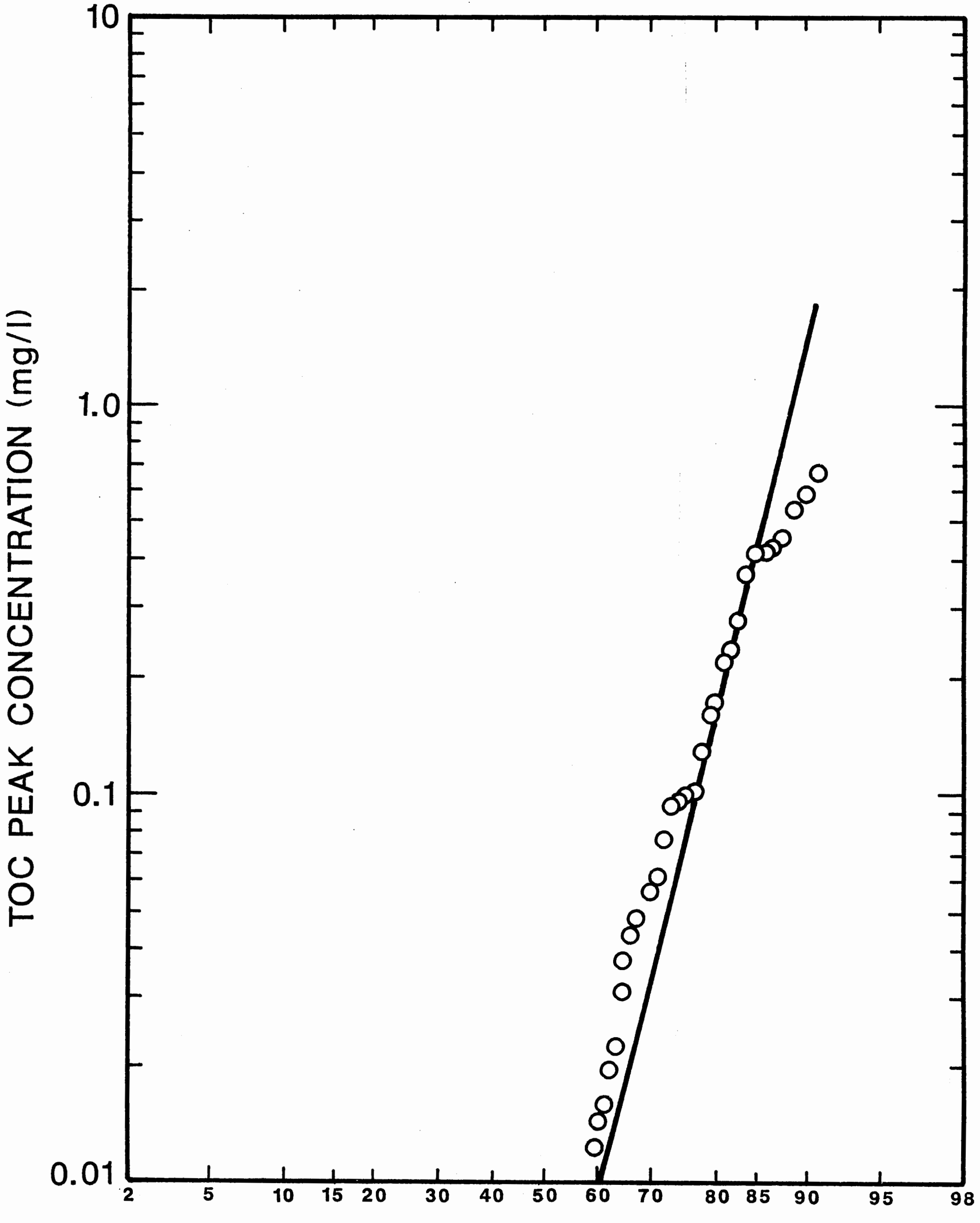

Figure 12. Distribution of TOC Peak Concentration (Wet Site) at 20 Years

TABLE II

PROBABILITY AT 5 YEARS FOR PEAK CONCENTRATION AND AFFECTED AREA

%time less than	TOC (mg/l) DRY	TOC (mg/l) WET	AREA FT^{2}x 10^5 DRY	AREA FT^{2}x 10^5 WET
10	0.05	0.0008	1.95	58.0
20	0.19	0.0038	2.23	67.5
30	0.51	0.011	2.45	73.0
40	1.20	0.029	2.65	78.2
50	2.60	0.068	2.80	83.5
60	5.80	0.16	3.00	88.3
70	14.00	0.40	3.18	94.0
80	37.00	1.25	3.40	100.0
90	150.00	5.00	3.70	109.0

TABLE III

PROBABILITY AT 10 YEARS FOR PEAK CONCENTRATION AND AFFECTED AREA

%time less than	TOC (mg/l) DRY	TOC (mg/l) WET	AREA $FT^2 x 10^5$ DRY	AREA $FT^2 x 10^5$ WET
10	0.024	0.000082	4.45	132.0
20	0.096	0.00041	4.85	146.0
30	0.26	0.00125	5.15	155.0
40	0.60	0.0036	5.40	163.0
50	1.35	0.0095	5.64	170.0
60	3.00	0.025	5.87	178.0
70	7.00	0.070	6.13	186.0
80	19.0	0.24	6.42	195.0
90	78.0	1.30	6.85	208.0

TABLE IV

PROBABILITY AT 20 YEARS FOR PEAK CONCENTRATION AND AFFECTED AREA

%time less than	TOC (mg/l) DRY	TOC (mg/l) WET	AREA $FT^2 x 10^6$ DRY	AREA $FT^2 x 10^6$ WET
10	0.0082	0.000005	0.98	23.0
20	0.035	0.000042	1.06	24.5
30	0.10	0.00021	1.12	25.6
40	0.25	0.00076	1.17	26.5
50	0.60	0.0025	1.22	27.4
60	1.4	0.0086	1.26	28.2
70	3.6	0.033	1.32	29.1
80	11.0	0.16	1.38	30.2
90	50.0	1.3	1.46	31.6

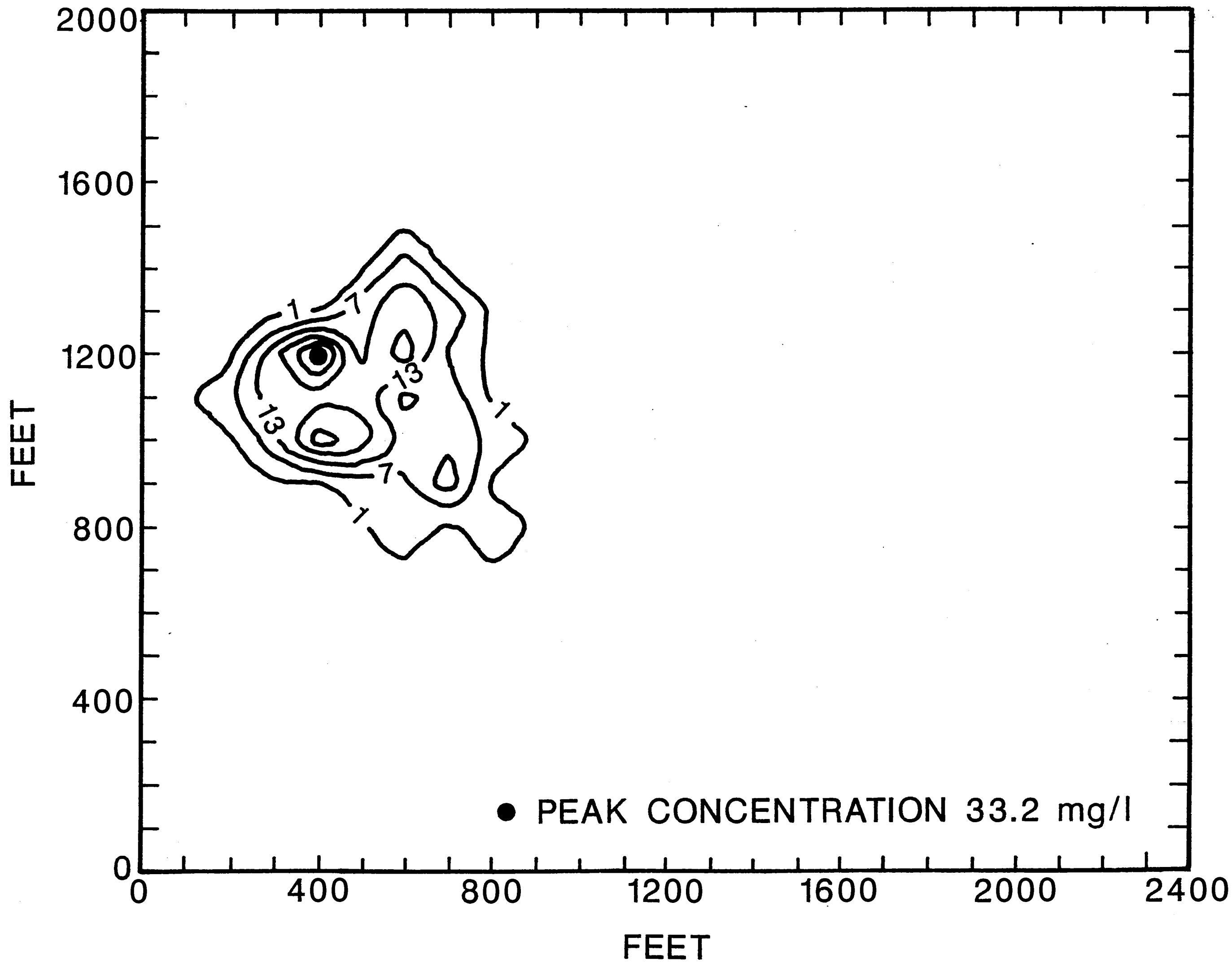

Figure 13. Contour Map of Dry Site Concentration (mg/l) at 5 Years

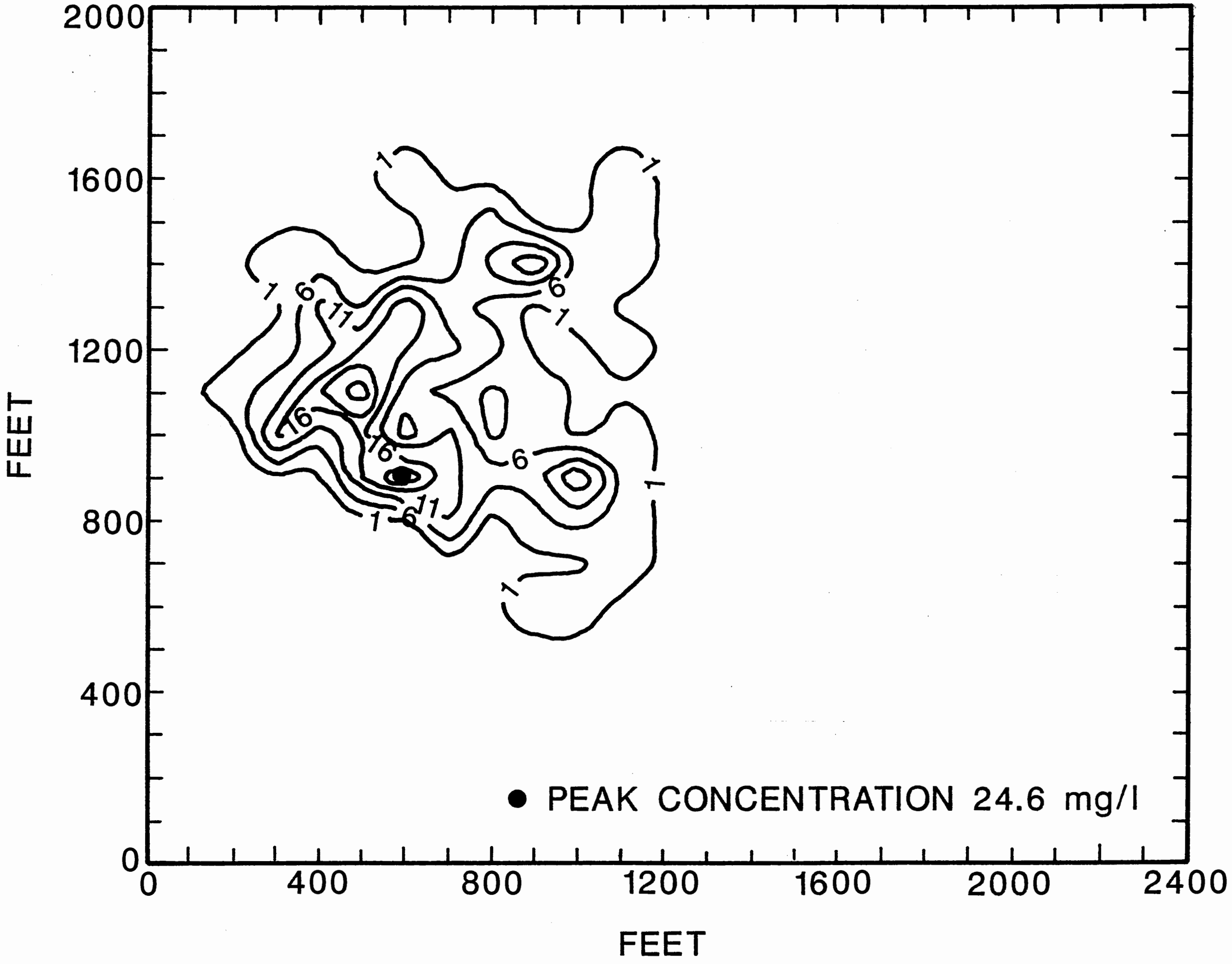

Figure 14. Contour Map of Dry Site Concentration (mg/l) at 10 Years

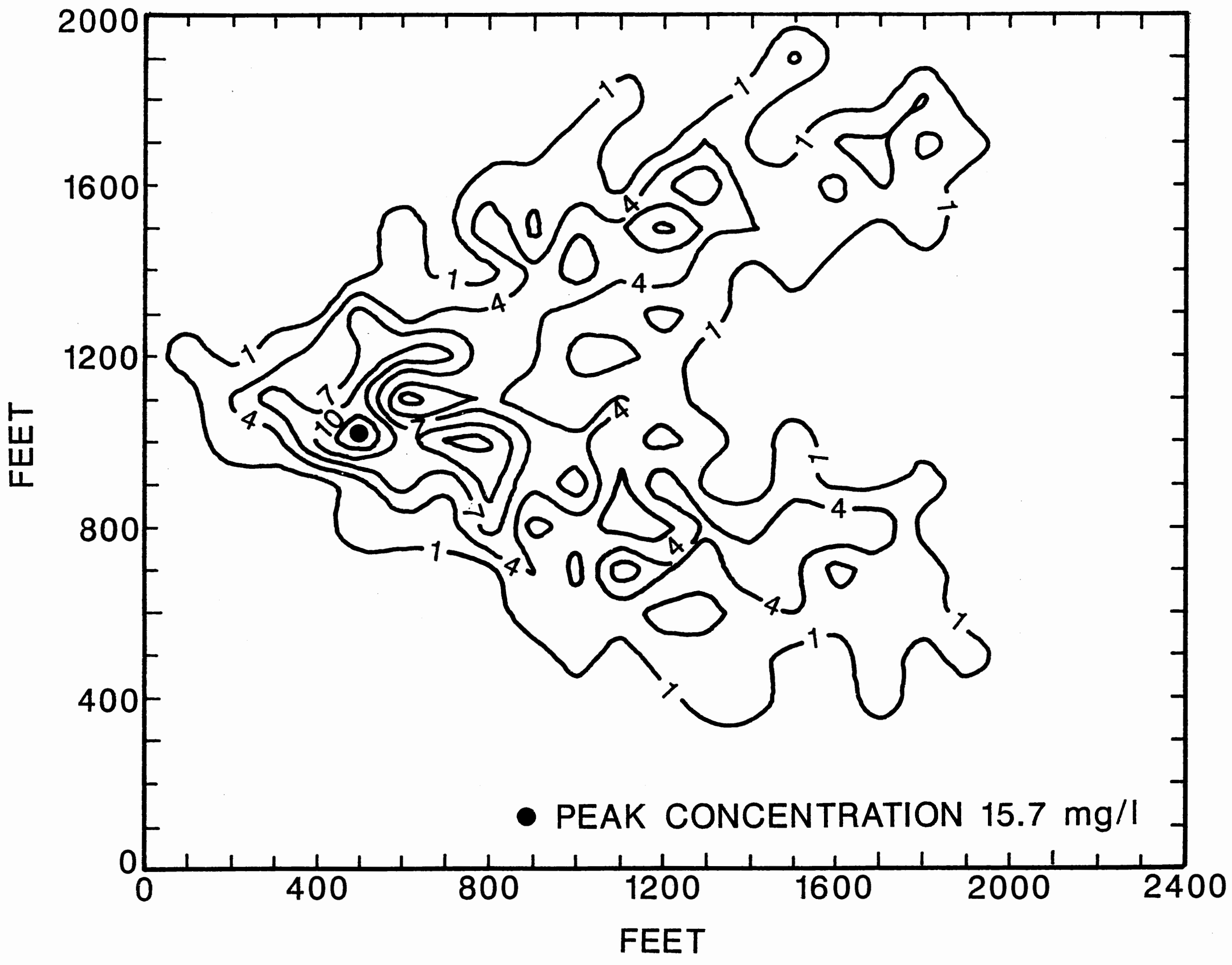

Figure 15. Contour Map of Dry Site Concentration (mg/l) at 20 Years

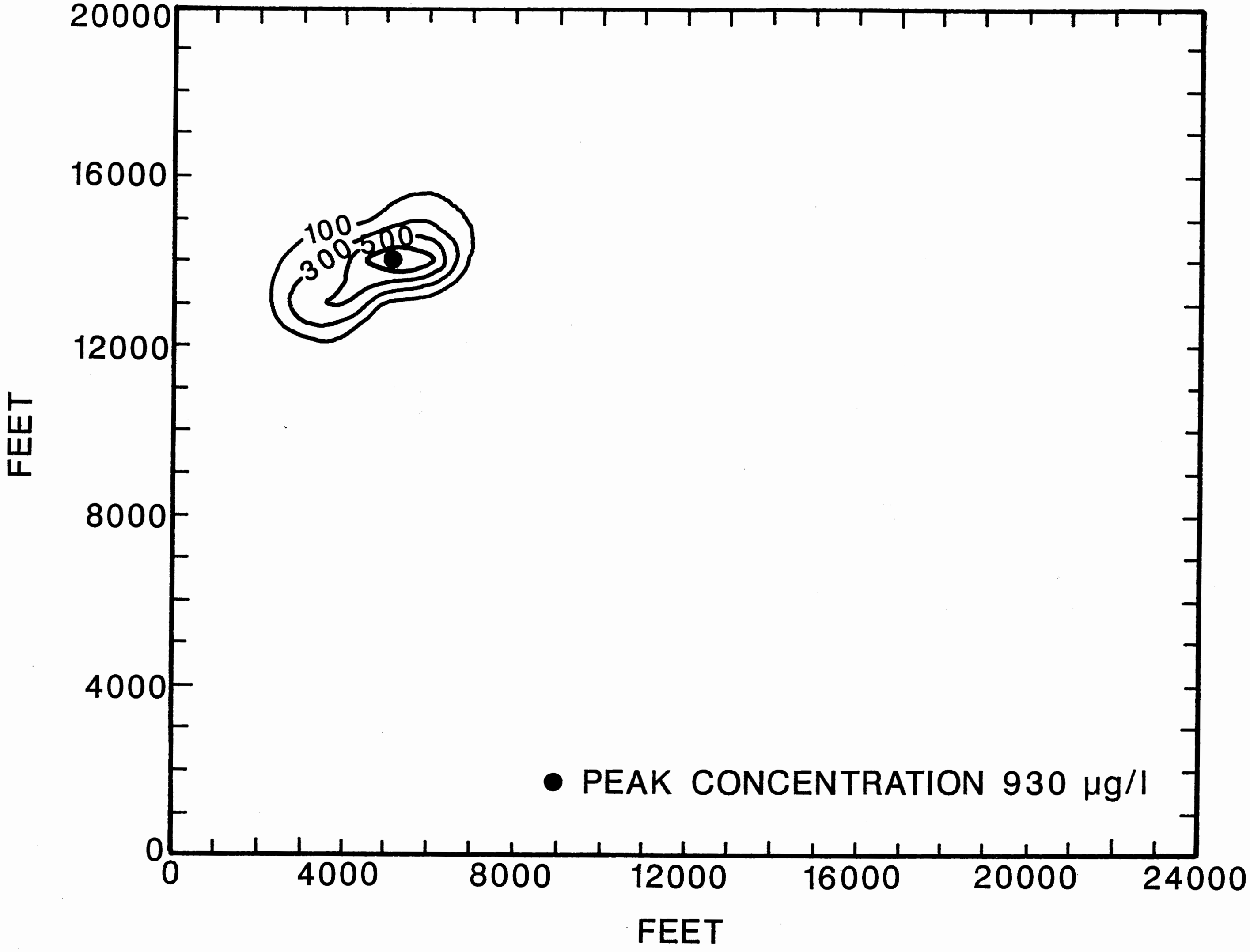

Figure 16. Contour Map of Wet Site Concentration (µg/l) at 5 Years

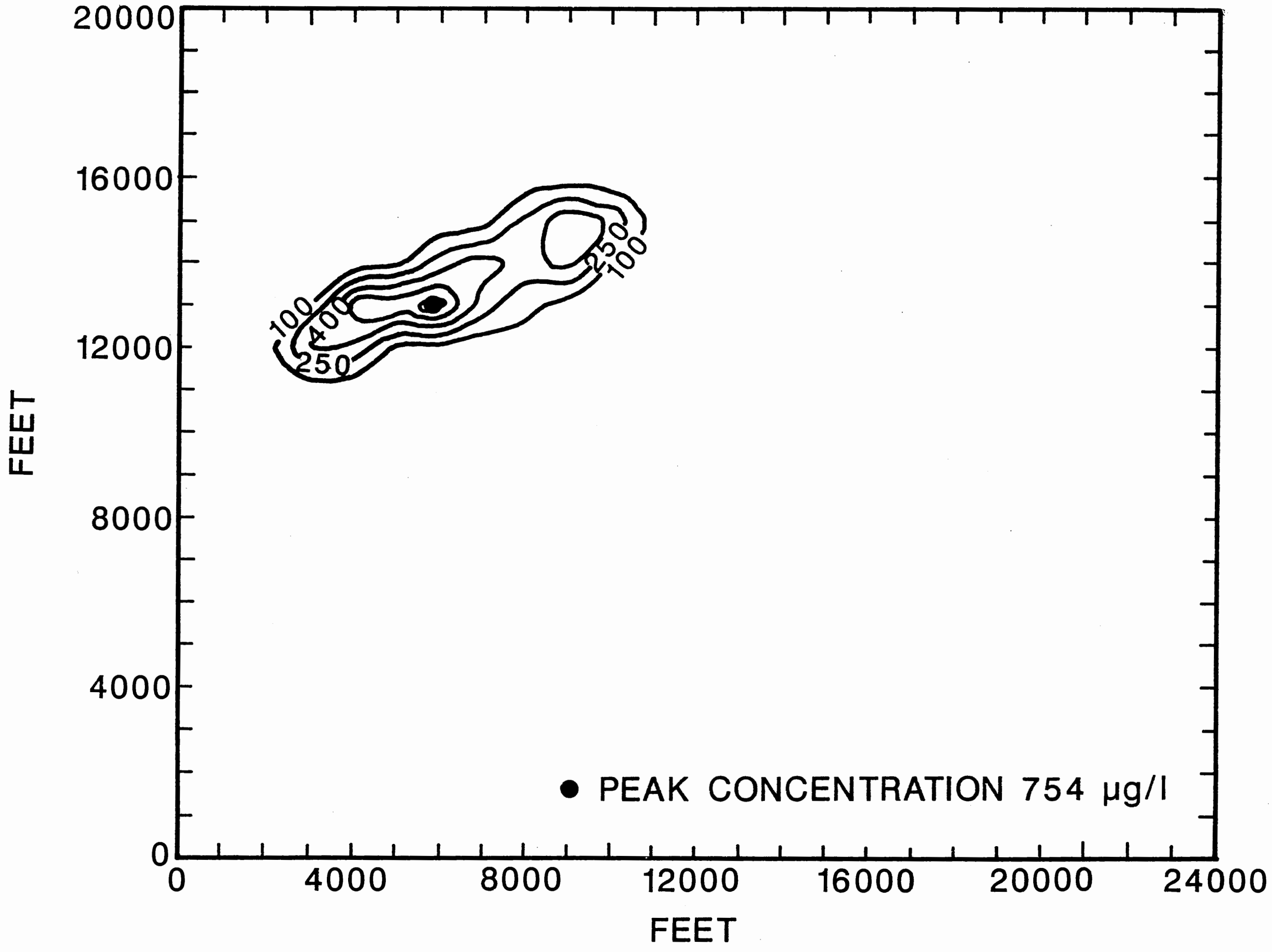

Figure 17. Contour Map of Wet Site Concentration (µg/l) at 10 Years

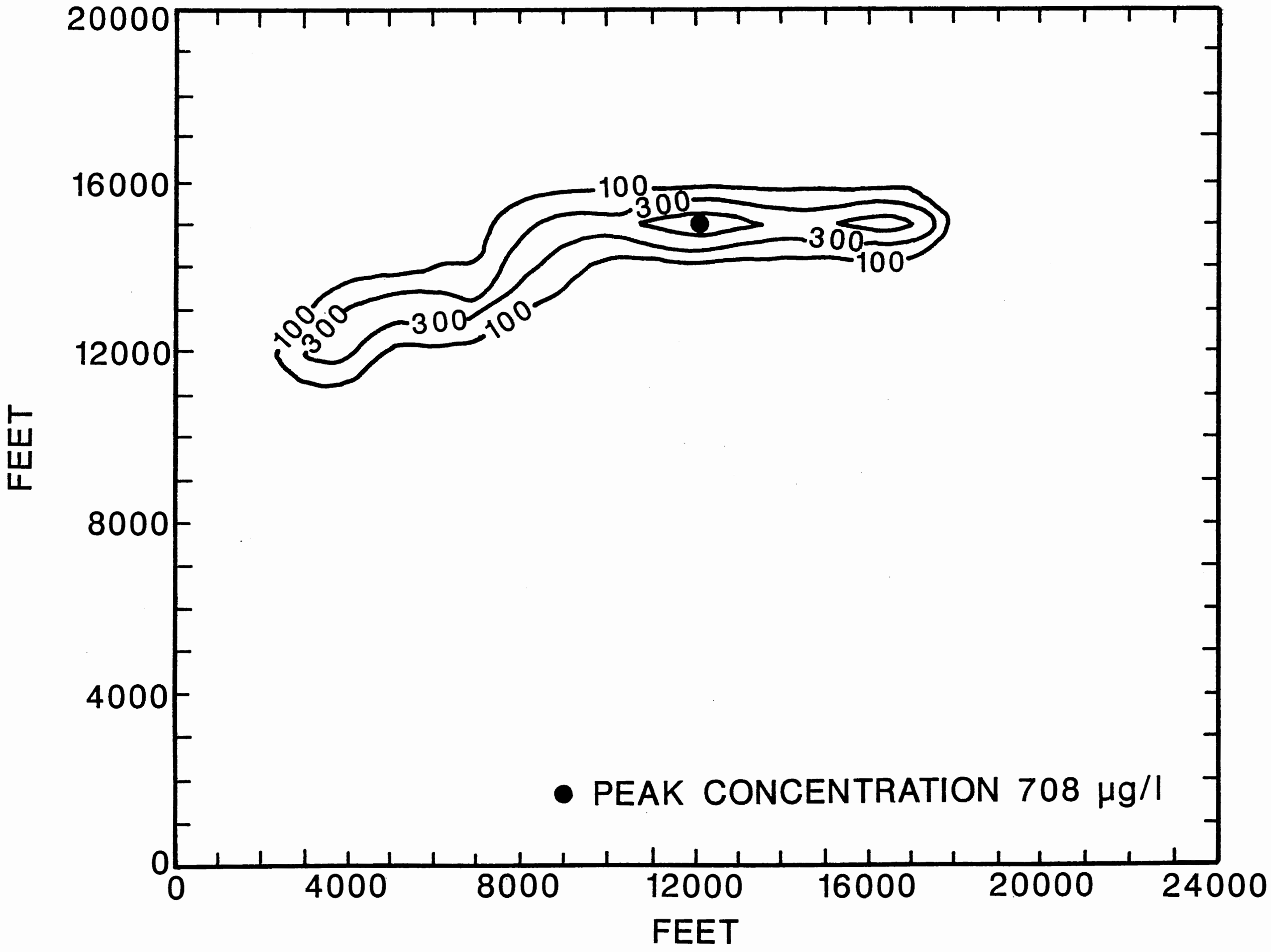

Figure 18. Contour Map of Wet Site Concentration (µg/l) at 20 Years

CHAPTER IV

DISCUSSION

Both the dry and wet sites would be considered at risk to groundwater contamination from the phenols produced during the UCG process. The magnitude of this risk can be determined by comparison of the results. It was found that as simulation time increased, peak concentration values decreased as was expected based on the biological decay, dispersion and retardance effects. For the dry site, after 5 years, 50% of the time the TOC peak concentration would be less than 2.6 mg/l, after 10 years it would be less than 1.35 mg/l and at 20 years it would be less than 0.60 mg/l (Fig. 19). The wet site peak concentration not only decreased with time but was substantially less than the dry values. After 5 years, 50% of the time, the TOC concentration was less than 0.0095 mg/l and at 20 years the concentration was less than 0.0025 mg/l (Fig. 19).

The opposite results were found for affected area values. The affected area increased with time but the wet site exhibited much higher contaminated area than the dry site. For the wet site after 5 years, 50% of the time, the affected area would be less than 8,350,000 ft^2 while at 10

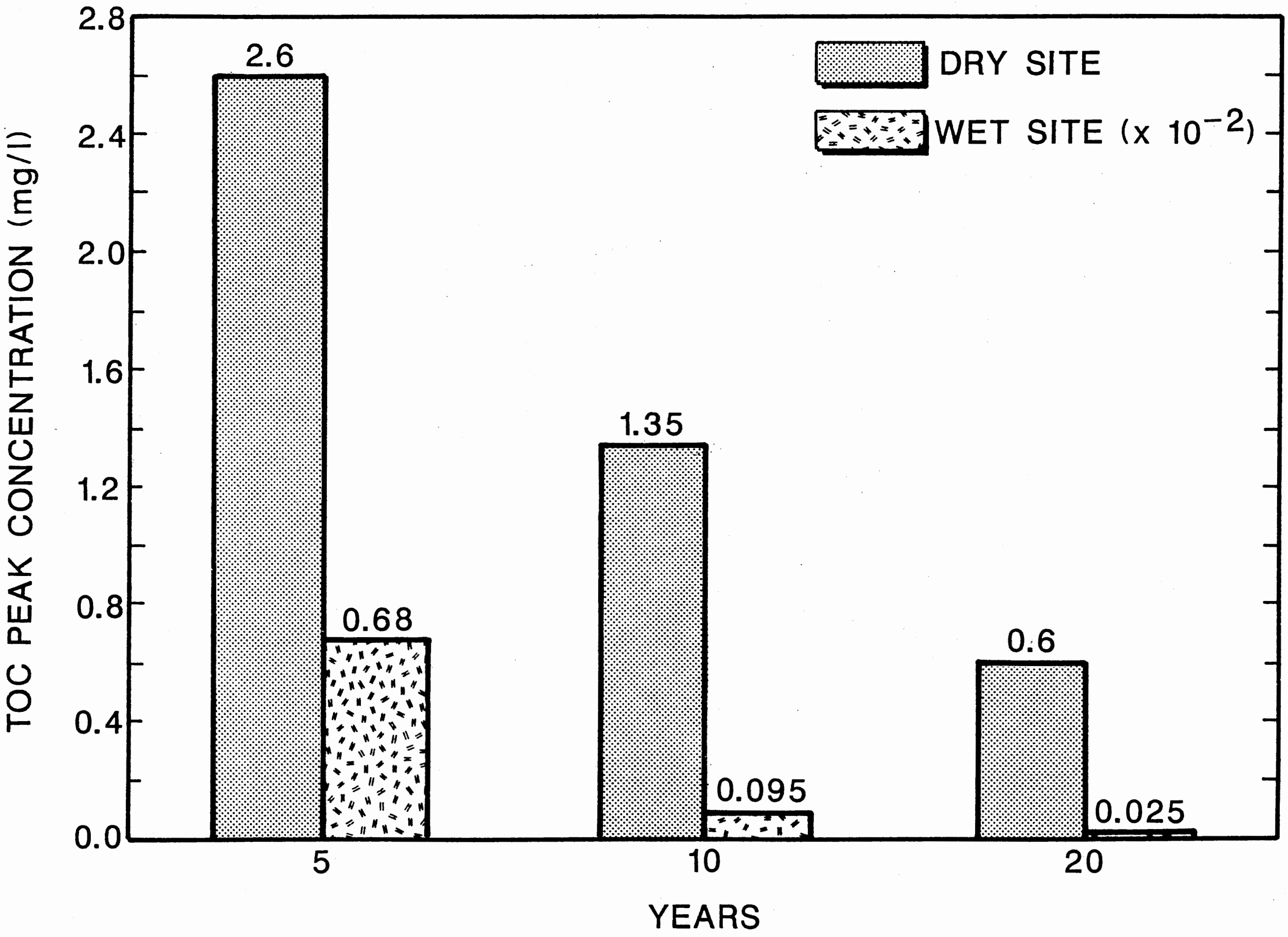

Figure 19. TOC Peak Concentration Results at 50 Percentile

years it would be less than 17,000,000 ft^2 and at 20 years it would be less than 27,400,000 ft^2 (Fig. 20). The dry site output distribution predicted that 50% of the time the contaminated area for 5 years would be less than 280,000 ft^2 at 10 years less than 564,000 ft^2 and a 20 years it would be less than 1,220,000 ft^2 (Fig. 20).

Examining the contour maps, figures 13 through 18, it should be noticed that the peak concentration is carried further away from the burn cavern by the wet velocity than the dry velocity but at a much lesser magnitude. This is attributed to the theory that a higher velocity migrates the contaminant more quickly through the aquifer (8).

Close examination of the plume plots should be made because the different scale and concentration units can be deceiving. The wet site plume width of approximately 2500 feet at 20 years isn't significantly greater than the dry site plume width of 1700 feet. As expected, the wider plume of the wet site more readily decreases the peak concentration, but recovery of the contaminants, if desired, becomes more difficult (8). It can also be seen that the distance of contaminant migration is much greater for the wet site at 14,000 feet at 20 years compared to the migration distance of 1500 feet for the dry site.

Though the results at 50% probability indicate that the wet site is at a greater risk for contaminated area and to a higher distance of migration, much of the concentration

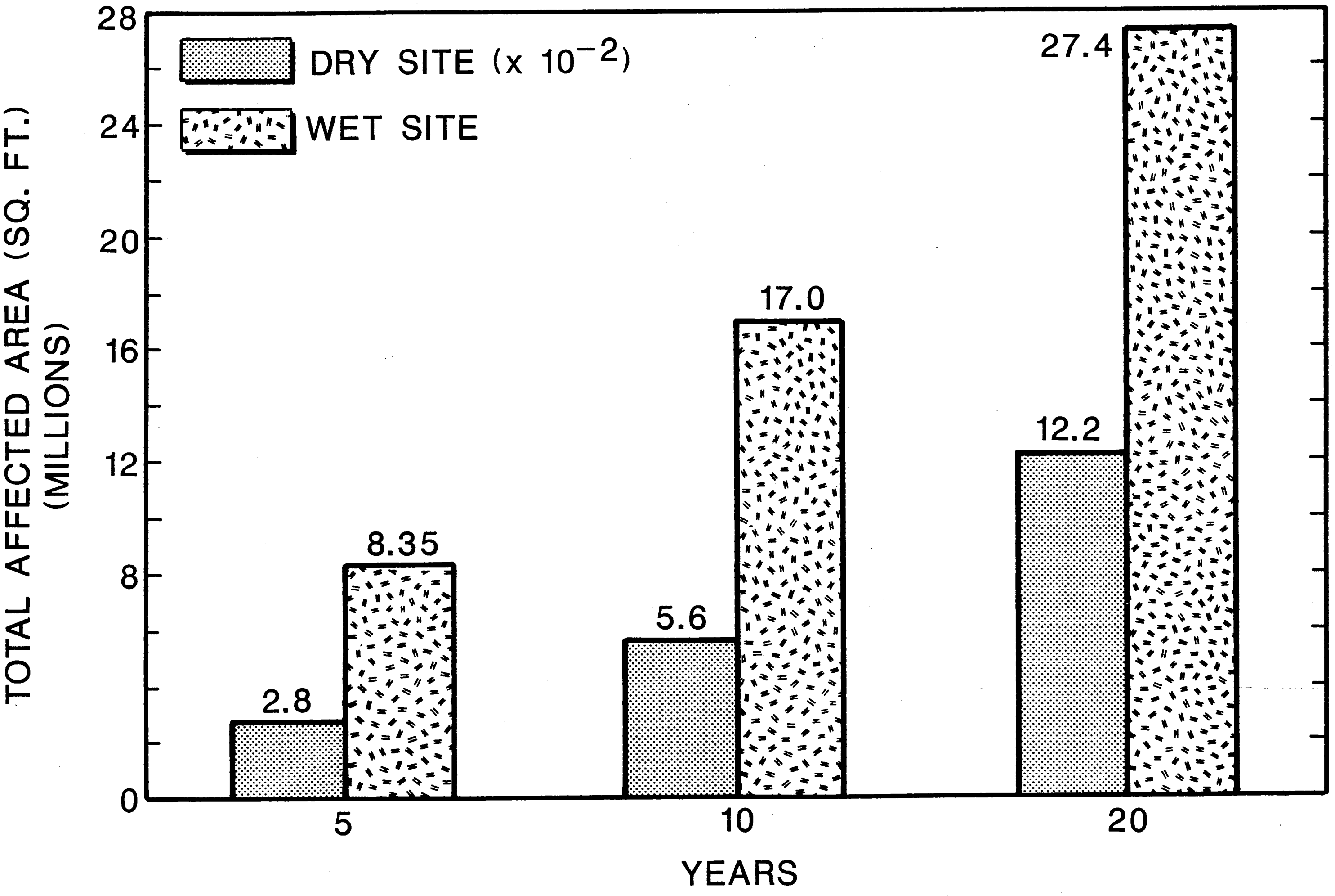

Figure 20. Total Affected Area Results at 50 Percentile

found at the wet site is insignificant, assuming a practical detection limit for the analysis techniques of contaminants approximates 1 μg/l or 0.001 mg/l. At 50% probability the 5 year concentration value for the wet site (0.068 mg/l) is detectable but at 20 years, 0.0025 mg/l, it is questionable if the contaminant could be detected. At 20 years there is over a 50% probability that the contaminant will not be detected in the aquifer at the wet site (Table IV).

This observation is favorable compared to the results of the dry site. Analysis of the dry site showed that peak concentration is at detectable levels for all probabilities except the value for the 10% level, 0.0082 mg/l, at 20 years (Tables II, III & IV). Based on these findings it appears that the natural restoration properties are more effective at the wet site than the dry site. Therefore the risk of significant contamination to the coal aquifer is greater at the dry site than the wet site.

CHAPTER V

SUMMARY

In summary, a procedure for evaluating the uncertainty of groundwater contamination has been applied to the Underground Coal Gasification process. A generic analysis of UCG groundwater contamination risk using site specific data as input was applied to a dry and wet site. Once the water in the resulting UCG cavern has reached regional groundwater flow levels, chemically altered contaminants, in particular phenols, flow into the groundwater system. The variables most affecting the contaminant transport are groundwater velocity, initial concentration, retardance, dispersion and biological decay.

The greatest uncertainty is associated with decay, retardance, concentration and dispersion. This uncertainty was handled by completing a Monte Carlo Simulation. In this study, dispersion was randomized by the "Random-Walk" Solute Transport Model (18). Initial concentration was randomized as input and then randomly generated by the model. Biological decay, for the source and the system, and retardance were randomly generated for input. The pollutant masses were then allowed to disperse, adsorb and decay along groundwater flow paths for 20 years. The repeated simulations produced data that were evaluated for a constant value at an appropriate probability level as assurance that the uncertainty had been regulated. Within each time period all the data were used to assess the risk by creating probability distributions for two conditions, peak concentration and affected area.

It was found that at the same probability level the wet site would have a higher value for affected area than the dry site. While for peak concentration the dry site output distributions resulted in higher values than for the wet site. Fifty percent of the time the concentration values at the wet site were found to be below detection limits.

It should be stressed that as with any modeling study, worth of the results is dependent on the input and the capabilities of the model. The results of modeling can be used to indicate additional data needed to improve predictions or strengthen conclusions. Modeling, used as a management tool, can be valuable in evaluating source control versus system control and analyzing cleanup and/or restoration procedures. Knowing the probability of extent and level of contamination can aid in the evaluation process.

REFERENCES

1. Bartel, L. C., "Site Characterization-Geophysical R & D Needs,"Proceedings of the Eighth Annual Underground Coal Conversion Symposium, 1982, pp. 449-455.

2. Carsel, R. F., Parrish, R. S., Jones, R. L., Hansen, J. L., and Lamb, R. L., "Characterizing the Uncertainty of Pesticide Leaching in Agricultural Soils", accepted in the Journal of Contaminant Hydrology, 1988.

3. Contractor, D. N., and Davidson, S. C., "Simulation of Groundwater Flow Regimes in a Coal Seam with UCG Cavities Using a Finite Element Model,"Proceedings of the Ninth Annual Underground Coal Gasification Symposium, 1983, pp. 512-515.

4. Dalton, V. A. and Campbell, J. H., "Laboratory Measurements of Groundwater Leaching and Transport of Pollutants Produced During Underground Coal Gasification," In Situ, 2(4), 1978, pp. 295-328.

5. Daniel, J., "Underground Coal Gasification," The Mining Claim, June, 1984.

6. Edgar, T. F., Humenick, M. J., Kaiser, W. R., and Charbeneau, R. J.,"Environmental Effects of In Situ Gasification of Texas Lignite," Report PB-81-171654, Mar., 1981.

7. Humenick, M. J., and Mattox, C. J., "Characterization of Condensates Produced During Underground Coal Gasification," In Situ, 6(1), 1982, pp. 1-17.

8. Humenick, M. J., and Novak, A. E., "Parametric Analysis of Pollutant Migration Following In Situ Gasification of Lignite, In Situ, 2(4), 1978, pp. 329-352.

9. Hutchinson, H. L., Boyd, R. M., and Fischer, D. D., "Hydrologic Characterization for Hanna III," Proceedings of the Third Annual Underground Coal Conversion Symposium, 1977.

10. Krakow, I., Lotus 1-2-3: Self Taught on the IBM PC, Prentice-Hall, New York, NY, 1985.

11. LaFleur, D. W., Grisak, G. E., Avis, J. D., Stetzenbach, K. J., and Thompson, G. M.,"Evaluation of the Porosity of the Hanna No.1 Coal Seam," US Department of Energy Report DE-AS20-83LC10987,1984.

12. Manahan, S. E., Bornhop, D., Farrier, D. S., Sheesley, D. C., and Poulson, R. E., "Interaction of Contaminated Water and Solid Material By-Products from In Situ Coal Gasification: Implications for Pollution Control Technology,"Proceedings of the Sixth Annual Underground Coal Gasification Symposium, 1980.

13. Mason, J. M., Oliver, R. L., Schreiber, J. D., Moody, C., Smith, P., and Healy, M. J., "Geohydrology of the Proposed Rocky Mountain 1 Underground Coal Gasification Site, Hanna, Wyoming," US Department of Energy, Laramie, Wyoming, 1987.

14. Mead, W., and Raber, E., "Environmental Controls for Underground Coal Gasification: Ground-Water Effects and Control Technologies," Lawrence Livermore Laboratory, 1980.

15. Mercer, J. W., Silka, L. R., and Faust, C. R., "Modeling Ground-Water Flow at Love Canal, New York," Journal of Environmental Engineering, Vol. 109, No.4, pp. 924-943.

16. McTernan, W. F., and Quimby, W. F., "Application of Groundwater Modeling Techniques to the Hanna, Wyoming, Underground Coal Gasification Site," US Department of Energy, Laramie, Wyoming, 1984.

17. Prickett, T. A., and Lonnquist, C. G., "Selected Digital Computer Techniques for Groundwater Resource Evaluation," Bulletin 55, Illinois State Water Survey, Champaign, Illinois, 1971.

18. Prickett, T. A., Naymik, T. G., and Lonnquist, C. G., "A 'Random-Walk' Solute Transport Model for Selected Groundwater Quality Evaluation," Bulletin 65, Ilinois State WAter Survey, Champaign, Illinois, 1981.

19. Schowengerdt, R. W., "Analysis of the Potential for Contaminant Migration at the Hanna Underground Coal Gasification Site, Hanna, Wyoming," US Department of Energy, Laramie, Wyoming, 1984.

20. Walters, E. A., and Niemczyk, T. M., "The Effect of Underground Coal Gasification on Groundwater," Department of Chemistry, University of New Mexico, 1983.

21. Way, S. C., and McKee, C. R., "Restoration of In-Situ Coal Gasification Sites from Naturally Occuring Groundwater Flow and Dispersion," In Situ, 5(2), 1981, pp. 77-101.

22. Yeh, G. T., "AT123D: Analytical Transient One-, Two- and Three-Dimensional Simulation of Waste Transport in the Aquifer System," Environmental Sciences Division, Department of Energy, Publication No. 1439, March, 1981.

APPENDIX A

OTHER APPLICATIONS

Introduction

There is an increasing concern for the impact of pesticide application on groundwater quality. There have been studies done on the probability that the pesticide will reach the groundwater (2) but the fate of the pesticide, if it reaches the saturated zone, must also be analyzed.

This study was completed to establish a procedure for evaluating the risks of groundwater contamination associated with the use of pesticides in Oklahoma. The procedure utilizes the numerical "Random-Walk" Solute Transport model revised to include biological decay (Appendix C) and the analytical AT123D Solute Transport model (22). The effects of natural control to the groundwater quality, biological decay, retardance and dispersion, were included.

The objectives of the work were to simulate the transport of pesticides through saturated aquifers. This problem involves a three dimensional movement of pesticides into and through the aquifer until the saturated thickness is filled with pesticide. Continued transport after this aquifer filling stage is also three dimensional but may in some cases be simulated by a two dimensional model if the pesticide concentration in the vertical is assumed homogeneous. In this way a surface area - two dimensional model can approximate this problem.

This report presents discussions concerning the linkage of the various saturated-unsaturated codes as well as presenting results which represent select conditions beneath Oklahoma winter wheat fields.

Modeling

Vertical Transport

Random-Walk Model

The two-dimensional Random-Walk model simulates a three dimensional problem. The 2D model is in the horizontal plane in the x and y directions and the third dimension is represented by the z component or the thickness of the aquifer, where homogeneity is assumed. This assumption has been appropriate when only flow was simulated. The vertical mixing of soluble contaminants as well as the movement of immiscible fluids or those of densities differing from water require that a depth or vertical dimension be included in the analysis. To observe transport in the vertical it is necessary to either use a 3 dimensional model or perform the two dimensional analysis in cross-section by turning the model on its side. This involves making x and z, length and thickness, the two directions modeled, while the y component or width becomes the thickness used. In this way, this thickness is simultaneously infinitely thin and representative of all comparable vertical slices through the aquifer.

The bottom of the aquifer, in the z direction, is modeled as a no flow boundary by setting the hydraulic conductivity and transmissivity equal to zero. The top of the aquifer or water table can also be modeled as a no flow barrier on either side of the contaminant source. This source is generated by either actual data or by linking the saturated zone Random-Walk code to a one or more dimensional unsaturated zone transport model. The source has units of mass per surface area, where the surface area is that equal to the original field plot receiving pesticides. The mass is that applied at the land surface less any transmission losses through the unsaturated zone.

The length of the finite difference grid in the z direction will be the same as the thickness of the saturated zone. The source is input as a line by utilizing the pollutant generation GENP(PL) subroutine. The length of the source line will be one side of the area to which the pesticide was applied. The width of the application area is depicted in the thickness term used by the model. The source area can either be the actual affected region or a unit area for comparison.

Velocities in both the x and z direction are required. The values can be determined based on the vertical hydraulic gradient, hydraulic conductivity in the x and z directions and porosity. The storage coefficients for both water table and confined aquifer conditions are required.

The thickness value can either be the actual width of the application area (y direction) or a unit width. The effect of this input will be detected in the concentration values. The length of the line source is the length of the source area in the x direction. The longitudinal and vertical components of dispersion are needed. For the model it is assumed that the pesticide is totally miscible, driven by dispersion.

After several attempts at modeling in the vertical plane, the AT123D model was preferred over Random-Walk. The vertical cross-section in Random-Walk created input data difficulties. The value R for recharge became the y velocity while the velocity the model calculates in the y direction is actually the recharge value. Since most geohydrologic data are recorded in the horizontal plane the validity of the vertical input data are questionable. When these features were coupled with the deficiencies associated with this 2 dimensional, quasi-3D approach, it was decided to use the true 3D model, AT123D.

AT123D Model

The AT123D model can simulate in one, two or three dimensions. The solute transport includes the effects of biological decay, retardance and dispersion. There are four types of source configurations: point, line, area and volume. The model can handle infinite or finite depth and width. The source can be released continuously, instantaneous or of finite duration.

The three dimensional modeling is accomplished by simulating vertical as well as horizontal flow of the aquifer. The results are presented in the horizontal plane as slices of the aquifer at various depths (z). The solute is assumed to be totally miscible and driven by dispersion in the vertical direction.

The application of AT123D to a contamination problem requires the geometry of the region, the dispersion coefficients, geohydrologic properties, retardation data, biological decay and source strength and configuration.

Linkage

The source concentration or amount of pesticide that will leach to the groundwater must be determined. The amount of pesticide, the crop and tillage practices are all factors that effect the amount of leaching as well as the pesticide characteristics (2). The various combinations of these factors creates an uncertainty in the source concentration. The use of an unsaturated zone transport model, such as the Pesticide Root Zone Model (PRZM) and a Monte Carlo Simulation was required to obtain pesticide loadings at the saturated zone (2).

Sample Problem

To illustrate the use and output of the AT123D model a sample simulation was made. Information on pesticide leaching in Oklahoma, obtained from previous work done at Oklahoma State University, was used to simulate vertical transport of a pesticide through the saturated zone.

Table V lists the input values used for the simulation. The source value represents the worst case of pesticide leaching to the water table. Though pesticide loads are given on an annual basis, application is not year round. A six month application time was assumed and the source rate was distributed over this time period using the finite duration source release option.

Flow and solute transport were simulated for 10 years. The results of the solute transport for the simulation are presented in Figures 21, 22, 23, 24 and 25, at depth intervals of 2 meters. Close examination of the results indicate that at 10 years, the pollutant has filled the saturated zone but at extremely low concentration levels. Figures 26 and 27 illustrate three-dimensionally the distribution of pesticide within the aquifer at 2 and 10 meters depth respectively. Figure 28 is a vertical cross-section of the aquifer through the center of the source area at 10 years.

To determine if these concentration values were signi-

TABLE V

INPUT VALUES - SAMPLE PROBLEM

Parameter	Value
Thickness	10 meter
Hydraulic Gradient	0.004
Hydraulic Conductivity	0.0025 m/hr
Porosity	0.20
Soil Bulk Density	1.6 gm/cc
Dispersion	
Longitudinal	10 meter
Transverse	1 meter
Vertical	1 meter
Source	
Area	1 Hectare
Location	x(0,100) y(50,150)
Rate	0.09 kg/ha/yr
Decay Constant	4.167E-05 /hr
Distribution Coefficient, Kd	0.014 m^3/kg

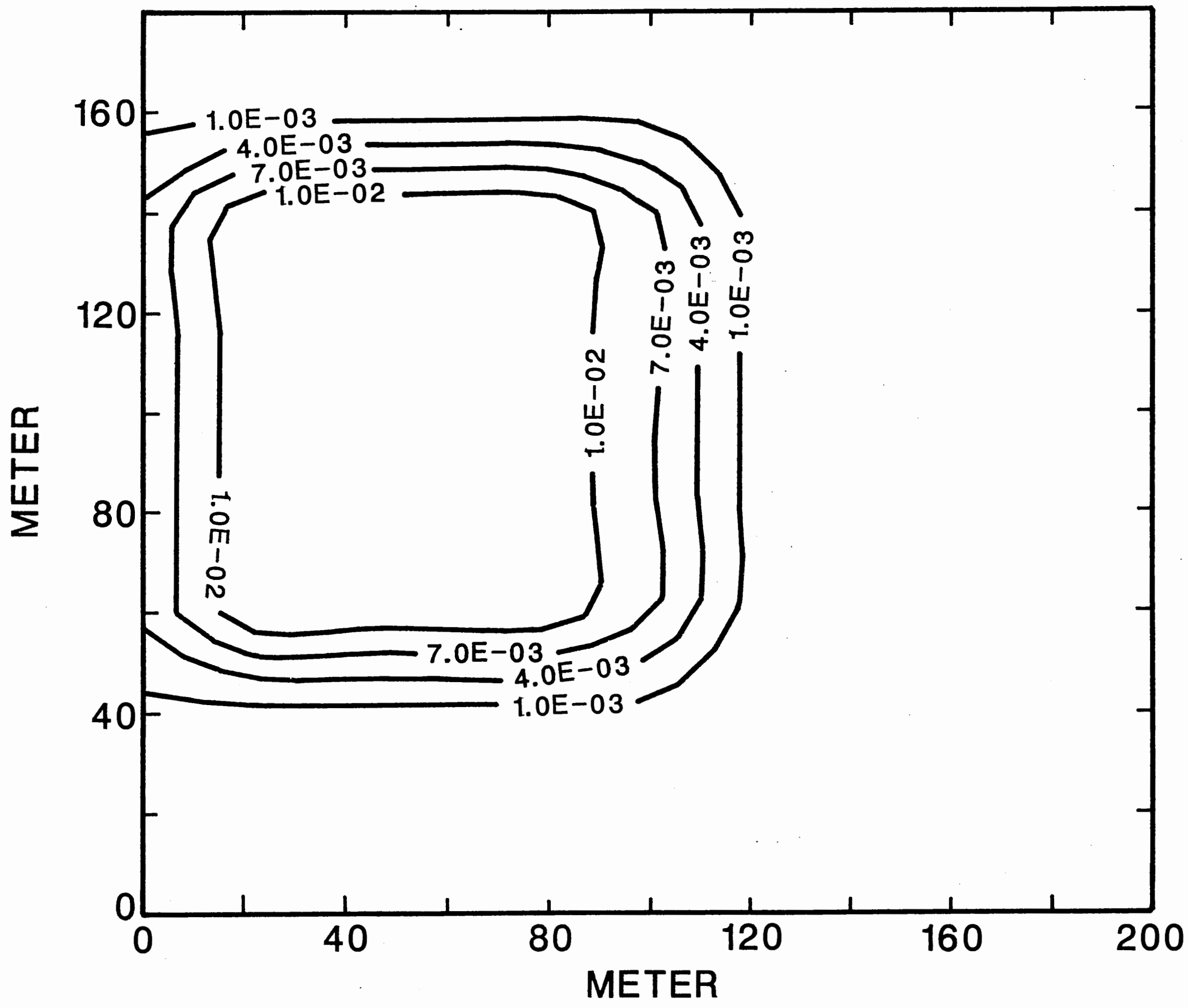

Figure 21. Contour Map of Pesticide Concentration (mg/l) at 2m Depth

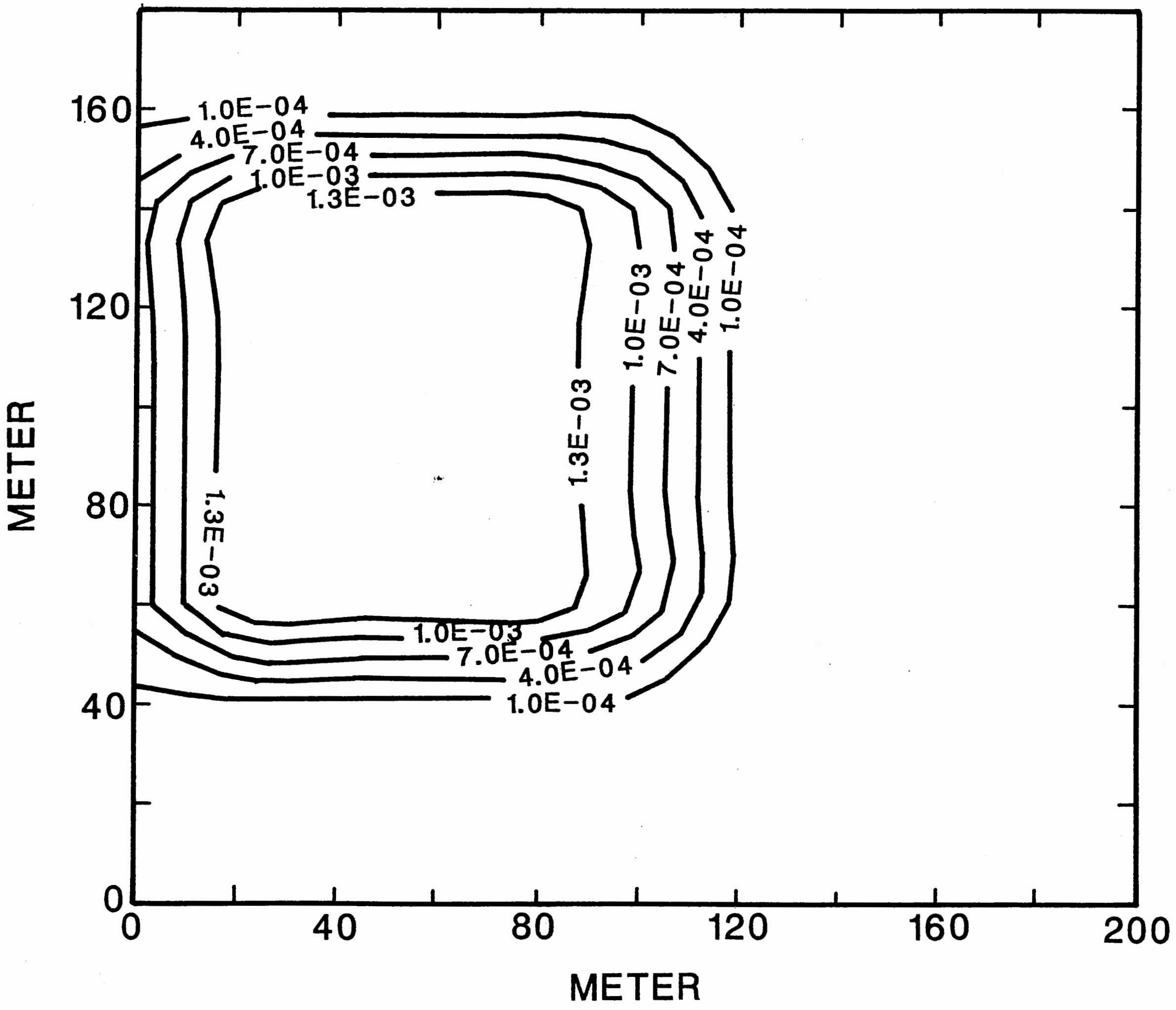

Figure 22. Contour Map of Pesticide Concentration (mg/l) at 4m Depth

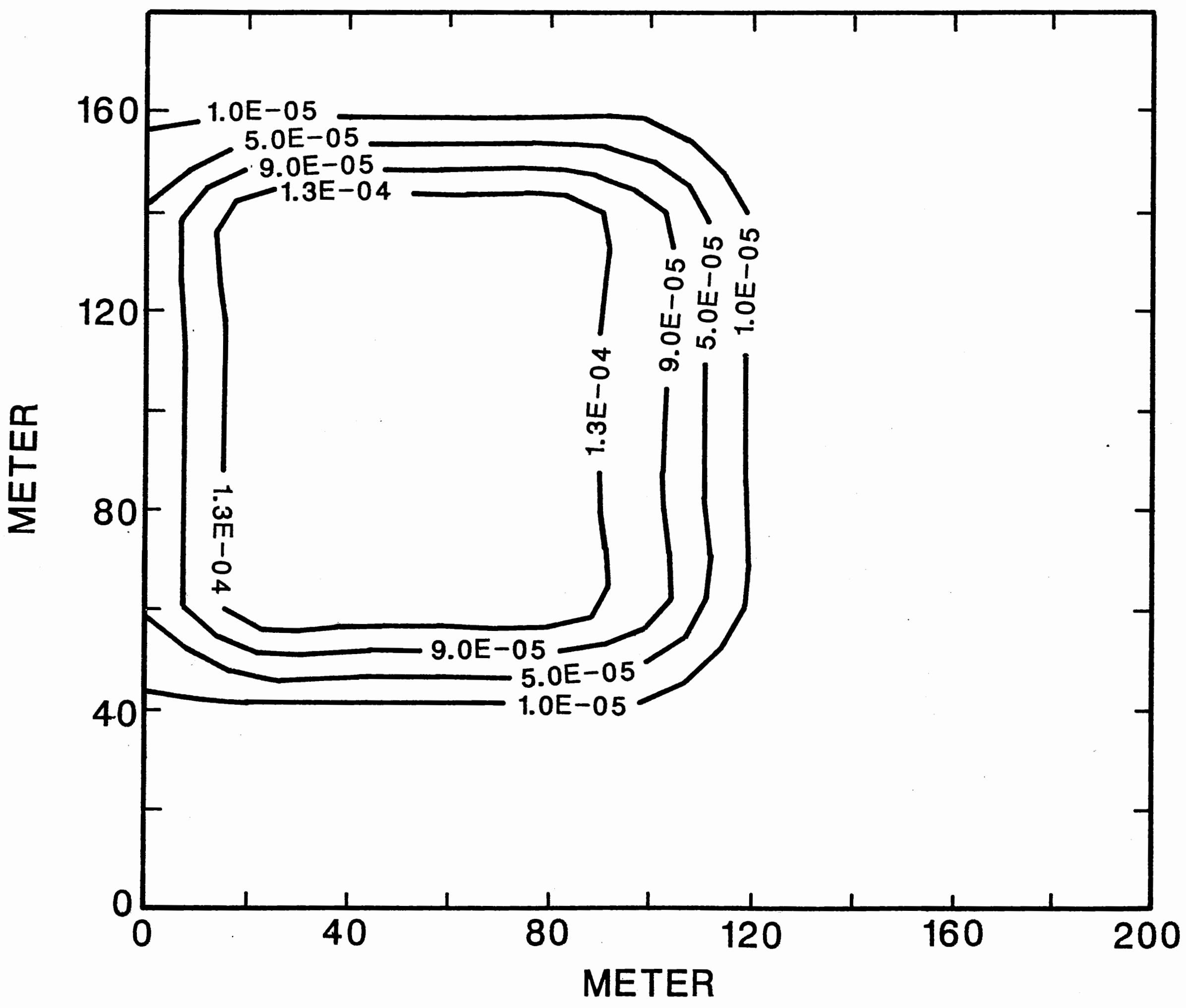

Figure 23. Contour Map of Pesticide Concentration (mg/l) at 6m Depth

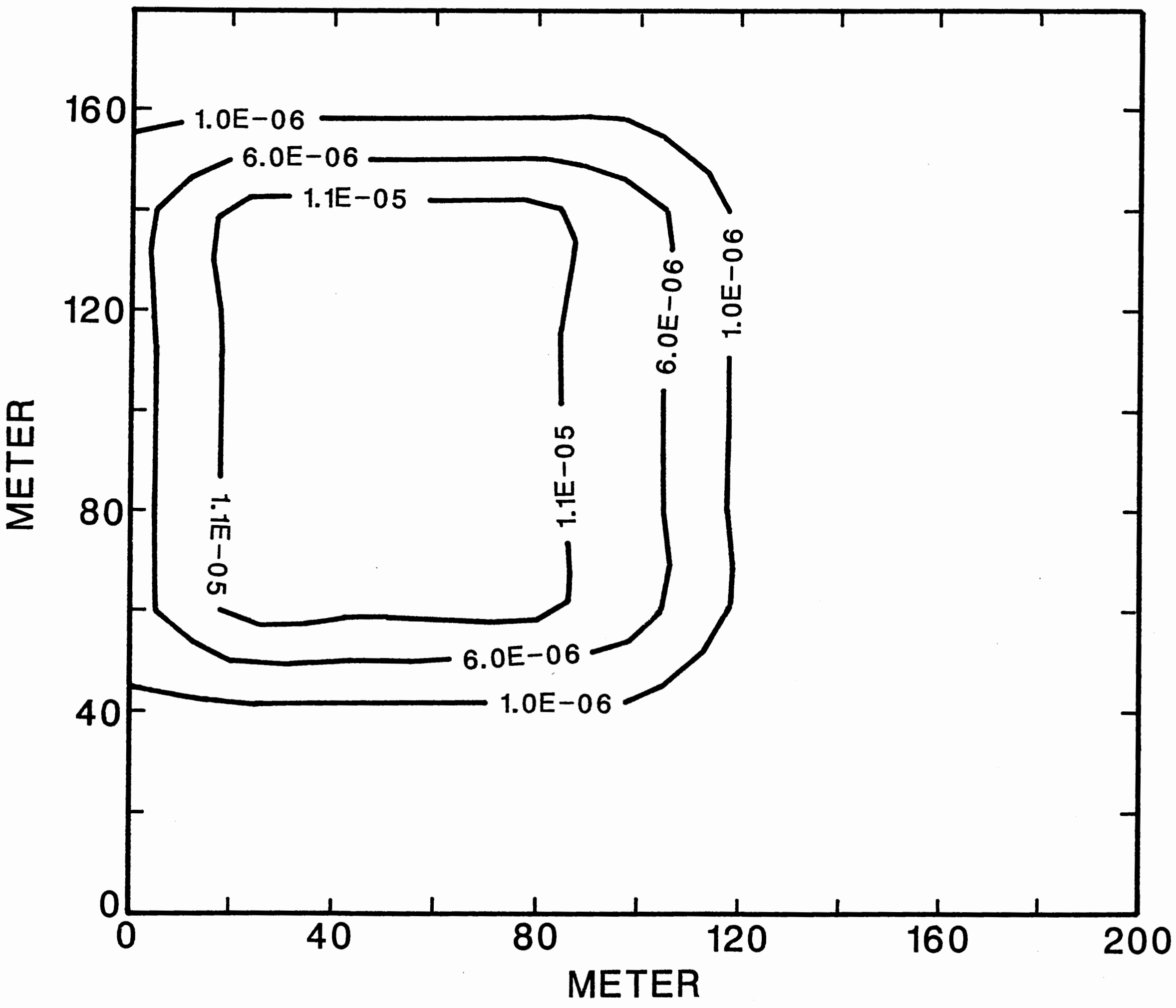

Figure 24. Contour Map of Pesticide Concentration (mg/l) at 8m Depth

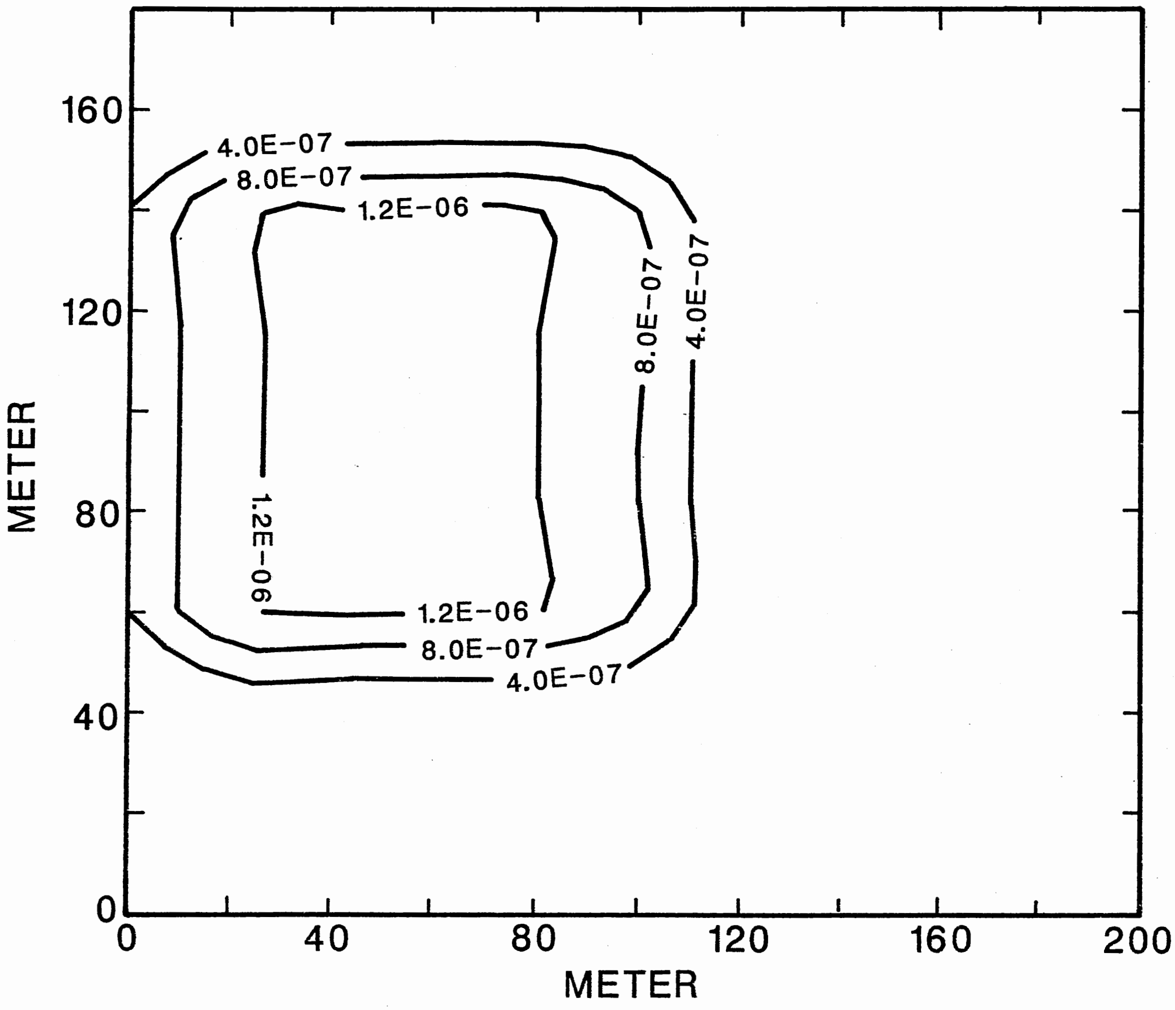

Figure 25. Contour Map of Pesticide Concentration (mg/l) at 10m Depth

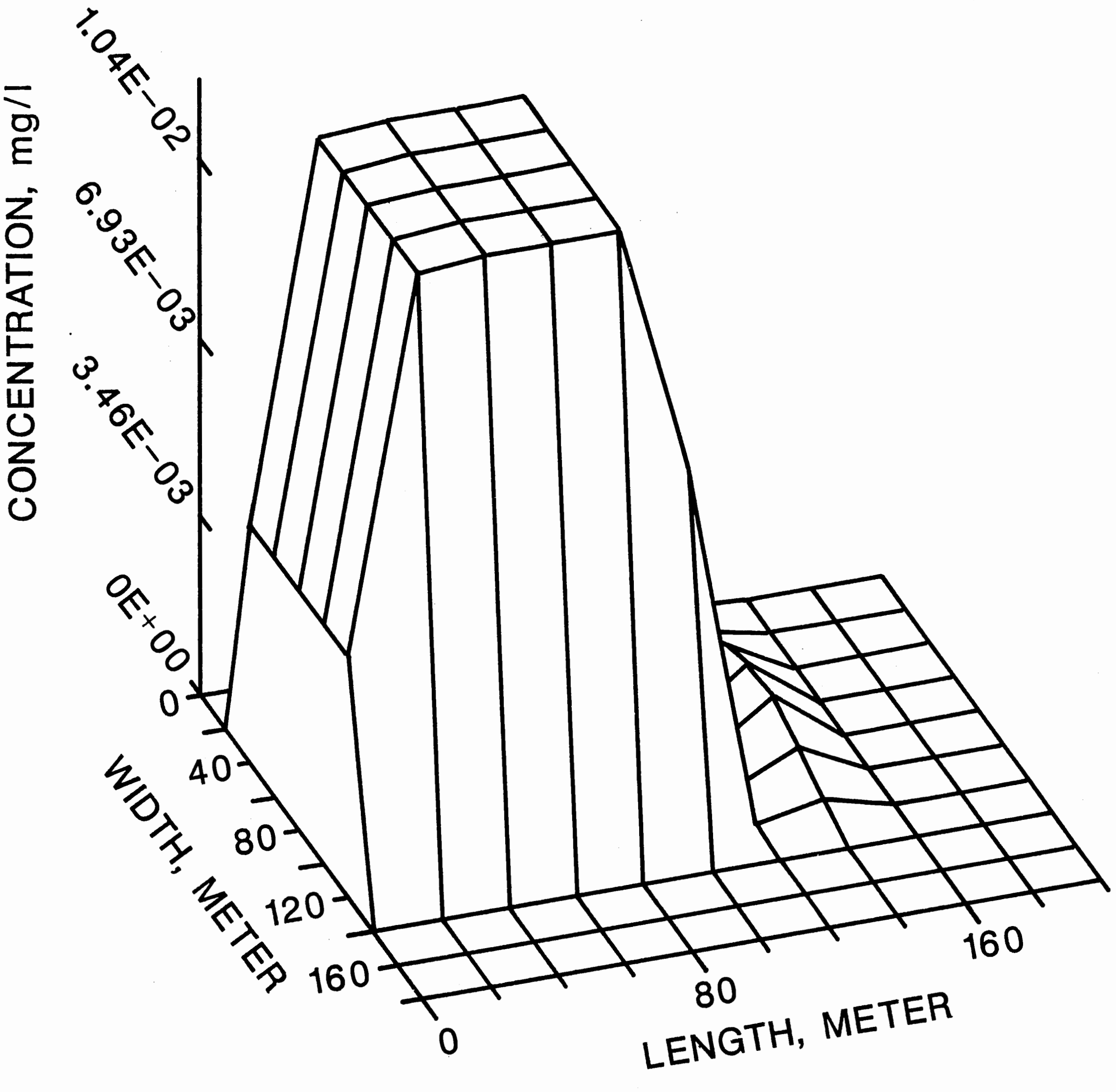

Figure 26. 3D View of Concentration at 2 Meter Depth

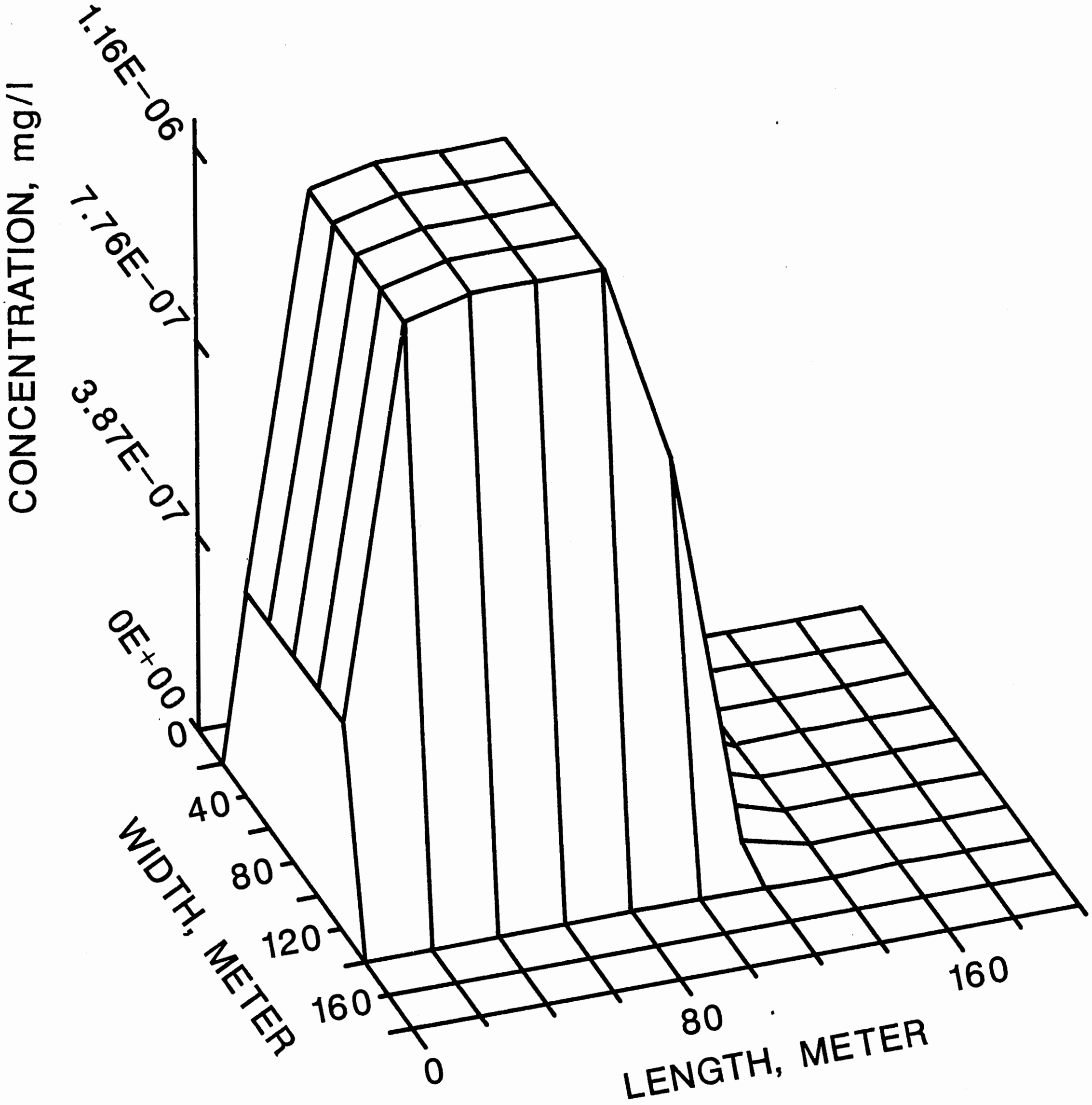

Figure 27. 3D View of Concentration at 10 Meter Depth

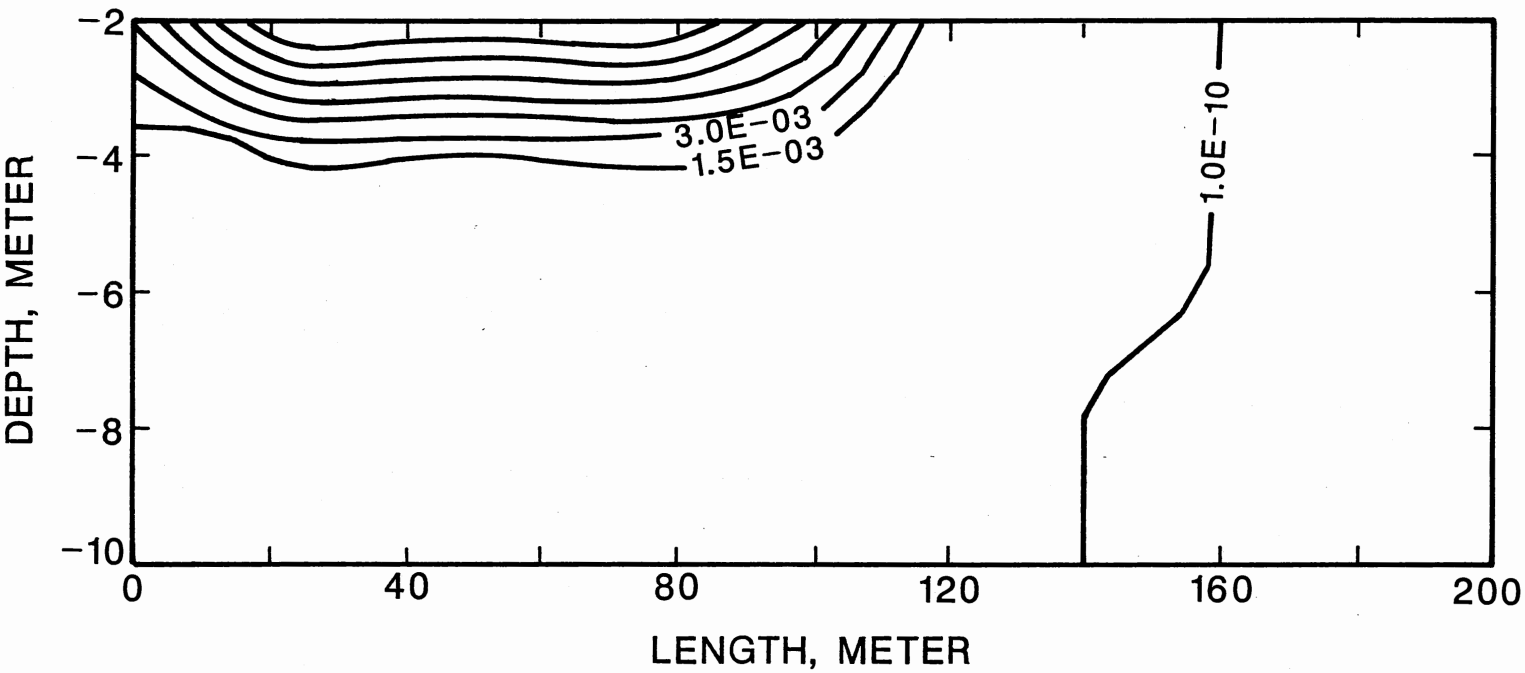

Figure 28. Vertical Cross−Section of Concentration (mg/l) at Center of Source

ficant, the EPA reference doses for typical leaching pesticides used in Oklahoma were accessed. The peak concentration found in the aquifer at the end of 10 years was used to determine the Reference doses. Reference doses have units of mg/kg-day and represent EPA's most current view of risk minimization in the consumption of drinking water. The dose is based upon a person of "average" size (i.e. 70 kg) consuming 2 liters of water per day with a chemical uptake efficiency of 50 percent. Table VI presents the EPA Reference Dose values together with the corresponding values determined from this simulation. The data presented in Table VI show that the Reference dose determined from the simulation is at or below the EPA recommended Reference Doses for pesticides used in Oklahoma.

TABLE VI

REFERENCE DOSES

Pesticide	EPA Recommended Reference Dose (mg/kg-day)	Calculated Reference Dose (mg/kg-day)
Dicamba	0.00013	0.00017
Carbofuran	0.005	0.00017
Propazine	0.005	0.00017
Atrazine	0.00035	0.00017
2,4-D	0.01	0.00017

APPENDIX B

UNDERGROUND COAL GASIFICATION PROCESS

For the possible environmental impacts resulting from the UCG process to be understood there should be some knowledge of the process itself. The gasification of solid coal converts the coal into a gas that can either be burned as a fuel or converted into higher valued products (liquid fuels or chemicals).

In UCG the coal seam itself is used as the reactor as opposed to a large reactor used for conversion at the surface. A minimum of two wells must be drilled into the coal seam, one well is used for injection while the other will be used for the production of the gaseous products (Fig. 29). For a more efficient burn, the coal seam should be prepared prior to the gasification. The purpose is to increase the permeability of the coal seam between the two wells. This increased permability may be accomplished by explosive fracturing, reverse burn linking, electrolinking, directional drilling or hydro-fracturing (14). The result is a gas-flow path or connection between the injection and the production wells. Depending on the amount of groundwater present dewatering may also be required before gasification begins.

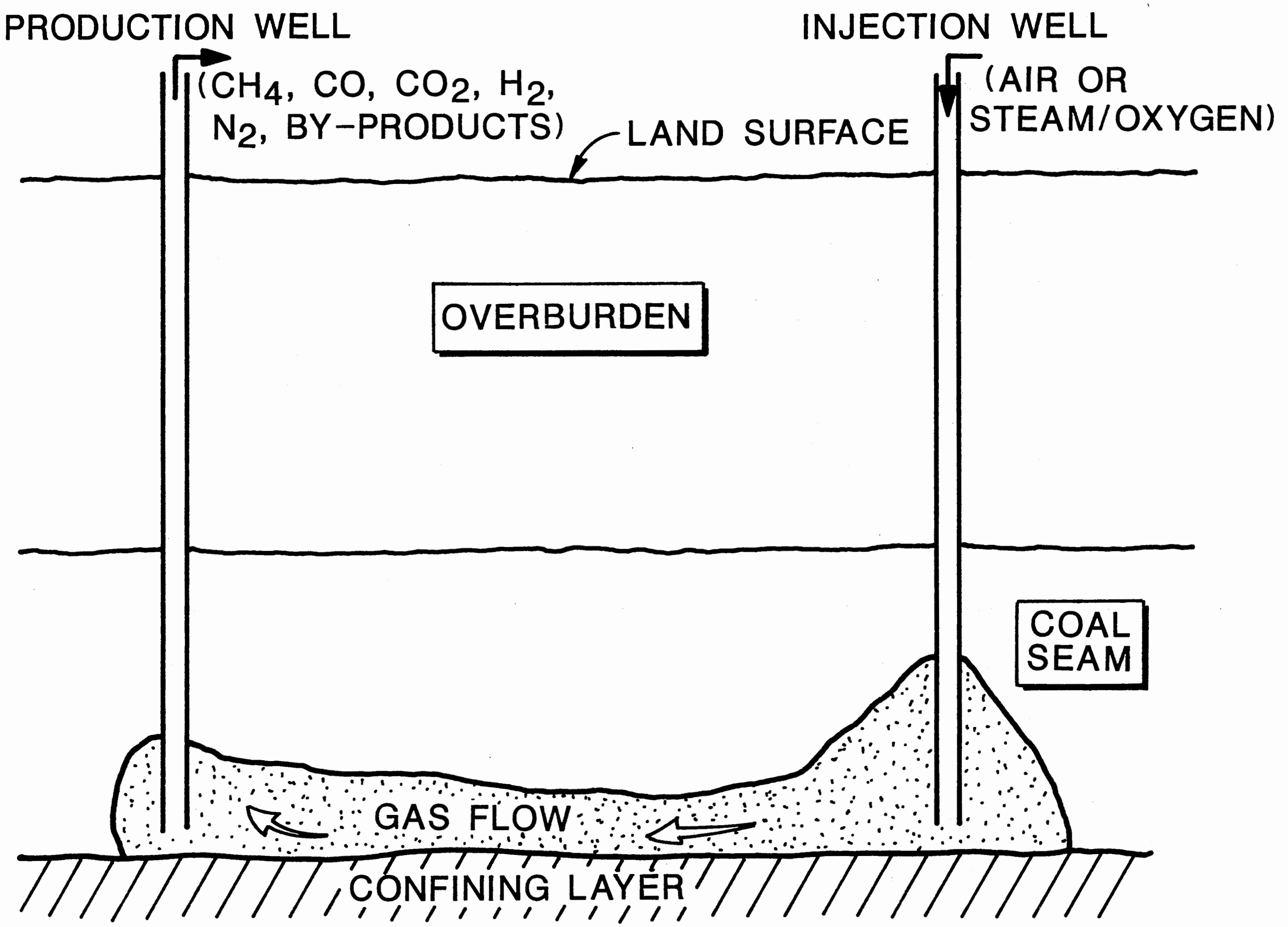

Figure 29. Schematic of UCG Phase

It is important to complete and connect the wells near the bottom of the well seam. Upon heating, coals tend to shrink and fall apart, creating a cavern or cavity. If the process is begun at the bottom of the seam then the coal collapses into the gasification zone and more of the coal seam is utilized. If the flow path is above the bottom of the seam, little gasification occurs below the gasification zone resulting in a less efficient burn.

The coal seam is ignited at the base of one of the wells, air or an oxygen/steam mixture is then injected to maintain the fire. As a result of the high permeability the fire slowly migrates in a broad front toward the production well. As the coal burns it produces heat and gas. Some of the coal is burned for the sole purpose of producing the heat that drives other reactions in the coal that actually produce the desired product gas. This product gas is primarily a mixture of methane, hydrogen, carbon monoxide and carbon dioxide.

The UCG process can be applied to both horizontal and dipping coal seams. Most of the U.S. coal sources lie in horizontal or moderately dipping seams. However there are some coal seams that are steeply dipping and not recoverable by conventional mining methods making the application of UCG very effective. In steeply dipping seams the wells are installed through the floor of the coal seams producing a more efficient reactor than in a horizontal seam (Fig. 30).

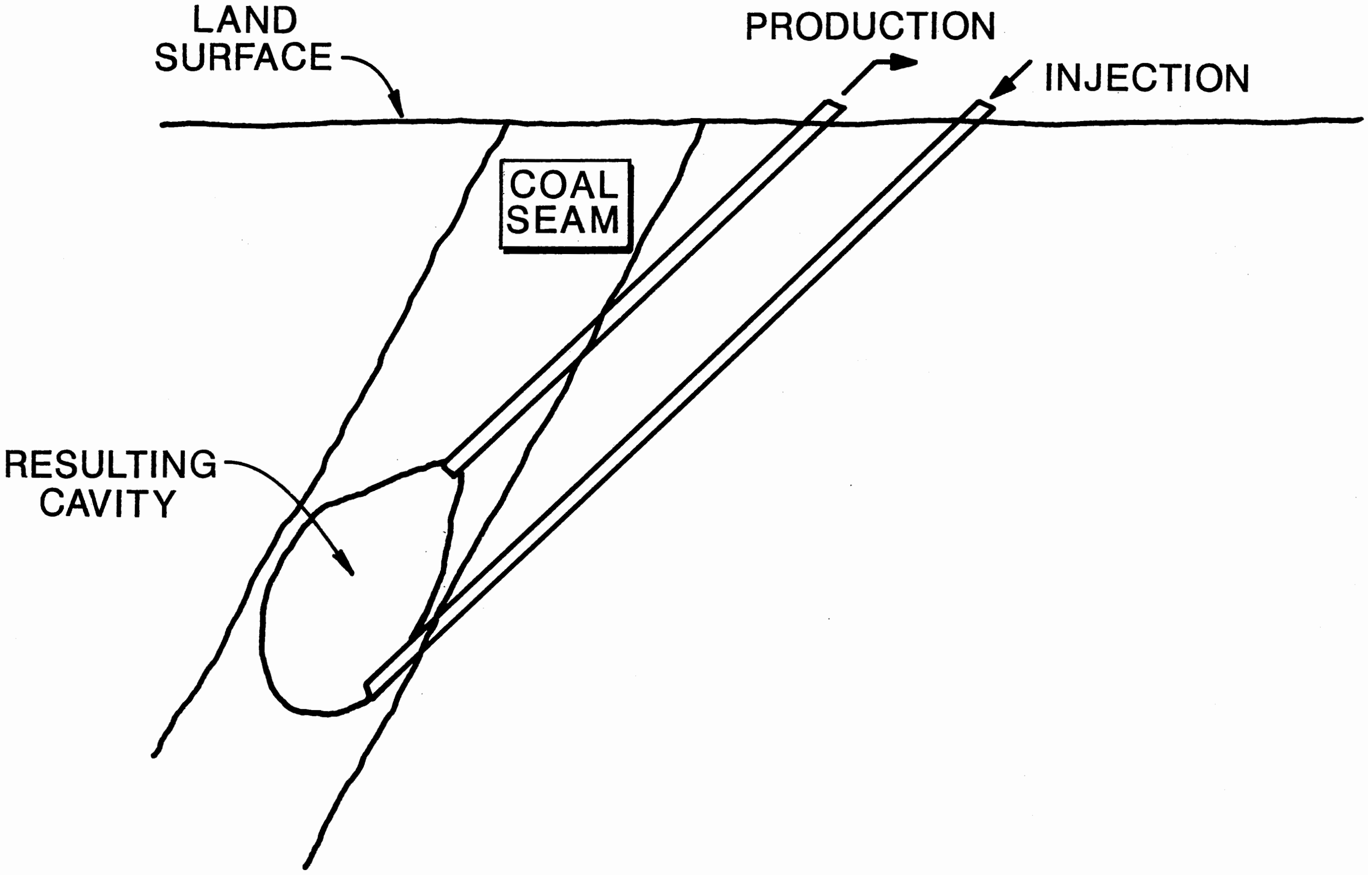

Figure 30. Schematic of UCG Process Steeply Dipping Coal Seam

A simple 2 well system has been described. For a commercial system there would be a large number of reactors (injection, production well pairs) that operate simultaneously. The raw products from the multiple reactors can then be blended at the surface to create various qualities of products. If air is injected, the product gas will contain significant quantities of nitrogen producing a low valued industrial fuel. If the gas is produced by the injection of a mixture of steam/oxygen it will have a higher heating value that could be used as direct replacement for natural gas as an industrial fuel (5).

Typically a coal seam is an aquifer. The possibility of groundwater contamination arises because some of the gasification reaction products and/or by-products remain underground in the vicinity of the reactors. Some of these potential contaminants include the organics: methane, ethane, benzenes, phenols and the inorganics: boron, flouride, bromide and sulfate. During the gasification process the water has been prevented from entering the reactor (cavity) by either product-gas pressure or dewatering operations altering the local flow patterns. Upon completion of gasification the groundwater returns to the cavity under local flow. As the cavity fills with water, leaching of inorganic compounds from the remaining ash and dissolving of organic species results (Fig. 31).

Once the water in the cavity reaches regional flow

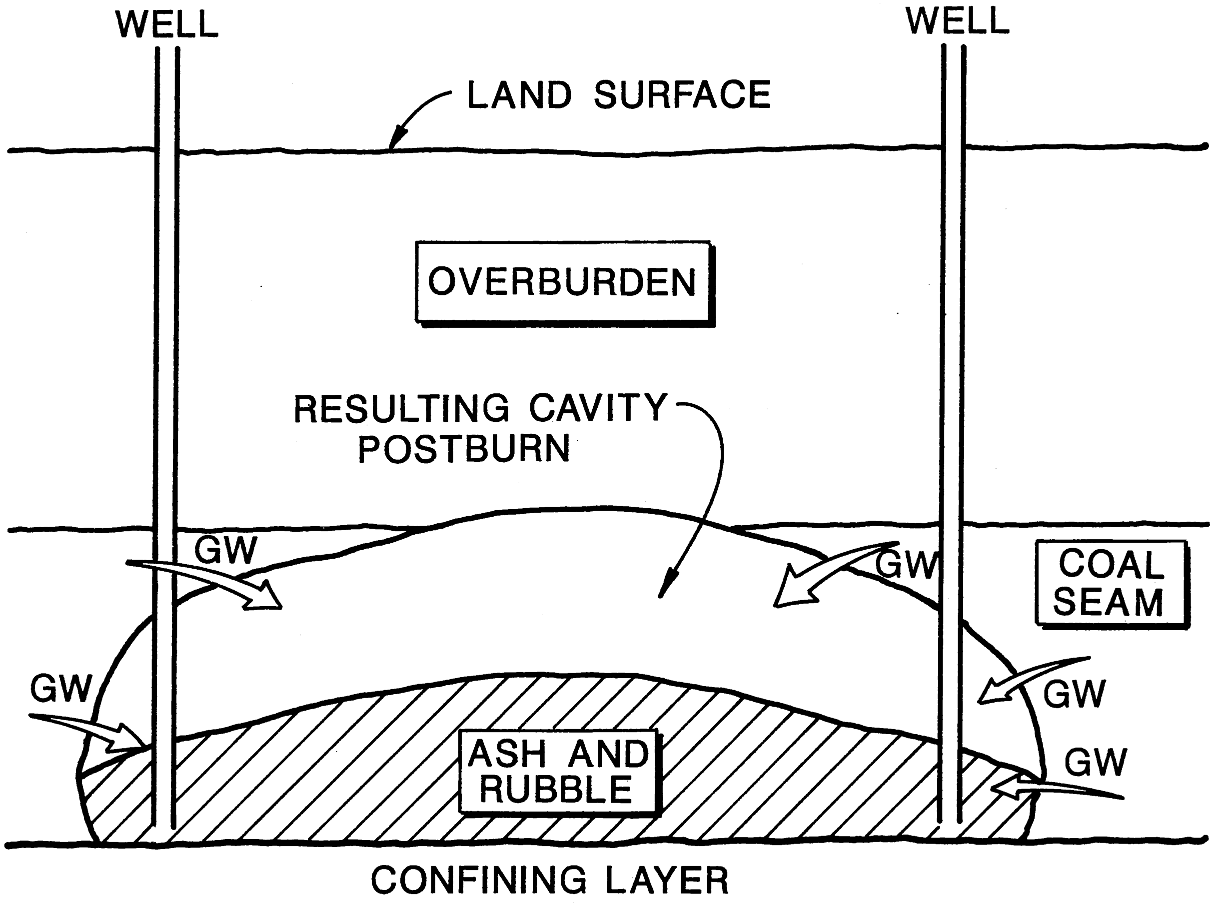

Figure 31. Local Groundwater Flow Postburn

levels a contaminated groundwater plume begins to move through the coal aquifer in the direction of flow (Fig. 32). The extent and strength of the plume is of major concern if it reaches surface waters or groundwaters used for domestic or agricultural purposes.

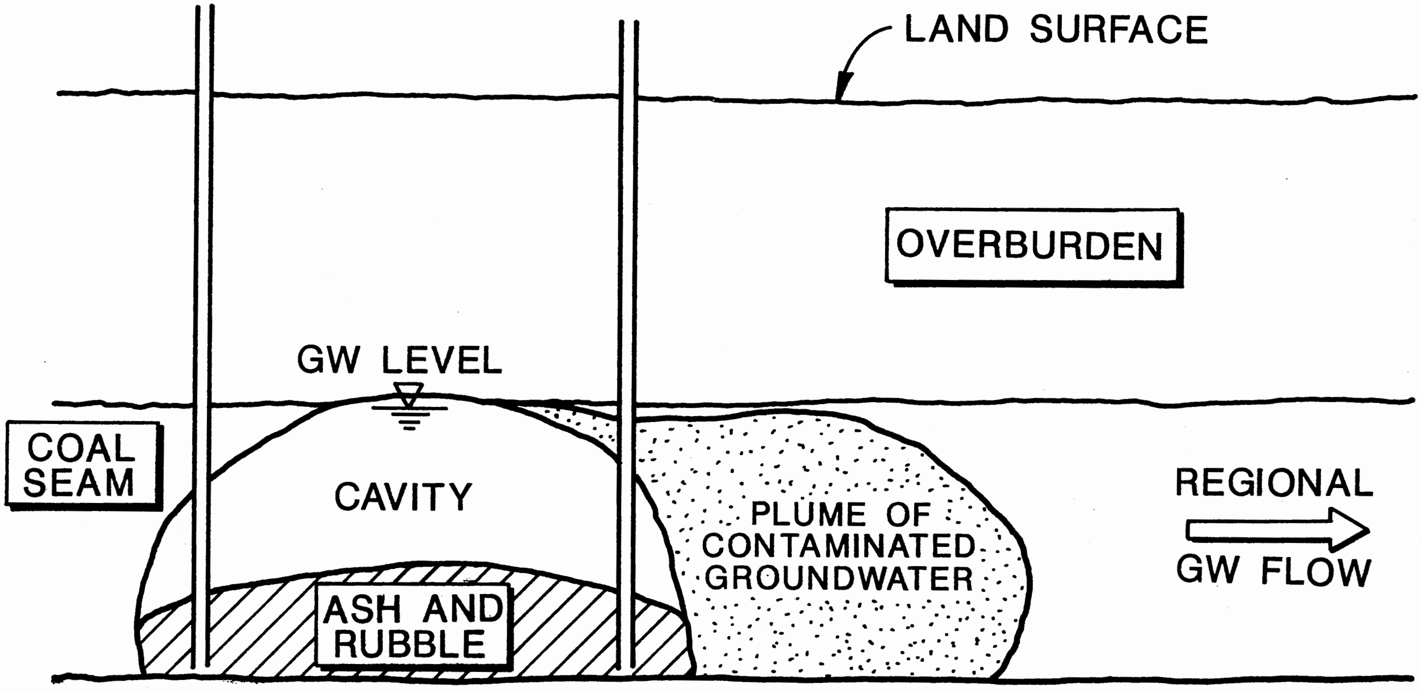

Figure 32. Export of Contaminants at Regional Water Levels

APPENDIX C

"RANDOM-WALK" USER MANUAL

Introduction

The model used for this study, "Random-Walk" Solute Transport Model for the microcomputer (18), was revised to include the effects of biological decay, at the source and in the system, on the contaminants within an aquifer. This appendix details the changes in the program code and the procedure for utilizing the revised model. This information should be used in conjunction with the original computer code and manuals, Bulletins 55 and 65, of the Illinois State Water Survey (17,18).

Code Changes

The effects of first order biological decay for the system are calculated by equation 1 and for the source by equation 2.

$$PM = PM \exp^{(-BD1*DELP)} \tag{1}$$

$$PL = PL \exp^{(-BD2*DELP)} \tag{2}$$

where

BD1 is the system biological decay factor, per day
BD2 is the source biological decay factor, per day
PM is the particle mass, lb/particle
PL is the pollutant load, lb
DELP is the time increment, days

The biological decay equations were added at the beginning of the source generation subroutine "GENP(PL)". The real variables BD1 and BD2 were added to the common statement "Trace". The new variables are read and written within the "Read and Write Pollution Parameters" section of the code. BD1 and BD2 are input as the last two entries on the pollution parameter card with the format F10.3.

The executable programs, RWBD.EXE and RWBDNN.EXE, are the compiled revised programs. The programs utilize a math co-processor chip to increase the speed of the simulation. If a math co-processor is not available the source programs, RWBD.FOR and RWBDNN.FOR, can be recompiled without using the math co-processor option.

Procedure

The "Random-Walk" job setup procedure discussed in Bulletin 65 should be followed but with the addition of the biological decay factors (18). It should be noted that because the effect of biological decay was added in the GENP(PL) subroutine it is the only source generation that can be used to evaluate decay.

If a constant velocity through out the aquifer system is desired then revisions to the job setup must be made. To calculate velocity the program first uses one of the flow subroutines, HSOLVE, HSOLV2 or HSOLV4, to determine the head distribution. From this distribution, the velocity is calculated. For constant velocity the head distribution should be directly input by use of node cards and the flow subroutine should not be utilized. The program will then use the input head distribution to calculate the desired velocity.

The first step is to accumulate the hydrologic and geologic parameters. Hydraulic conductivity or permeability should be determined in both the major and minor directions. Since the desired velocity in the X and Y direction is known, the unknown is the hydraulic gradient required to achieve this velocity.

The grid cell size, X and Y, is predetermined based on the size of the aquifer and the degree of discretization desired. The hydraulic gradient, dH/dL, in the X direction is based on the length of X and in the Y direction on the length of Y. This reduces the unknown to dH or the change in head term. Solve for the dH term in both directions by equation 3.

$$dH = V\alpha dL/7.48K$$

where

dH is the change in head, ft
V is the interstitial velocity (x or y), ft/day

K is the permeability (x or y), gal/day/ft^2
dL is the length of cell (ΔX or ΔY), ft
α is the effective porosity

Based on the dH required and cell size, a head distribution map is created using the difference in elevation at each node as the change in head. The elevation for each node is then input by the use of the node cards. Every value on the node card must be entered even if it is the same as the default value previously entered. Be careful to note that the velocity vectors are determined using the Chapeau function and that the permeability in the X direction is PERM2 and in the Y direction is PERM1. Reversing the two values will give a different velocity than desired.

The input of the head distribution may require numerous node cards. To avoid printing the node cards for each simulation, use the executable program, RWBD.EXE, only to check the input values on the node cards. Once the values on the node cards are correct use the executable program, RWBDNN.EXE, in which node cards are not printed, to make multiple simulations.

A print routine should be added to the calculation of the average linear velocities in the main section of the program as a check to assure that the desired velocity is being produced by the program. This print out is only used as an initial check and should not be done for each of the simulations.

VITA 2

Tina V. Garner

Candidate for the Degree of

Master of Science

Thesis: APPLICATION OF MONTE CARLO TECHNIQUES TO THE DETERMINATION OF GROUNDWATER CONTAMINATION RISK IN SATURATED TWO-DIMENSIONAL AQUIFER SYSTEMS

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