DEVELOPMENT OF A SIMPLIFIED METHOD FOR ESTIMATING THE TIME REQUIRED TO REMEDIATE A CONTAMINATED AQUIFER

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ABSTRACT

Groundwater flow and solute transport models are useful for planning groundwater remediation systems. The groundwater flow model provides information on the hydraulic impact of the proposed system (e.g., extent of contaminant capture, pumping rates, etc.). The solute transport model provides information on spatial distribution of the contaminant with time. The latter is very useful for estimating the approximate time to remediate the aquifer. This is of practical interest since this is equivalent to the design life of the pump and treat system. Often, however, due to project constraints, a solute transport model may not be developed for the site.

This paper describes a quick and inexpensive method for estimating the time required to remediate a contaminated aquifer. As a part of this study, the new method was implemented in a computer program called CLEAN. The program requires as input: average groundwater seepage velocity, retardation factor, longitudinal dispersivity, decay constant, target aquifer clean-up concentration, and a set of starting concentrations and associated spatial coordinates along a critical pathline.

The method involves solving a finite-difference form of the one-dimensional advection dispersion equation along a critical pathline. The program automatically creates the finite-difference grid using the appropriate grid spacing and time step size to control numerical dispersion and oscillation. To verify the accuracy of the finite difference solution, the model was compared to a one-dimensional analytical solution. The program used to solve the analytical solution is called STRIP1B. The CLEAN solution showed excellent agreement with the analytical solution.

As an example, the method was used to estimate the required design life of a pump and treat system designed to remediate groundwater contaminated with trichloroethylene (TCE) at a U.S. Government facility in the State of Washington. Estimates of clean-up times from CLEAN and MT3D, a widely used numerical solute transport model, were obtained for comparison. The two-dimensional MT3D analysis utilized groundwater flow information generated by the U.S. Geological Survey code MODFLOW. At low values of longitudinal dispersivity (20 feet), CLEAN tended to underestimate clean-up time relative to MT3D. Conversely, at high values of longitudinal

dispersivity (360 feet), CLEAN tended to overestimate clean-up time relative to MT3D. Nevertheless, given the wide range of uncertainty in dispersivity, as well as numerous other parameters required in the numerical solute transport model, the results produced by CLEAN are quite reasonable. Considering also, its ease of use, the method is a potentially useful tool for estimating aquifer clean-up time.

INTRODUCTION

The purpose of this paper is to describe a method for estimating the time to remediate an aquifer system without the use of a complicated numerical solute transport model. The paper describes the technical approach and numerical implementation of the new method, and gives an example of its use with an actual groundwater contamination problem. Potential limitations of the method are also discussed.

APPROACH

Figure 1A shows a contaminant plume in an idealized aquifer system. The characteristics of the plume in Figure 1A are commonly observed at hazardous waste sites (1). The plume tends to be long and narrow with the maximum concentration, C_{max}, located at the up gradient end of the plume near the origin of the contaminant source. The outer extent of the plume is defined by the required clean-up level, C_{cu}. For the purpose of the method development, it is further assumed that groundwater flow is horizontal, that the aquifer type is confined or unconfined, that the aquifer hydraulic conductivity is relatively high so that advective transport dominates, and that the contaminant concentration does not vary with depth.

Migration of the contaminant plume shown in Figure 1A can be described by the two-dimensional form of the advection-dispersion equation (2):

$$\frac{R\partial C}{\partial t} = \frac{\partial}{x_i}\left(D_{ij}\frac{\partial C}{\partial x_j}\right) - \frac{\partial}{\partial x_i}(v_i C) - \lambda RC + \frac{q}{\theta}C \quad \text{(Eq1)}$$

where, C is concentration, t is time, R is retardation factor, x_i is the distance along the respective Cartesian coordinate axis, D_{ij} is the hydrodynamic dispersion coefficient, v is the fluid velocity, λ is the decay constant, and q is the volumetric flux of water per unit volume of aquifer representing sources and sinks.

In Figure 1B, a groundwater recovery well has been placed at the down gradient end of the plume. The figure shows a flow pathline bisecting the center of the plume, extending from the up gradient plume fringe, through the point of maximum concentration, and terminating at the recovery well. This pathline will be referred to here as the critical pathline. A one-dimensional form of equation 1, may be used to estimate the concentration distribution along the critical pathline, and to estimate the time to reduce the plume's maximum concentration to below the target clean-up level, C_{cu}. The one-dimensional form of the advection-dispersion equation is given below:

$$\frac{R\partial C}{\partial t} = \frac{\partial}{\partial x}\left(D\frac{\partial C}{\partial x}\right) - \frac{v\partial C}{\partial C} - \lambda RC + \frac{q}{\theta}C \qquad \text{(Eq2)}$$

where $D = \alpha_L v + D_m$ is the dispersion coefficient in the direction of flow, α_L is longitudinal dispersivity, D_m is the diffusion coefficient, and θ is aquifer porosity.

Equation 2 assumes that transverse dispersion (lateral and vertical) is zero. The use of equation 2 can be justified, based on the fact that transverse dispersion in the idealized aquifer system will be small relative to longitudinal dispersion. Transverse dispersivity is often assumed to be from 1/5 to 1/10 of the longitudinal dispersivity (3). Transverse dispersion is further inhibited because the groundwater flow converges toward the recovery well. Assuming that vertical dispersion within the aquifer is negligible is also a reasonable assumption. Typically the vertical dispersivity is on the order of 1/50 to 1/100 of the longitudinal dispersivity (3).

The applicable problem domain is illustrated in Figure 1C. Initial and boundary conditions are presented below:

$$C(0,t) = 0$$

$$C(x,0) = C_o(x)$$

$$q_w(x_w,t) = qC(x_w,t), \quad \partial C(x_w,t)/\partial x = 0$$

where C_o is the initial concentration, q_w is the mass flux of solute into the well, q is the volumetric water flux, and x_w is the x coordinate at the location of the recovery well. It is also assumed that the source of contamination is removed at $t = 0$.

Figure 1C also illustrates the concentration distribution with time. Concentration is shown for the initial time (t_o), two intermediate times (t_1 and t_2) and the clean-up time (t_{cu}) when the maximum concentration has dropped to the value of C_{cu}.

CODE DEVELOPMENT

A finite-difference form of equation 2 was developed and implemented in a computer program called CLEAN. Use of a numerical solution (as opposed to an analytical solution) allows the initial distribution of contamination along the critical pathline to be specified by the user. The system of difference equations are solved implicitly using the efficient Thomas algorithm described by Wang and Anderson (4). The computer program automatically determines the maximum time step and grid spacing to be used based on the Peclet and Courant numerical criteria. These criteria provide the conditions necessary to avoid numerical dispersion and oscillation problems.

During execution, the program performs the following steps:

1. Reads average groundwater seepage velocity, retardation coefficient, longitudinal dispersivity, decay constant, target aquifer clean-up level, and a set of starting concentrations and associated spatial coordinates along the critical pathline.
2. Determines the maximum time step and grid spacing;
3. Calculates and assigns initial concentrations to the finite-difference nodes using a cubic spline interpolation technique.
4. Solves the transport equation successively with time until the maximum concentration is less than C_{cu}.

It should be noted that the overall grid length is set equal to twice the distance between the up gradient plume fringe and the recovery well. The additional length is added upstream of the plume, and the initial concentration along this reach is set to zero. This allows for the possibility of upstream dispersion if x_{max} is close to x_{cu}, and C_{max} is large.

To verify the accuracy of the finite-difference solution, CLEAN was compared with the results of the computer program STRIP1B (5). STRIP1B calculates the analytical solution of the one-dimensional transport problem for a constant relative concentration of 1 at the left boundary. This boundary condition was also used in the CLEAN model. Comparison of the two models at $t = 1$, 5 and 10 years, indicated excellent agreement.

APPLICATION

As an example of the use of CLEAN for estimating aquifer clean-up time, the model was applied to an actual contaminated site. A two-dimensional solute transport model was also applied to the site to verify that the CLEAN results are reasonable.

Figure 2 illustrates an actual situation which currently exists at a U.S. Government facility in the State of Washington. The trichloroethylene (TCE) plume originated from a near-surface dump site located within the northern portion of the plume. The maximum observed concentration of 1800 ug/L occurs within the

1000 ug/L contour (not shown). Figure 2 indicates the location of a recovery well which is extracting groundwater at a rate of 170 gallons per minute (gpm).

As part of the remedial design, a two-dimensional groundwater flow model was developed for the site. The computer model MODFLOW (6) was used. The flow model was calibrated to non-pumping aquifer conditions, then used to evaluate various plume recovery and reinjection alternatives. Table 1 lists the model size and range of data used in the flow model for the site as a whole, and in the plume area specifically.

Table 1. Characteristics of the Two-Dimensional Flow Model

	Site	Plume Area
Rows	48	
Columns	41	
Area (acres)	1000	30
Hydraulic Conductivity (feet/day)	45 - 120	45 - 80
Aquifer Recharge (inches/year)	2.5 - 9.6	4.8
Bottom of Aquifer Elevation (feet)	35 - 70	46 - 62

Using the solute transport computer model MT3D (7), a series of runs were made to evaluate the time required to lower the TCE concentration to 5 ug/L. The runs involved varying the longitudinal dispersivity over the range of values reported by Gelhar et al. (8) for a plume scale of 2,500 feet. Transverse dispersivity (α_T) was maintained at 1/10 of the longitudinal dispersivity (α_L). The retardation factor, decay constant and diffusion coefficient were set to 4.6, 0 and 0, respectively, for all runs.

The average seepage velocity along the critical pathline is required as input to CLEAN. There are two ways of estimating the coordinates of the critical pathline and the magnitude of the seepage velocity. One way is to plot groundwater equipotential contours and streamlines. Once the critical pathline has been determined, the average hydraulic gradient is estimated. The hydraulic gradient is then multiplied by the hydraulic conductivity and divided by the aquifer porosity. This approach is, however, not recommended as it may lead to large errors in the seepage velocity estimate. This is because the seepage velocity varies along the critical pathline due to well drawdown. Seepage velocity variations may also results due to variations in hydraulic conductivity and porosity.

The preferred method to approximate the coordinates of the critical pathline and the magnitude of the average seepage velocity is particle tracking. In this study, the groundwater flow and particle tracking model FLOWPATH (9) was used. The characteristics of the flow model were identical with the MODFLOW model discussed above. FLOWPATH was used instead of a particle tracker linked with MODFLOW, because of its user friendliness and graphical capabilities. Initially, a capture zone analysis was performed to determine the critical pathline. In this analysis, particles are seeded around the well and allowed to travel in reverse away from the well. The critical pathline as determined by FLOWPATH is shown in Figure 2. It should be noted that the bend in the pathline towards the west is due to the influence of a reinjection well located approximately 2,500 feet east of the plume. After the critical pathline was determined, a single particle was released on the critical pathline positioned at the up gradient end of the plume (Figure 2). Using the time-related pathline option in FLOWPATH, the time for the particle to reach the recovery well was determined by trial and error. After determining the particle travel time, the seepage velocity was calculated by dividing the path length by the travel time. The average seepage velocity estimated by this method was 1.1 ft/day.

The initial concentration distribution entered into CLEAN was obtained from Figure 2. Concentrations were read from the contour map along the critical pathline. A total of fourteen

C-x pairs were entered into CLEAN. The number of C-x pairs used in this example was arbitrary, more or less pairs could have been used. It is important for the user to inspect the concentration distribution along the finite-difference grid to be sure that it looks reasonable. The cubic spline interpolation scheme used in CLEAN may oscillate about specified values giving an unacceptable starting concentration distribution. If this problem occurs, it is easily corrected by adding more C-x pairs to the data set. The retardation factor, decay constant and diffusion coefficient were set to 4.6, 0 and 0, respectively, for all runs.

Results

Figure 3 shows the concentration distribution along the critical pathline calculated by CLEAN at t = 0, 10, 30 and 50 years, and $\alpha_L = 100$ feet. The time required for the concentration to drop below the C_{cu} value of 5 ug/L all along the critical pathline was 64 years. The Figure illustrates how the maximum concentration drops rapidly during the early part of the simulation. With time, the concentration decreases at a decreasing rate. During the last 14 years of the simulation, for example, only a 30 ug/L drop in the maximum concentration occurred.

Table 2 lists the CLEAN and MT3D estimated clean-up times for α_L = 20, 33, 100, 200 and 360. For $\alpha_L = 100$, the two models were in good agreement. However, relative to MT3D, CLEAN underestimated clean-up time for low values of dispersivity and overestimated clean-up time for high values. The lack of agreement in the two models may be due to numerous factors. From Table 1, we see that the numerical computer model simulated aquifer heterogeneities, spatial variations in recharge and aquifer bottom elevation, two-dimensional flow and transverse dispersion, whereas the CLEAN model did not take into account any of these factors.

Table 2. CLEAN and MT3D Estimated Clean-up Times For Different Values of Dispersivity

Computer Model	α_L	α_T*	Time (Years)
CLEAN	20	-	39
MT3D	20	2	51
CLEAN	33	-	45
MT3D	33	3.3	53
CLEAN	100	-	64
MT3D	100	10	62
CLEAN	200	-	78
MT3D	200	20	67
CLEAN	360	-	97
MT3D	360	36	70

*Because CLEAN solves the one-dimensional advection dispersion equation, α_T is not required as input.

In addition to the simulations performed and presented in Table 2, a run was made in which the initial concentrations were reduced by a factor of 4. The estimated clean-up time by CLEAN and MT3D were 41 and 45 years, respectively, for a value $\alpha_L = 33$. This result suggests that for lower initial concentrations, CLEAN may perform better, probably because transverse dispersion is reduced and solute transport tends to behave more one-dimensional.

Discussion

The range over which longitudinal dispersivity was evaluated (20 to 360 feet) was based on data presented by Gelhar et al. (1985) for a plume scale of approximately 2500 feet. Varying dispersivity over the reported range resulted in a 30 year variation in the clean-up time estimate using MT3D. In addition to dispersivity, uncertainty exists in numerous parameters that influence solute transport and consequently, the estimated clean-up time. When one considers the inherent uncertainty in the system being modeled, the deviations in the CLEAN and MT3D results becomes less significant.

CLEAN and MT3D results becomes less significant.

For virtually all simulations performed, the CLEAN model performed the calculations in under 1-minute on a 486, 50 MHz personal computer. MT3D, on the other hand averaged 30 to 60 minutes per run, and one MT3D run required 3.5 hours to complete. Also, in terms of model set up, MT3D took a significantly greater time than did the CLEAN model.

MODEL LIMITATIONS

From the example problem, it is evident that the CLEAN estimate of clean-up time may not match exactly the estimate produced by a two-dimensional solute transport model. Therefore, results from CLEAN must be viewed as "ball park" estimates only. The method described here is based on numerous assumptions. The user should be aware of these assumptions and consider how violation of any assumptions might affect the result.

The method described here is limited to a single pumping well located at the down gradient end of the plume. In many case, however, multiple pumping wells are used. In fact, the final design for the site considered in the example problem, added two more wells within the TCE plume. During operation of a multi-recovery well system, each of the wells within the contaminant plume has its own capture zone. For this reason, it may be possible to perform a CLEAN analysis on each well separately. In this case, the clean-up time for the site would be equal to the longest clean-up time required by any of the individual pumping wells.

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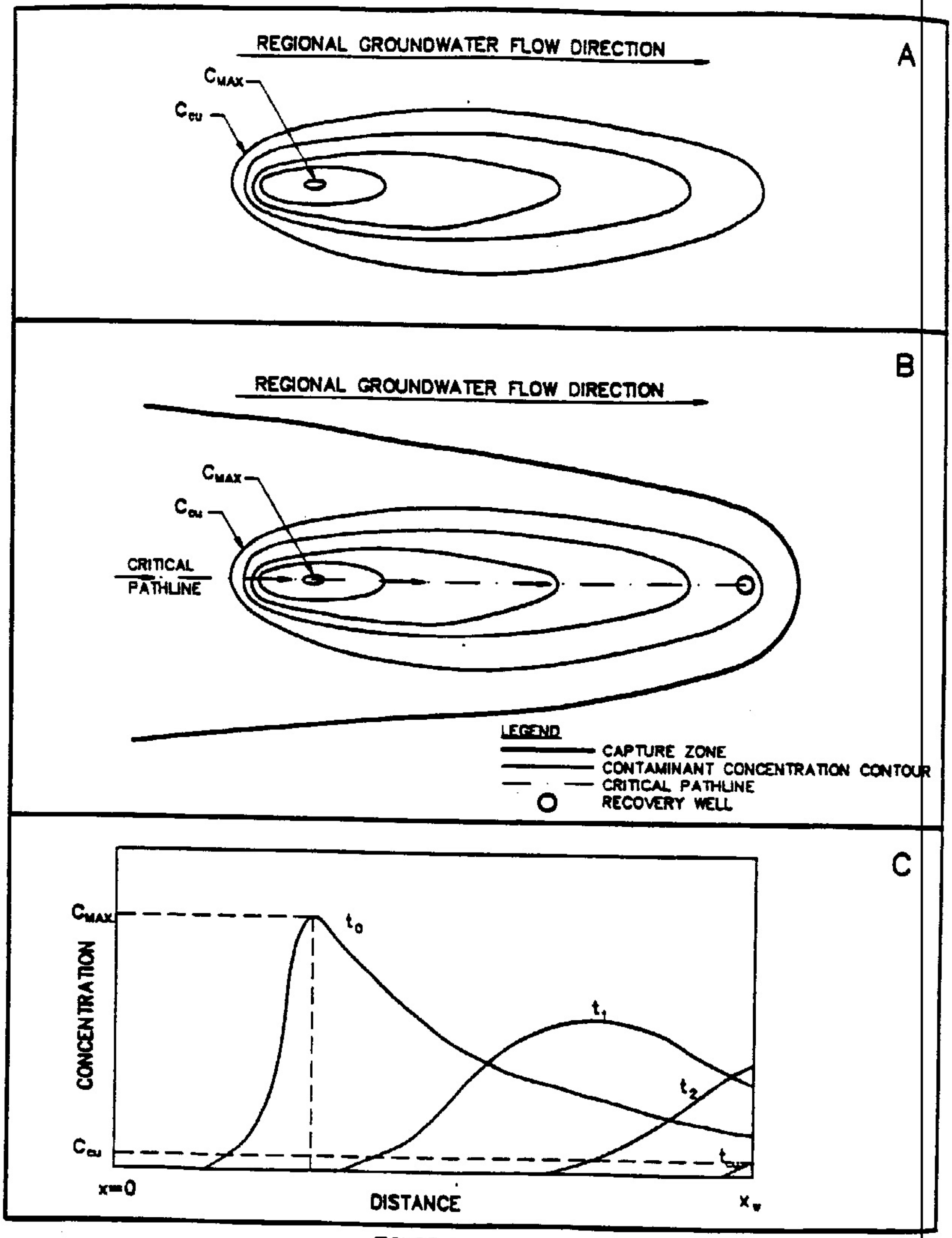

FIGURE 1

A. TYPICAL GROUNDWATER CONTAMINANT PLUME. B. GROUNDWATER CONTAMINANT PLUME WITH PUMPING. C. CONCENTRATION DISTRIBUTION ALONG THE CRITICAL FLOW PATH.

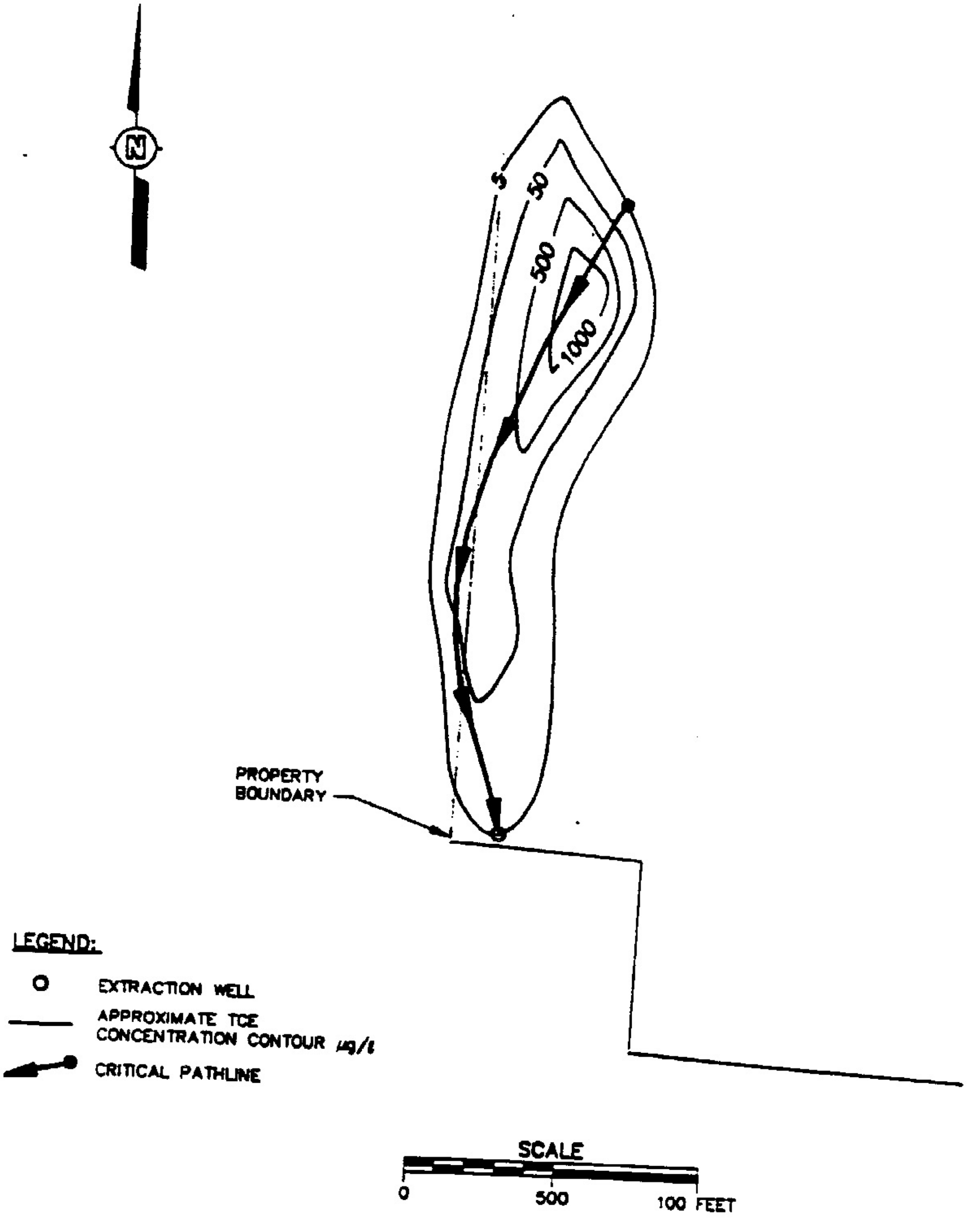

FIGURE 2

GROUNDWATER TCE DISTRIBUTION

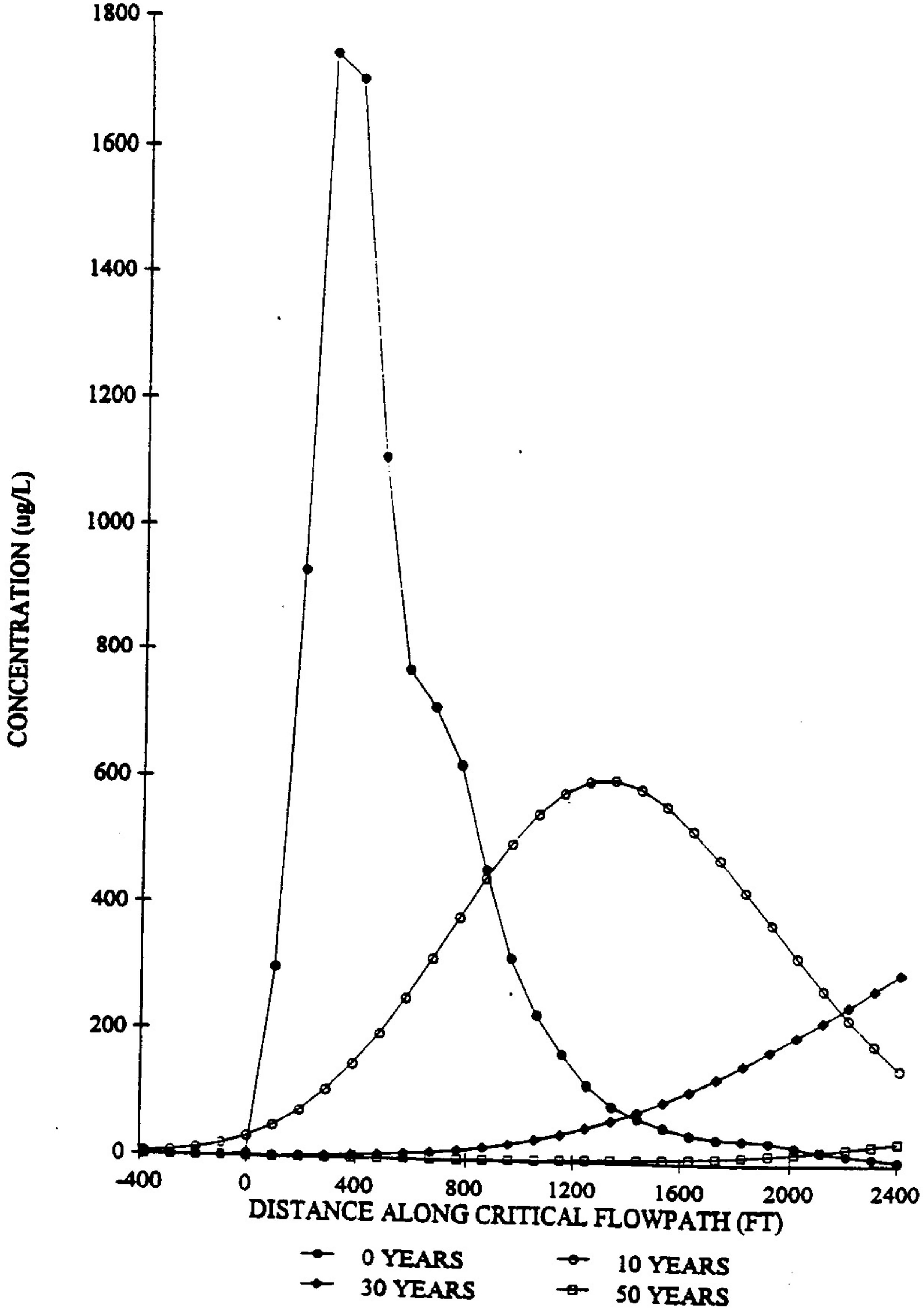

FIG. 3 EXAMPLE PROBLEM PREDICTED CONCENTRATION DISTRIBUTION