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FIELD APPLICATION OF PARAMETER IDENTIFICATION IN GROUNDWATER CONTAMINANT TRANSPORT MODELING: A CASE STUDY

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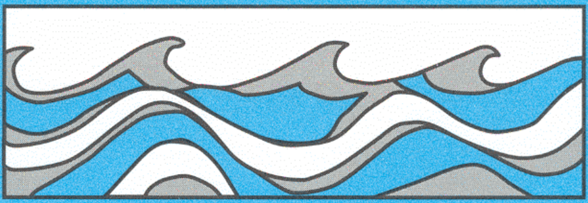

Water Resources Series
Technical Report No. 105
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Project Completion Report Submitted to

The State of Washington Water Research Center

and

The U.S. Department of the Interior

Water Research Center Project A-145-WASH

U.W. Department of Interior Grant No. G1259-05

For the Period

May 1, 1986 to March 31, 1987

June 1987

ABSTRACT

The application of a parameter identification (PI) algorithm in groundwater contaminant transport modeling is attempted in this study. The computer code used was a combination of an ordinary least square optimization routine and the United States Geological Survey's Method of Characteristics Code (USGS-MOC). In working with engineers and scientists from Washington State Department of Ecology and the consulting firm Golder and Associates, a suitable field problem with adequate monitoring data was selected. Using available observations, the transmissivity and dispersivity were calibrated by both the PI approach and the more conventional trial-and-error approach. The calibrated parameters were then used by USGS-MOC in simulation of remedial action effects. It was found that although the PI procedure allowed a more objective and efficient search of suitable model parameters, the parameters found by the PI routine in even a well-monitored site may not be physically plausible. The determination of proper parameters by a PI method must still be determined with significant user intervention.

KEYWORDS: Groundwater, Contamination, Water Pollution Sources, Parameter Identification, Simulation Model, Data Requirements

ACKNOWLEDGEMENTS

The activities on which this report is based were financed in part by the Department of the Interior, U. S. Geological Survey through the Washington State Water Research Center. The support is greatly appreciated. The work could not have been completed without the contribution and support from the staff at Washington Department of Ecology (WDOE), and Golder and Associates. We would particularly like to thank Dennis Erickson and Will Abercrombie of WDOE and Greg Laird of Golder and Associates for their input to this project. The gracious assistance by Kim Scattarella for his work on the graphics and typing work by Margo Behler are appreciated.

The contents of this publication do not necessarily reflect the views and policies of the Department of the interior, nor does mention of trade names or commerical products constitute their endorsement by the United States Government.

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CHAPTER 1

INTRODUCTION

Groundwater contamination is becoming an increasingly prevalent problem faced by engineers, planners, and public officials in this country. Although only a relatively small percentage of the available groundwater is contaminated, the problem has become rather severe in many parts of the country. Washington State may be particularly susceptible to groundwater contamination because of the large percentage of state residents who depend on groundwater for their source of drinking water. Nearly 40 percent of the state's population use groundwater as their source of drinking water. A recent study by the Washington State Department of Ecology showed that the drinking water of one in every seven residents now is believed to be threatened by (certain kinds of) contamination.

In the past two decades, engineers and scientists have developed a large number of mathematical models to simulate groundwater movement and contaminant transport through the substrata. Several authors have summarized the various mathematical models used in the study of groundwater movement and contaminant transport (see e.g., Anderson, 1979; Faust and Mercer, 1980; and Javandel et al., 1984). Solution techniques used in these models include finite difference (e.g. Remson et al., 1971), finite element (e.g. Pinder and Gray, 1977), method of characteristics (Reddel and Sunada, 1970), and random walk (Prickett et al., 1981) methods. Although there are numerous different numerical solution techniques, every model requires the input of site specific parameters which must be calibrated by matching field observations with model predictions. A model is of little practical value unless it is adequately calibrated.

There are two different approaches to calibrate a model. The first is a trial-and-error process in which the parameter values are varied until the observed conditions match the model predictions as closely as possible. This approach is used in almost all present modeling studies. This calibration process requires repeated model simulation runs and is quite time consuming. The results of this calibration method are highly dependent on the user's experience and can vary from user to user.

The second approach to model calibration involves the use of a computer search algorithm which finds model parameter values by minimizing the differences between model solutions and available field observations. This procedure is known in groundwater modeling as parameter identification (PI), (Yeh, 1986). The procedure can be coded in any model so that selected parameter values can be found from an initial estimate and numeric lower and upper bounds of the parameter (Strecker and Chu, 1986). The advantages of this calibration method are that it helps to reduce the number of model calibration runs and it minimizes to a certain extent the variation in calibration results by different users. Parameter identification is not without its problems. The approach has been shown to be ill-posed (Yeh, 1986) and it works well only with abundant, high quality data (Sadeghipour and Yeh, 1984; Yeh and Sun, 1984; Chu, et al., 1987). Most of the present PI applications involved only groundwater flow modeling (Yeh, 1986; Strecker and Chu, 1986).

The objective of this study to apply a particular PI procedure to an appropriate field situation involving groundwater contamination. Specifically, this study investigates the applicability and limitations of the PI technique for field problems as compared to the more conventional trial-and-error calibration approach. This objective required the selection of a field problem which had adequate boundary conditions and a reasonable amount of monitoring data. Once such a site was identified, the model was calibrated using both the parameter identification technique and a trial-and-error approach for comparison purpose. Simulation runs using calibrated parameters from both approaches were also compared and analyzed in this study.

The United States Geological Survey's Method of Characteristics (USGS-MOC) model (Konikow and Bredehoeft, 1978) was selected as the basic groundwater contaminant transport model for the study. Numerous applications of the USGS-MOC model are available in the literature (see e.g. Konikow, 1977; Warner, 1979; Bedient et al., 1984; Freeberg, et al., 1987). This model was chosen because of its excellent documentation, its widespread usage, and available PI software developed for it (Strecker and Chu, 1986). The model with the built-in parameter identification procedure is referred to as PI-MOC in this report. With PI-MOC, selected model parameters needed by USGS-MOC can be found by a quadratic programming routine which minimizes the sum of the squared deviations between observations and model predictions. Because of the large number of references on general PI methodology (see Yeh, 1986) and PI-MOC (Strecker et al., 1985; Strecker and Chu, 1986), they will not be repeated here for brevity.

This report will first describe the site selection process. The PI-MOC application and parameters determined by the PI calibration for the selected site are then presented. Finally, results of simulation runs using parameters determined by the PI technique and trial-and-error approach are presented and compared. Conclusions from this study are given at the end of the report.

CHAPTER 2

SITE SELECTION

The field site selection process involved reviewing numerous groundwater contamination cases in Washington with personnel from the Washington State Department of Ecology and the consulting firm of Golder and Associates. Each site was evaluated to determine how well the USGS-MOC and PI-MOC models could be applied. Specifically, the research required the site to have well-defined flow boundaries, known contaminant source, some estimates of site specific aquifer and hydrologic parameters, and a reasonable amount of monitoring data. Such requirements effectively narrowed the choices of field problems to two. A description of the two sites and the final choice for the study are given below.

2.1) Tacoma Site

The city of Tacoma operates 13 wells to supplement surface water supply during summer months. The wells can provide up to 45 million gallons per day of water supply. Chlorinated hydrocarbons were first detected at Well 12A in the summer of 1981. Since that time, several studies have identified the source of the contamination and a number of remedial actions have been undertaken (Laird, 1985).

The underlying materials that characterize the site are glacial in origin. Predominantly, the site is composed of recessional outwash of fairly high permeability underlain by low permeability glacial till and high permeability advance out wash. Throughout the site the thickness and composition of the underlying material varies widely. There may also be lacustrine and ice contact deposits which further complicate the site's geology. Such materials are usually difficult to characterize in terms of hydrogeologic parameters because of the heterogeneous nature of the deposit.

Griffin et al. (1962) presented a detailed regional water table map of the Tacoma site which shows Well 12A to be located near a groundwater divide. Seasonal recharge and well withdrawal schedules cause the hydraulic boundary conditions and groundwater flow patterns to vary widely throughout the year. The presence of seasonally varying hydraulic boundary conditions and groundwater flow patterns severely complicates site characterization.

From a modeling point of view, the Tacoma Well 12A site is a very complicated one. Although the source of contamination has been determined, monitoring data on the spread of contaminant are sparse. Laird (1985) attempted to implement and calibrate the USGS-MOC code for the site, but concluded that because of the complicated hydrogeologic boundary conditions and shortage of data, the results were unreliable for practical engineering and planning uses. This site was eventually excluded from further study.

2.2) Site X

The second site reviewed will be referred to as Site X in this report because of ongoing investigation by the Washington State Department of Ecology (WDOE). Actual maps of the area are given in Figures 1 and 2. These maps show the general relationship of the site to several important hydrologic boundaries. A close-up view of the site is given in Figure 2. The site has been used as a solvent recycling plant from 1980 to present. It processed up to 1000 gallons of waste per week until 1984 when contamination (due to leakage of a storage sump) was first detected. Contaminants present in the substrata include a variety of organic solvents such as trichloroethene and tolulene (Erickson, 1986).

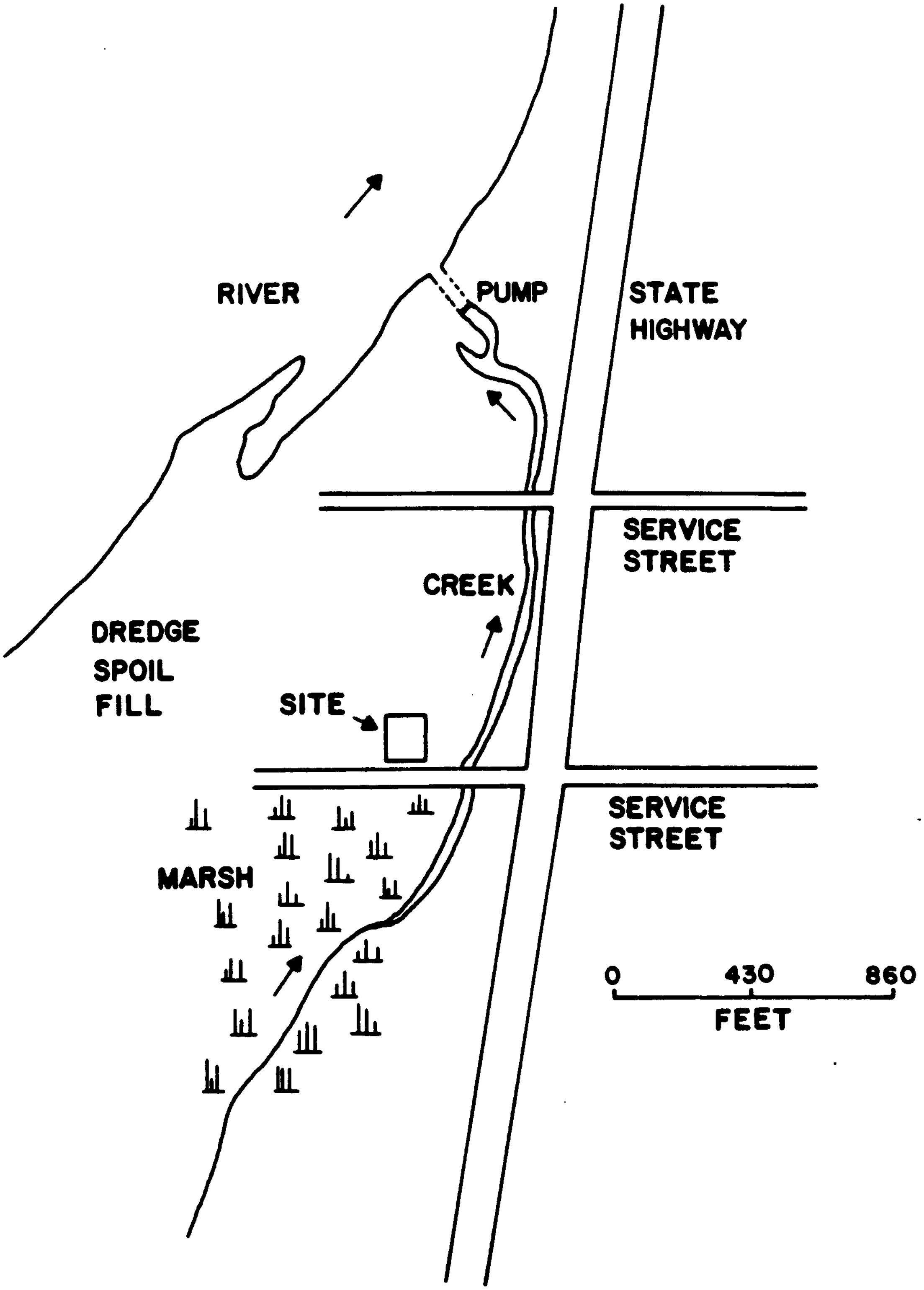

Figure 1 Vicinity Map of Site

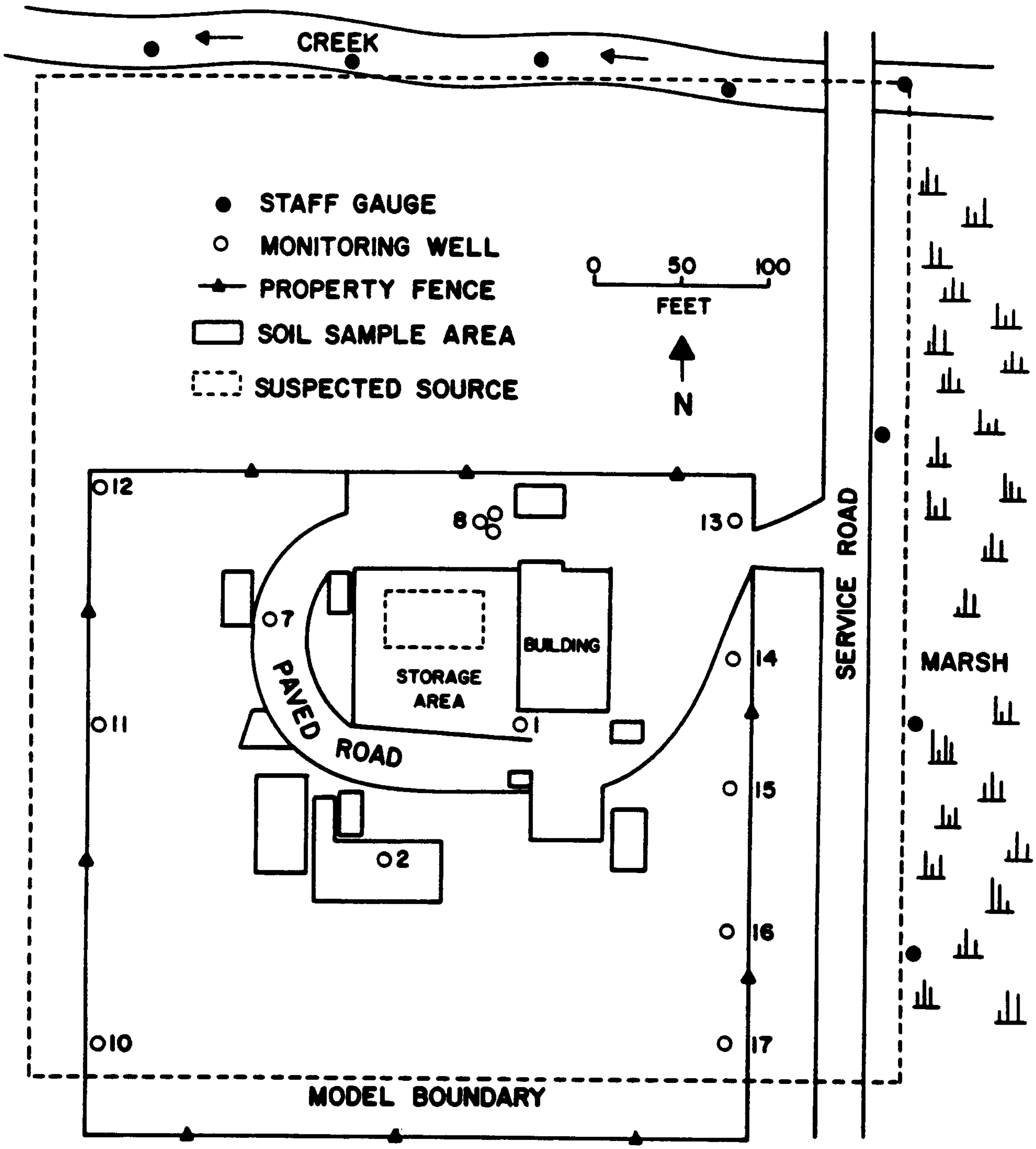

Figure 2 Close-up Map of Site X

The material underlying the site and adjacent area consists of uniform, well sorted, fine to medium grained dredged spoils overlying native alluvial silt. Below these layers are Quaternary alluvium. The dredged spoils, produced from channel dredging of the river shown in Figure 1, create an unconfined aquifer. The underlying alluvial silt is comparatively impermeable and allows very little vertical movement of water into lower layers. A number of cross-sections through the site are shown in Figure 3. The sand is of fairly uniform thickness at the site and the lower silt layer has been shown to be continuous on site (Erickson, 1986). Soil borings taken by the U.S. Army Corps of Engineers show that silt extends to a depth of about 50 feet (Erickson, 1986). No contamination has been detected in the aquifer which lies below the alluvial silt.

Groundwater flow direction has been determined through extensive monitoring of wells at the site. Twelve observation wells were installed in 1985 and monitored monthly for one year. The locations of these wells are shown in Figure 2. The creek and the swamp, located on the north and east edges of the study area respectively, form two constant head boundaries. From the analysis of the data, it was concluded that both the creek and the swamp are hydraulically connected to the aquifer during most of the year. Monitoring data also indicate that these features act as hydraulic sinks and groundwater flows towards these boundaries.

After reviewing the available information, Site X was determined to be an ideal site for USGS-MOC and PI-MOC applications. Previous studies of the site have identified the location and extent of contamination. A sufficient amount of monitoring data exists for model calibration. The site has well-defined flow boundaries and the aquifer is made up of relatively homogeneous material. Site specific aquifer parameters have also been reported in previous studies.

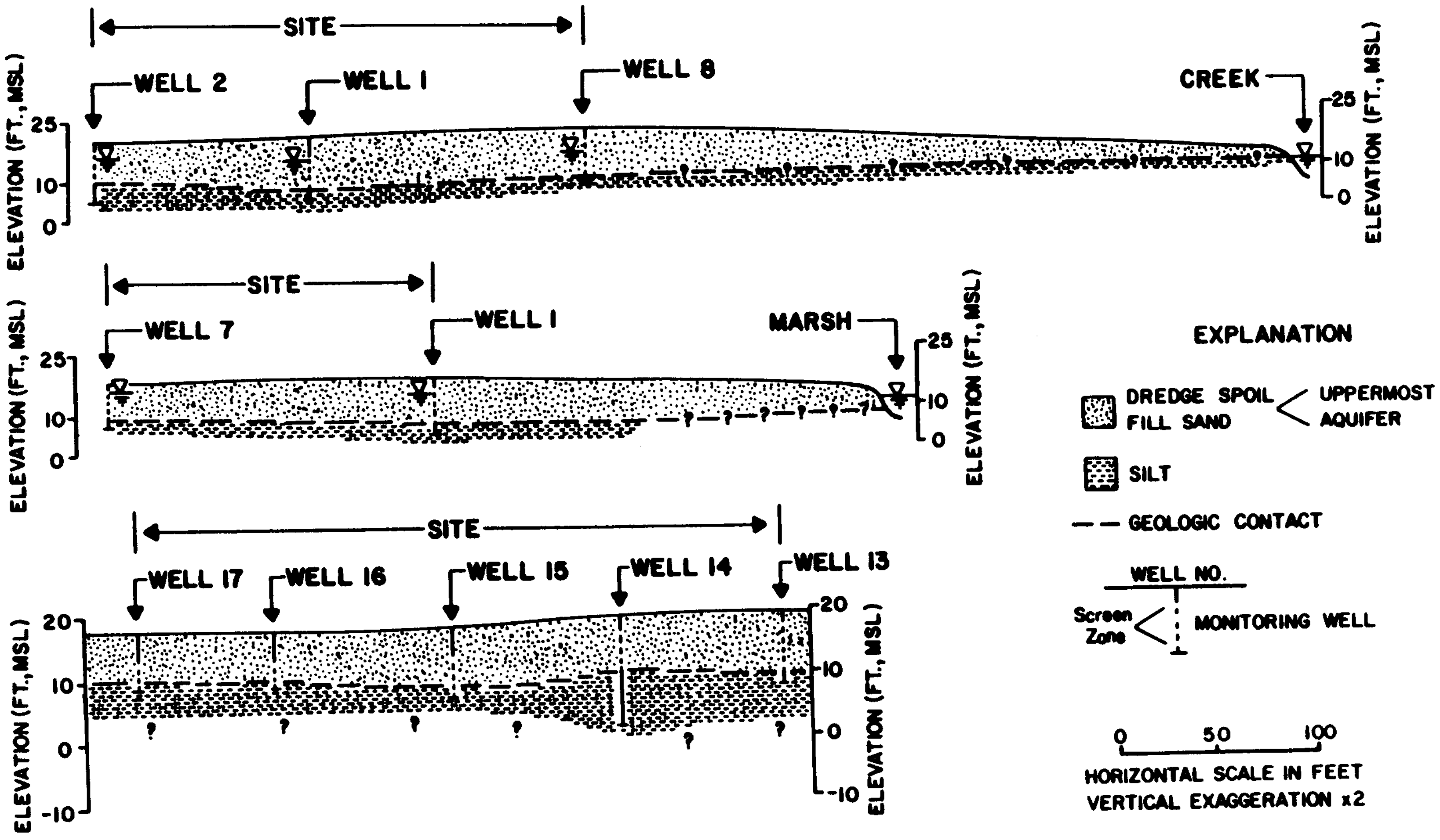

Figure 3 Selected Cross Sections at Site X

CHAPTER 3

PI-MOC APPLICATION

3.1) Parameter Identification and USGS Method of Characteristics Model

In a previous study, a generalized parameter identification (PI) algorithm was incorporated into the USGS Method of Characteristics (MOC) code (Konikow and Bredehoeft, 1978). The revised code was referred to as PI-MOC by Strecker and Chu (1986). PI-MOC allows the users to choose particular parameters that are to be identified by the PI algorithm. The algorithm finds optimal parameters by a constrained least square formulation. The formulation, development, and some applications of the PI-MOC model can be found in a number of previous publications (Strecker et al., 1985; Strecker and Chu, 1986; and Chu et al., 1987), and will not be repeated here for brevity.

3.2) Input Parameters for Site X

Modeling of groundwater movement and contaminant transport at Site X first required the determination of several parameters. Some of these parameters such as specific yield, saturated thickness, source location, and effective porosity were obtained from previous investigations done on the site. These parameters, which are given in Table 1, were not adjusted during model calibration and the subsequent simulation runs. Other information such as dispersivity and contamination scenario were inferred from results collected in previous studies and from field inspection.

The areal extent modeled is indicated in Figure 2. This area was extended beyond Site X's boundaries to correctly model the influence of the creek and marsh (see Figure 2). Previous studies in the area had determined the creek and swamp to be hydrologically connected and that the water level in the creek significantly influences areal groundwater flow.

TABLE 1 Input Parameters for Modeling Site X by USGS-MOC

Delta X	50 feet
Delta Y	50 feet
Longitudinal dispersivity	10 feet
Ratio of transverse to longitudinal dispersivity	0.30
Ratio of Tyy to Txx	1.00
Saturated thickness	6-10 feet
Effective porosity	0.25
Specific yield (transient case)	0.20
Specific yield (steady-state case)	0.00

3.3) PI-MOC Applications

In the PI-MOC application, the code was used to calibrate only model transmissivity values. Although PI-MOC can be used to calibrate dispersivities from contaminant concentration data (Strecker and Chu, 1986), this option was not used because of the lack of good water quality data. Instead, the dispersivities will be manually adjusted as explained later. This particular parameter identification scenario requires the input of observed groundwater table at specific locations. Instead of incorporating the seasonally variation in PI-MOC, stationary water table data in one appropriate time period were used for a steady-state calibration. The location of the monitoring wells and staff gauges where data were observed are given in Figure 2.

Even with the almost homogeneous material (constant hydraulic conductivity) at the site, the input transmissivity to USGS-MOC is not constant because of the variable aquifer thickness (See Figure 3). To reflect this variation in transmissivity, the aquifer was divided into a number of zones, each with a constant transmissivity. The zoning patterns and an initial estimate of zonal transmissivity values were input to PI-MOC. The number of zones used in this study varied from one to four (see Second Column of Table 2). Although the selection of zonal pattern has been shown to effect the outcome of PI calibration (Chu, Strecker, and Lettenmaier, 1987), zone selection was relatively straightforward for Site X. Since the aquifer at Site X is composed of rather homogeneous materials, transmissivity should vary with aquifer thickness. Figure 4 shows the aquifer thickness map which was constructed from soil samples and well log data. Transmissivity patterns used for two, three, and four zones are shown in Figures 5a, 5b, and 5c respectively.

FIGURE 4. Aquifer Thickness (in Feet) for Modeling Area (Zeros denotes no flow region)

0	0	0	0	0	0	0	0	0	0	0	0	0
0	6	6	6	6	6	6	6	6	6	6	6	0
0	7	7	7	7	7	7	7	7	7	7	6	0
0	8	8	8	8	8	8	8	8	8	7	6	0
0	10	10	10	10	10	10	10	10	8	7	6	0
0	10	10	10	10	10	10	10	10	8	7	6	0
0	10	10	10	10	10	10	10	10	8	7	6	0
0	10	10	10	10	10	10	10	10	8	7	6	0
0	10	10	10	10	10	10	10	10	8	7	6	0
0	10	10	10	10	10	10	10	10	8	7	6	0
0	10	10	10	10	10	10	10	10	8	7	6	0
0	10	10	10	10	10	10	10	10	8	7	6	0
0	0	0	0	0	0	0	0	0	0	0	0	0

FIGURE 5. Transmissivity map for 2, 3, and 4 Zones

```
          Creek                                Creek                                  Creek
0 0 0 0 0 0 0 0 0 0 0 0 0           0 0 0 0 0 0 0 0 0 0 0 0 0           0 0 0 0 0 0 0 0 0 0 0 0 0
0 2 2 2 2 2 2 2 2 2 2 2 0           0 3 3 3 3 3 3 3 3 3 3 3 0           0 4 4 4 4 4 4 4 4 4 4 4 0
0 2 2 2 2 2 2 2 2 2 2 2 0           0 2 2 2 2 2 2 2 2 2 2 3 0           0 3 3 3 3 3 3 3 3 3 3 4 0
0 2 2 2 2 2 2 2 2 2 2 2 0           0 1 1 1 1 1 1 1 1 1 2 3 0           0 2 2 2 2 2 2 2 2 2 3 4 0
0 1 1 1 1 1 1 1 1 2 2 2 0  Marsh    0 1 1 1 1 1 1 1 1 1 2 3 0  Marsh    0 1 1 1 1 1 1 1 1 2 3 4 0  Marsh
0 1 1 1 1 1 1 1 1 2 2 2 0           0 1 1 1 1 1 1 1 1 1 2 3 0           0 1 1 1 1 1 1 1 1 2 3 4 0
0 1 1 1 1 1 1 1 1 2 2 2 0           0 1 1 1 1 1 1 1 1 1 2 3 0           0 1 1 1 1 1 1 1 1 2 3 4 0
0 1 1 1 1 1 1 1 1 2 2 2 0           0 1 1 1 1 1 1 1 1 1 2 3 0           0 1 1 1 1 1 1 1 1 2 3 4 0
0 1 1 1 1 1 1 1 1 2 2 2 0           0 1 1 1 1 1 1 1 1 1 2 3 0           0 1 1 1 1 1 1 1 1 2 3 4 0
0 1 1 1 1 1 1 1 1 2 2 2 0           0 1 1 1 1 1 1 1 1 1 2 3 0           0 1 1 1 1 1 1 1 1 2 3 4 0
0 1 1 1 1 1 1 1 1 2 2 2 0           0 1 1 1 1 1 1 1 1 1 2 3 0           0 1 1 1 1 1 1 1 1 2 3 4 0
0 1 1 1 1 1 1 1 1 2 2 2 0           0 1 1 1 1 1 1 1 1 1 2 3 0           0 1 1 1 1 1 1 1 1 2 3 4 0
0 0 0 0 0 0 0 0 0 0 0 0 0           0 0 0 0 0 0 0 0 0 0 0 0 0           0 0 0 0 0 0 0 0 0 0 0 0 0

       2-Zone 2                            3-Zone 3                            4-Zone 4
       1-Zone 0                            2-Zone 2                            3-Zone 3
       0-Zone 0                            1-Zone 1                            2-Zone 2
                                           0-No flow                           1-Zone 1
                                                                               0-No flow
          a.)                                 b.)                                 c.)
```

The PI-MOC model also requires the input of numeric upper and lower bounds and initial estimate of transmissivity values in each zone. These values are listed in columns three, four, and five in Table 2. The upper and lower bounds on transmissivity were determined from physical characteristics of the material and from pump test data. Upper and lower bounds of transmissivity are the only constraints in the optimization formulation in PI and therefore represent the only bounds on the solution domain. Low, medium, and high

TABLE 2. Summary of PI Calibration Runs

Run	Number of Transmissivity Zones	Initial Parameter Estimate	Upper Bound	Lower Bound	Solution	Objective
1	1	T1=.005	T1=.01	T1=.001	no solution	----
2	2	T1=.003 T2=.002	T1=.01 T2=.01	T1=.0001 T2=.0001	no solution	----
3	3	T1=.003 T2=.002	T1=.05 T2=.05	T1=.0001 T2=.0001	T1=.05 T2=.008	4.76
4	3	T1=.006 T2=.001 T3=.001	T1=.01 T2=.008 T3=.006	T1=.0010 T2=.0001 T3=.0001	T1=.0100 T2=.00066 T3=.0060	22.40
5	3	T1=.0010 T2=.0001 T3=.0001	T1=.01 T2=.008 T3=.006	T1=.0010 T2=.0001 T3=.0001	T1=.0100 T2=.0022 T3=.0014	29.30
6	3	T1=.008 T2=.006 T3=.004	T1=.01 T2=.008 T3=.006	T1=.0010 T2=.0001 T3=.0001	T1=.01 T2.006 T3=.006	65.00
7	3	T1=.006 T2=.001 T3=.001	T1=.01 T2=.008 T3=.006	T1=.0001 T2=.00001 T3=.00001	T1=.0100 T2=.00066 T3=.0060	22.40
8	3	T1=.006 T2=.001 T3=.001	T1=.01 T2=.008 T3=.006	T1=.0010 T2=.0008 T3=.0006	T1=.01 T2=.001 T3=.003	41.70
9	4	T1=.006 T2=.001 T3=.001 T4=.001	T1=.01 T2=.008 T3=.006 T4=.004	T1=.0001 T2=.0001 T3=.0001 T4=.0001	T1=.0100 T2=.0007 T3=.0060 T4=.0040	25.60
10	4	T1=.0010 T2=.0001 T3=.0001 T4=.0001	T1=.01 T2=.008 T3=.006 T4=.004	T1=.0001 T2=.0001 T3=.0001 T4=.0001	T1=.0100 T2=.0060 T3=.0060 T4=.0001	41.40
11	4	T1=.008 T2=.006 T3=.004 T4=.002	T1=.01 T2=.008 T3=.006 T4=.004	T1=.0001 T2=.0001 T3=.0001 T4=.0001	T1=.0100 T2=.0060 T3=.0040 T4=.00066	39.90
12	4	T1=.006 T2=.001 T3=.001 T4=.001	T1=.01 T2=.008 T3=.006 T4=.004	T1=.0010 T2=.0008 T3=.0006 T4=.0001	T1=.0100 T2=.00083 T3=.0060 T4=.0040	40.90

initial estimates for transmissivity were used in PI-MOC runs. If the PI procedure is robust, different initial estimates should not significantly affect the PI solutions.

3.4) PI-MOC Results

Each PI-MOC run was for a steady-state simulation period of one half year. The PI algorithm finds the optimal parameters by an iterative procedure (Strecker and Chu, 1986). Parameter values are improved (measured by the value of the objective function) in each successive iteration. The model parameters in each case studied were determined in four iterations. The objective value of the optimization (which is the sum of squares of the differences between predicted and observed water tables at all the monitoring wells) and the parameters found at the end of the fourth iteration for each case are given in the last column of Table 2. The objective value at each iteration for Run 4 in Table 2 is shown in Figure 6. As shown by Figure 6, most of the improvement in the parameter estimation occurs in the first two iterations.

The various runs in Table 2 were designed to show the effects of zonal patterns and initial parameter estimates on PI-MOC. The use of one zone of transmissivity did not produce satisfactory solutions. One zone of transmissivity for this site also is not physically plausible. The observed water table gradient increases near the constant head boundaries (where the Marsh and the Creek are). For an aquifer with relatively constant hydraulic conductivity, this is possible only with a decrease in aquifer thickness and transmissivity near these boundaries. Available cross section at the site (Figure 3) confirm this decrease in aquifer thickness. The use of one transmissivity zone does not reflect the change in the water table gradient observed at the site.

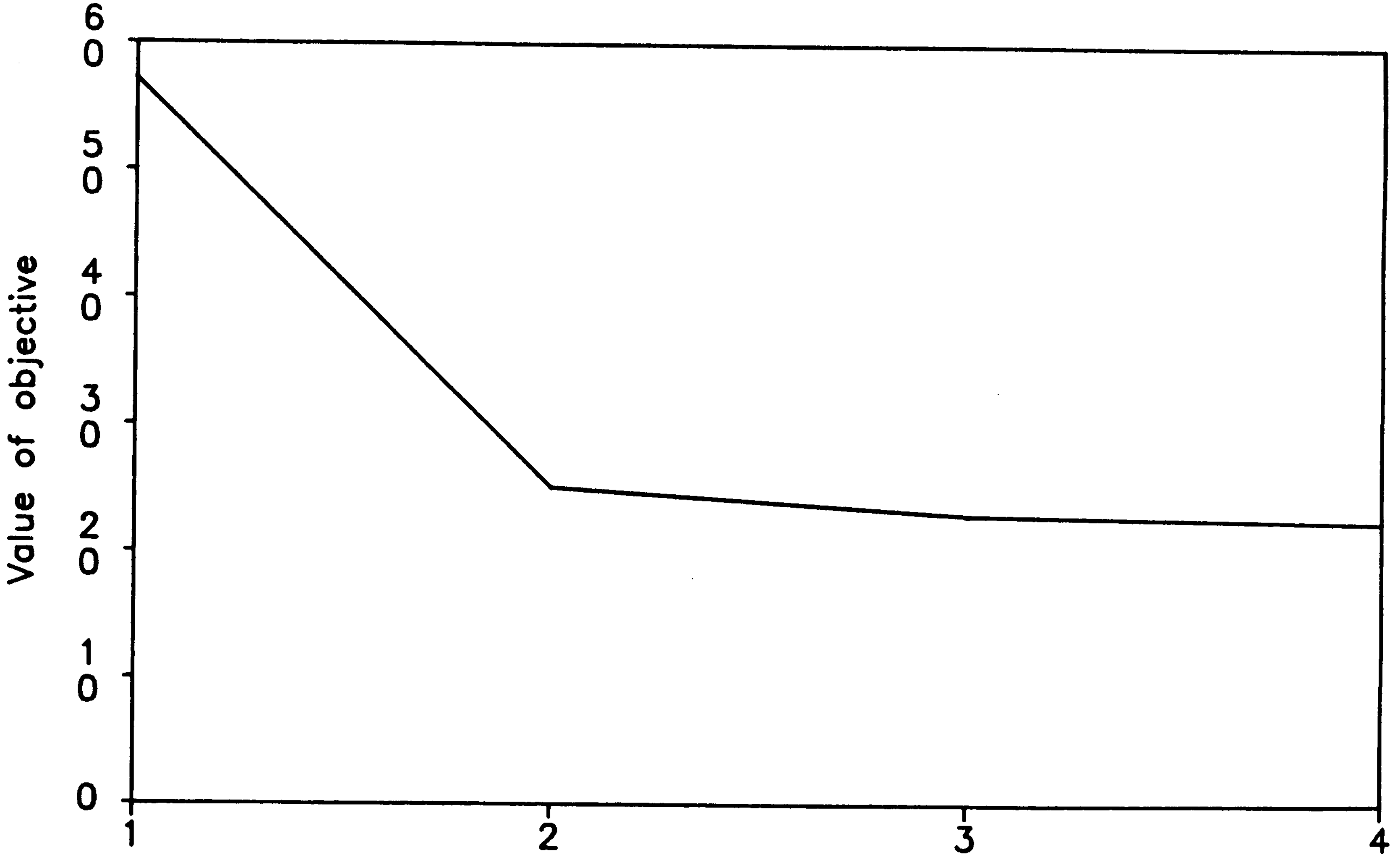

Figure 6 Value of Objective for Run number 4

Runs 2 and 3 assumed two zones of transmissivity. This transmissivity pattern is shown in Fig 5a. For a physically plausible upper bound of 0.01 ft^2/s, Run 2 could not reach a convergent solution in four iterations. Relaxing this upper bound to 0.05 ft^2/s (Run 3) did produce a convergent solution for transmissivity but the values were considered too high. Earlier studies of the site have estimated the transmissivity of the site to range from .01 to .0002 ft^2/s with the most likely value as .006 ft^2/s (Erickson, 1986).

The use of three transmissivity zones in PI-MOC did produce a solution that was within the upper and lower bounds (See runs 4 through 8 in Table 2). The configuration of these transmissivity zones is shown in Figure 5b. Runs 4 through 6 show the effect of initial parameter estimation on the solution. As shown in the last column of Table 2, different parameters were found by the PI scheme using a medium, low, and high initial estimation of parameter values. The run with medium initial parameter estimate produced the smallest objective value in the optimization. The behavior of objective value for this run is shown in Figure 6.

Runs 7 and 8 show the effect of the parameter lower bound on the PI-MOC solution. Run 7 results show that relaxing the parameter lower bound does not affect the final parameter values by PI-MOC. Run 8 results show that tightening the lower parameter bound does affect the PI-MOC solution. The effect can be seen in Figure 7, where the objective valued ceased to improve after second iteration because of a more restrictive solution domain.

Runs 9 through 12 assumed 4 zones of transmissivity for the site. Configuration of these transmissivity zones is given in figures 5c. Runs 9 through 11 show the effect of initial parameter estimation on the solution. As in the three zone case, the medium initial parameter estimate produced the PI solution with minimum objective value. The tightened lower parameter bound in

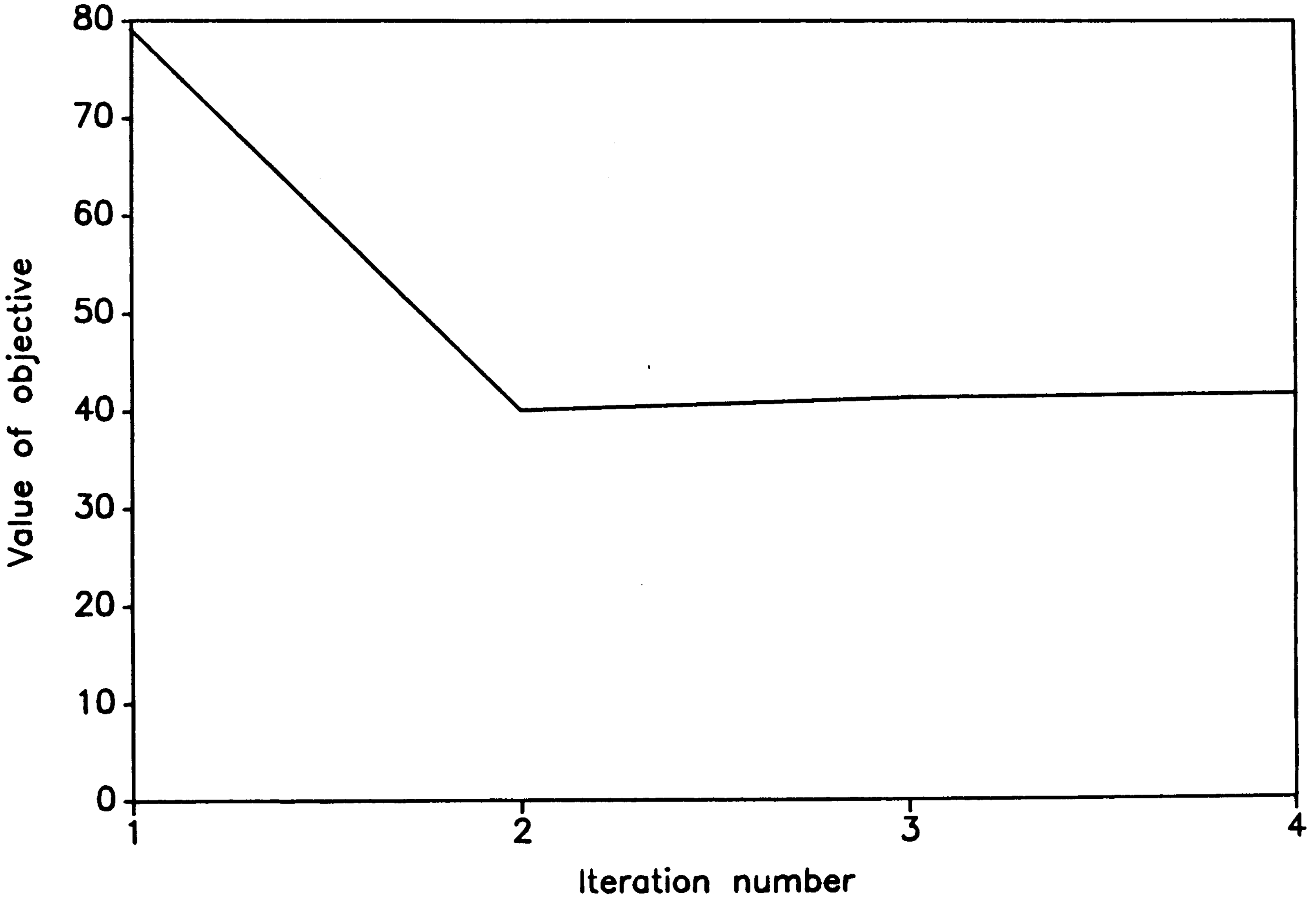

Figure 7   Value of Objective for Run Number 8

Run 12 produced unstable behavior in the objective values as was observed in the 3 zone case (Run 8) which were not acceptable in this study.

In terms of the objective value, Runs 4 and 9 for the three- and four-zone cases produced the best PI-MOC results. The zonal transmissivity values found by PI-MOC in both cases, however, were physically implausible. Since the aquifer is of relatively constant hydraulic conductivity, transmissivity values should decrease as the aquifer thickness decreases. Thus, transmissivities should decrease from zones 1 to 3 and zones 1 to 4. Runs 4 and 9 both show a zone of abnormally low transmissivity between zones of higher transmissivities.

In summary, the PI-MOC algorithm is effective in finding a set of parameters to minimize the defined objective function, but it is unable to recognize the fact that transmissivity in a homogeneous aquifer should vary with depth, unless provided by predefined zoning patterns. Initial parameter estimation also was shown to affect the parameter values determined by PI-MOC. Efficient as they are, PI algorithms should always be used with thoughtful human judgment.

CHAPTER 4

USGS-MOC APPLICATION

4.1) Objective of Application and Input Parameters

The objectives of the USGS-MOC application here were: 1) to attempt an independent trial-and-error calibration of transmissivity in USGS-MOC model for the site without the use of PI technique, and 2) to compare the results of simulation runs using transmissivities obtained from the two calibration methods (PI and trial-and-error). The same input parameters listed in Table 1 were used here.

4.2) Water Table Calibration

The USGS-MOC model was calibrated "manually" by changing the transmissivity values until the predicted water table contours compared favorably with the observed water table contours. An one-half year steady-state calibration period was used again. The manual calibration took approximately 15 runs of the USGS-MOC. The final transmissivity map is shown in Figure 8.

Comparisons of water table contours produced by USGS-MOC with parameters obtained from the two calibration techniques are shown in Figures 9a-9d. Figure 9a shows the observed water table data provided by the Washington State Department of Ecology. Figures 9b and 9c show the water table data produced by USGS-MOC using transmissivity determined from PI-MOC assuming three and four zone characterization respectively. Figure 9d show water table data produced by USGS-MOC using transmissivity determined from manual calibration. All three cases (Figures 9b, 9c, and 9d) produce water table elevations that are in good agreement with the observed conditions (Figure 9a).

FIGURE 8. Map Determined by Trial-and-Error Calibration (ft*ft/sec)
(Zeros denote no flow boundary)

0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.0000	0.0010	0.0010	0.0010	0.0010	0.0010	0.0010	0.0010	0.0010	0.0010	0.0010	0.0010	0.0010
0.0000	0.0015	0.0015	0.0015	0.0015	0.0015	0.0015	0.0015	0.0015	0.0015	0.0015	0.0010	0.0000
0.0000	0.0050	0.0050	0.0050	0.0050	0.0050	0.0050	0.0050	0.0050	0.0050	0.0015	0.0010	0.0000
0.0000	0.0100	0.0100	0.0100	0.0100	0.0100	0.0100	0.0100	0.0100	0.0050	0.0015	0.0010	0.0000
0.0000	0.0100	0.0100	0.0100	0.0100	0.0100	0.0100	0.0100	0.0100	0.0050	0.0015	0.0010	0.0000
0.0000	0.0100	0.0100	0.0100	0.0100	0.0100	0.0100	0.0100	0.0100	0.0050	0.0015	0.0010	0.0000
0.0000	0.0100	0.0100	0.0100	0.0100	0.0100	0.0100	0.0100	0.0100	0.0050	0.0015	0.0010	0.0000
0.0000	0.0100	0.0100	0.0100	0.0100	0.0100	0.0100	0.0100	0.0100	0.0050	0.0015	0.0010	0.0000
0.0000	0.0100	0.0100	0.0100	0.0100	0.0100	0.0100	0.0100	0.0100	0.0050	0.0015	0.0010	0.0000
0.0000	0.0100	0.0100	0.0100	0.0100	0.0100	0.0100	0.0100	0.0100	0.0050	0.0015	0.0010	0.0000
0.0000	0.0100	0.0100	0.0100	0.0100	0.0100	0.0100	0.0100	0.0100	0.0050	0.0015	0.0010	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

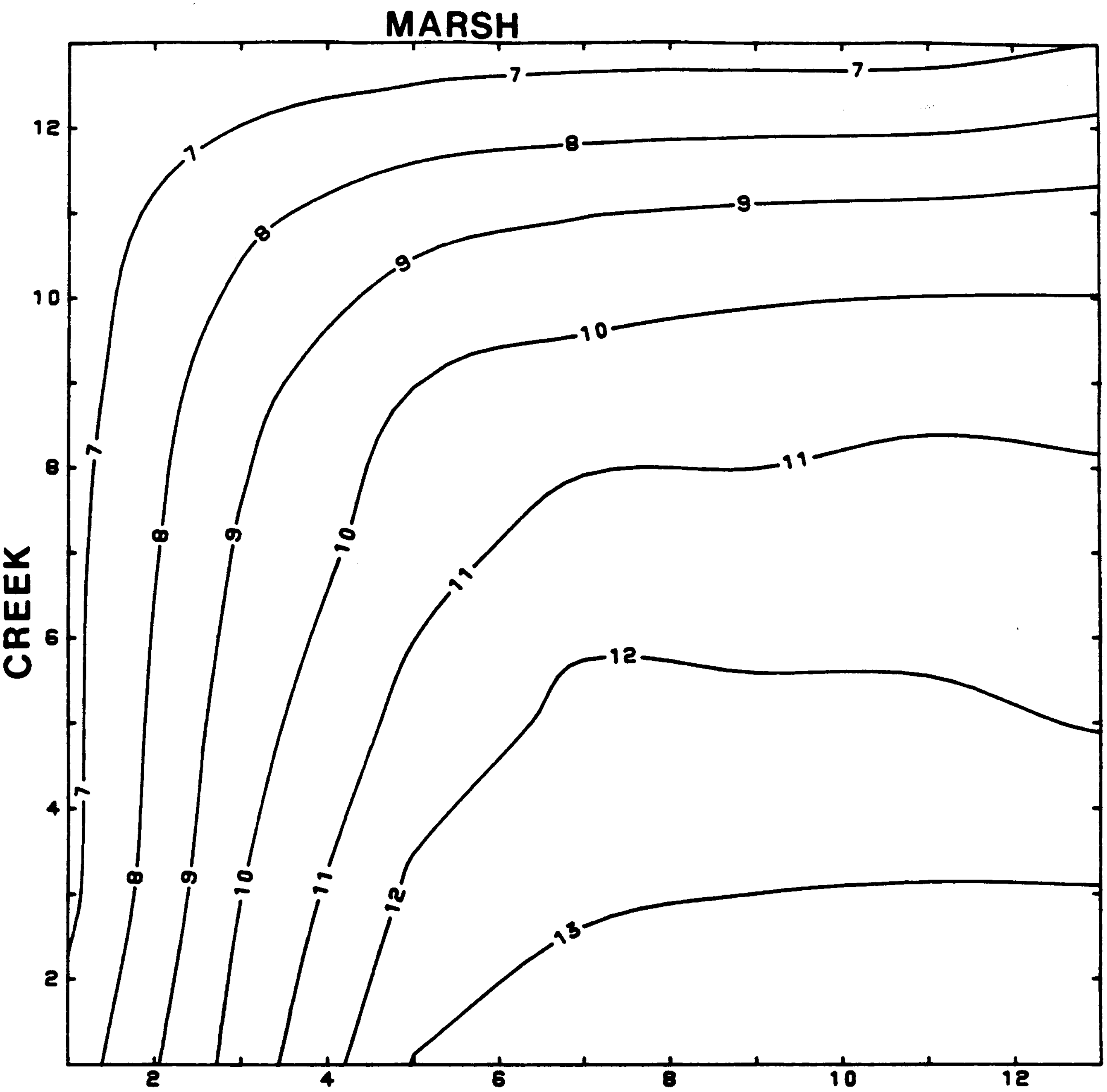

Figure 9a Observed Water Table Contours for the Calibration Period (based on data from Washington Department of Ecology)

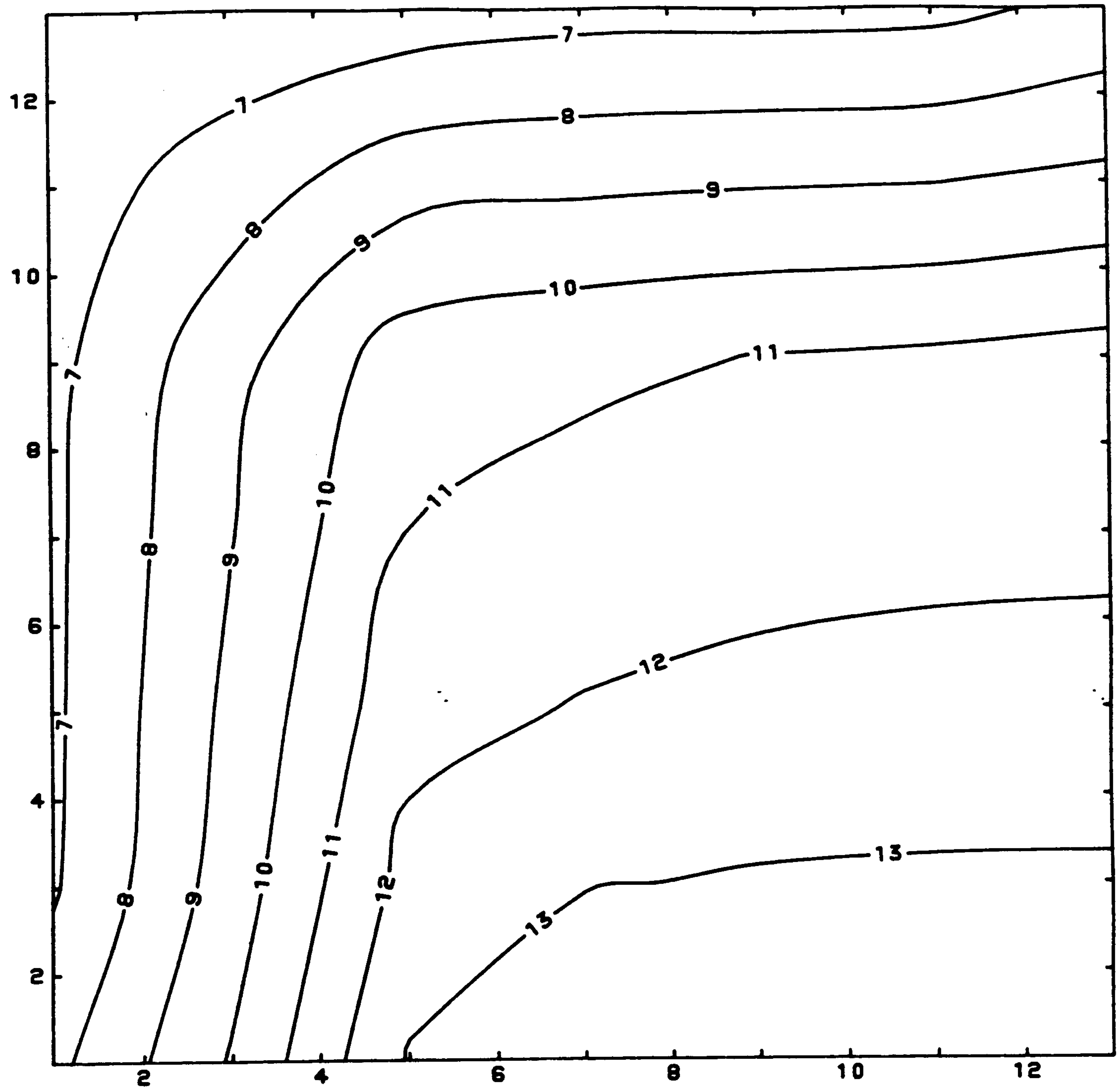

Figure 9b Water Table Contours Produced by USGS-MOC Using Transmissivity Determined from PI-MOC Assuming Three Zone Characterization

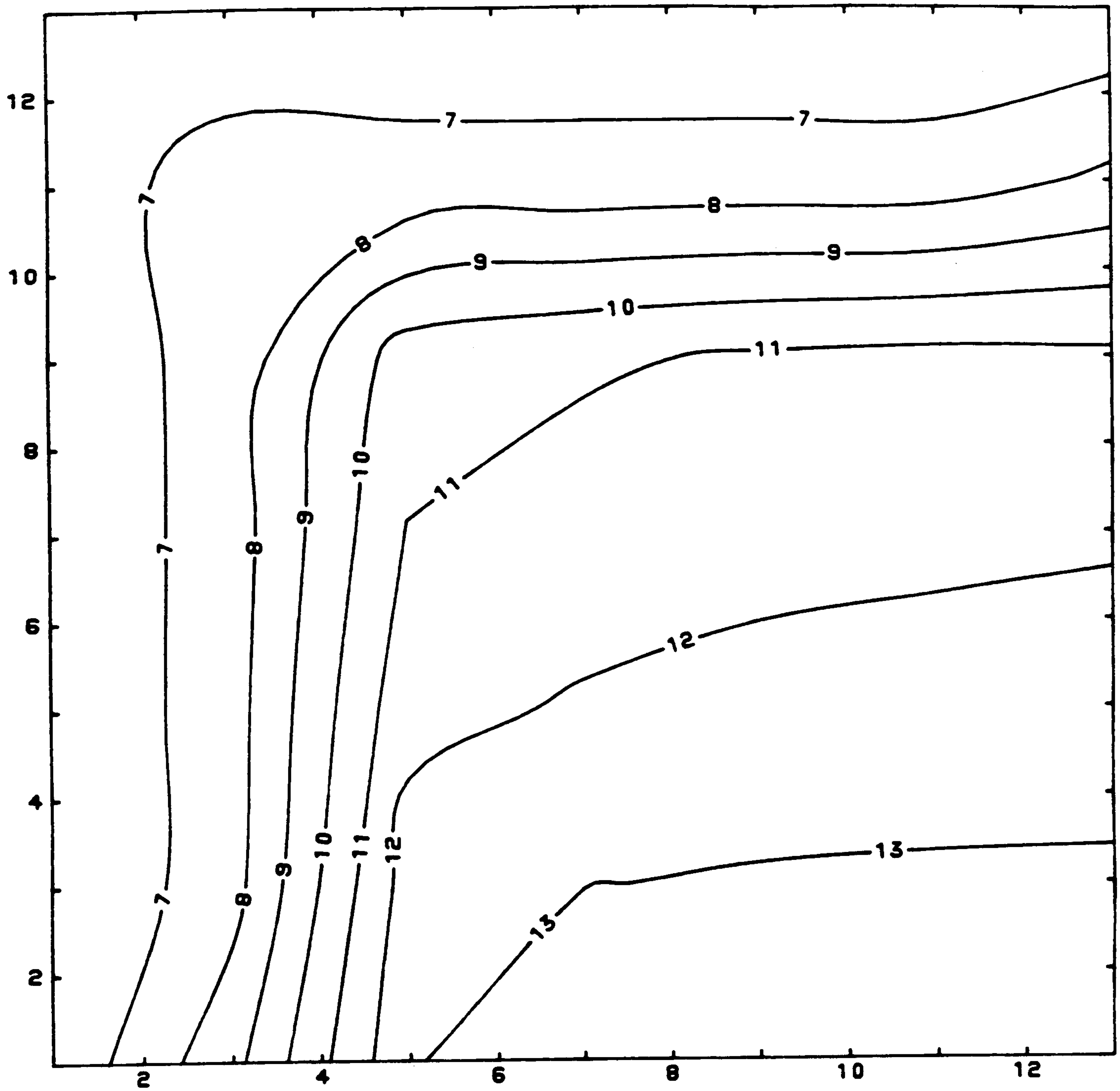

Figure 9c Water Table Contours Produced by USGS-MOC Using Transmissivity Determined from PI-MOC Assuming Four Zone Characterization

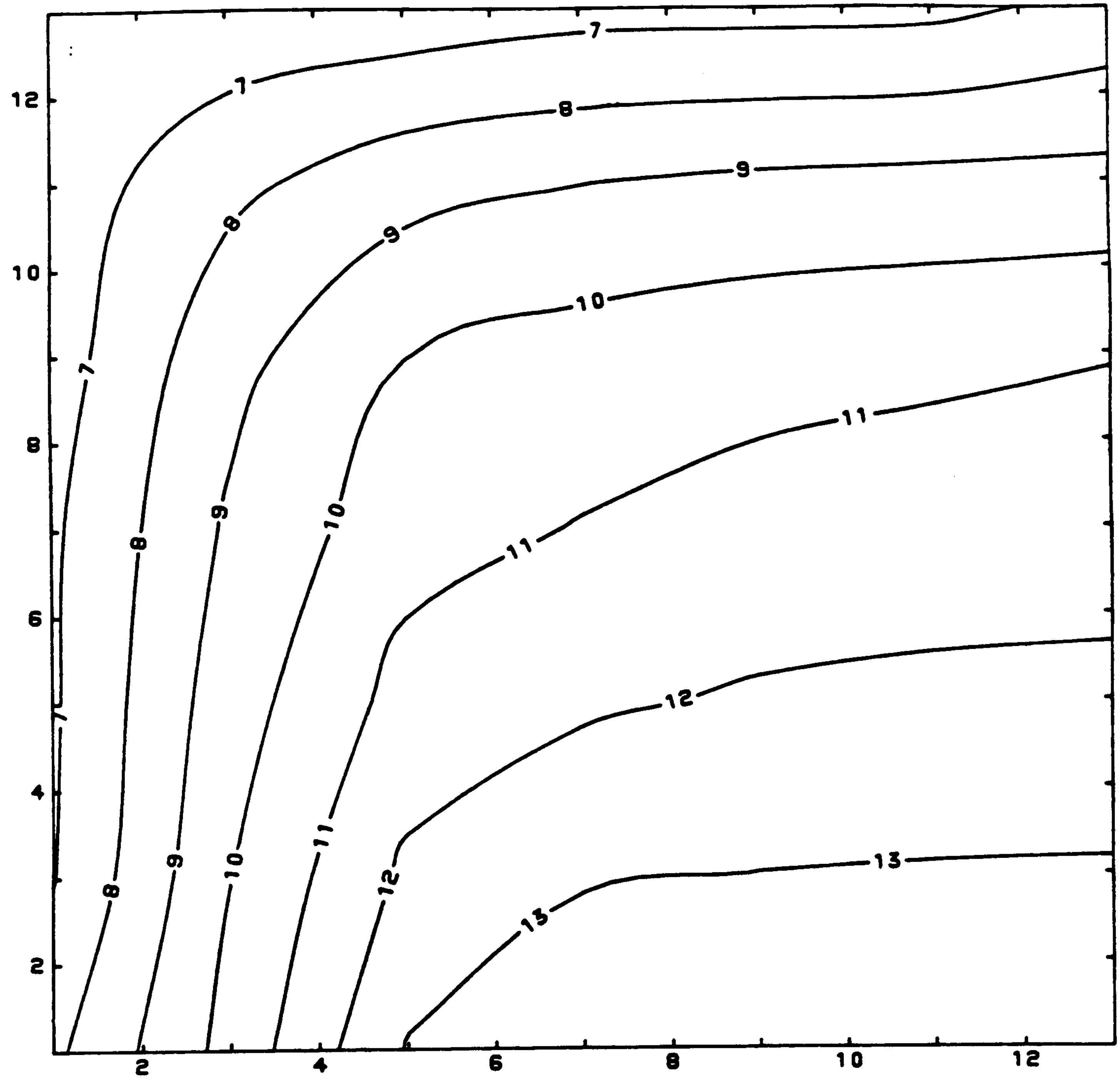

Figure 9d   Water Table Contours Produced by USGS-MOC Using Transmissivity Determined by Trial-and-Error Calibration

4.3) Contaminant Plume Characterization

Although present data were not adequate for an accurate calibration of dispersion coefficients in USGS-MOC, it was felt that a reasonable dispersivity value could be inferred from the general shapes of the contaminant plume.

The contamination scenario was inferred from the site's history of usage (Erickson 1986). Most of the contamination of groundwater occurred during the four year period of 1981 to 1984 by the leaky storage sump and improper waste handling (Erickson 1986). This contamination was modeled in USGS-MOC as a continuous injection well (at a rate of 0.001 ft^3/sec), which best characterizes the continuous nature of contamination at the site. Location of the source was taken from earlier investigation (Erickson, 1986) and is shown in Figure 2.

Using the transmissivities determined from trial-and-error calibration, a number of simulation runs were made to investigate the effects of input dispersivity values on the shapes of the contaminant plume. The results of using longitudinal dispersivity values of 1, 10, and 100 are shown in Figures 10a, 10b, and 10c respectively. The plume generated by a longitudinal dispersivity of 1 (Figure 10a) was too narrow in that it did not reach some monitoring wells where contamination was detected. The plume generated by a longitudinal dispersivity of 100 (Figure 10c) showed an exaggerated spread that appeared to move up gradient from the source, which was not observed in the field. The dispersivity value of 10 (Figure 10b) produced the most reasonable plume shape and was eventually adopted for further simulation.

4.4) Further Simulation Runs

After the dispersivity value was estimated, the USGS-MOC model was used to simulate contaminant transport at the site over the period of 1981 to 1984 (a hindcast). Because of the period covered in these runs, transient

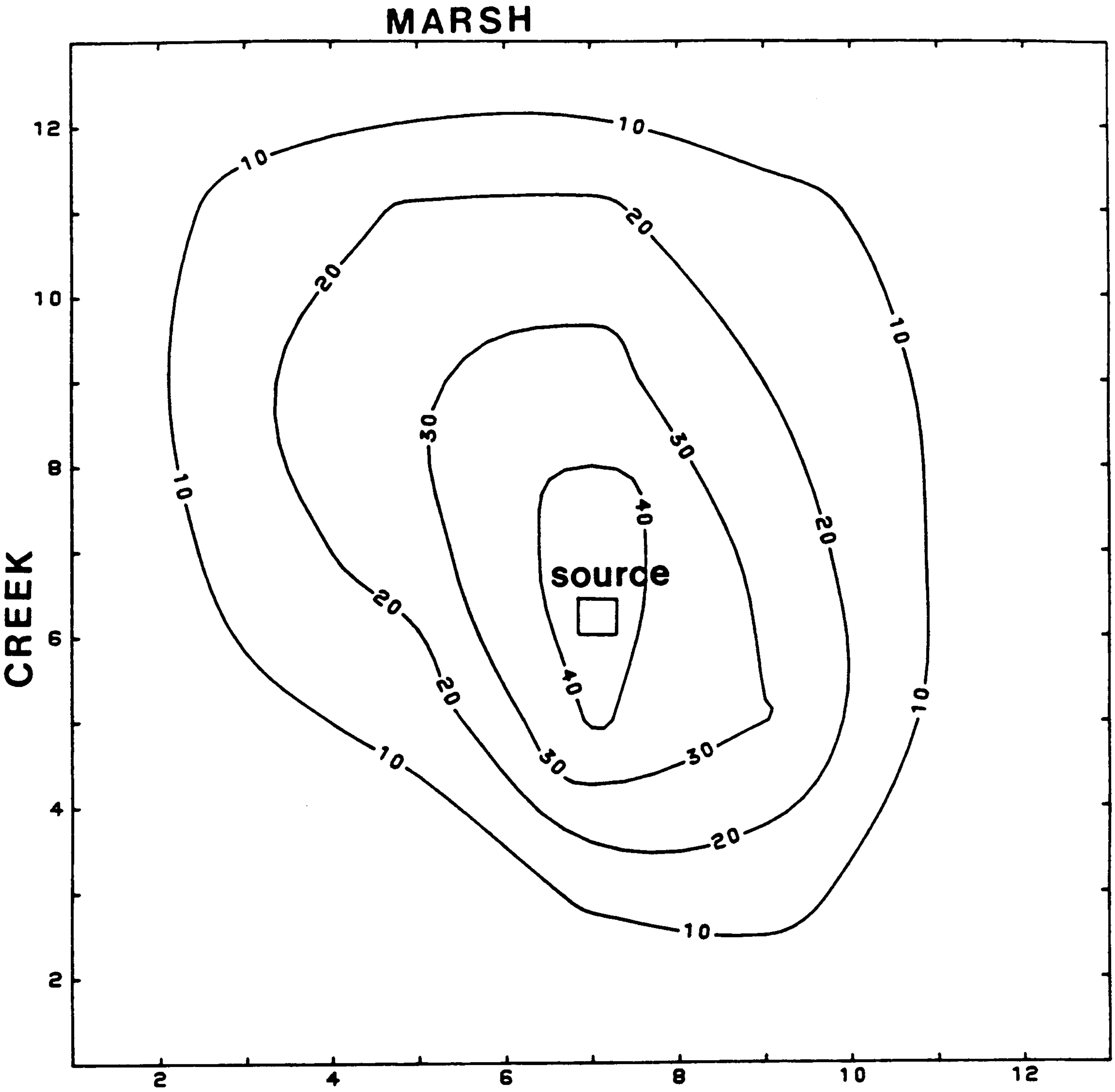

Figure 10a Contaminant Plume From an Input Longitudinal Dispersivity of 1 (Source Concentration = 1000 units)

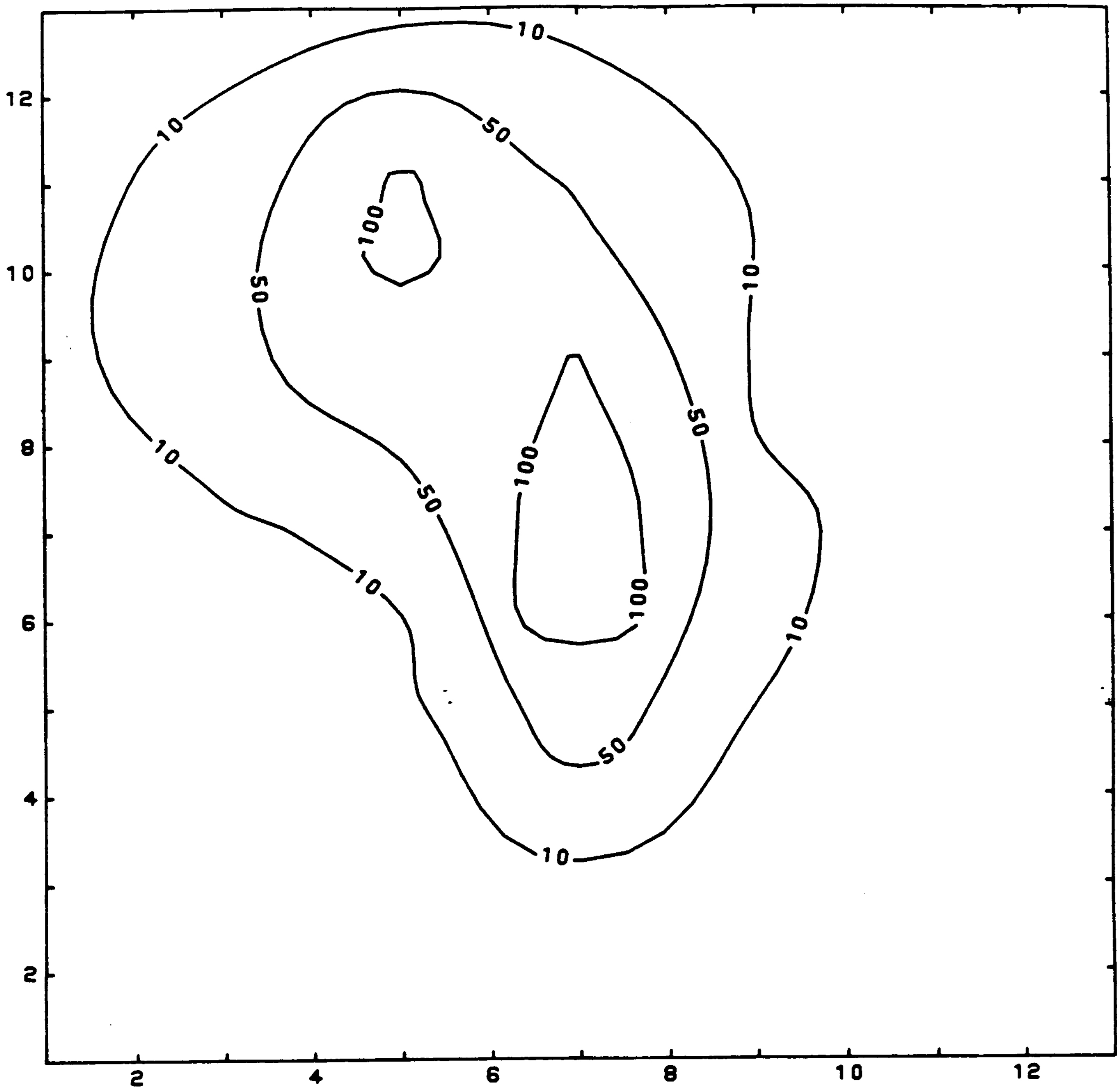

Figure 10b Contaminant Plume From an Input Longitudinal Dispersivity of 10 (Source Concentration = 1000 units)

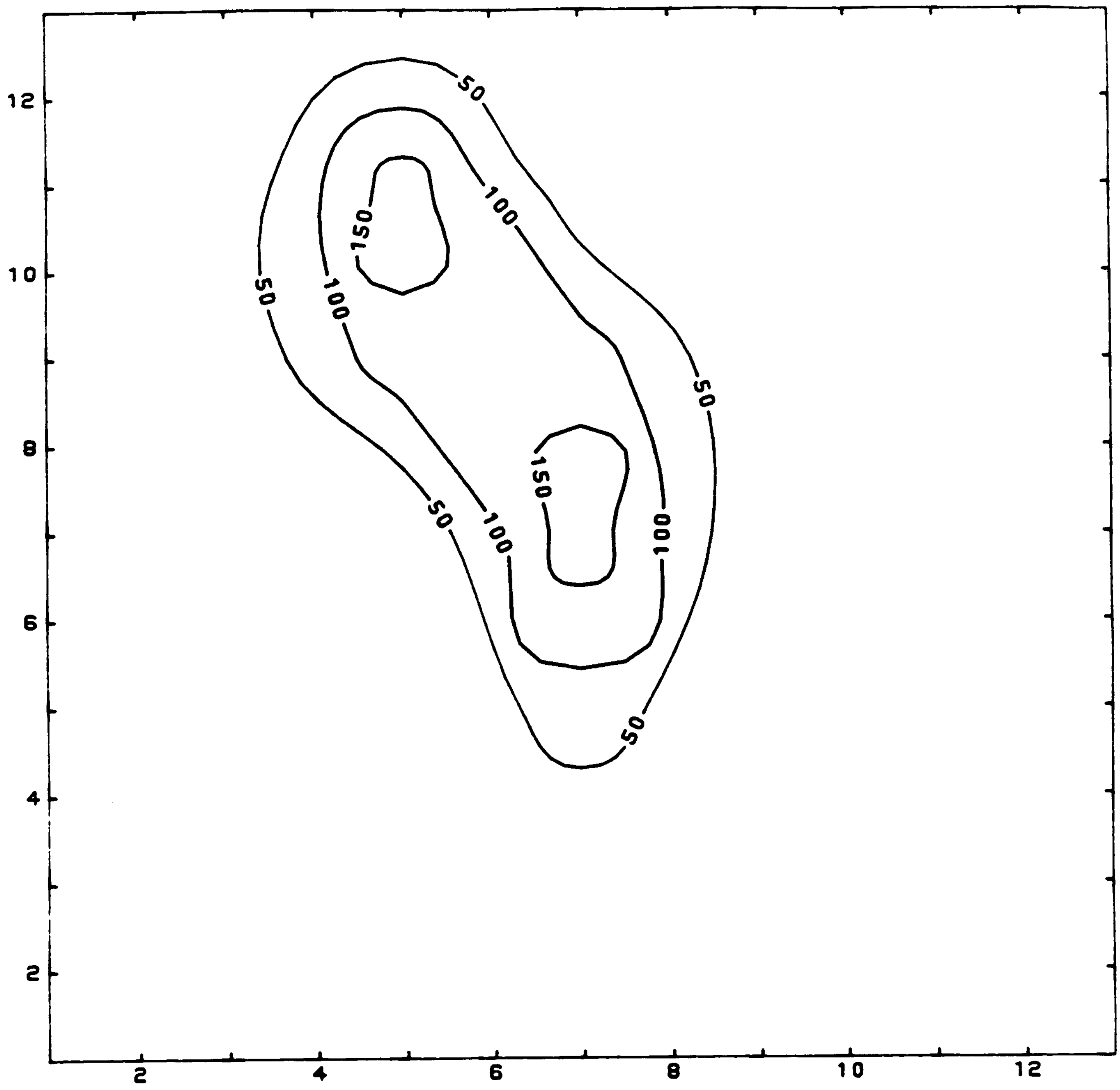

Figure 10c Contaminant Plume From an Input Longitudinal Dispersivity of 100 (Source Concentration = 1000 Units)

simulations must be made. The input storage coefficient value used in these runs is given in Table 1. A summary of these runs is given in Table 3. The contaminant plumes calculated from the model using parameters determined from both calibration techniques at the end of the four year simulation are shown in Figures 11, 12, and 13.

TABLE 3. Summary of USGS-MOC Modeling Runs

Case no.	Period (years)	Transmissivity	Background Contaminant Concentration	Chem. Mass Balance Error (percent)	Mass Balance Error (percent)
1.	0.5000	Manual	None	-22.34	.7900
2.	4.0000	PI-3 Zones	None	15.2-32.7	-.0134-.48
3.	4.0000	PI-4 Zones	None	4.1-30.2	-.006-.22
4.	4.0000	Manual	None	12.6-33.3	-.026-.144
5.	2.0000	PI-4 Zones	Yes	-33.- -37.	-.041-1.44
6.	2.0000	Manual	Yes	-33.- -35.	-.07-2.08

The general shape of the plume is similar for each run. The major differences are in contaminant concentration. The runs using PI-calibrated parameters produced slightly higher contaminant concentrations within the site. This is due to the presence of a low transmissivity zone identified by PI-MOC (see Cases 4 and 9 in Table 2) within the model domain which slows the movement of contaminant in the aquifer. Table 3 shows the range of mass balance and chemical mass balance errors estimated by the model for each run. The exact concentration values and concentration differences between the various model runs are relatively unimportant because of the large chemical mass balance

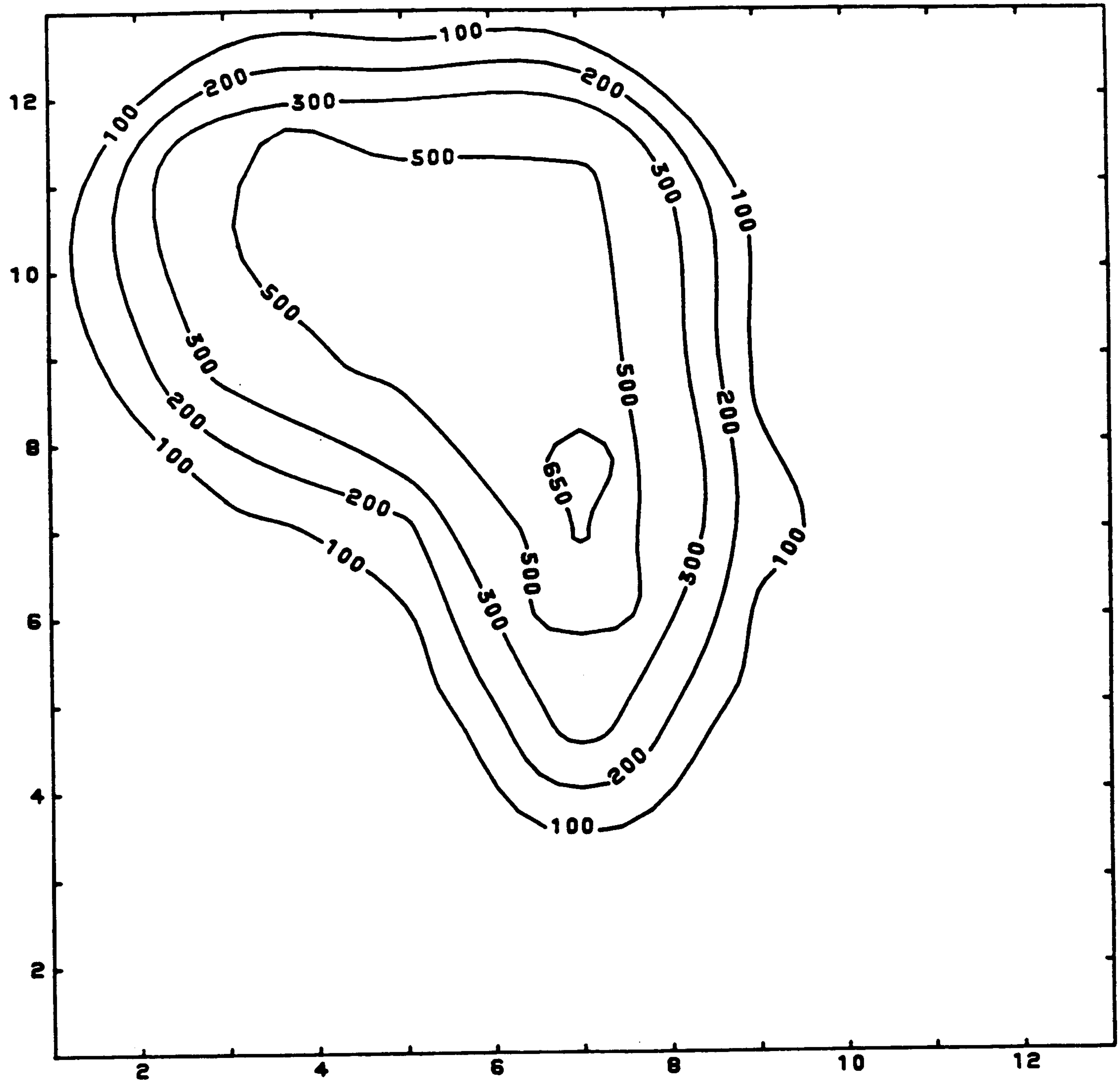

Figure 11 Contaminant Plume at the End of Four Year Simulation with Transmissivity Determined by Trial-and-Error Method (Longitudinal Dispersivity = 10, Source concentration = 1000 units)

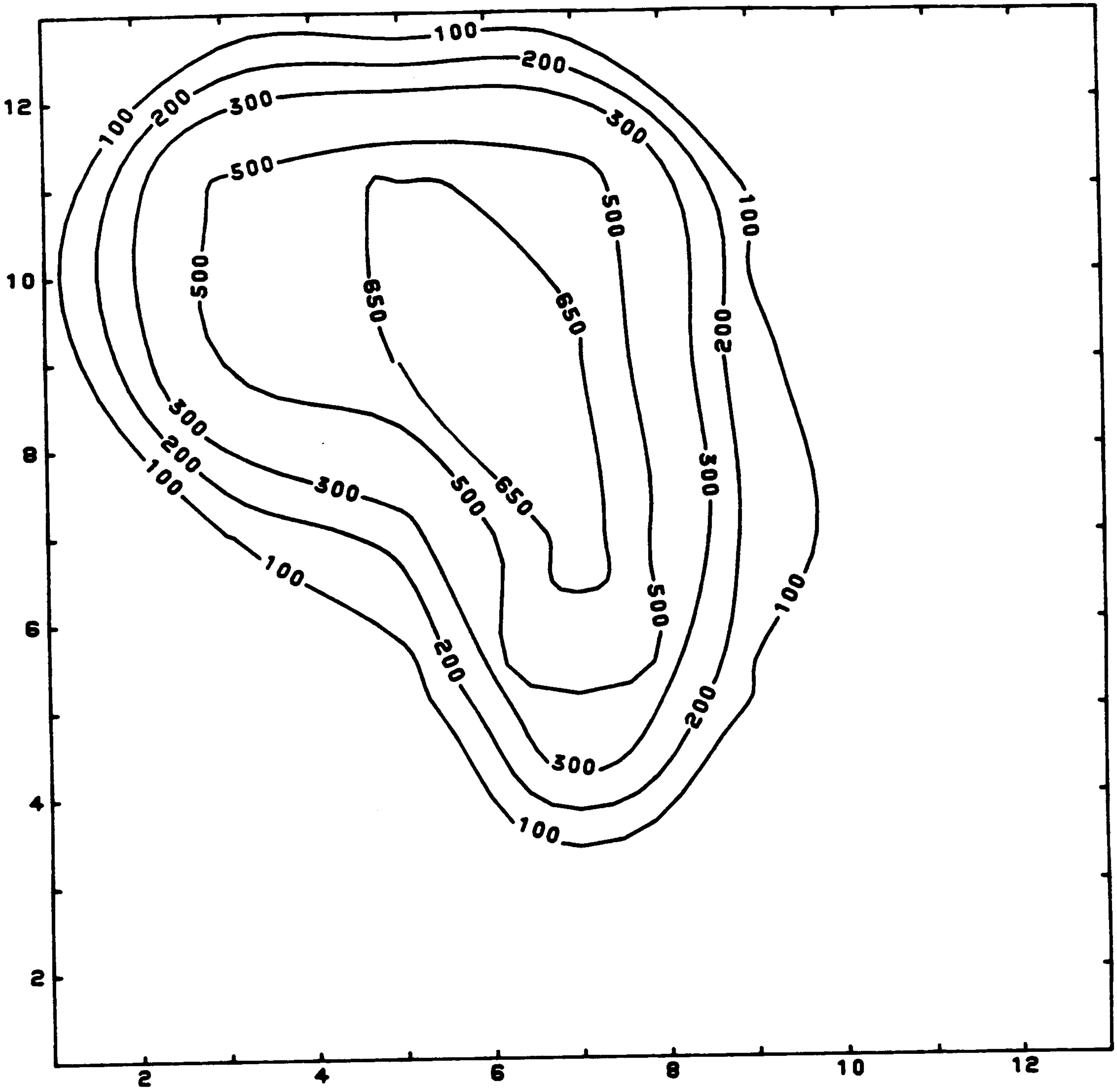

Figure 12 Contaminant Plume at the End of Four Year Simulation with Transmissivity Determined by PI-MOC Assuming Three-Zone Characterization (Longitudinal dispersivity = 10, source concentration = 1000 units)

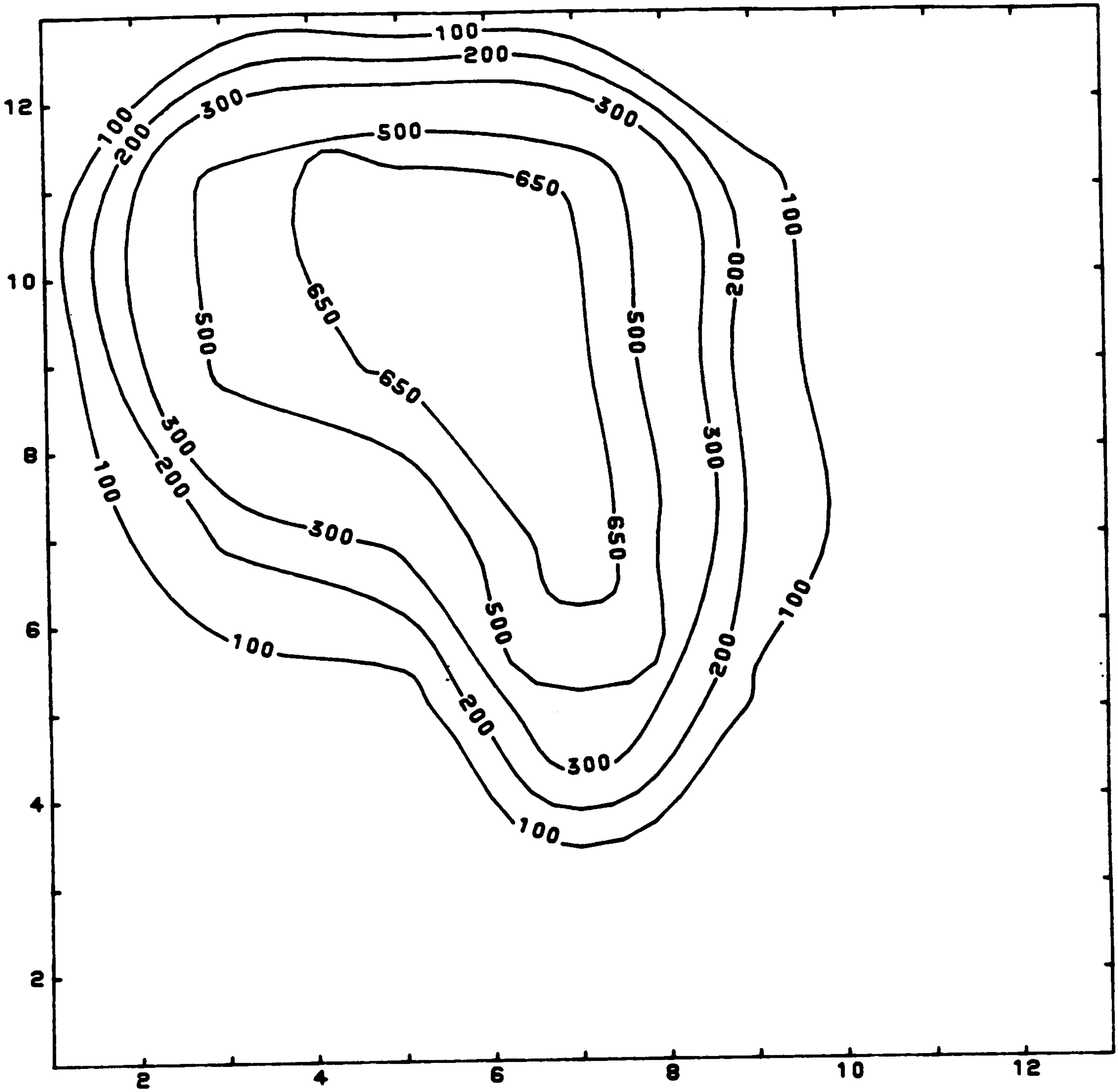

Figure 13 Contaminant Plume at the End of Four Year Simulation with Transmissivity Determined by PI-MOC Assuming Four-Zone Characterization (Longitudinal dispersivity = 10, Source concentration = 1000 units)

errors in nearly all the runs. The simulation study once again suggests that the USGS-MOC model should be used to characterize the contaminant plume rather than the contaminant concentration at specific locations (Chu, Strecker, and Lettenmaier, 1987).

Using the contaminant concentrations at the end of the four year simulations as background concentrations, the model was further run for two more years to simulate the behavior of the plume after the source was removed (leakage stopped). Runs using both manually calibrated and PI-calibrated parameters predicted rapid disappearance of the plume after the source removal (See Figures 14a, 14b, 15a, 15b and 15c). The results from using the PI-calibrated parameters showed a slower plume disappearance which was again due to the presence of a low transmissivity zone within the model domain. For all cases simulated, virtually all contaminants migrated out of the area within one year. This was expected since groundwater velocities across most of the modeling area were on the order of 300 feet/year.

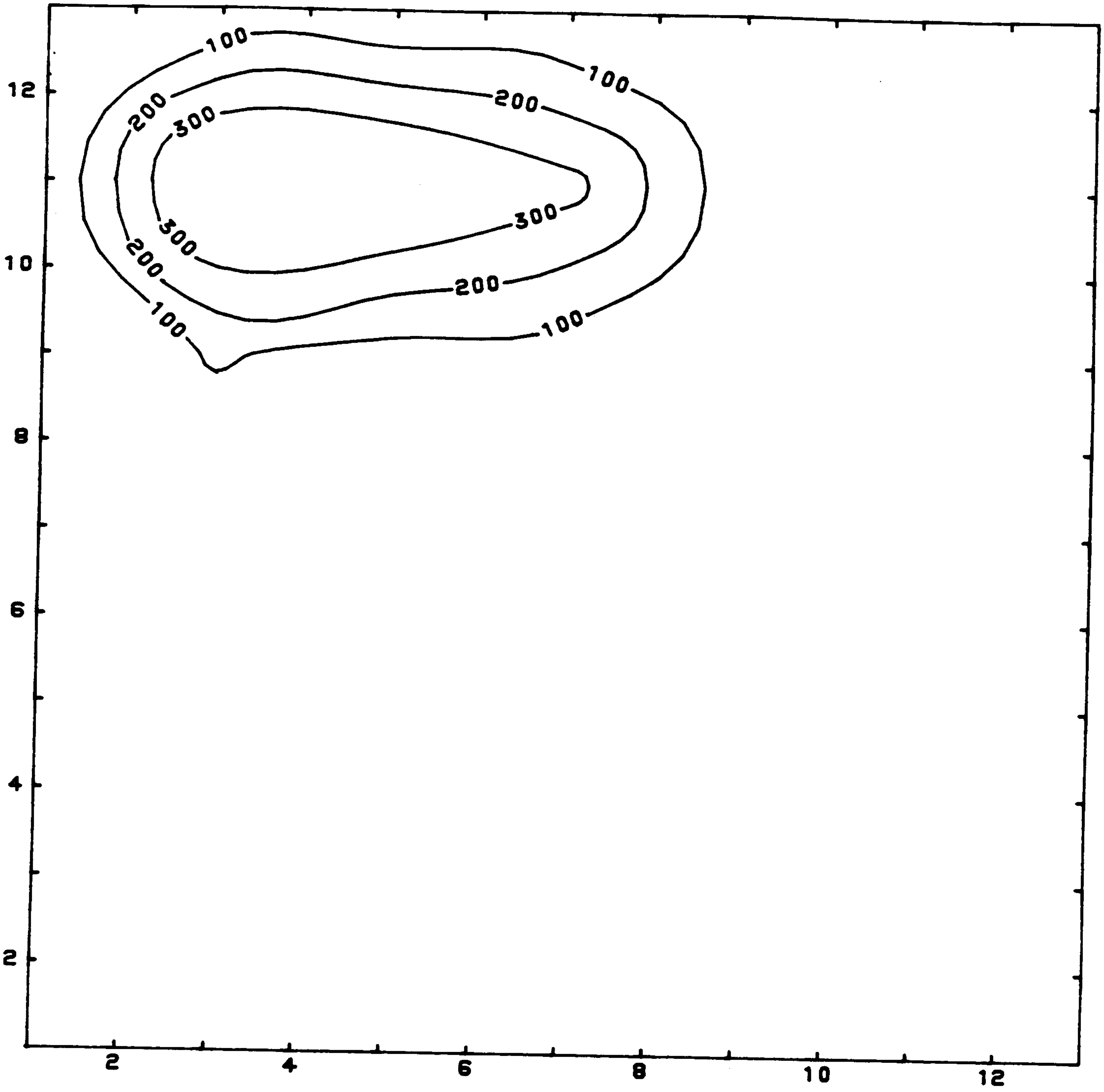

Figure 14a Contaminant Plume at 0.285 Year (Using transmissivity from trial-and-error calibration, longitudinal dispersivity = 10)

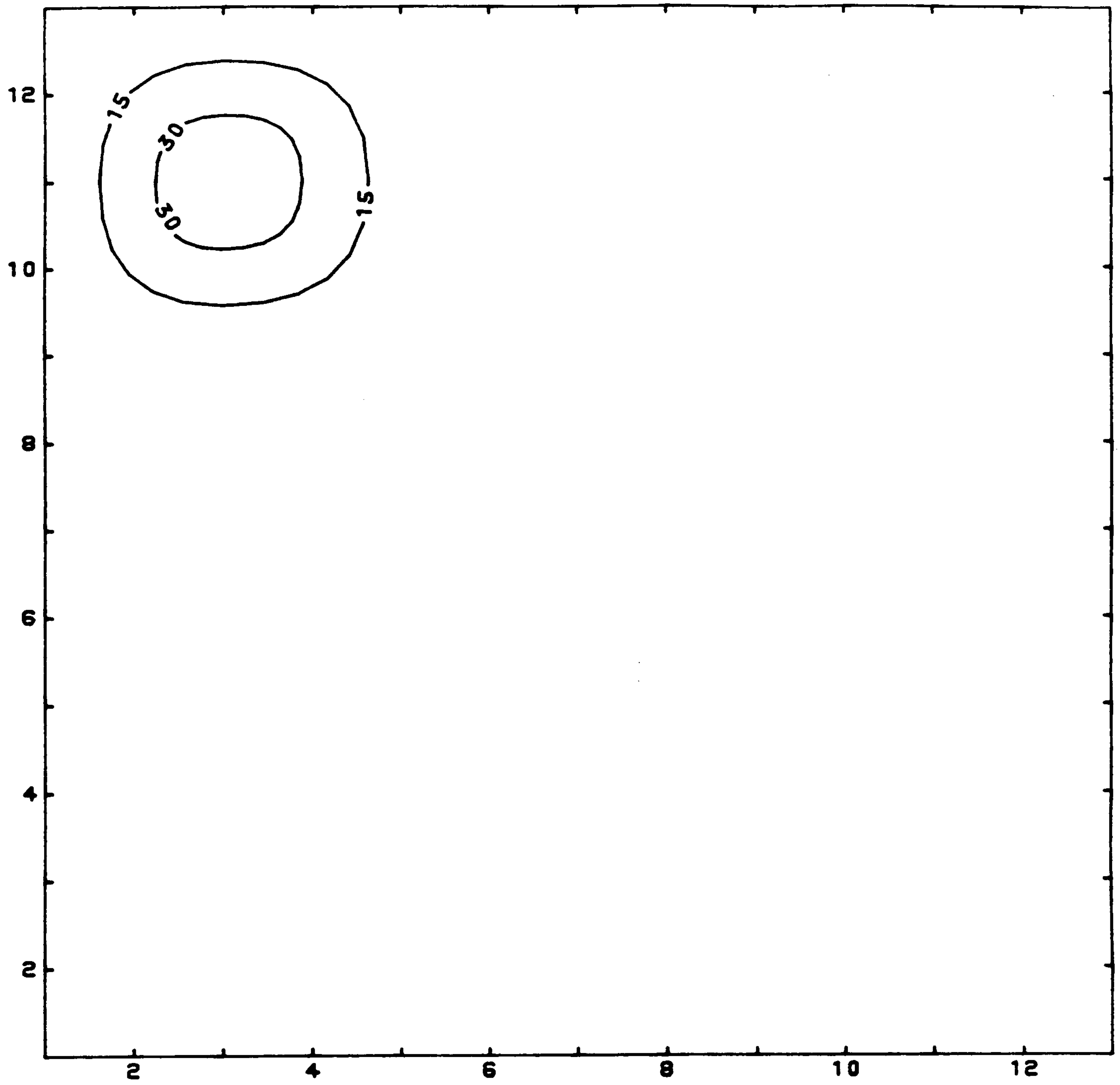

Figure 14b Contaminant Plume at 0.570 Year (Using longitudinal dispersivity = 10)

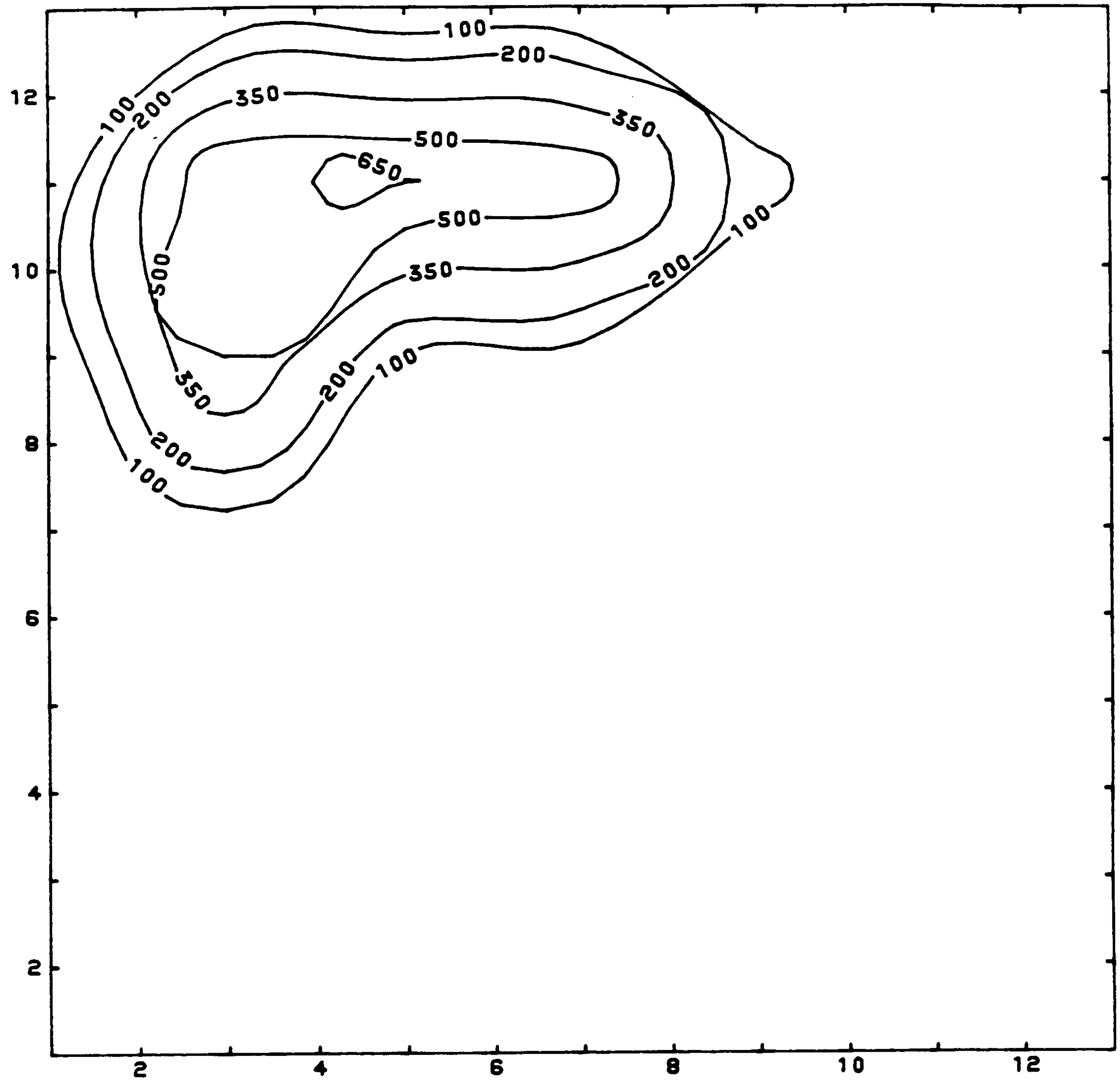

Figure 15a Contaminant Plume at 0.285 Year (Using transmissivity from PI-MOC assuming four-zone characterization, longitudinal dispersivity = 10)

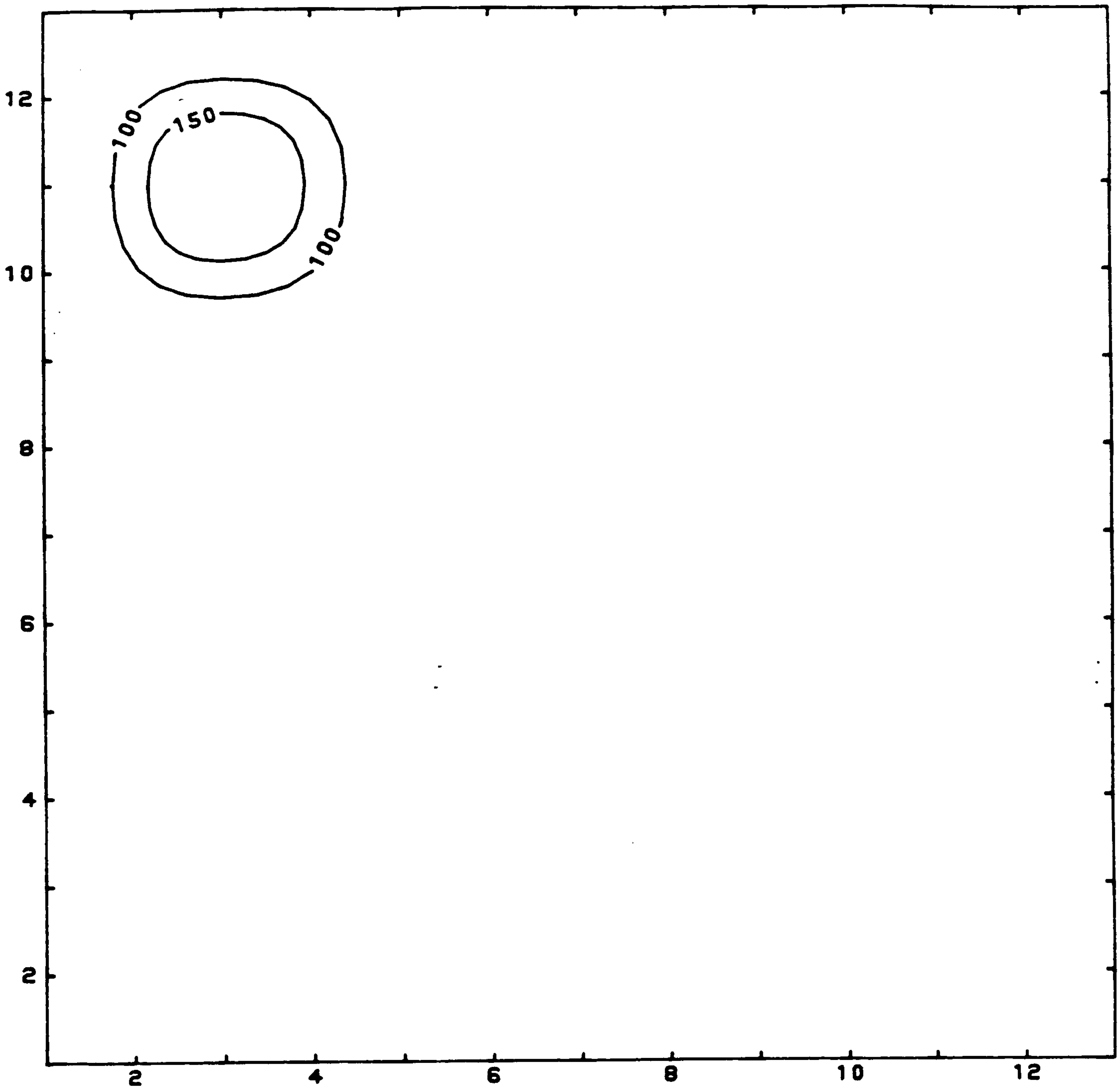

Figure 15b Contaminant Plume at 0.570 Year (Using transmissivity from PI-MOC assuming four-zone characterization, longitudinal dispersivity = 10)

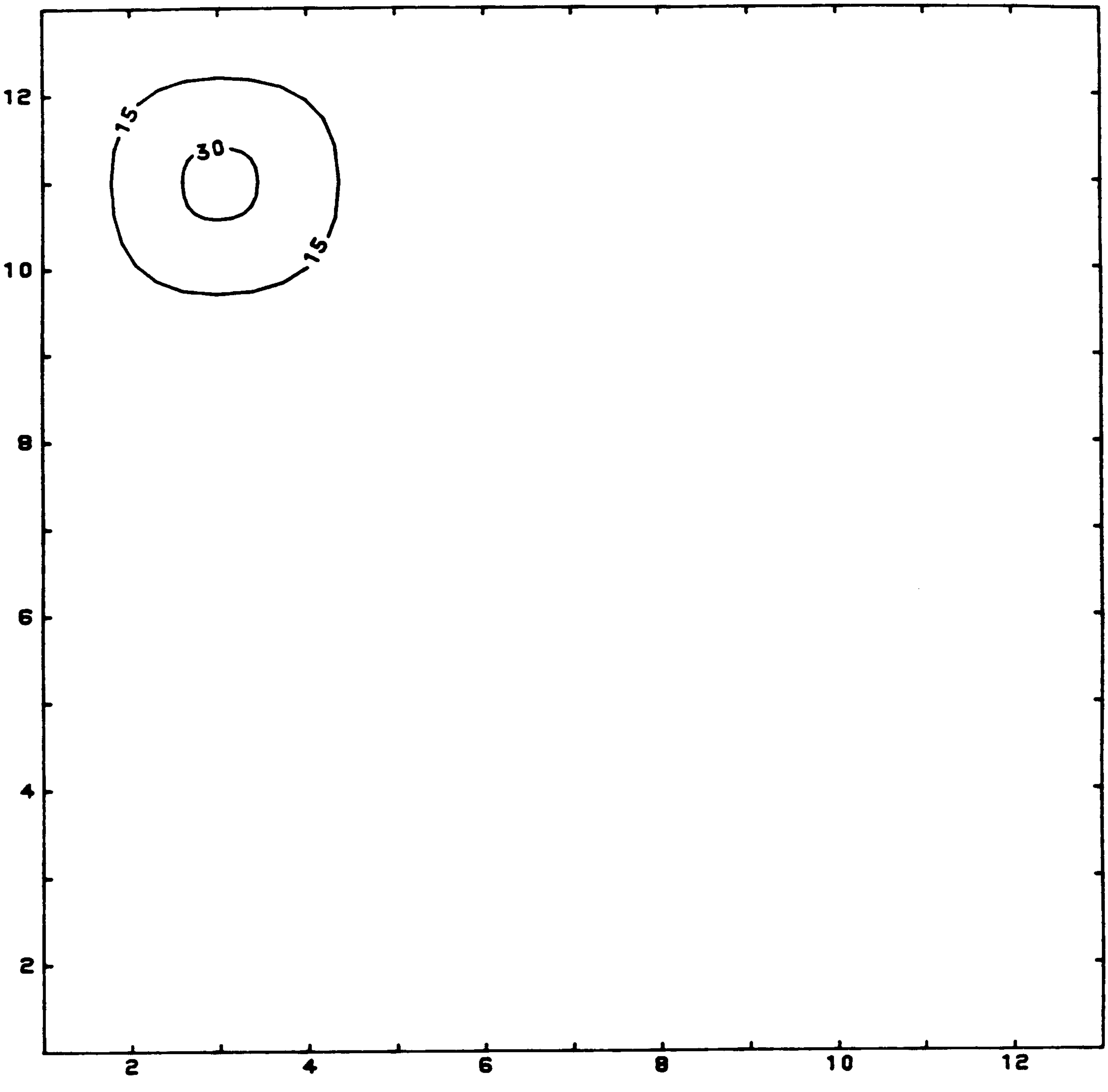

Figure 15c Contaminant Plume at 0.855 Year (Using transmissivity from PI-MOC assuming four-zone characterization, longitudinal dispersivity = 10)

CHAPTER 5

SUMMARY

The objectives of this nine month study were to apply the parameter identification (PI) technique in groundwater modeling to a field problem and to compare the results of the PI application with those from the more conventional trial-and-error (manual) calibration technique. The study objective required the selection of a field site in cooperation with the staff from the Washington State Department of Ecology and a local consulting firm. After careful screening, a site with proper boundary conditions and sufficient monitoring data was chosen for applications.

In the application to the field problem, the PI technique was shown to be very effective in finding desirable model parameters. However, the results from the method are sensitive to upper and lower parameter bounds and initial parameter estimates. The proposed PI procedure simply seeks a minimum objective value from a set of initial estimates in a feasible region (parameter bounds). The optimal parameters found by the optimization may not be physically plausible. Although this problem can be dealt with in PI by examining the covariance matrix of the estimated parameter (Yeh and Yoon, 1976), the optimized parameter values were only visually inspected here.

In field problems such as the one studied here, the presence of random errors will render the objective function nonconvex. The fact that the final parameter values in PI-MOC depended on the initial estimates was an indication that the PI procedure was only able to find a local optimum from the nonconvex objective function.

Through a series of simulations for the selected site, the study found that the parameters determined by the PI technique and the trial-and-error approach will produce very similar predictive results when used by the USGS-MOC model. Although the parameters can be found in a more efficient and objective manner by the PI approach, the resulting parameter structure must be examined carefully for further application.

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