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E. A. Jacobson
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March 1990

Prepared for the U.S. Department of Energy
under Contract DE-AC06-76RLO 1830

Pacific Northwest Laboratory
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AN INITIAL INVERSE CALIBRATION OF THE GROUND-WATER FLOW MODEL FOR THE HANFORD UNCONFINED AQUIFER

E. A. Jacobson[(a)]
M. D. Freshley

March 1990

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SUMMARY

Large volumes of process cooling water have been discharged to the ground at the Hanford Site. These discharges have impacted ground-water flow and contaminant movement in an unconfined aquifer located in a sequence of fluvial, lacustrine, and glaciofluvial sediments that were deposited on top of the Columbia River basalts.

Ground-water flow and contaminant transport models of the unconfined aquifer were developed during the 1970s and applied to assess the impacts of site operations on flow and transport in the aquifer. At that time, a two-dimensional ground-water flow model of the unconfined aquifer was calibrated with an iterative routine that was applied to estimate the distribution of transmissivity in the aquifer. Recently, an inverse calibration method developed by Neuman (1980) and modified by Jacobson (1985) was applied to data from the unconfined aquifer to improve the model calibration.

The inverse calibration method includes all information available about estimates of transmissivities, measured hydraulic heads, boundary conditions, and discharges to and withdrawals from the aquifer. The effects of including areal recharge and prescribed head or prescribed flux along the Cold Creek boundary in the inverse calibration were investigated. Results of these calibrations demonstrated that the application with prescribed head along the Cold Creek Valley and varying areal recharge across the Hanford Site yields the best fit with measured water levels.

The best fit of the transmissivity distribution estimated with the inverse calibration was used in a two-dimensional model of ground-water flow in the unconfined aquifer based on the Coupled Fluid, Energy, and Solute Transport (CFEST) code. The CFEST code was applied to simulate water-level changes over a 6-year period from 1980 to 1985. At the end of the simulation, the predicted water levels were compared with measured water levels for December 1985. The water levels predicted with CFEST were also compared with water levels predicted with the Variable Thickness Transient (VTT) code over the same time period. In general, the water levels predicted with CFEST and the transmissivity distribution from the inverse calibration more closely match the observed water levels than the water levels predicted with VTT and the previous calibration.

CONTENTS

SUMMARY iii

INTRODUCTION 1

BACKGROUND 5

INVERSE CALIBRATION METHOD 9

DEVELOPMENT OF THE HANFORD INVERSE CALIBRATION MODEL 13

- SELECTION OF STEADY-STATE TIME PERIOD 13
- PREPARATION OF THE HYDRAULIC HEAD DATA 15
- PREPARATION OF THE TRANSMISSIVITY DATA 18
- PREPARATION OF BOUNDARY CONDITIONS 19
- PREPARATION OF DISCHARGE DATA 22

RESULTS OF THE HANFORD INVERSE CALIBRATION MODEL 25

APPLICATION OF THE INVERSE CALIBRATION RESULTS 37

CONCLUSIONS 41

REFERENCES 43

FIGURES

1 Location of Hanford Site in Southeastern Washington State 2

2 Subregion CFEST Finite-Element Grid 7

3 Distribution of Hydraulic Conductivities Used with the CFEST Code . 8

4 Discharges to Cooling Water Ponds for 1968 to 1983 14

5 Water Level History for Well 699-45-42 14

6 Water Level History for Well 299-W19-1 15

7 Water Table Map for December 1979 16

8 Map of Well Locations of Water Level Data Employed in the Inverse Calibration 17

9 Map of Measured Transmissivities Based on Aquifer Tests 20

10 Zonation of Transmissivity for Inverse Calibration 21

11 Distribution of Areal Recharge to the Unconfined Aquifer Estimated for Inverse Calibration Applications 26

12 Water Levels Predicted by Applications of the Inverse Calibration Model for Case 3 28

13 Inverse Estimates of Transmissivity for Case 3 29

14 Coefficients of Variations for Case 3 30

15 Water Levels Predicted by Application of the Inverse Model for Case 4 31

16 Inverse Estimates of Transmissivity for Case 4 33

17 Coefficients of Variation for Case 4 34

18 Water Levels Predicted with CFEST for December 1985 38

19 Water Levels Predicted with VTT for December 1985 40

TABLE

1 Summary of Major Discharges to Ground at Facilities in 200 East and 200 West Areas 23

INTRODUCTION

Large volumes of process cooling water are discharged to the ground from U.S. Department of Energy (DOE) nuclear fuel processing operations in the central portion of the Hanford Site in southeastern Washington (Figure 1). Over the years, these large volumes of waste water have recharged the unconfined aquifer at the Site. This artificial recharge has affected ground-water levels and contaminant movement in the unconfined aquifer.

Ground-water flow and contaminant transport models developed during the 1970s have been applied to assess the impacts of site operations on the rate and direction of ground-water flow and contaminant transport in the unconfined aquifer at the Hanford Site. Previous modeling efforts at the Hanford Site are described in DOE (1987). A model based on the Variable Thickness Transient (VTT) code (Kipp et al. 1972) was calibrated and used to simulate ground-water flow in the unconfined aquifer. The Multicomponent Mass Transport (MMT) code (Ahlstrom et al. 1977) and the TRANSS code (Simmons, Kincaid, and Reisenauer 1986) were applied to simulate contaminant transport. Recently, the Coupled, Fluid, Energy, and Solute Transport (CFEST) code (Gupta et al. 1982) was calibrated to more current Hanford data to improve model capabilities. The development of the ground-water flow models based on the VTT and CFEST codes is further described in Evans et al. (1988).

The inverse calibration method developed by Neuman (1980) and modified by Jacobson (1985) was applied to improve calibration of a ground-water flow model of the unconfined aquifer at the Hanford Site. Initial application of the inverse method to the unconfined aquifer is described in Evans et al. (1988). All information about estimates of hydraulic properties of the aquifer (transmissivities), hydraulic heads, boundary conditions, and discharges to and withdrawals from the aquifer is included in the inverse method to obtain an initial calibration of the ground-water flow model. Use of the inverse method provides an improved calibration of the two-dimensional ground-water flow model based on CFEST.

The purpose of this report is to provide a description of the inverse method, its initial application to the unconfined aquifer at Hanford, and to present results of the initial inverse calibration. As background

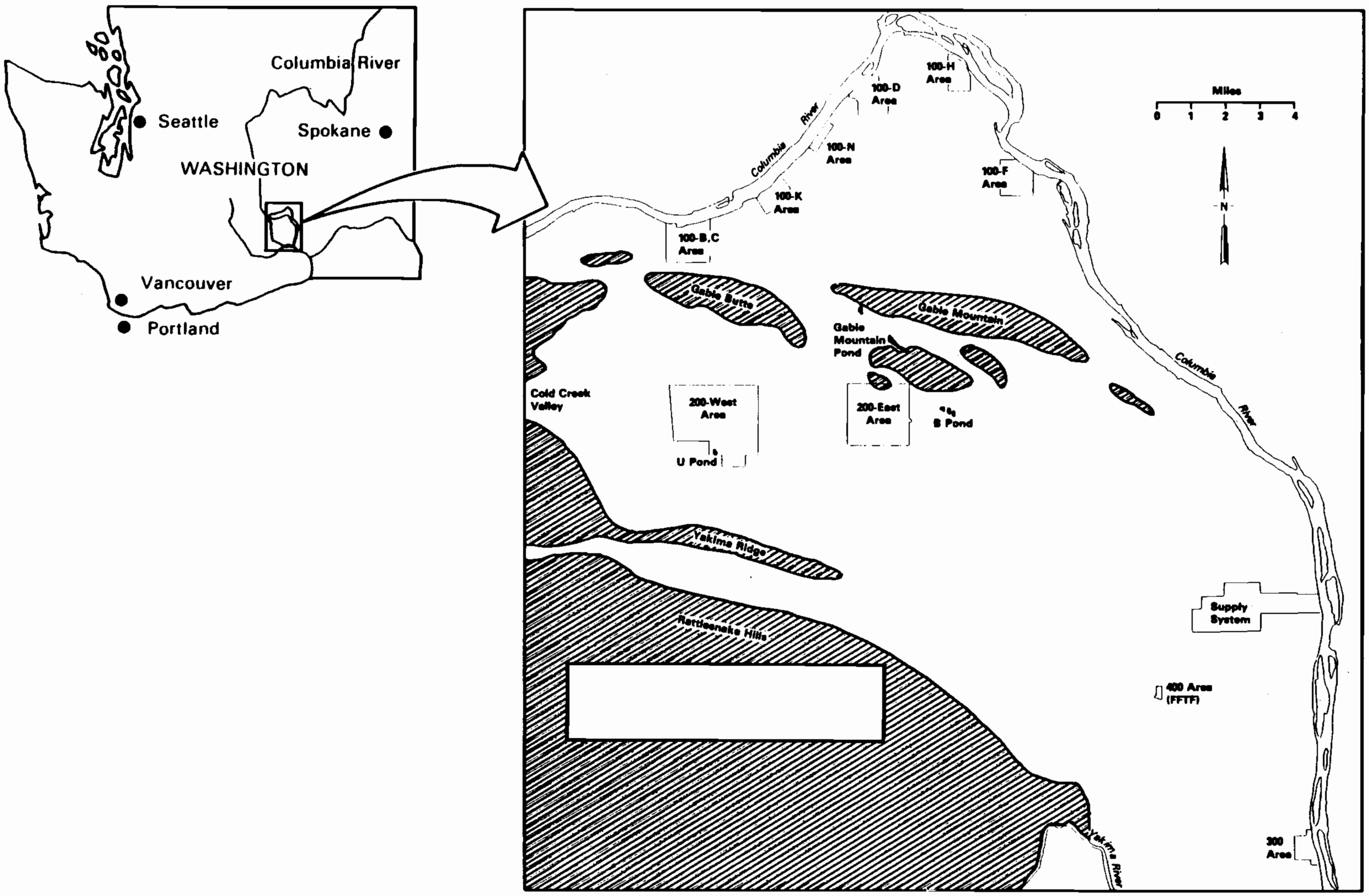

FIGURE 1. Location of the Hanford Site in Southeastern Washington State

information, a previous calibration of the ground-water flow model of the Hanford Site unconfined aquifer based on the VTT code is briefly described. Water levels were simulated from 1980 to 1985 with models based on the VTT and CFEST codes. The simulation with the VTT code is based on a transmissivity distribution resulting from calibration with a previous method. The simulation with the CFEST code is based on a transmissivity distribution resulting from the inverse calibration method. The two simulations were conducted to apply the results of the steady-state inverse calibration method with time-varying data and to compare the results from a model calibrated with the inverse calibration method with results from a model that was applied previously at Hanford.

BACKGROUND

A two-dimensional model of ground-water flow in the unconfined aquifer at the Hanford Site was developed in the 1970s. The model was based on the VTT ground-water flow code developed by Kipp et al. (1972) and was calibrated with an iterative routine developed by Cearlock, Kipp, and Friedrichs (1975).

The iterative technique applied by Cearlock, Kipp, and Friedrichs (1975) is based on an equation obtained by numerical integration of the Boussinesq equation, which describes ground-water flow in unconfined aquifers along instantaneous streamlines of flow. The streamlines, or flow paths, for the unconfined aquifer were based on a hand-contoured water table map for 1973. The iterative technique was implemented to estimate the transmissivity distribution for the unconfined aquifer. A transmissivity value obtained from aquifer test data was needed in each stream tube, which is defined by bounding streamlines. For stream tubes in which no transmissivity data were available, the spatial distribution of transmissivity could not be calculated. In these portions of the model area, the transmissivity values were estimated by interpolation. The resulting transmissivity distribution was input to the VTT model along with estimates of storage coefficients, recharge to and discharge from the aquifer, and boundary conditions to predict water levels in the unconfined aquifer from 1968 to 1973.

The calibration of the ground-water flow model based on the VTT code with the iterative routine (Cearlock, Kipp, and Friedrichs 1975) yielded reasonable predicted water levels over most of the study area. The water levels calculated for 1973 with the calibrated VTT model were within several feet of the hand-contoured water levels except at four locations. Predicted water levels were smaller than the hand-contoured water levels by up to 34 ft at locations east of Umtanum Ridge and by 22 ft at locations northeast of Rattlesnake Mountain. Predicted water levels to the east of the 200-West Area were up to 13 ft smaller than the hand-contoured values. A small region of the study area southeast of Gable Mountain also had predicted water levels up to 21 ft smaller than the hand-contoured values.

The large differences in predicted and measured water levels in some areas may be related to some fundamental assumptions and approximations used in the iterative routine. The transmissivities estimated with the iterative routine were based solely on the stream tubes and did not directly consider recharge to and discharge from the aquifer and flux boundary conditions. In addition, in some areas where initial transmissivity estimates were not available, the stream tube technique could not be applied and the distribution of transmissivity in those portions of the aquifer had to be interpolated from nearby areas.

Input data were transferred from the existing two-dimensional model based on VTT to the ground-water flow portion of the CFEST code (Gupta et al. 1982). Evans et al. (1988) describes the selection of the CFEST code and its application to the unconfined aquifer. The hydraulic conductivity distribution used in the model based on VTT was transferred to the model based on CFEST by interpolation of finite difference nodal values to finite elements. The irregularly spaced finite-element grid allows more realistic boundary conditions and increased discretization in areas of rapid changes in transmissivity, or near liquid waste facilities (i.e., artificial recharge areas).

The finite-element grid for the ground-water flow model of the unconfined aquifer based on the CFEST code is shown in Figure 2. The finite-element grid was designed to provide detail in areas of high waste disposal (artificial aquifer recharge) and areas of rapid changes in hydraulic conductivity. The grid was designed to ensure that changes in hydraulic conductivity are adequately represented, i.e., values are not averaged over large elements in areas of rapid change. Although the node spacing for the CFEST grid in some locations is much greater than the 2000-ft node spacing of the VTT finite difference grid, all pertinent changes in hydraulic conductivity are well represented (Figure 3). Larger elements were used where detail is not required.

The transfer of data from the model based on the VTT code to the CFEST code did not include calibration of the model based on CFEST. The inverse method developed by Neuman (1980) and modified by Jacobson (1985) was applied to data from the unconfined aquifer to improve the CFEST model calibration. Application of the inverse method to the unconfined aquifer at the Hanford

Site is based on the finite-element grid and boundary conditions for the two-dimensional CFEST ground-water flow model.

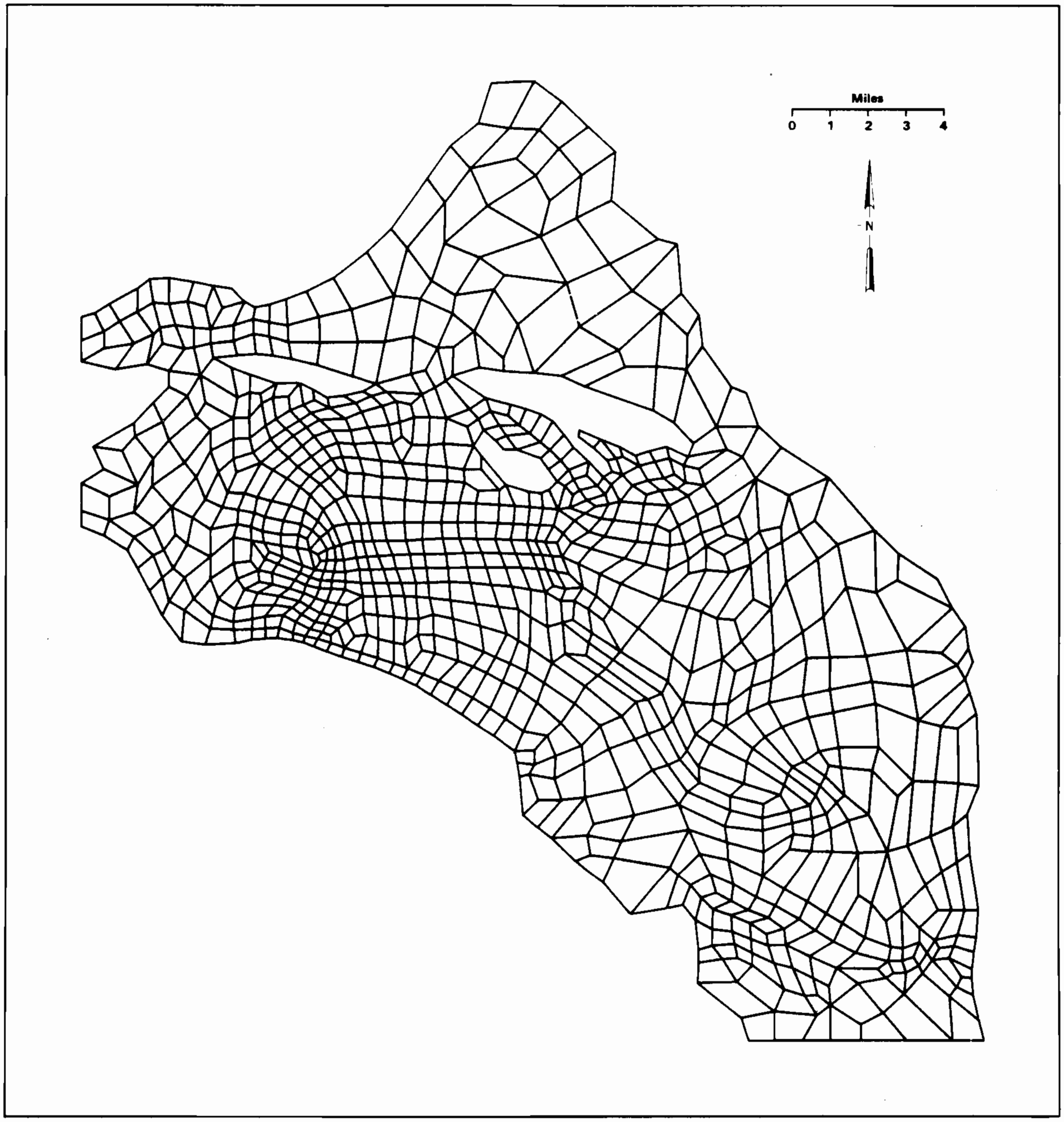

FIGURE 2. Subregion CFEST Finite-Element Grid

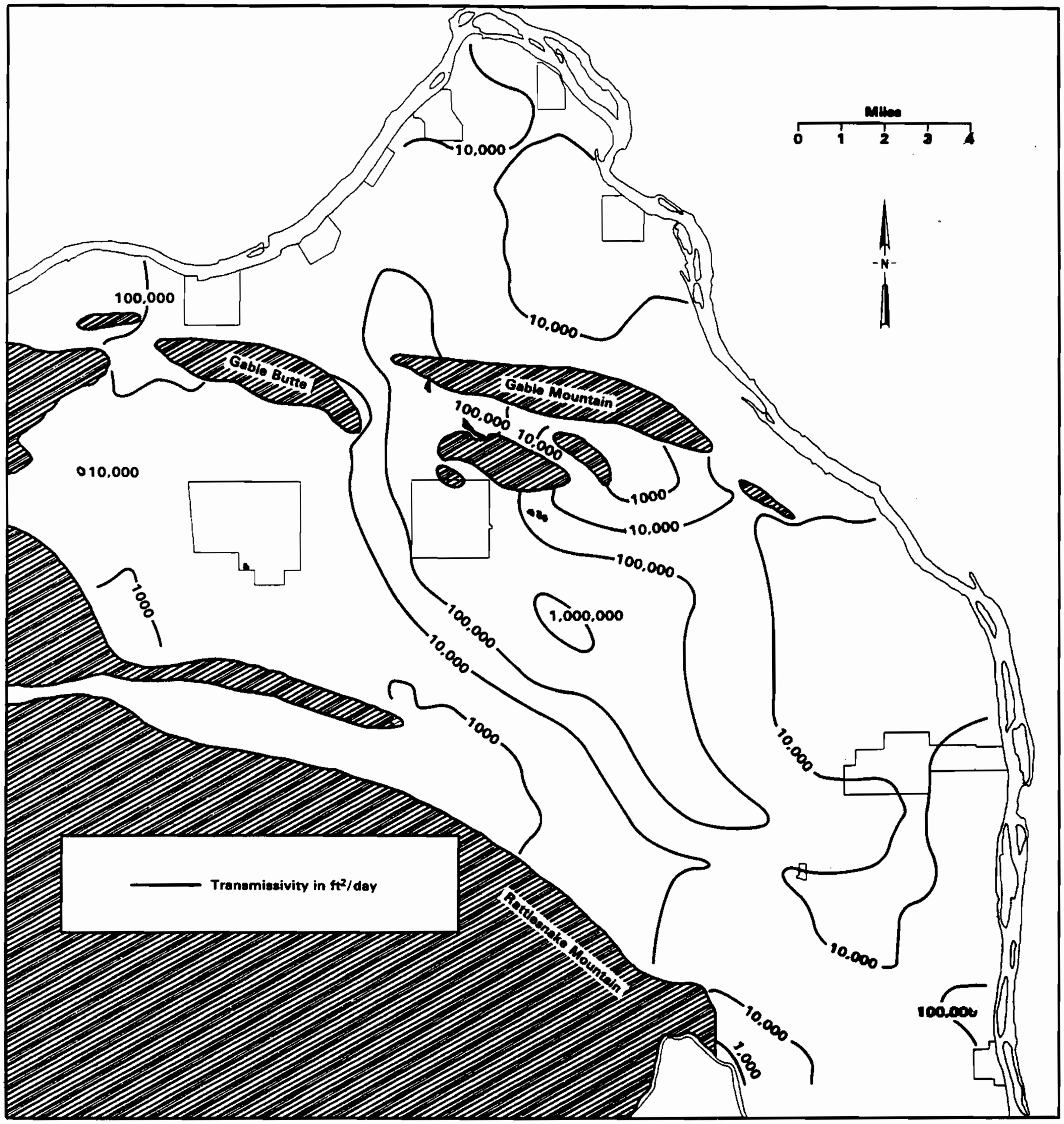

FIGURE 3. Distribution of Transmissivities Used with the CFEST Code

INVERSE (PARAMETER ESTIMATION) CALIBRATION METHOD

Before applying a numerical model to calculate the steady-state, hydraulic-head distribution in a ground-water system, the aquifer parameters such as transmissivities, pumping and recharge rates, and boundary conditions must be known. However, measurements of aquifer properties and knowledge of recharge and pumping rates and boundary conditions are usually insufficient to fully model flow systems, and some sort of calibration is required. The traditional approach for calibrating a steady-state, ground-water flow model has been to select boundary conditions, estimate sources and sinks, and modify the estimates of transmissivity by a trial-and-error procedure until the predicted hydraulic heads are reasonably close to the measured hydraulic head data. Although such a trial-and-error procedure may yield a reasonable representation of the measured head data, the estimates of the transmissivity are not unique, and their associated uncertainty cannot be determined.

During the past few years, automated, rather than trial-and-error, procedures for calibrating numerical models have been used to determine aquifer characteristics. These automated procedures account for past water level data, boundary conditions, pumping rates, previous knowledge of transmissivities and estimates of the recharge rates. Methods of estimating aquifer characteristics with the aid of automated procedures are referred to as "inverse" or "parameter estimation" methods. Since 1975, several inverse (parameter estimation) methods (Yeh and Yoon 1976; Cooley 1977, 1979, 1982, 1983; Neuman and Yakowitz 1979; Neuman 1980; Jacobson 1985) have been developed.

A statistically based inverse method developed by Neuman (1980) and modified by Jacobson (1985) for steady-state, two-dimensional ground-water flow problems was applied to the data from the unconfined aquifer at Hanford. Neuman's (1980) method was selected over other inverse methods because it uses prior information and any available statistical data. In Neuman's method, the governing equation for steady-state, two-dimensional flow in the region R, subject to some known boundary conditions, is written as:

$$\nabla \bullet T \nabla h - q = 0 \qquad (1)$$

where h = hydraulic head

T = transmissivity

q = recharge to and discharge from aquifer

∇ = two-dimensional gradient operator.

Applying a finite-element method to Equation (1) yields a set of linear equations written in matrix form as:

$$\underline{\underline{A}}(\underline{T})\ \underline{h} = \underline{Q} \tag{2}$$

where $\underline{T}$ = vector representing transmissivities defined as constant values in various zones

$\underline{\underline{A}}$ = square matrix containing information about grid; is a function of $\underline{T}$

$\underline{Q}$ = vector containing the source and sink terms and boundary flux information at nodal points

$\underline{h}$ = vector of hydraulic heads at nodal points.

The statistical inverse method developed by Neuman (1980) is based on prior information on transmissivities as well as observed hydraulic heads. Prior information on transmissivities may include estimates of transmissivity based on aquifer testing and estimates of aquifer thickness based on geologic information. The spatial distribution of transmissivity determined with the statistical inverse method produces hydraulic heads that are reasonably close to observed heads while keeping the inverse estimates of transmissivity reasonably close to the prior estimates. In addition, Neuman's inverse method considers all statistical information about the prior estimates of transmissivity and hydraulic heads in calculating the new estimates of transmissivity.

Statistical information on prior estimates of transmissivity and hydraulic head can be derived by the geostatistical technique called kriging. The kriging technique has been used by Clifton and Neuman (1982) and Jacobson (1985) to interpolate the transmissivity and hydraulic head data to obtain estimates at node points where no data are available and to yield their associated estimation errors and covariance, which is a measure of correlation between estimation errors. The kriged estimates of transmissivity and the covariance of the estimation errors are used as prior information, while the kriged estimates of hydraulic head are used as "observed" hydraulic heads for the inverse method. Including statistical information about the prior estimates of the transmissivities and the kriged hydraulic heads in the parameter estimation method allows development of a statistically calibrated ground-water flow model. If no prior statistical information is available, the inverse method can still be applied; however, the result would not be considered a statistically calibrated model.

In modeling ground-water flow systems where the spatial coverage of hydraulic head measurements is limited (i.e., no data exist in parts of the study area), application of an interpolation technique such as kriging may not be possible. In these cases, the inverse method can be applied with measured hydraulic head values at well locations. In the past, inverse solution methods required that well locations correspond to node points. This requirement may lead to irregular grids because of the spatial distribution of wells. The method developed by Neuman (1980) permits use of hydraulic head data anywhere in the grid, not necessarily at node points; thus, a regular grid can be imposed over the study area. Jacobson (1985) applied this approach to data from an unconfined aquifer in southern Arizona.

DEVELOPMENT OF THE HANFORD INVERSE CALIBRATION MODEL

Several steps had to be completed before Neuman's (1980) inverse method, as modified by Jacobson (1985), could be applied to the Hanford unconfined aquifer. Because the method is designed to examine only steady-state conditions, an appropriate period of time was selected when discharges to the aquifer and corresponding water-level responses were relatively constant. Once the period of time was selected, data representative of that period were prepared for input to an inverse calibration model. Data processed for the model included hydraulic heads, transmissivities, boundary conditions, and discharges to ground.

SELECTION OF STEADY-STATE TIME PERIOD

A review of cooling water discharge information at the major disposal facilities within the 200-East and 200-West Areas suggests that, compared with other periods of time, the discharges remained relatively constant from 1976 through 1979 (Figure 4). Major disposal facilities include U Pond, located in the 200-West Area, and B Pond and Gable Mountain Pond, which are located near the 200-East Area. In general, the water levels in wells monitoring the unconfined aquifer near these ponds reflect the relatively constant trend in the discharge data from 1976 through 1979. This trend is illustrated in the hydrograph for a well (699-45-42) near B Pond and Gable Mountain Pond (Figure 5) and the hydrograph for a well (299-W19-1) near U Pond in 200-West Area (Figure 6).

Based on our review of discharge and water-level information, we selected 1979 as the most appropriate time for the inverse calibration. Because discharges and water levels remained constant from 1976 through 1979, 1979 represented the closest approximation to steady-state conditions within recent Hanford operations.

Although water level measurements were collected in June and December of 1979, the December measurements were selected for the inverse calibration because these data are closer to the end of the steady-state period. In addition, the influence of changing river level was less in December when the river was lower and more constant than in June.

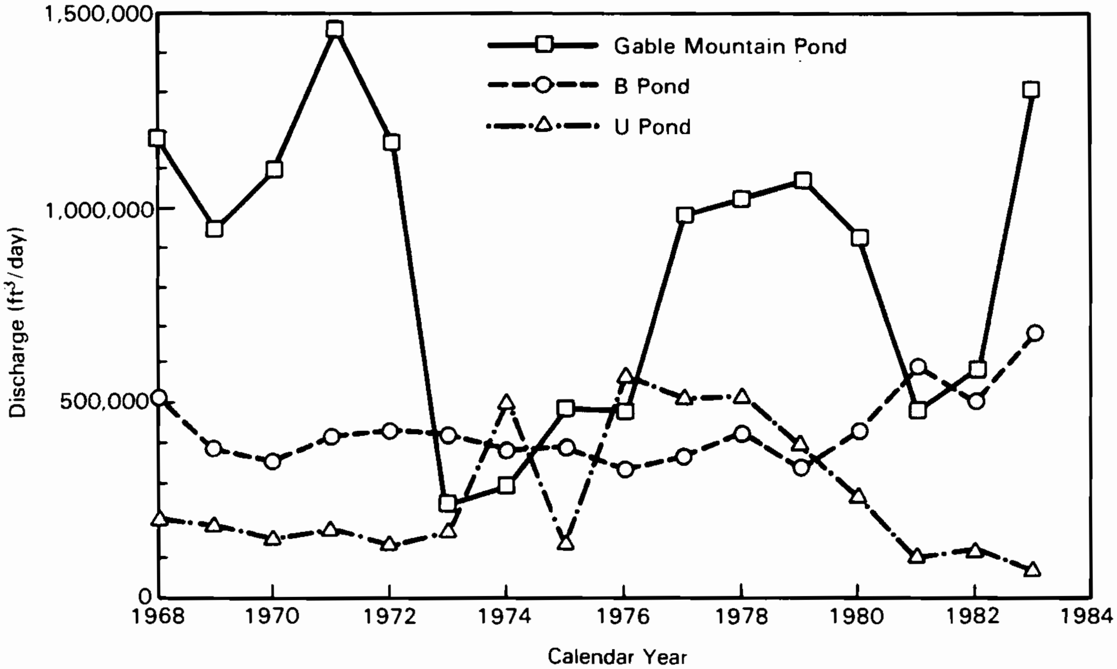

FIGURE 4. Discharges to Cooling Water Ponds for 1968 to 1983

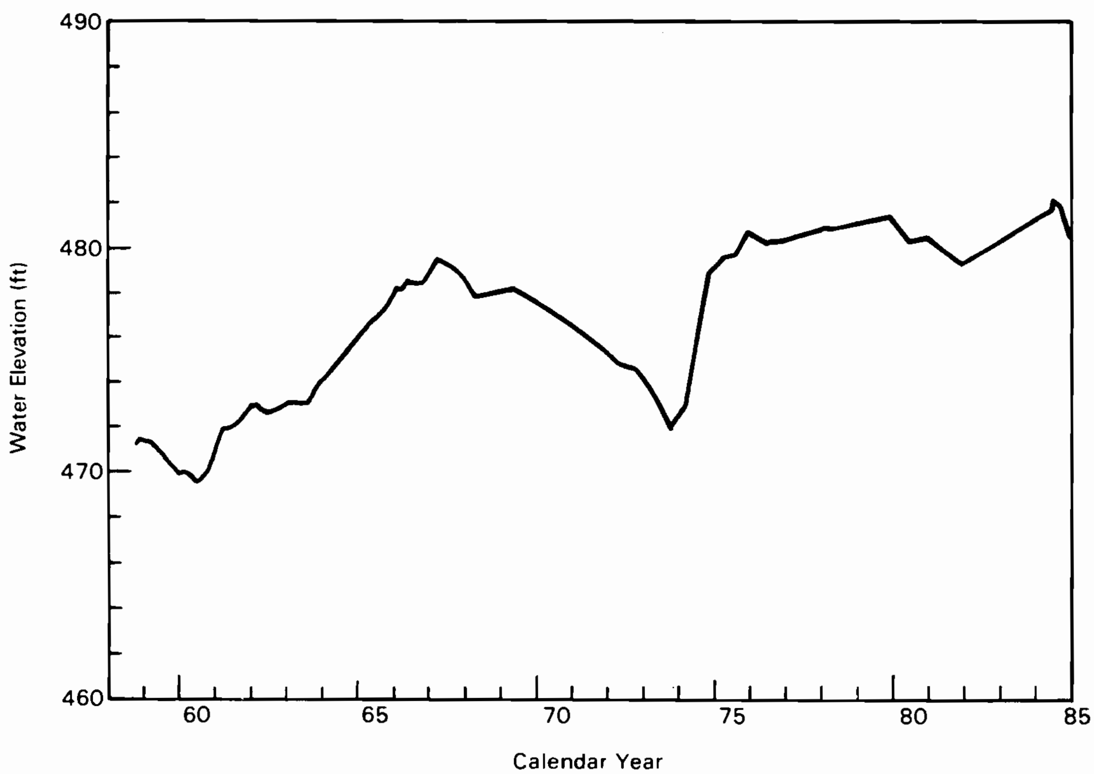

FIGURE 5. Water Level History for Well 699-45-42

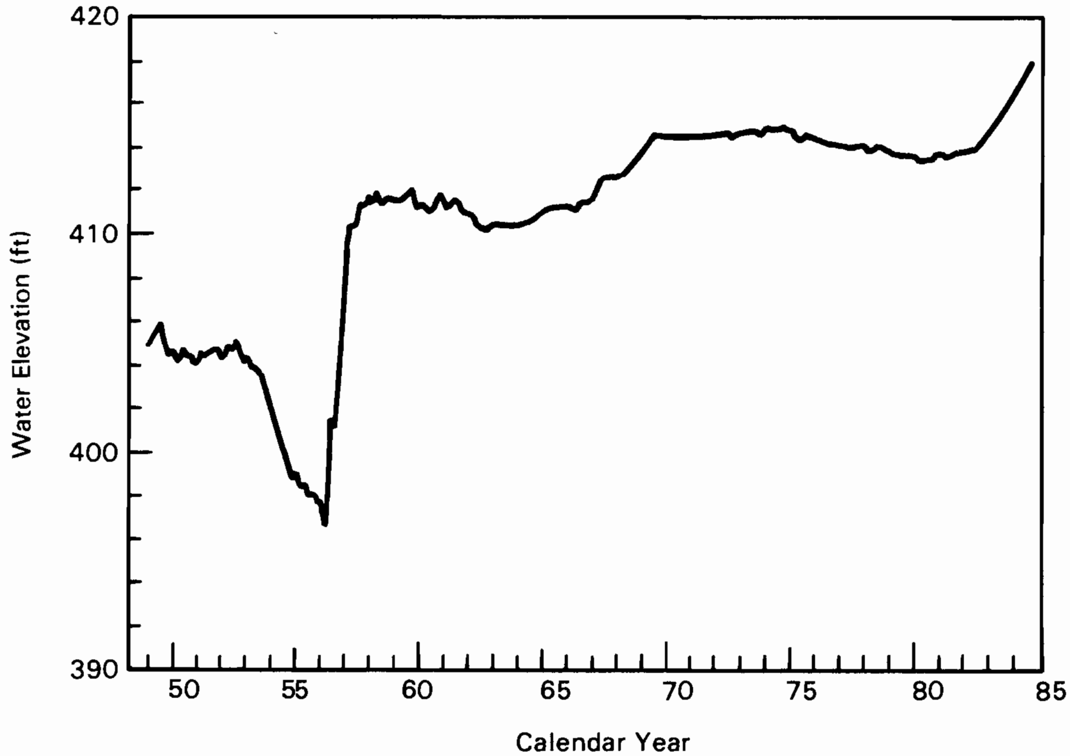

FIGURE 6. Water Level History for Well 299-W19-1

PREPARATION OF THE HYDRAULIC HEAD DATA

Water level data collected in December 1979, shown in Figure 7, were reviewed for trends and outliers. Water level measurements from wells that were obvious outliers, or from wells strongly influenced by changes in river stage, were not included in data used for the inverse calibration. A few wells were not included because their screened intervals are open to a large portion of the unconfined aquifer and these measurements may not reflect the water table, particularly where vertical hydraulic gradients are likely to occur. Of the 278 wells included in the original list of hydraulic head measurements for December 1979, 214 were used for the inverse calibration. The locations of the wells used are shown on Figure 8.

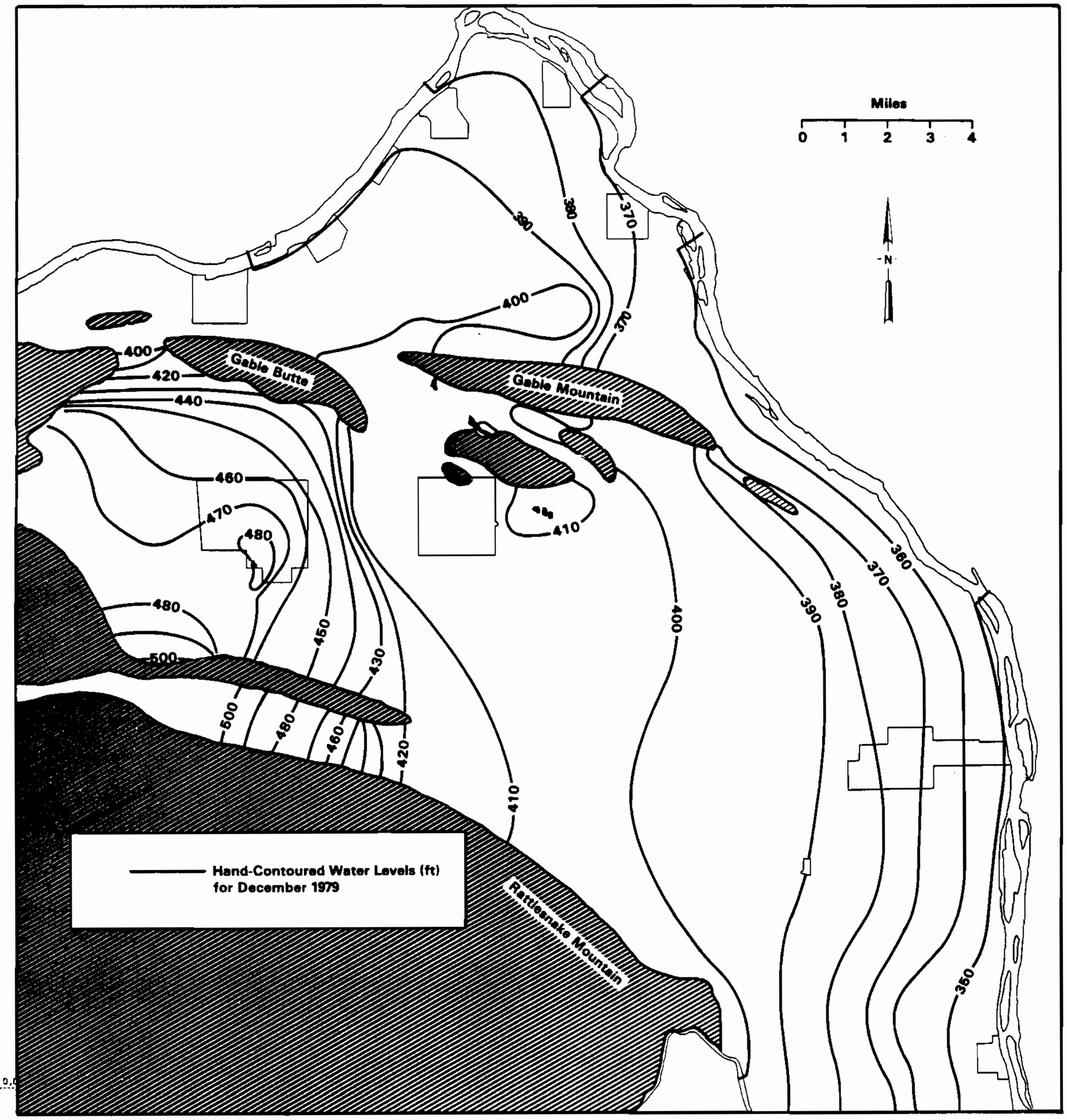

FIGURE 7. Water Table Map for December 1979 (contours in ft)

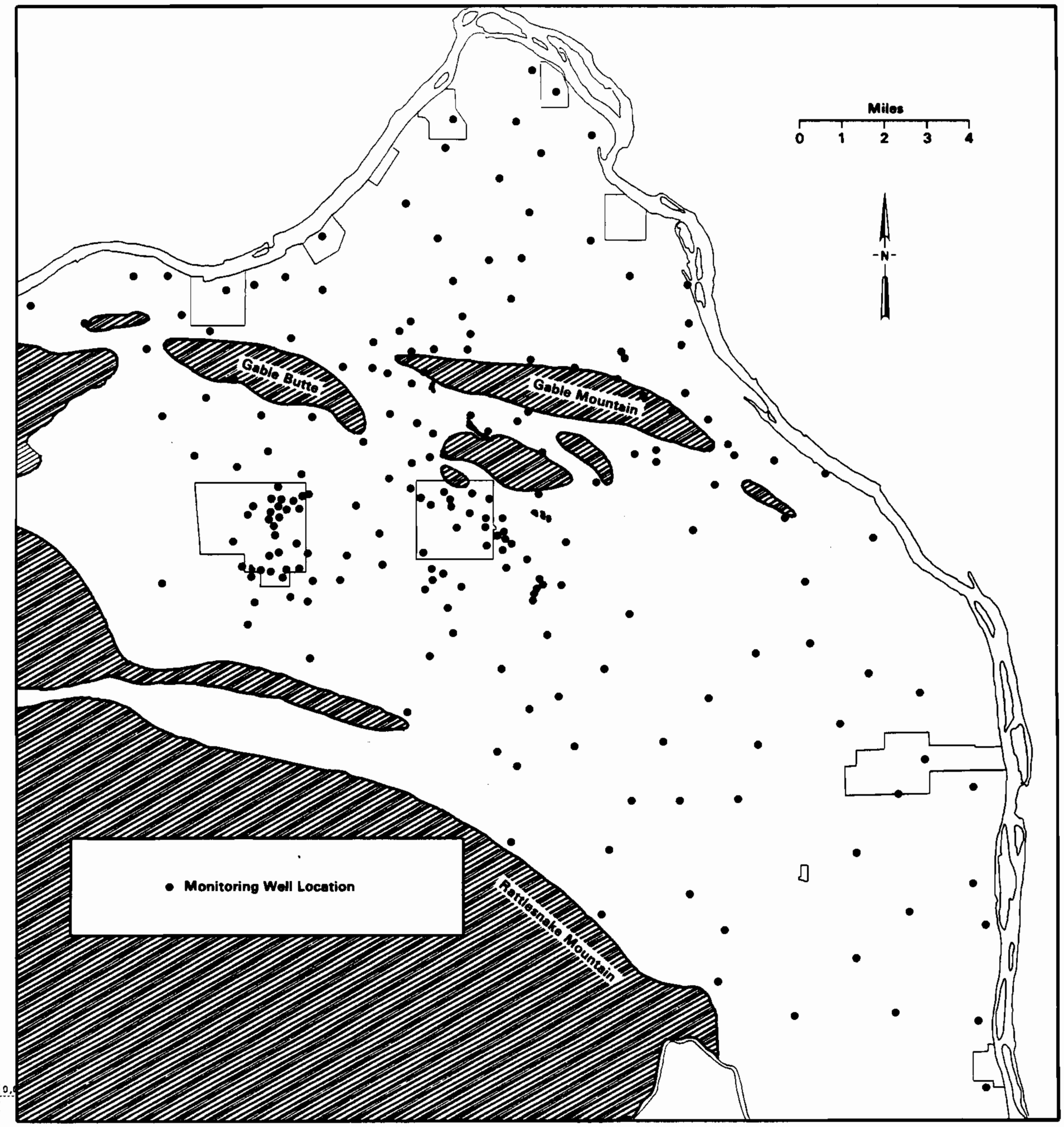

FIGURE 8. Map of Well Locations of Water Level Data Employed in the Inverse Calibration

To apply the statistical inverse method to the unconfined aquifer at Hanford, estimates of hydraulic heads and their associated estimation errors at all node points are needed as input data. An attempt was made to interpolate the hydraulic heads by kriging, but kriged estimates of hydraulic head could not be obtained when the entire study area was considered because of the complex nature of the hydraulic head distribution. The large volumes of cooling water discharged to the ground and the large variations in transmissivity make it difficult to define a semivariogram for the distribution of hydraulic head, which is necessary for kriging.

Because kriging the hydraulic heads was unsuccessful, two aspects of the inverse method could not be addressed. First, because estimates of hydraulic head from kriging were not available at node points, only measured hydraulic head data at well locations were used in the inverse calibration. Secondly, because no statistical information about the measured hydraulic heads is available, the statistical aspects of the inverse calibration could not be considered at this time.

PREPARATION OF THE TRANSMISSIVITY DATA

Neuman's (1980) inverse method is based on a finite element approach where transmissivity is assumed to be constant in each element. If several elements have the same transmissivity, they are treated as a zone of constant transmissivity. Transmissivity values obtained from aquifer tests are generally viewed as point measurements because they represent an average value over the aquifer close to the well.

Estimates of transmissivity have been made from aquifer tests conducted on the Hanford Site since 1945 (Bierschenk 1959). The transmissivity data through 1972 were included in the calibration of the VTT ground-water flow model for the unconfined aquifer at Hanford (Cearlock, Kipp, and Friedrichs 1975). Results from tests on wells completed in the Hanford unconfined aquifer and reported in Bierschenk (1959), Kipp and Mudd (1973), Deju and Summers (1975), and Graham et al. (1981) were reviewed for their applicability to the inverse calibration procedure. In addition to the reported aquifer tests in the published documents, unpublished aquifer test data were reviewed and reanalyzed where required. Tests from a total of 52 wells in the unconfined aquifer (Figure 9) were determined to be applicable for the inverse calibration procedure.

The number of data points available was insufficient for kriging because a semivariogram could not be defined. Because the transmissivity data could not be kriged, the distribution of transmissivity obtained from calibration of the VTT model (Cearlock, Kipp, and Friedrichs 1975) was adapted as an initial estimate for the inverse calibration. No statistical information was available about the prior estimates of transmissivity; thus, only the prior estimates with no statistical information were included in the inverse calibration.

A zonation pattern (Figure 10) and prior estimates of transmissivities were developed based on the distribution of transmissivities obtained in the VTT model calibration (Cearlock, Kipp, and Friedrichs 1975) and transferred to the CFEST finite-element grid. The zonation pattern was developed to reflect areas of similar values of transmissivity. The prior estimates of transmissivity resulting from the inverse method were calculated for each zone by taking the arithmetic average of the logarithm of the transmissivity values from the VTT calibration for all elements in the zone. In the inverse calibration procedure, these prior estimates of transmissivity are treated as constant in each zone. A contour map of transmissivities calculated by assigning the prior estimates of transmissivity to the center of each element is similar to the overall spatial variation of prior transmissivities illustrated in Figure 3.

PREPARATION OF BOUNDARY CONDITIONS

Boundary conditions for the inverse calibration were the same as those applied to the ground-water flow model of the unconfined aquifer based on the VTT code and transferred to the more recent model based on the CFEST code. Prescribed head conditions were assumed along the Columbia River and Yakima River boundaries. The prescribed head was equal to the yearly average river level at each boundary node during 1979. Prescribed fluxes were specified along the Cold Creek and Dry Creek Valleys to incorporate inflow of ground water from these valleys to the study area. The contribution from spring

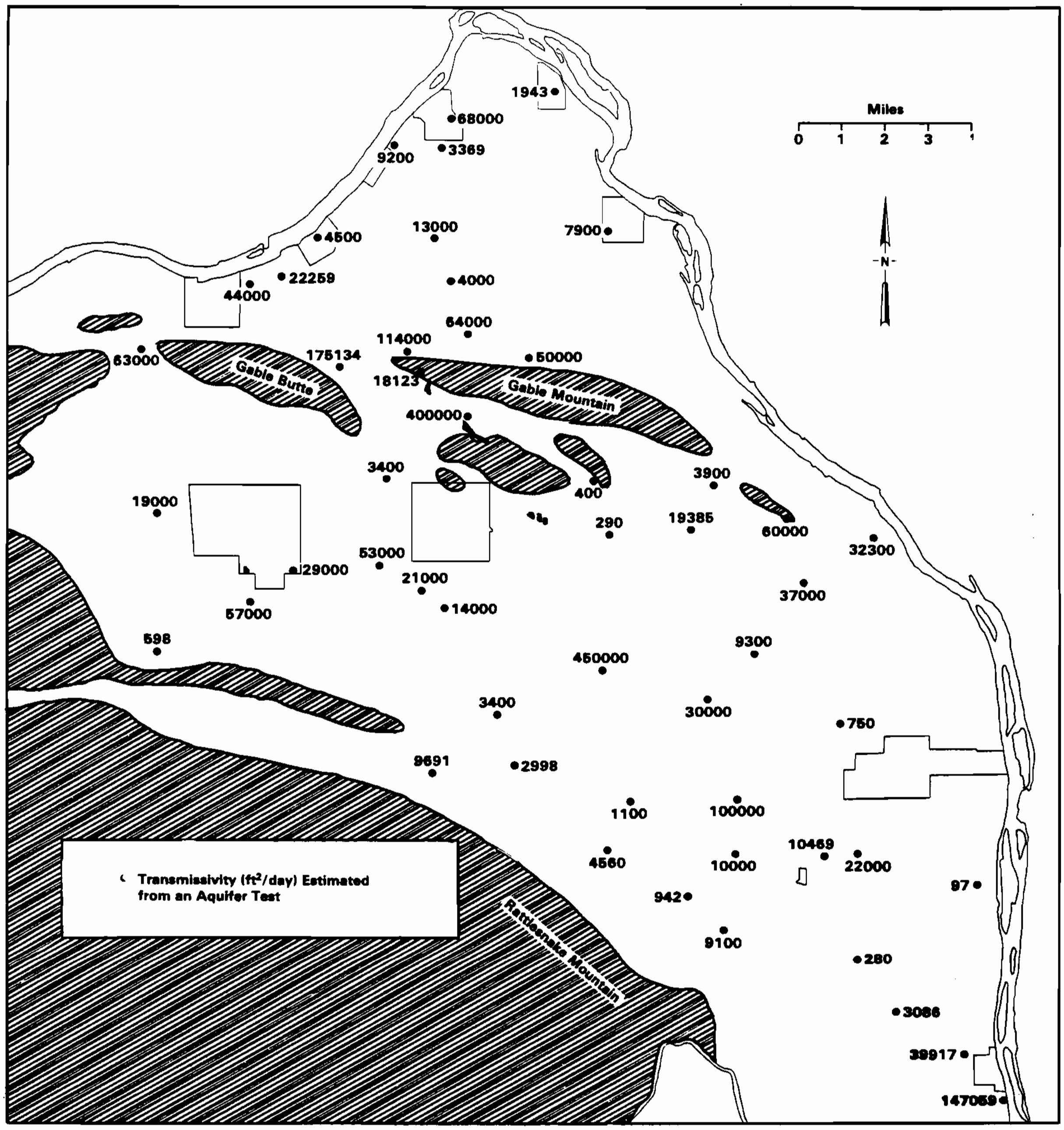

FIGURE 9. Map of Measured Transmissivities (in ft^2/day) Based on Aquifer Tests

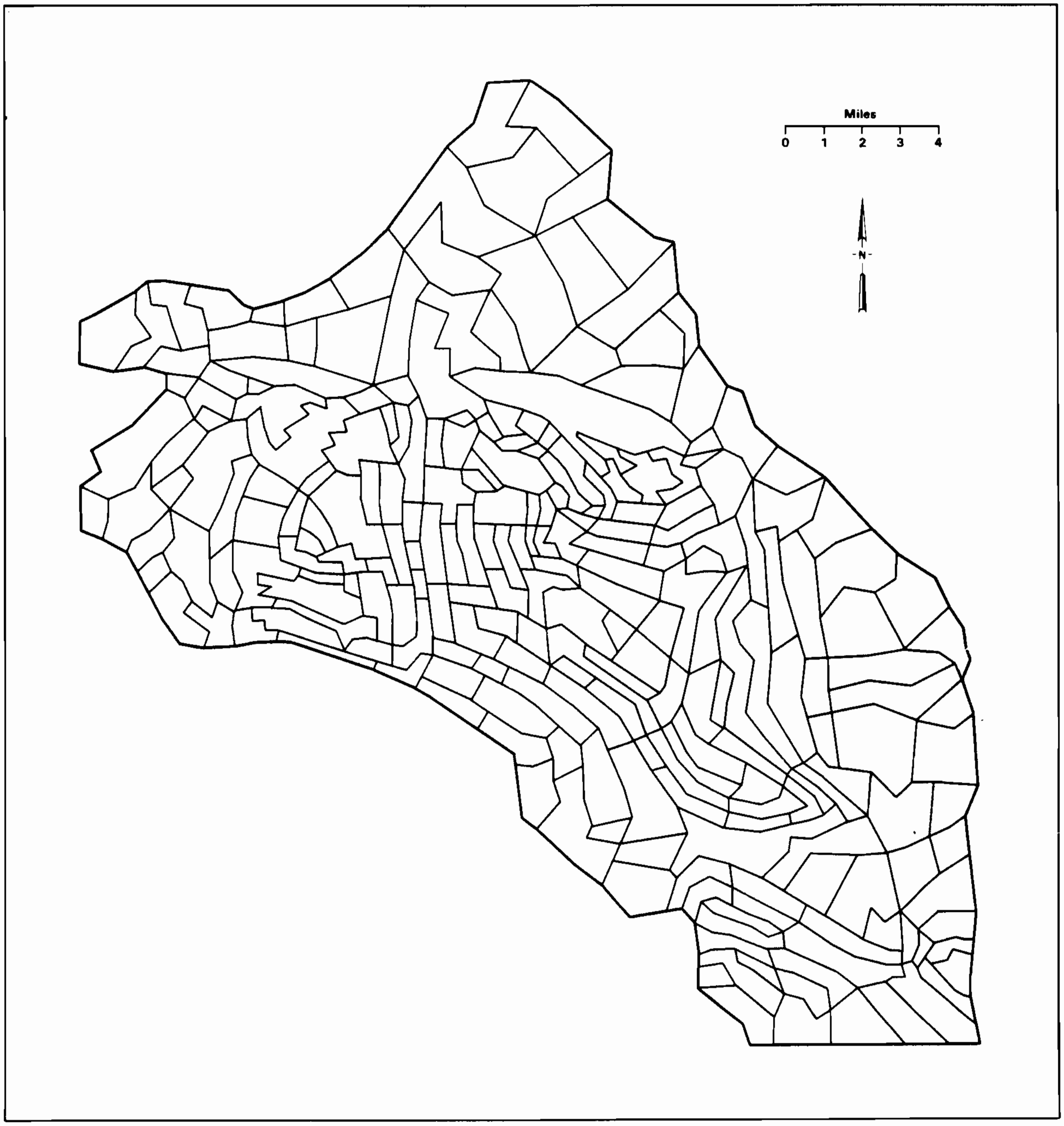

FIGURE 10. Zonation of Transmissivity for Inverse Calibration

discharges along the northeast side of Rattlesnake Mountain was also accounted for by specified flow rates. The amounts of water contributed by the inflow boundaries are 321,945 ft^3/day from Cold Creek Valley and 47,014 ft^3/day from Dry Creek Valley and Rattlesnake Mountain Springs. These flow rates are from previous calibration of the VTT flow model. No-flow conditions were assumed in areas where the aquifer is bordered by basalt outcrops and subcrops (basalt intersecting the water table) near Gable Mountain and Gable Butte.

PREPARATION OF DISCHARGE DATA

Estimates of waste water discharged to the ground in 1979 were obtained from Sliger (1980), which contains a summary of the radioactive liquid waste discharged to the ground in the 200 Areas for 1979. This information is provided annually by the operating contractor at the Hanford Site. Corrections were made in the discharge estimates reported by Sliger (1980) based on comparison of inflow to the operating areas with discharges to the major disposal facilities. The resulting discharge estimates for each facility are listed in Table 1.

TABLE 1. Summary of Major Discharges to Ground at Facilities in 200-East and 200-West Areas

Facilities	Discharge, ft^3/day
200-West Area	
U Pond (216-U-10)	164,364
West Area Ash Pit	1,648
216-U-12	12
216-T-1	404
216-T-4-2	499
216-S-10	19,271
216-S-19	5,210
216-S-25	2,210
200-East Area	
Gable Mountain Pond (216-A-25)	1,084,668
B Pond (216-B-3)	245,144
East Area Ash Pit	2,473
216-A-30	15,227
216-A-37-1	1,904
216-B-55	6,367
216-B-62	1,560
216-B-63	31,122
216-C-7	0.13

RESULTS OF THE HANFORD INVERSE CALIBRATION MODEL

A finite-element grid with 966 nodes and 878 elements (Figure 2) developed for the CFEST Hanford model was used in the application of the inverse method to the data from the unconfined aquifer at Hanford. The spatial distribution of transmissivity was represented by 240 zones with constant transmissivity in each zone (see Figure 10). As discussed previously, the initial (prior) values of transmissivity were based on the calibration of the VTT code (Cearlock, Kipp, and Friedrichs 1975).

Four different applications of the inverse method to the unconfined aquifer at the Hanford Site were investigated. These applications (cases) differed in treatment of the boundary condition along the Cold Creek Valley (i.e., either prescribed head or prescribed flux) and in areal recharge. Areal recharge is not included in existing ground-water flow models of the unconfined aquifer. The objective of varying the applications was to investigate how changes in the Cold Creek Valley boundary conditions and the addition of areal recharge affect calibration of the ground-water model for the unconfined aquifer. The Cold Creek Valley boundary contributes a significant volume of ground-water flow to the unconfined aquifer, and thus is an important component in calibration and applications of the model.

In the first application of the inverse method (Case 1), the flux prescribed at the Cold Creek boundary was the same as that used in existing models, and no areal recharge was included. This application yielded water levels that were unreasonably high (greater than 600 ft) in the Cold Creek Valley. Thus, the initial inverse application (Case 1) did not yield a good calibration to the expected water levels in this region.

The effects of including areal recharge with the prescribed flux boundary condition in the Cold Creek Valley were considered in a second application of the inverse model (Case 2). The spatial distribution of areal recharge used in this application is illustrated in Figure 11. These recharge estimates represent one possible spatial distribution based on knowledge of the soil and vegetation types on the Hanford Site; they are in no way assumed to be definitive. The goal of the second inverse application

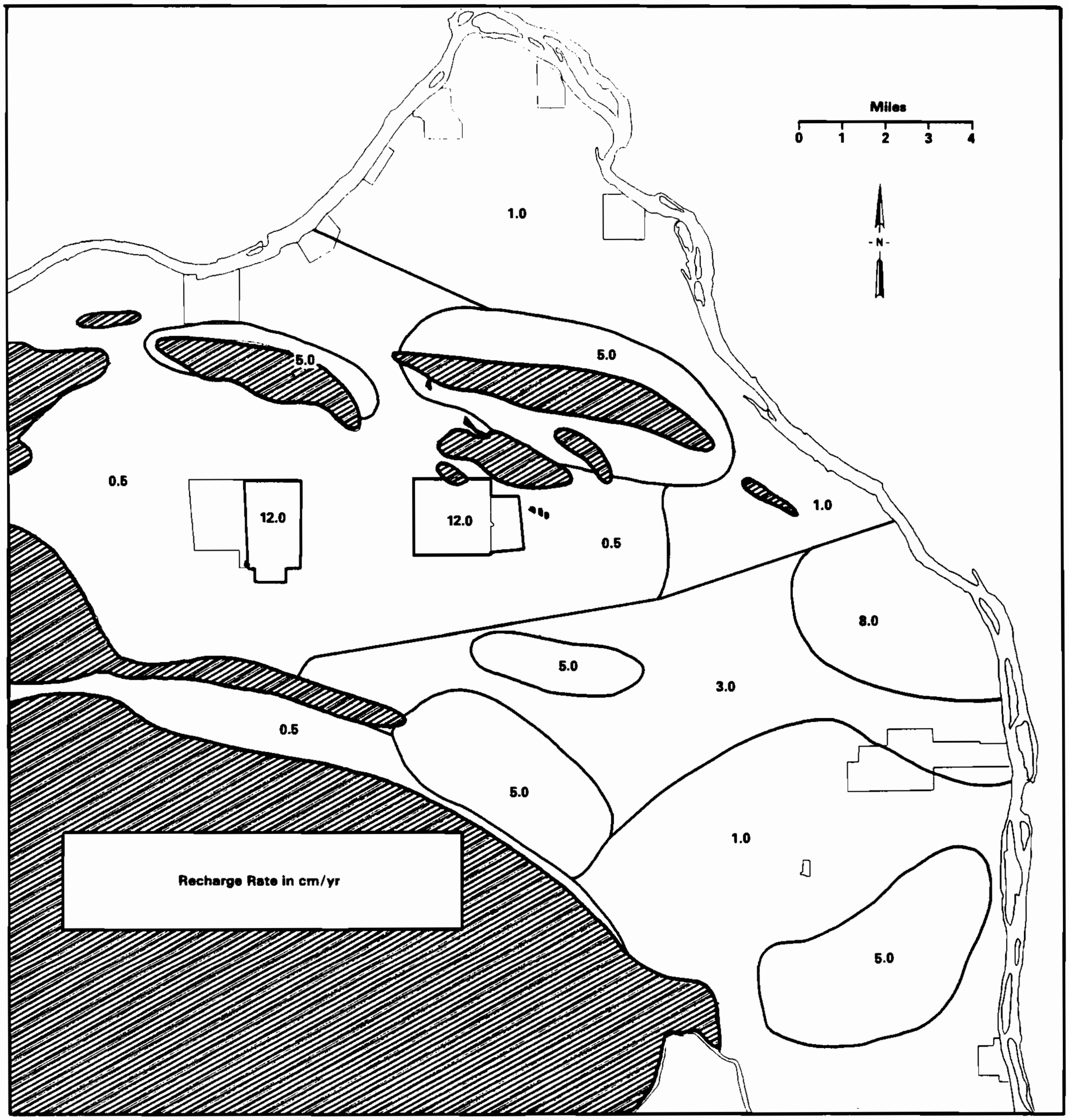

FIGURE 11. Distribution of Areal Recharge to the Unconfined Aquifer Estimated for Inverse Calibration Applications

was to investigate the effect of including areal recharge on the estimates of transmissivity resulting from the model calibration. The recharge values in the distribution vary from 12 cm/yr to 0.5 cm/yr, where the larger value represents 75% of the precipitation. The water levels computed from the Case 2 inverse application (with prescribed flux boundary condition along the Cold Creek Valley and areal recharge) were unreasonably high in the region of Cold Creek Valley. Thus, the Case 2 application of the inverse calibration model does not yield a good calibration to the water levels in this region.

The two remaining applications of the inverse model (Cases 3 and 4) were made to examine the effect of using a prescribed head boundary condition in Cold Creek Valley. The Case 3 application included no areal recharge while the Case 4 application included the areal recharge illustrated in Figure 11.

The water levels calculated by the Case 3 inverse application with a prescribed head boundary condition in the Cold Creek Valley and no areal recharge are illustrated in Figure 12. The water level predicted in the Cold Creek Valley are reasonable because of the prescribed head conditions. The Case 3 inverse application reduced water levels at well locations (i.e., the average residual) from -8.4 ft to -0.19 ft, calculated from the initial and Case 3 inverse estimates of transmissivity, respectively. The overall trends in Case 3 inverse estimates of transmissivity, illustrated in Figure 13, are similar to the initial estimates (see Figure 3). However, the largest transmissivity value has increased to over 1,500,000 ft^2/day. A measure of the uncertainty in the inverse estimates of transmissivity is the coefficient of variation, which is defined as the standard deviation divided by the mean. The coefficients of variation for the Case 3 transmissivity are contoured in Figure 14. Over large regions of the study area, the coefficients of variation are around 0.30, which means the inverse estimation error is 30 percent of the transmissivity estimate. In general, Case 3 yielded a reasonable calibration for the Hanford unconfined aquifer because of the small average residual and the reasonable water levels in the Cold Creek Valley.

For the Case 4 application, which had a prescribed head boundary condition along the Cold Creek Valley and the areal recharge estimates from Figure 11, the computed water levels (Figure 15) along the Cold Creek Valley are reasonable. Water levels in other portions of the study area do not

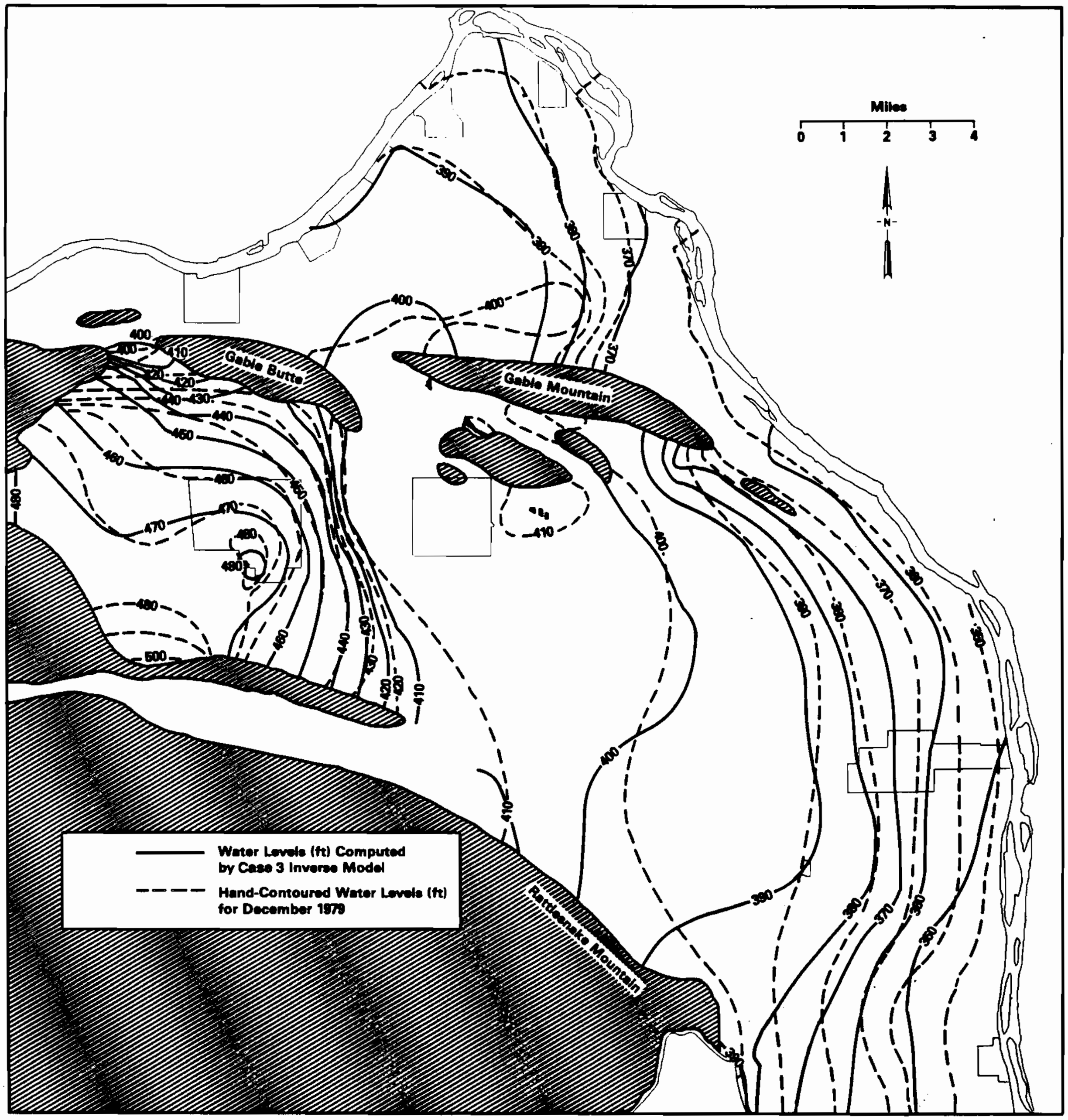

FIGURE 12. Water Levels Predicted by Application of the Inverse Calibration Model for Case 3

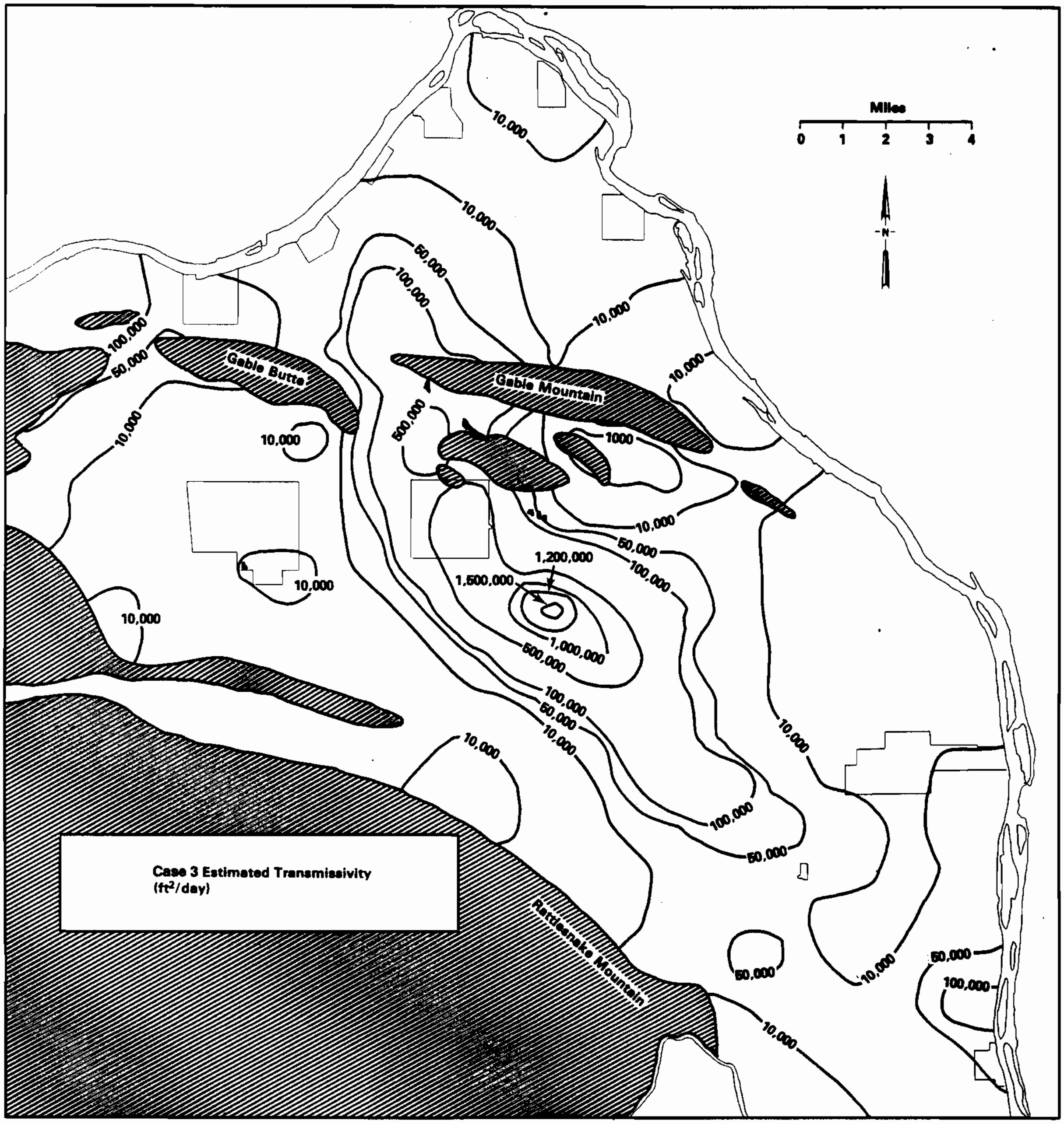

FIGURE 13. Inverse Estimates of Transmissivity for Case 3

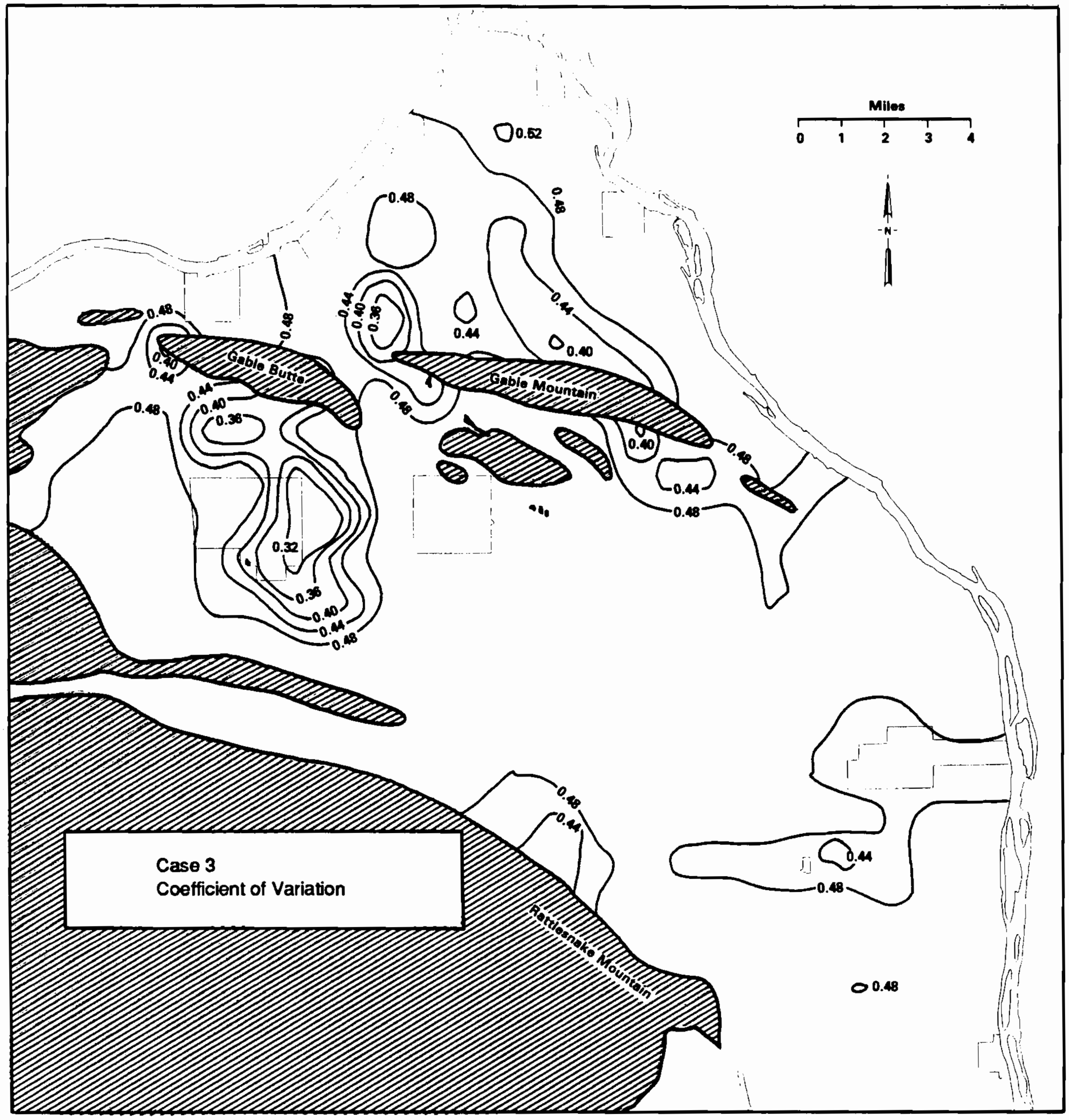

FIGURE 14. Coefficients of Variation for Case 3

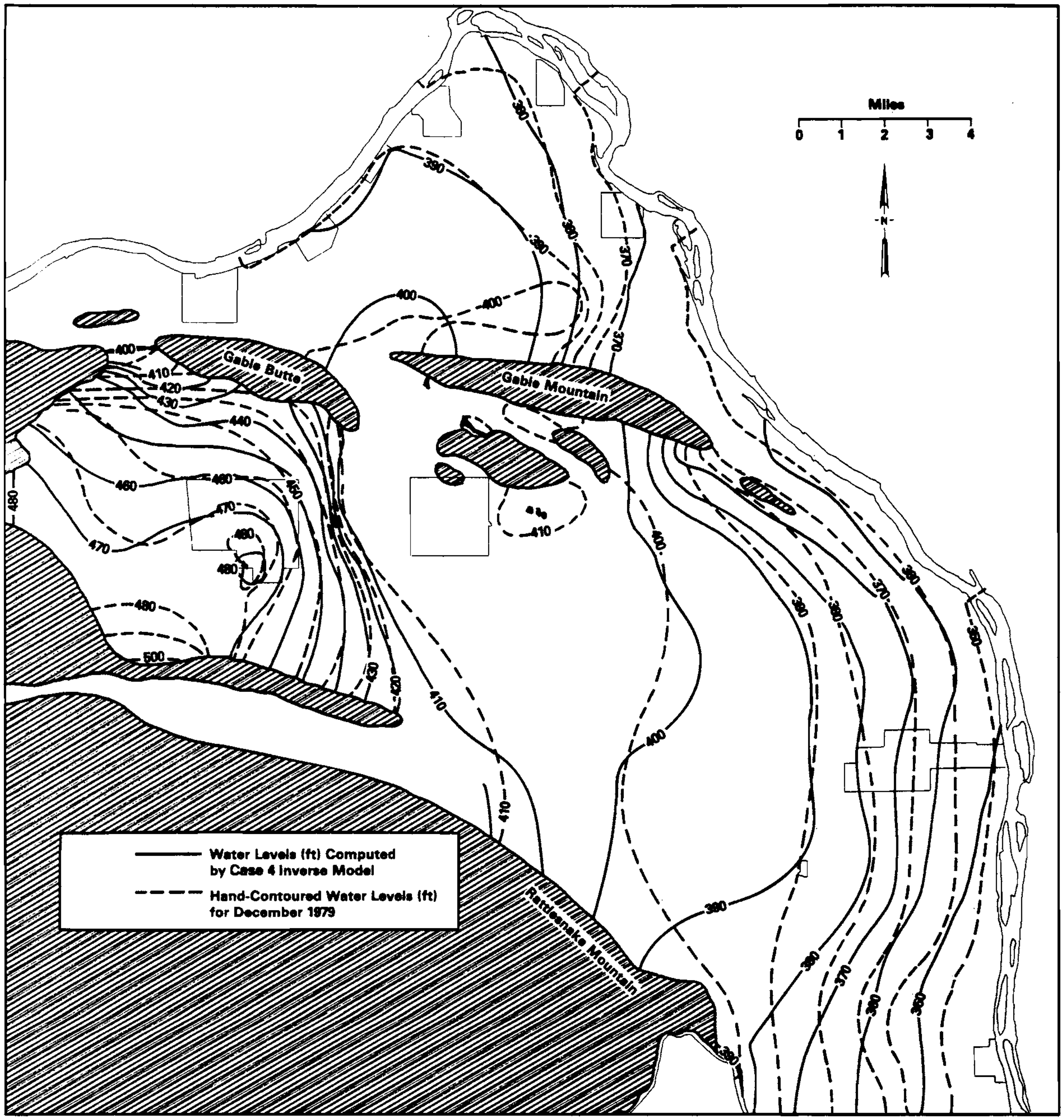

FIGURE 15. Water Levels Predicted by Application of the Inverse Calibration Model for Case 4

differ significantly from those obtained by the Case 1 inverse application. The average residual decreased from 2.2 ft to 0.14 ft, based on the initial and inverse estimates of transmissivity, respectively. The Case 4 inverse estimates of transmissivity, presented in Figure 16, show that overall trends in the estimated transmissivities are similar to the previous inverse results and the initial values. The largest transmissivity value, over 1,200,000 ft^2/day, is less than the corresponding value obtained in the Case 3 application, which had the same boundary condition along the Cold Creek Valley. The coefficients of variation associated with the inverse estimates of transmissivity for Case 4 are illustrated in Figure 17 and show patterns similar to these in previous cases. However, the overall values of the coefficients of variation are smaller than those computed in Case 3 with the same boundary condition.

The water levels computed with the prescribed head boundary condition along the Cold Creek Valley (Cases 3 and 4) more closely approximated the observed water levels than the levels computed with the prescribed flux boundary condition. For Cases 3 and 4 the average residuals were small (i.e., -0.19 and 0.14 ft for the cases without and with areal recharge, respectively), and the computed water levels along the Cold Creek Valley were reasonable.

Water levels at well locations were used in the fitting procedure for the inverse applications; thus, a direct comparison with hand-contoured water levels may not be appropriate but provides an overall indication of the fit of predicted values to measured values. A comparison of water levels for Case 3 (no areal recharge) with hand-contoured water levels for December 1979 (Figure 12) indicates that the general trends (e.g., steep gradient to the east of the 200-West Area) have been reproduced by the inverse results. A comparison of the water levels for Case 4 (areal recharge) with the hand-contoured water levels (Figure 15) suggests that the overall match of predicted and observed water levels is better for the Case 4 results than for the Case 3 results.

The two inverse applications with the prescribed head boundary condition along the Cold Creek Valley and varying areal recharge yielded a better fit with the measured water levels than the application without areal recharge.

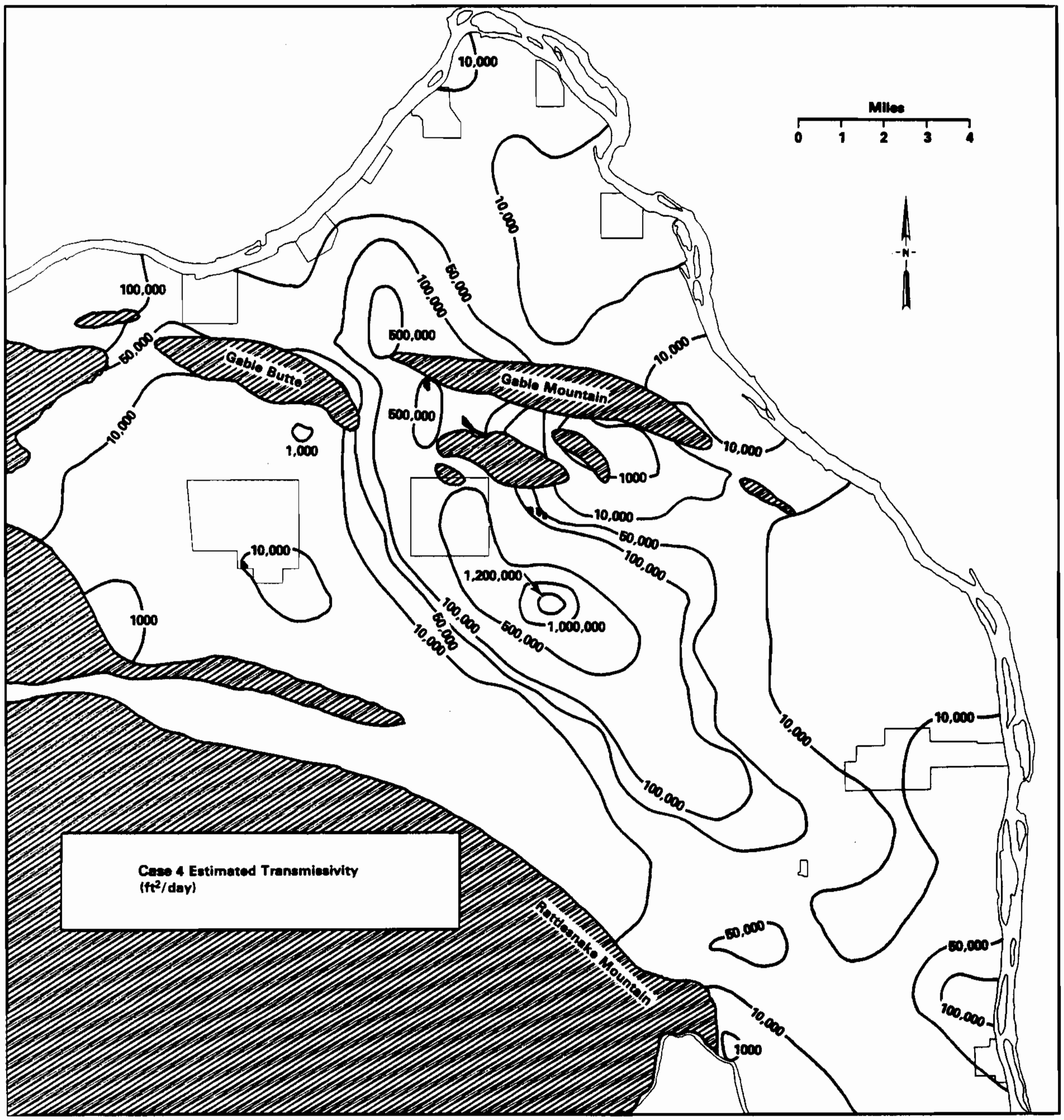

FIGURE 16. Inverse Estimates of Transmissivity for Case 4

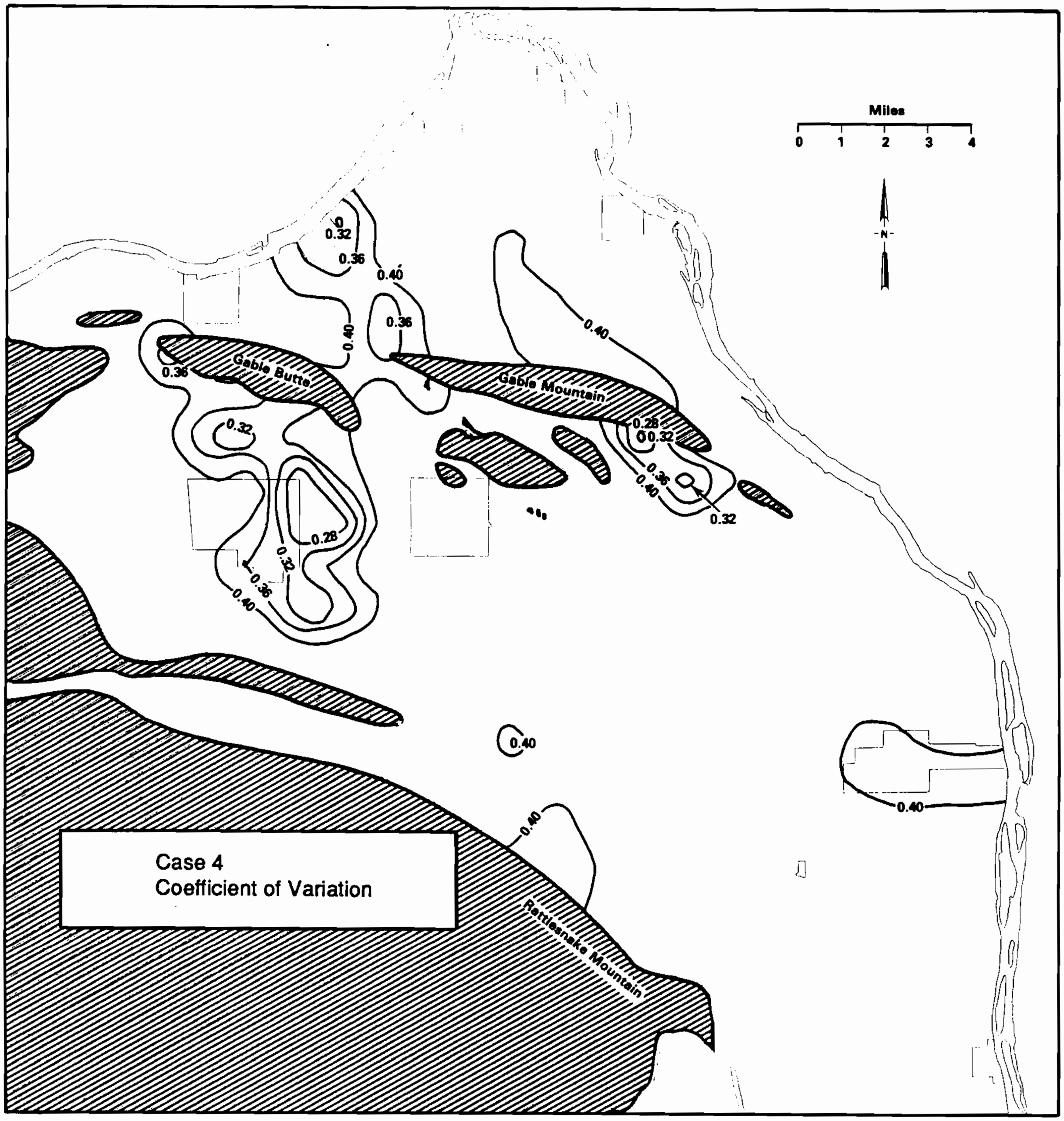

FIGURE 17. Coefficients of Variation for Case 4

In addition, the boundary flux along the Cold Creek Valley calculated by the inverse results assuming prescribed head along that boundary (311,000 ft^3/day) is of the same magnitude as the value assumed in the calibrated VTT model (322,000 ft^3/day). However, the prescribed flux in the VTT model was evenly distributed among three nodes, whereas the prescribed flux estimated with the constant head boundary in the CFEST model is not evenly distributed. More than half of the flux enters at one node.

APPLICATION OF THE INVERSE CALIBRATION RESULTS

The results of the inverse calibration were applied in a two-dimensional model of ground-water flow in the unconfined aquifer to determine how well the predicted water levels matched observed water levels. The transmissivity distribution from the inverse application with prescribed head in the Cold Creek Valley and areal recharge (Case 4) was input to the CFEST code, and the model was applied to simulate water level changes over a 6-year period from 1980 to 1985. Water levels predicted with the model based on the CFEST code were compared with measured water levels. They were also compared with water levels predicted with a model based on the VTT code to provide a benchmark with a previous model of the unconfined aquifer calibrated with an iterative method (Cearlock, Kipp and Friedrichs 1975).

The CFEST code was applied to simulate ground-water flow in the unconfined aquifer with the same boundary conditions as used in the inverse calibration. The transient simulations require that the distribution of storage coefficients in the unconfined aquifer be specified. The number and distribution of storage coefficient measurements for the unconfined aquifer is limited, so the constant value of 0.1 assumed for the model based on VTT (Kipp et al. 1972) was also used in the CFEST model. The liquid waste discharges to the ground for the transient simulation are from Aldrich and Sliger (1981), Sliger (1982, 1983), and Aldrich (1984, 1985, and 1986). A monthly time step was used in the transient simulation.

At the end of the simulation, the water levels predicted with the CFEST model were compared with measured water levels for December 1985 (Figure 18). The predicted and observed contoured water levels are in close agreement, based on visual inspection. The differences between the observed and predicted water levels may result from errors in estimating the transmissivity distribution, the lack of a defined spatial distribution for the storage coefficient, or errors in the data on discharges to ground at disposal facilities.

The water levels predicted with the VTT model for December 1985 compared with observed water levels for the same time period are illustrated in

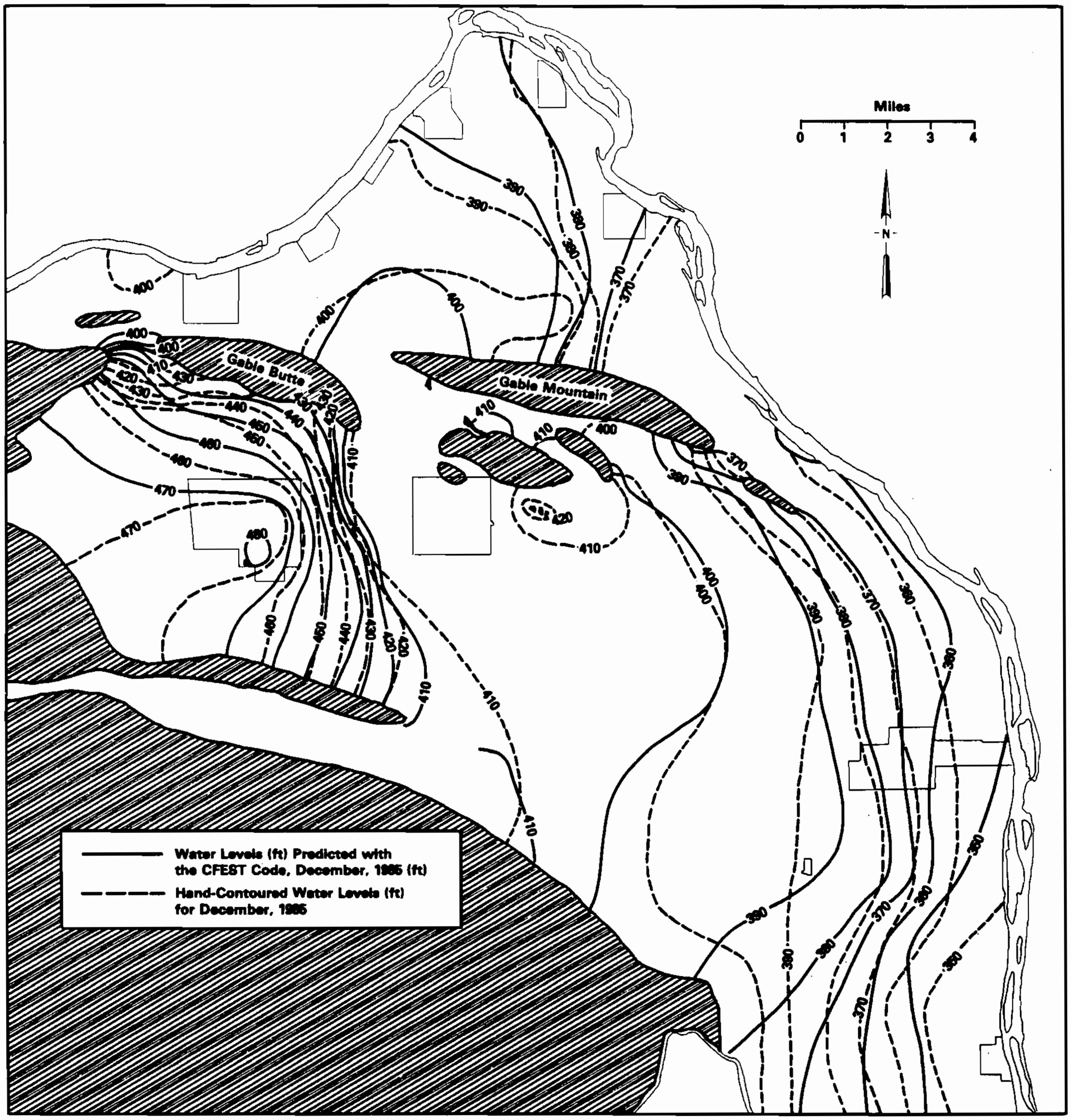

FIGURE 18. Water Levels (in ft) Predicted with CFEST for December 1985

Figure 19. The water levels predicted with VTT at the end of the 5-year simulation are in general agreement with the observed water levels. By comparison of Figures 18 and 19, it can be seen that the water levels predicted by the CFEST model with the inverse estimates of transmissivity are in closer agreement with the observed water levels than those predicted with the VTT model and the iterative calibration for the same 5-year period. For example, in the east-central portion of the study area, the water level gradient and magnitude are reproduced more accurately by the CFEST model based on the inverse estimates of transmissivity. In addition, in the central portion of the study area (see the 400-ft contour), the CFEST predictions indicate the water table is flat, whereas the VTT predictions show a slowly changing gradient. Thus, the large transmissivity estimate of 1,200,000 ft^2/day in the central part of the area (see Figure 16) obtained by the inverse calibration may yield a more accurate representation of the water level gradient than the smaller value used in the VTT model (see Figure 3). Both the VTT and CFEST water level predictions reproduce the water level gradient near the 200 Area. However, in a visual comparison, the CFEST predictions appear to match the hand-contoured water level observations better than the VTT predictions.

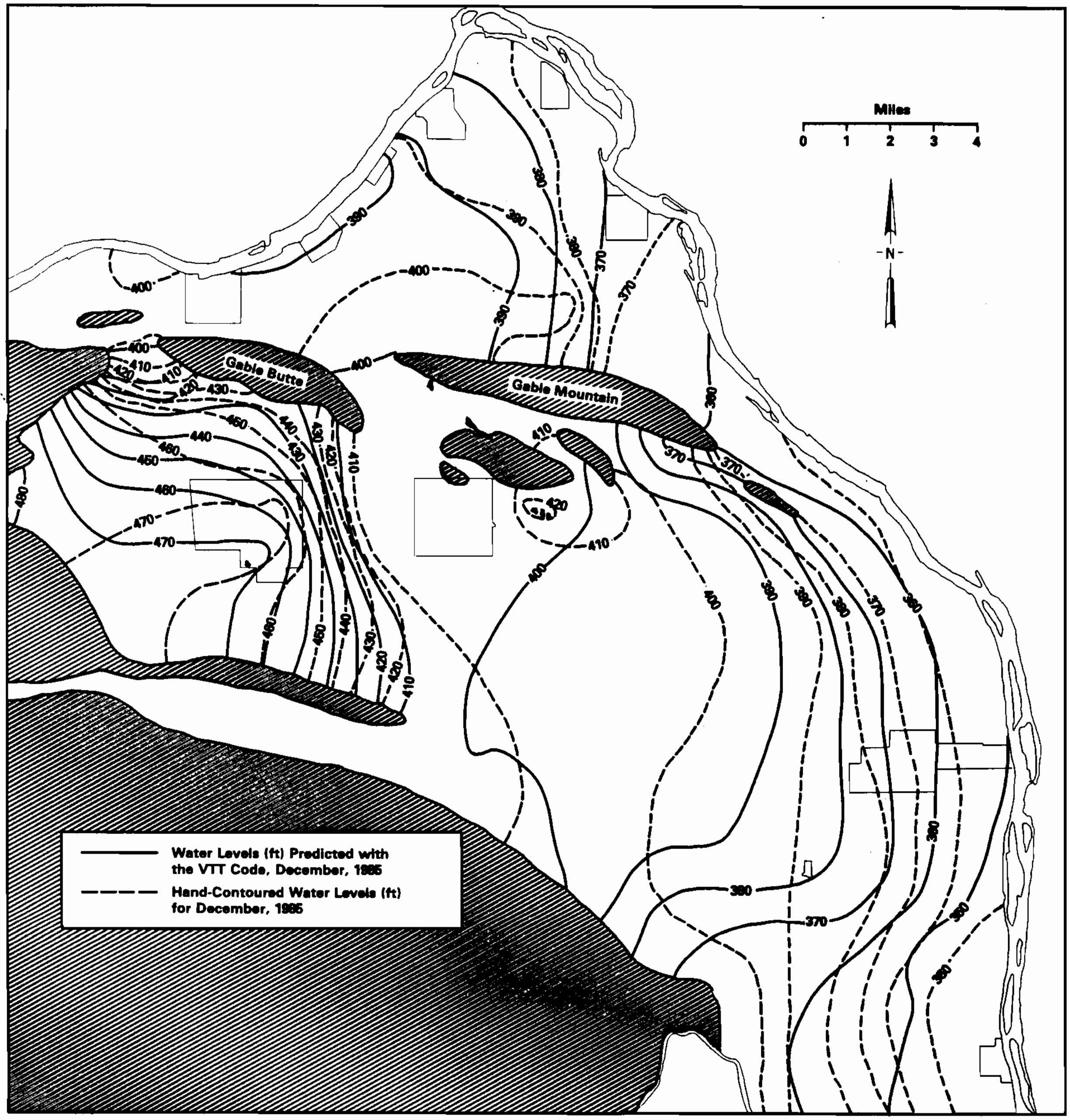

FIGURE 19. Water Levels (in ft) Predicted with VTT for December 1985

CONCLUSIONS

The results of applying the inverse calibration method to the ground-water flow model of the Hanford unconfined aquifer suggest that the water levels computed by the inverse calibration with a prescribed head boundary condition along the Cold Creek Valley provided the closest overall match to observed water levels. These results also suggest that the inverse calibration that includes areal recharge across the site results in a slightly better fit with observed data than the application without areal recharge.

In the simulations of transient conditions from 1980 through 1985, the water levels predicted with the model based on the CFEST code more closely matched observed water levels than the predictions with the model based on the VTT code. The transmissivity distribution from the inverse application with prescribed head along the Cold Creek Valley and areal recharge was used with CFEST, and the transmissivity distribution from previous calibration of the model with the iterative method was used with the VTT code. The differences between the observed and predicted water levels for both the CFEST and VTT simulations may be caused by errors in estimating the transmissivity distributions used, the assumed constant storage coefficient of 0.1, or errors in the data on discharges to ground at disposal facilities applied in the models.

REFERENCES

Ahlstrom, S. W., H. P. Foote, R. C. Arnett, C. R. Cole, and R. J. Serne. 1977. Multicomponent Mass Transport Model: Theory and Numerical Implementation (Discrete-Parcel Random-Walk Version). BNWL-2127, Pacific Northwest Laboratory, Richland, Washington.

Aldrich, R. C., and G. J. Sliger. 1981. Radioactive Liquid Wastes Discharged to Ground in the 200 Areas During 1980. RHO-CD-80-34 4Q, Rockwell Hanford Operations, Richland, Washington.

Aldrich, R. C. 1984. Radioactive Liquid Wastes Discharged to Ground in the 200 Areas During 1983. RHO-HS-SR-83-3 4QLIQ P, Rockwell Hanford Operations, Richland, Washington.

Aldrich, R. C. 1985. Radioactive Liquid Wastes Discharged to Ground in the 200 Areas During 1984. RHO-HS-SR-84-3 4QLIQ P, Rockwell Hanford Operations, Richland, Washington.

Aldrich, R. C. 1986. Radioactive Liquid Wastes Discharged to Ground in the 200 Areas During 1985. RHO-HS-SR-85-3 4QLIQ P, Rockwell Hanford Operations, Richland, Washington.

Bierschenk, W. H. 1959. Aquifer Characteristics and Ground-Water Movement At Hanford. HW-60601, Hanford Atomic Products Division, General Electric Company, Richland, Washington.

Cearlock, D. B., K. L. Kipp, and D. R. Friedrichs. 1975. The Transmissivity Iterative Calculation Routine - Theory and Numerical Implementation. BNWL-1706, Pacific Northwest Laboratory, Richland, Washington.

Clifton, P. M., and S. P. Neuman. 1982. "Effects of Kriging and Inverse Modeling on Conditional Simulation of the Avra Valley Aquifer in Southern Arizona." Water Resour. Res., 18(4):318-324.

Cooley, R. L. 1977. "A Method of Estimating Parameters and Assessing Reliability for Models of Steady State Groundwater Flux, 1, Theory and Numerical Properties." Water Resour. Res., 13(2):318-324.

Cooley, R. L. 1979. "A Method of Estimating Parameters and Assessing Reliability for Models of Steady State Groundwater Flow, 2, Application of Statistical Analysis." Water Resour. Res., 15(3):603-617.

Cooley, R. L. 1982. "Incorporation of Prior Information on Parameters Into Nonlinear Regression Groundwater Flow Models, 1, Theory." Water Resour. Res., 18(4):965-976.

Cooley, R. L. 1983. "Incorporation of Prior Information on Parameters Into Nonlinear Groundwater Flow Models, 2, Applications." Water Resour. Res., 19(3):662-676.

Deju, R. A., and W. K. Summers. 1975. Transmissivity and Hydraulic Conductivity of Saturated Sedimentary Rocks in the Hanford Reservation. CA-168-RA-D5, Atlantic Richfield Hanford Company, Richland, Washington.

DOE. 1987. Final Environmental Impact Statement; Disposal of Hanford Defense, High-Level, Transuranic and Tank Wastes Hanford Site, DOE/EIS-0113, U.S. Department of Energy, Richland Operations Office, Richland, Washington.

Evans, J. C., D. I. Dennison, R. W. Bryce, P. J. Mitchell, D. R. Sherwood, K. M. Krupka, N. W. Hinman, E. A. Jacobson, and M. D. Freshley. 1988. Hanford Site Ground-Water Monitoring for July Through December 1987. PNL-6315-2, Pacific Northwest Laboratory, Richland, Washington.

Gee, G. W., and R. R. Kirkham. 1984. Arid Site Water Balance: Evapotranspiration Modeling and Measurements. PNL-5177, Pacific Northwest Laboratory, Richland, Washington.

Graham, M. J., M. D. Hall, S. R. Strait, and W. R. Brown. 1981. Hydrology of the Separations Area. RHO-ST-42, Rockwell Hanford Operations, Richland, Washington.

Gupta, S. K., C. T. Kincaid, P. R. Meyer, C. A. Newbill, and C. R. Cole. 1982. A Multi-Dimensional Finite Element Code for the Analysis of Coupled Fluid, Energy, and Solute Transport (CFEST). PNL-4260, Pacific Northwest Laboratory, Richland, Washington.

Jacobson, E. A. 1985. A Statistical Parameter Estimation Method Using Singular Value Decomposition With Application to Avra Valley Aquifer in Southern Arizona. Dissertation, Department of Hydrology and Water Resources, University of Arizona.

Kipp, K. L., and R. D. Mudd. 1973. Collection and Analysis of Pump Test Data for Transmissivity Values. BNWL-1709, Pacific Northwest Laboratory, Richland, Washington.

Kipp, K. L., A. E. Reisenauer, C. R. Cole, and L. A. Bryan. 1972. Variable Thickness Transient Groundwater Flow Model: Theory and Numerical Implementation. BNWL-1703, Pacific Northwest Laboratory, Richland, Washington.

Neuman, S. P. 1980. "A Statistical Approach to the Inverse Problem of Aquifer Hydrology: 3. Improved Solution Method and Added Perspective." Water Resour. Res., 16(2):331-346.

Neuman, S. P., and S. Yakowitz. 1979. "A Statistical Approach to the Inverse Problem of Aquifer Hydrology, 1, Theory." Water Resour. Res., 15(4):845-860.

Simmons, C. S., C. T. Kincaid, and A. E. Reisenauer. 1986. A Simplified Model for Radioactive Contaminant Transport: The Transs Code. PNL-6029, Pacific Northwest Laboratory, Richland, Washington.

Sliger, G. J. 1980. Radioactive Liquid Waste Discharged to Ground in the 200 Areas During 1979. RHO-CD-79-34 4Q, Rockwell Hanford Operations, Richland, Washington.

Sliger, G. J. 1982. Radioactive Liquid Wastes Discharged to Ground in the 200 Areas During 1981. RHO-HS-SR-81-3 4QLIQ, Rockwell Hanford Operations, Richland, Washington.

Sliger, G. J. 1983. Radioactive Liquid Wastes Discharged to Ground in the 200 Areas During 1982. RHO-HS-SR-82-3 4QLIQ P, Rockwell Hanford Operations, Richland, Washington.

Yeh, W. W-G., and Y. S. Yoon. 1976. "A Systematic Optimization Procedure for the Identification of Inhomogeneous Aquifer Parameters." In Advances in Groundwater Hydrology, pp. 72-82, American Water Resources Association, Minneapolis, Minnesota.

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