

INVESTIGATION OF CONTAMINANT TRANSPORT
PARAMETERS IN MICHIGAN AQUIFERS

BY

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PROJECT REPORT

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INTRODUCTION

This report describes the preliminary results of an investigation into contaminant transport processes at selected locations within the state of Michigan. The primary purpose was to determine parameter values used to describe the hydrodynamic dispersion processes at specific locations with existing contamination problems. An additional objective was to examine the adsorption characteristics of specific contaminants. Previously obtained field data was analyzed in order to accomplish these objectives.

Two sites were selected in the preliminary phase of the investigation: 1) A styrene spill from a train derailment near Pearl, Michigan in May 1979; 2) Contamination resulting from waste disposal practices at Ott/Story Chemical Company near Muskegon, Michigan. The Pearl site is characterized by a one time spill with subsequent attempts at a cleanup of the styrene that was released. All pertinent information regarding data collected at that site has not been received at the present point in time and only a preliminary analysis has been made; the final project report will deal with this site in more detail. It presently appears that the "local" nature of the problem

will make it difficult to obtain a meaningful analysis. Additional complications arise because of the tendency for styrene to polymerize and be retained in the unsaturated zone only to enter the groundwater system after rises in the groundwater table.

The Story Chemical site analysis has been more tractable and the remainder of this report deals with this subject. The contamination apparently resulted primarily from seepage from waste lagoons on-site during the 1960's and 70's. The wastewater contained relatively high concentrations of chloride ions in addition to a number of organic compounds. Large enough concentrations of contaminants have apparently entered the water table aquifer to have some density effect since the highest contaminant concentrations are found at or near a clay layer serving as an effective bottom to the aquifer. However, no indication is present that this influence has been important in determining the migration routes of the contaminants. The chloride data have been used in the analysis of aquifer dispersivities because of their relative abundance and the fact that chloride ions are not significantly adsorbed in the soil matrix. Analytical procedures are used to obtain estimates of the aquifer dispersivities and the resultant values are used in a numerical solution of the groundwater flow at the site to provide additional verification. Data on specific organic chemicals is also examined to attempt to define adsorption characteristics in the

aquifer system. These results are presented herein along with interpretations justified within the uncertainty of the available data.

DATA BASE

A number of different sources of information were obtained from the Michigan Department of Natural Resources files. These include the following reports or other sources of information:

1. Williams and Works Engineering report to the Ott Chemical Company, Nov. 1966 entitled "Water Supply and Waste Water Disposal."

2. Miscellaneous data provided by Williams and Works to the Ott Chemical Company providing interpretation of groundwater quality samples at or near the company location. These are in the form of contour plots of phenol and chloride concentrations and range in time from 1971 to 1975.

3. A report entitled "Report of Groundwater Quality and Storage of Wastes at Story Chemical Corp., Muskegon, Michigan based on a survey conducted March 8-9, 1977." Concentrations of various chemicals at selected observation wells are included in this report which is assumed to have been produced by the D.N.R.

4. Portions of a report by Keck Consulting Services to the DNR entitled "Hydrogeological Investigation, Story Chemical Company, . . ." November 10, 1977. This includes chloride concentrations at various observation wells from 1965 to 1977.

5. Summary sheets of water quality data from the Muskegon County Health Department obtained July and August, 1977. Various chemical parameters are analyzed.

6. D.N.R. report entitled "Hydrogeological study of Groundwater Contamination in the Area of the Former Story Chemical Company." This includes sampling with depth at seven observation wells, primarily in 1978.

7. D.N.R. Report entitled "1979 Hydrogeological Study of the Groundwater Contamination in the Area of the Former Story Chemical Company." Results of sampling at various observation wells is presented.

8. Report by Keck Consulting Services to D.N.R. entitled "Ott/Story Chemical Groundwater Contamination Study," September 6, 1979.

9. Ott/Story Chemical Company Hydrogeological Investigation; Phase A-6: Computer Simulation July 3, 1980 and related correspondence to Gary Klepper (D.N.R.) of October 22, 1980, and December 4, 1980.

10. Appendix to previous report "Review of Data: Phase A-4."

While it is probable that there is additional information available regarding hydrogeologic conditions at the site, the above data provides a reasonably continuous record of chloride concentrations in the groundwater aquifer from 1965 to 1980, phenol concentrations from 1975 to 1980, and various other organic chemicals at irregular intervals.

Groundwater levels are provided in various of the above reports and References 8-10 contain information on aquifer characteristics. These data were used to generate the results presented in this report. A previous numerical simulation, (9)*, was performed in which the groundwater flow in the area was computed. This was used as a starting point for the present numerical simulation in which contaminant transport is also included. Changes in the simulation details from the previous report are documented and justified by interpretation of the available data. The major difference in the present approach is the inclusion of the water quality data in the problem interpretation.

CONTAMINATION PLUME ANALYSIS

Since there was considerable information on chloride concentrations in the aquifer, this source provided the most information regarding transport parameters. Although chlorides may be present from additional sources (notably road de-icing operations) the chloride concentrations in the contaminant plume are so large this source is relatively easy to identify compared to other minor fluctuations in background levels. Chloride concentrations in the plume in excess of 2000 mg/l were not unusual compared to background levels of less than 10 mg/l. A considerable number of samples where adjacent observation wells sampled both shallow and

*In the remainder of this report, information referenced is indicated by the numbers assigned above.

deep portions of the aquifer indicated that higher chloride concentrations were found at greater depth. This could be due to either density effects or the natural recharge diluting the near surface waters. In fact, probably both effects are present. Consideration of this fact resulted in a decision to only analyze deep well chloride concentrations since data for shallow observation wells may be distorted by further migration of chlorides towards deeper levels with distance away from the source. On the other hand, concentrations in deep observation wells were relatively large at or near the chemical company site indicating vertical movement was fairly rapid and deep well concentrations should not be affected significantly by three dimensional effects.

Selected plots of chloride contours are presented in Figs. 1-6 for deep observation wells. Sources of data are indicated on the figures which cover the span in time of available information. These data, along with other information available, support the following general conclusions:

- A. Early in the time period covered by the data, a substantial amount of the contamination problem was confined to the immediate site. 1965 data appear to indicate a general movement from the waste lagoons to the pumping wells on-site. The effect of pumping on-site seems to have been to deflect the plume somewhat to the southwest.

- B. Recharge ponds do not appear to be a significant source of contamination at any point in time.
- C. After the mid 1970's, chloride concentrations have been dropping at the upstream end of the plume with the cessation of waste discharge and the aquifer system appears to be flushing itself.

Plots of phenol concentrations for the years of 1975, 1977, and 1979 are given in Figs. 7-9. Since the time record on this data is not as long, it is more difficult to draw conclusions. A critical assumption is that these compounds entered the aquifer system at the same time as the chloride contamination. Inherent in this assumption are the following two considerations; (1) phenol and chloride concentrations in the source were directly proportional to each other and (2) the distance from the source to the water table is short enough that adsorption in the unsaturated zone is not a critical element of this problem. If these assumptions are valid, then the following general conclusions may be made:

Phenolic compounds are relatively strongly absorbed in the aquifer media and are retarded significantly in their horizontal movement. This is evidenced by a buildup in concentrations at the Little Bear Creek tributary only beginning to be evidenced in the late 1970's. Concentrations are still rising relatively close to the site during the time period in question. This contaminant may be expected to persist in the aquifer for a considerable length of time.

The validity of the above conclusions will be further addressed during the presentation of the results of the numerical simulation.

Miscellaneous measurements for other organic chemicals related to the Story Chemical Company operation were investigated to determine their transport in the aquifer system. Sufficient information on benzene, toluene, and aromatic amines was obtained to be able to estimate their distribution; the results are provided in Figs. 10-12. If the same assumptions as made regarding the movement of phenols is made, it is possible to determine their relative adsorption characteristics. In order of relative mobility, aromatic amines appear to be the most mobile with benzene the least. All are more mobile than phenols and may be expected to flush from the system more rapidly. There is such little data that these conclusions can only be regarded as very tentative; they will be discussed later in the presentation of the numerical results. Insufficient data is available on the concentrations of other compounds to be able to draw any general conclusions on their rate of movement in the groundwater system. It can be anticipated that this is due to several factors including: low concentrations of specific compounds; large retardation factors and very little movement with lack of data at the various observation wells; and difficulties with analytical procedure due to the presence of many unknown contaminants.

Additional test results are available for 1978 and 1979 for ammonium ion NH_3^- , but they will not be analyzed in any detail. The very high PH of the contaminated water will likely have a significant influence on the chemistry that may not be repeated at other potential contamination sites. The available data however seem to indicate NH_3 movement with very little adsorption effects in this particular plume.

MODEL FORMULATION

Since the above conclusions are only qualitative in nature, an attempt was undertaken to quantify them as well as fulfill the basic objectives of this investigation. In order to do this, a numerical model was formulated which solved the simultaneous problems of groundwater flow and contaminant transport. The U.S. Geological Survey "Method of Characteristics" program* was selected as the modeling tool because of relative familiarity with its use and some degree of confidence in its ability. Although this program is not formulated to be able to analyze flow with adsorption, it is possible to transform some input parameters and obtain a solution if a linear, reversible adsorption isotherm (i.e. that the use of retardation factors is valid) is assumed. Details are discussed in the following sections. Parameter identification for this model was accomplished by a variety of techniques as outlined in the following pages. The result

*Computer Model of Two-Dimensional Solute Transport and Dispersion in Ground Water," by L. F. Konikow and J. D. Bredehoeft, Techniques of Water-Resources Investigations of the U.S.G.S. Chapter C2 Book 7.

is a model that is believed to provide a realistic description of the general aquifer behavior at the Ott/Story Chemical site and allows more specific conclusions regarding the contaminant transport parameters for this location. A more thorough analysis of the problem may well yield a model that better reproduces details of the contaminant migration in the system as this was not the present objective of the model formulation.

Modeling Philosophy

The numerical model was not constructed with the intent of reproducing the observed contamination profiles as closely as possible. Instead, it was used as an aid in sorting out the various influences in the problem and the determination of the appropriate transport parameters. As such, unless additional detail was deemed to be of critical importance to the results obtained, it was not included in the formulation. It is also possible that additional data, known to exist but not available at the time of the model formulation, would alter the specific formulation somewhat. On the other hand, the uncertainty in various details of the actual problem probably renders additional complexity unjustifiable in most instances.

The first attempt was to reconstruct the groundwater flow in the area. The starting point for this part of the simulation was the previous study by Keck Consulting Services (9) and the 1979 data on water table elevations (8).

Adjustments to the previous simulation results were made as outlined and justified in a subsequent section until a reasonable reproduction of the water table levels was obtained. Steady state groundwater flow conditions were assumed throughout the analysis as the only justifiable approach given other uncertainties in the problem resolution. From the groundwater flow model, the contaminant transport model was used to attempt to reproduce the detail of the chloride plume. Only one adjustment as discussed later was made to the initial simulation.

This change was required only because the initial run was known to oversimplify the source detail from the beginning and the final description is one that was visualized as the most appropriate from the outset of the modeling effort. Considerable detail regarding temporal and spatial distribution of groundwater pumping at the site and contaminant discharge is not included in the model. This is because this detail is both not accurately known and not felt to be of critical importance to the assessment of aquifer parameters. On that basis, only one release scenario was investigated; however it is felt to be reasonably consistent with the known detail at the site. Once the contaminant plume simulation was obtained, the effect of retardation on the expected plume behavior was investigated. The sensitivity of the model to the various transport parameters is investigated, and finally, the results obtained are interpreted in light of the available data and appropriate conclusions are drawn.

Parameter Identification

The initial information on the groundwater flow portion of the problem were taken from the previous numerical simulation by Keck Consulting Services (9). Specifically, these are tabulated in Table 1 along with the source for the parameter estimate. The saturated thickness of the aquifer for the present simulation was taken as 70 ft from the well

Table 1 - Hydraulic Parameters for Local Aquifer

Parameter	Estimated Value	Source
Hydraulic Conductivity	66.8 ft/day	small scale pump tests described in (10)
Specific Yield	0.1	estimate
Local Groundwater Recharge	10 inches/year	estimate from (4)
Specified piezometric head boundary conditions	variable	water table contours from previous hydro-geologic investigation (4)

log data given in (8). The discussion of the Keck numerical solution provides additional detail on this. Of the above parameters in Table 1, only the groundwater recharge rate was kept as in the previous simulation. Since no better estimate of this rate was available, it was not considered

to be a variable subject to analysis. The additional parameters were adjusted as deemed necessary, but still consistently with available information. The small scale pump tests conducted by Keck Consulting Services (10) were at such low flow rates that the storativity coefficient was more nearly due to that of a confined aquifer situation when the well logs clearly indicate an unconfined aquifer. This behavior is often noted for small drawdowns in water table aquifers and requires a longer pumping time to make an accurate assessment of the actual specific yield. The pump test results were interpreted by assuming an effective aquifer thickness of the screen length of the pumping well and dividing the computed transmissivity by that length to obtain hydraulic conductivity. In actuality, the vertical distance influenced by the pumping will be greater than the screen length, so a somewhat lower hydraulic conductivity than the value in Table 1 would be expected. Previous studies cited in (9) gave hydraulic conductivities of between 20 and 60 ft/day and support the above conclusion. No estimate was available for the specific yield, but it is understood that the value of 0.1 was selected on the basis that it provided a conservative estimate or "factor of safety" in the results obtained from the numerical simulations. A further attempt to rationalize the values of these two parameters

was obtained from the chloride concentration profiles (2) and the time of travel of the chloride peaks. Although this procedure is suspect due to the lack of resolution in chloride data, it did point out some inconsistencies in the previous parameter values. The Darcy velocity could be estimated from the local hydraulic gradient given by $q = K \Delta\phi/\Delta\ell$ and the seepage velocity by

$$v = \frac{\Delta\ell p}{\Delta t}$$

Here K is the hydraulic conductivity, $\Delta\phi/\Delta\ell$ is the water table slope obtained from the contours given, $\Delta\ell p$ is the distance the concentration peak moves in time Δt . Nearly all of these calculations clearly indicate a specific yield $S_y = q/v$ much greater than physically expected. Figure 13 indicates a sample calculation. A specific yield of 0.73 is much greater than can be physically expected. The difficulty now is that the determination of K and S_y cannot proceed independently from these data since a reduction in K will produce a proportional reduction in S_y . Subsequently, a value for S_y of 0.25 was assumed and a hydraulic conductivity of 32 ft/day was estimated. The approach was to take as large a value of specific yield as physically realistic and determine what hydraulic conductivity would give a good match between the Darcy and seepage velocities.* This approach may

* Note the recent report "Management Options Contaminated Ground Water Plume Ott/Story Chemical Company" by Keck Consulting Services and Snell Environmental Group Inc., June 1981, estimates a larger specific yield than 0.1 and also notes the possibility of a lower hydraulic conductivity.

be subject to considerable question, but the reduction of hydraulic conductivity appeared to give a much better simulation of water table levels as discussed later. These values were used without modification in the numerical simulation. The transverse dispersivities were also estimated from the same data on chloride profiles. There was never adequate enough resolution of the leading edge of the plume to attempt an estimate of the longitudinal dispersivity so in all analyses a value three times that of the lateral dispersivity was assumed. This approach is simply consistent with known variations of the two components from previous studies. The lateral dispersivity was estimated by an analytical procedure which requires a large number of assumptions:

- Molecular diffusion effects are negligible;
- Steady release of a point source of contaminant;
- Two dimensional contaminant transport;
- Negligible longitudinal dispersion;
- Uniform ground water flow.

Of the above, the second and last are the most critical assumptions for the specific problem, but the effect of these influences was mitigated by the approximate procedure used. For the above assumptions, the lateral concentration profile is given by

$$C = C_{\max} e^{-y^2/4\alpha_T x}$$

where y is lateral distance from the peak concentration C_{\max} , x is longitudinal distance from the source, and α_T is the transverse dispersivity. Then by definition

$$\sigma^2 = 2\alpha_T x$$

where σ^2 is the variance of the lateral concentration distribution. The effect of the point source approximation is removed by taking the derivative

$$\frac{d\sigma^2}{dx} \approx \frac{\Delta\sigma^2}{\Delta x} = 2\alpha_T$$

and observing the rate of growth of the plume width. The uniform flow assumption is partially negated by measuring distance along the plume travel path. The concentration profiles taken directly from (2) between 1974 and 1975, a plume profile in 1976 from (4) and the present estimate of the plume location ((9), correspondence of October 22, 1980) were used to estimate the transverse dispersivity. In all cases except the last, a Gaussian profile was approximated through the plume data, and a total width of 4σ was estimated. In the latter case, a width of 4σ for the plume outline was assumed. This procedure was repeated for two or three locations along the plume and corresponding values of α_T were computed. Figures 14-16 demonstrate example calculations and Table 2 summarizes the computed results. From these data, a value for α_T of 20 ft was estimated

Table 2. Estimates of Lateral Dispersivity
(distances in ft)

Date (source)	X_1	X_2	σ_1	σ_2	α_T	Average
Nov. 1974 (2)	1070 1860	1860 2670	200 275	275 325	22.5 18.5	20.5
May 1974 (2)	1160 1740	1740 2760	250 295	295 350	21.1 17.4	18.8
Jan. 1975 (2)	1290 2275	2275 3140	230 288	288 346	15.3 21.3	18.1
1976 (4)	700	2650	275	400	21.1	
1980 (8)	1415	3200	350	450	22.4	
					Average	20.2

with only a small amount of scatter in the computed results. This value and a longitudinal dispersivity of 60 ft were taken as the baseline values in the numerical simulations although a sensitivity analysis was performed. These values are consistent with previously reported values for similar aquifer systems* and so are presumed to be fairly reliable estimates for those parameters. A retardation factor was only estimated for phenols since that was the compound for which the most data was available and also since it appeared to be the least mobile of the specific chemicals investigated. Only a crude estimate of the retardation factor was obtained and used in the numerical solution to observe its influence. The considerations involved in this analysis were as follows:

According to (4), little chloride movement off site was detected in 1965. This would place the beginning of the plume migration problem some time in the middle to late 1960's. Assume phenols were present in the initial waste discharge. By 1975 they have shown high concentration (17 mg/l) in observation well 17 (Fig. 17) and continue upwards to values of 22 mg/l in 1977 and 38 and 43.5 mg/l in 1979. In 1980 levels of 27 mg/l were detected, indicating peak concentrations have possibly arrived at the site. On the other hand values of only

*J.J. Fried "Groundwater Pollution," Developments in Water Science," Volume 4, Elsevier Publishing Co., 1975.

3 or 4 mg/l are detected further downgradient at observation wells A & C in 1978 and 1979. Chloride levels were high in well 17 in 1968 and never got much larger than that. From this, the relative time of movement to well 17 could be approximately 5 years for chloride and perhaps 15 years for phenols, giving a retardation factor of approximately 3. This value would give a time of movement for peak concentrations of perhaps 30 years or more to observation wells A and C.

This value of retardation factor was used in the numerical model discussed later to observe whether results consistent with the observed data could be generated.

NUMERICAL SIMULATIONS

A series of numerical simulations were performed to obtain some additional information regarding the transport parameters at the Ott/Story Chemical Company Site. Basically the approach was similar to that used in the previous simulation by Keck Consulting Services (9). The grid with 400 ft spacing between nodes was used in the simulation effort to be consistent with the previous analysis.

WATER TABLE SIMULATIONS

Specified head boundaries were applied at all exterior nodes (actually one node in from the boundary as shown in Fig. 18) and along Little Bear Creek and tributary as in

Fig. 19. Most of the boundary nodes are far enough removed from the contamination site that a significant change in boundary head only influences the interior heads a relatively minor amount. Calculations are much more sensitive to the heads specified along the creeks and these represent a critical element of the simulation. The U.S.G.S. model has the capability of performing a steady state computation with only boundary heads specified. In this procedure, all interior heads are left unspecified and are computed in the simulation. The interior water table elevations so computed were then compared to available water level observations (8). One difficulty with the available data is that there were two types of observation wells; one with screens at depth and another which sampled the water table location directly. There appears to be a significant component of vertical flow as adjacent wells show approximately 1.6 ft difference in head between deep and shallow observation wells at a considerable distance from the creek. Scatter in water levels essentially adjacent to the creek indicate that significant vertical velocity components must exist and therefore large changes in head with depth. Interpretation of the available data becomes difficult near the creek which is unfortunately the most critical area from the standpoint of supplying boundary conditions. An initial head distribution along the creek was selected however as given in Fig. 20 and never altered during subsequent calibration attempts.

Initial runs with a hydraulic conductivity of 66.8 ft/day yielded results that appeared to predict piezometric heads too low at the interior locations of the grid. Lowering the hydraulic conductivity to 32 ft/day raised interior heads by approximately 1.5 ft and yielded much more satisfactory water table comparisons. On the basis of this and the previous discussion, the lower value of hydraulic conductivity is recommended for future simulations. The final simulation selected gave the groundwater contours shown in Fig. 21, and yield as good as an agreement with the available data as appears reasonable to expect. This basic data was then used in all further simulations of the site.

CONTAMINANT PLUME SIMULATIONS

After much consideration of the possible source descriptions, a somewhat simplified approach was taken. This is again consistent with the modeling philosophy of transport parameter simulation and does not reflect accurate histories of contaminant plume movement. Future simulations for management decisions, should they be performed, may want to consider better descriptions of the source. It was decided that the two most important considerations were probably source location and the influence of pumping at the site. The U.S.G.S. model offers the alternatives of concentrating contaminants at a point (injection well) or over a grid cell

which in this case is 400 ft square. Since this is on the order of the size of the original waste ponds, the latter option was used and a single node slightly downgradient of the actual ponds was used as the source location. Its position is indicated in Fig. 19. A source concentration of 3000 (arbitrary units) was used to check chloride concentration profiles since this is representative of maximum chloride concentrations in mg/l observed. The Williams and Works data (2) seem to indicate a drop in chloride concentrations near the source in the early 1970's and a gradual decrease continues over time. The source was assumed to be in effect for 10 years (e.g. from 1958 to 1968 or some similar description) and then completely removed thereafter. Although it is known that the contamination continued after that point, the relative amounts of contamination input in the two periods is unknown and it was primarily desired to observe the computed plume movement. Again, this description could be criticized for various reasons but there seems to be some merit in such a description. Finally, rather than attempt to specify recharge and pumping rates at the Story Chemical site directly, specified heads were used as source conditions. The Williams and Works data (1) indicate an approximate 1 ft rise in head below the waste ponds and drawdowns of up to 8 or 9 feet below that level at nearby pumping wells. The effect of pumping wells was included in a crude sense only because the early data seemed to show

that the contamination moved in response to pumping and migrated more to the southwest than otherwise expected. Pumping wells were assumed at two nodes as indicated in Fig. 19 and heads of 9 ft lower than that below the waste ponds were specified. The waste pond head was determined by taking the result of the water table simulation at that node and simply adding 1 ft to it. After the initial 10 year period, the construction of the recharge ponds on site apparently effectively stopped the pumping well influence, so these effects were removed from the simulation after 10 years. Again, it should be emphasized that these steps were performed because a great deal of source information was not available and only the qualitative effects of the source were felt necessary to examine transport parameters. It should be mentioned that the above description was selected in advance of any model calibration attempts and does not represent any attempt to reproduce the plume location or behavior.

RETARDATION EFFECTS

The effects of absorption were included in the numerical solution to examine movement of some of the other chemical compounds in the aquifer. Although the U.S.G.S. model does not include adsorption effects, this can be included in a relatively straight forward manner. The general equation

for contaminant transport as solved by the U.S.G.S. program is

$$\frac{\partial C}{\partial t} = - \nabla \cdot \left(\frac{q}{n} C \right) + \nabla \cdot (D_h \nabla C) + S_o$$

i.e. no chemical reaction or adsorption terms are given. Here C is contaminant concentration, q is the specific discharge vector, n is the effective porosity, D_h is the hydrodynamic dispersion tensor, and S_o represents sources or withdrawals of fluid. If the adsorption process is considered to be given by a linear reversible isotherm, the above equation is modified by multiplying the time derivative term by a retardation factor R_d .* Since we don't have any information to the contrary, this approach is assumed in this study. Dividing all sides of the equation by R_d implies that if the effective porosity is multiplied by R_d and the dispersion coefficient is divided by R_d , all flow terms in the above equation will be adjusted properly to account for adsorption. Also, it is important to note that the U.S.G.S. program uses a separate term for aquifer storativity and effective porosity so no conflict arises in the solution of the flow equation. Since a recharge rate is not being directly specified in the numerical simulation, the source term S_o is not modified and the amount of water

* "Hydraulics of Groundwater," J. Bear, McGraw Hill Inc., 1979.

entering the system is the same in an adsorbing and non-adsorbing case.

PLUME SIMULATION RESULTS

An initial set of runs was performed to investigate the sensitivity of the lateral dispersivity in the solution relative to the source description. A baseline run with no pumping well effects was run for a simulation period of 8 years with the contaminant source located as discussed previously. The lateral and longitudinal dispersivities were taken to be 20 and 60 ft respectively. Additional runs with the dispersivities doubled and halved; a comparison of the results is given in Fig. 22 in which the location of the 100 (corresponding approximately to mg/l of chloride) contour is plotted. It can be seen that the groundwater mounding at the source provides a relatively rapid initial spreading and dispersion effects downgradient are more or less as expected; higher coefficients give greater plume extent. A similar run with the simulated effect of pumping included as previously described and the original dispersivities is indicated in Fig. 23. The major conclusion to be drawn from Figs. 22 and 23 is that determination of α_T by comparison with the plume extent by means of a numerical simulation is not likely to be very adequate. The difficulty is that the source details apparently have a much larger influence on the plume extent than do the magnitude of the dispersivities

within a reasonable range of their variation. From this, it is recommended that the original value of 20 ft for the lateral dispersivity be accepted as a best estimate for the site in question until such time as better evidence may become available.

With the above considerations, the plume simulation was continued in time with the source detail outlined previously. Figures 24-26 give details of the plume profiles for times of approximately 10, 15 and 20 years respectively. Included for comparison sake is information of the actual plume detail estimated for 1968, 1973, and 1978-79 which are felt to be roughly corresponding points in the time history of the plume development. Results of these comparisons are quite reasonable although it is clear that an altered description of the source detail could probably resolve the plume location better in the vicinity of the chemical plant site. In particular, the removal of the source at $t = 10$ years is obviously in error as the simulated plume has moved nearly off site by the end of 20 years. A more nearly correct simulation would be to continue the source after 10 years with some reduced concentration level without influence of on site pumping included.

The most significant discrepancy between the numerical and measured plume profiles is the lack of agreement between the two on the location of the northeastern plume boundary.

It would be easy to advance the argument that so little observation well data is available in the vicinity of the plume boundary that the lack of agreement is due to insufficient field data. However, it is also realistic to expect that this discrepancy is real and due to the specified heads along the Little Bear Creek tributary in the numerical solution. The computed groundwater profile in this vicinity seems to agree very well with the 1979 water level data presented in Fig. 21 but it should be noted that the previous simulation by Keck (9) would have resulted in a plume deflected more to the south as it enters Little Bear Creek and Tributary, as indicated by Fig. 27 which was a run made in early 1981 without all the detailed information now available. Basically, Fig. 27 reproduces the Keck groundwater flow simulation with a source at the location indicated and no pumping well influence. The correct description of the groundwater flow in this vicinity may well lie in between the two simulations, but the present approach locates the plume boundary more adequately.

The effect of contaminant retardation was studied by comparison with the phenol data. A retardation factor of 3 was used in the simulation as previously estimated. The results of simulations are presented for 10, 15 and 20 year periods in Fig. 28-30. For comparison, phenol data from 1975-79 are included in Figs. 29 and 30. Since the contaminant has not moved as rapidly in this case due to

adsorption, details of the source become much more critical. Given the lack of detail presently incorporated in the numerical simulation, a surprisingly good agreement is obtained. The important conclusion is that a retardation factor of 3 seems to be realistic for this particular compound in the given aquifer system. A detailed investigation for the other parameters (benzene, toluene, and aromatic amines) was not conducted due to lack of detailed data, but it is relatively clear that their retardation factors should be corresponding smaller. This can be incorporated into a later phase of the present investigation if desired.

The phenol simulation was extended in time beyond the present to estimate the flushing from the aquifer system under natural conditions. Note that the contamination was turned off in this simulation at an approximate date of 1968 when it actually is known to continue up through the middle 1970's to some extent. The 1 mg/l (approximately estimated by comparison of maximum phenol concentrations observed in Fig. 7-9 with computed values) contour is shown to develop in time in Fig. 31. The obvious implication of the 15 year maximum flushing time estimated (9) for this site has very little to do with the persistence of chemical constituents in the present aquifer as the retarded pollutant plume is barely "reaching" the Little Bear Creek tributary after this time. An estimated natural flushing time for

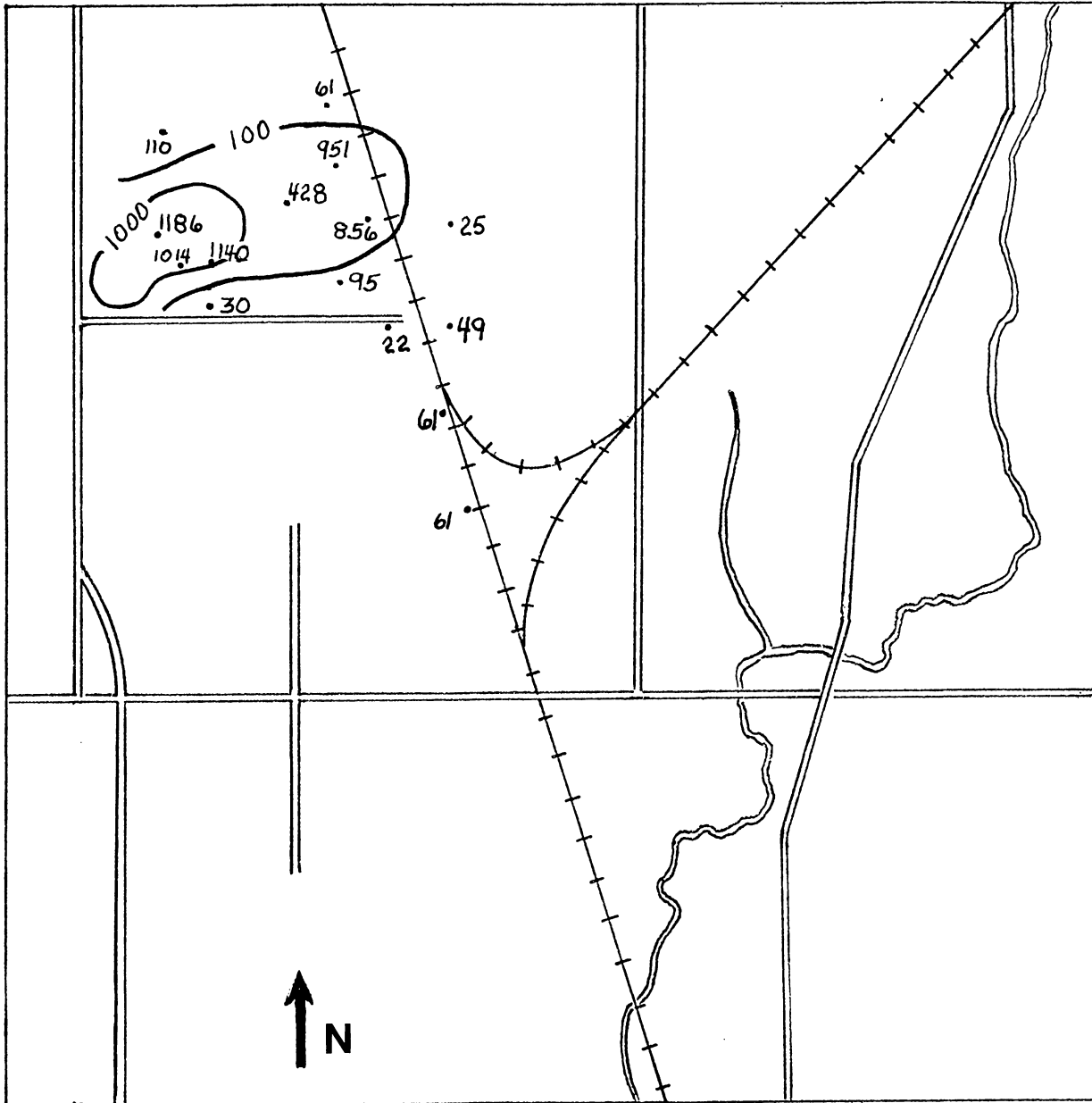
phenolics would be more on the order of 50 years, provided that reasonable estimates regarding the pollutant behavior has been made in this study. It must also be considered likely that other chemical constituents have been more strongly adsorbed than the ones investigated. There are some rather significant consequences with respect to management options on site cleanup inherent in these results.

CONCLUSIONS

The numerical model and simulations described herein were not intended to develop detailed description of the plume behavior, but comparisons of actual data appear to yield surprisingly good agreement with the numerical results. Therefore, with some minor modifications of the source description, it is felt that this model could be used to evaluate management options presently under consideration at the site. The results of this study have produced the following conclusions:

1. A realistic estimate of the lateral dispersivity is 20 ft for the sand aquifer in question. Available data seems to be in strong support of this value.
2. No information could be generated to estimate the longitudinal dispersivity directly, but the comparison of the phenol data with the corresponding numerical simulation lends support for the value of 60 ft adopted.
3. A retardation factor of approximately 3 appears to be appropriate for the adsorption of phenols in this aquifer.

4. Retardation factors lower than that for phenols would be required to describe the apparent movement of benzene, toluene, aromatic amines, and ammonium through the aquifer. The latter two appear to be subject to negligible adsorption in the contamination plume. Benzene appeared to be more strongly absorbed than toluene but an insufficient data base prohibits determinations of retardation factors with any degree of confidence.
5. Adjustments to the previous numerical simulation of groundwater flow at the site appear to be necessary to yield satisfactory agreement between the observed and computed plume detail.
6. Long natural "flushing" times for the aquifer in excess of 100 years may be expected for some of the organic chemicals present.



Scale 1" = 1200 ft

Figure 1. 1965 Chloride Concentrations in Deep Observation Wells. (concentrations in mg/l) from Keck (4).

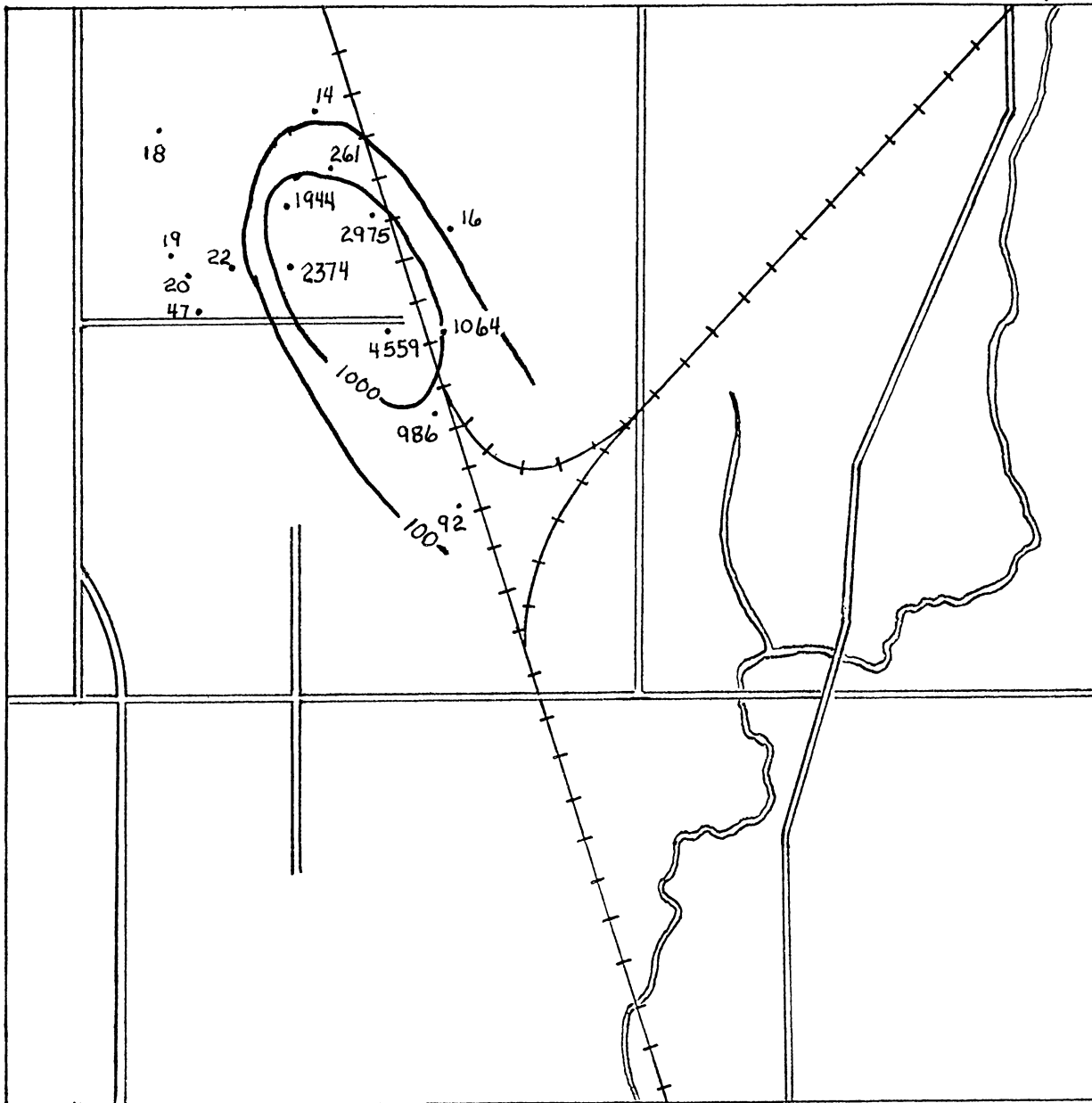


Figure 2. 1968 Chloride Concentrations in Deep Observation Wells. (concentrations in mg/l) from Keck (4).

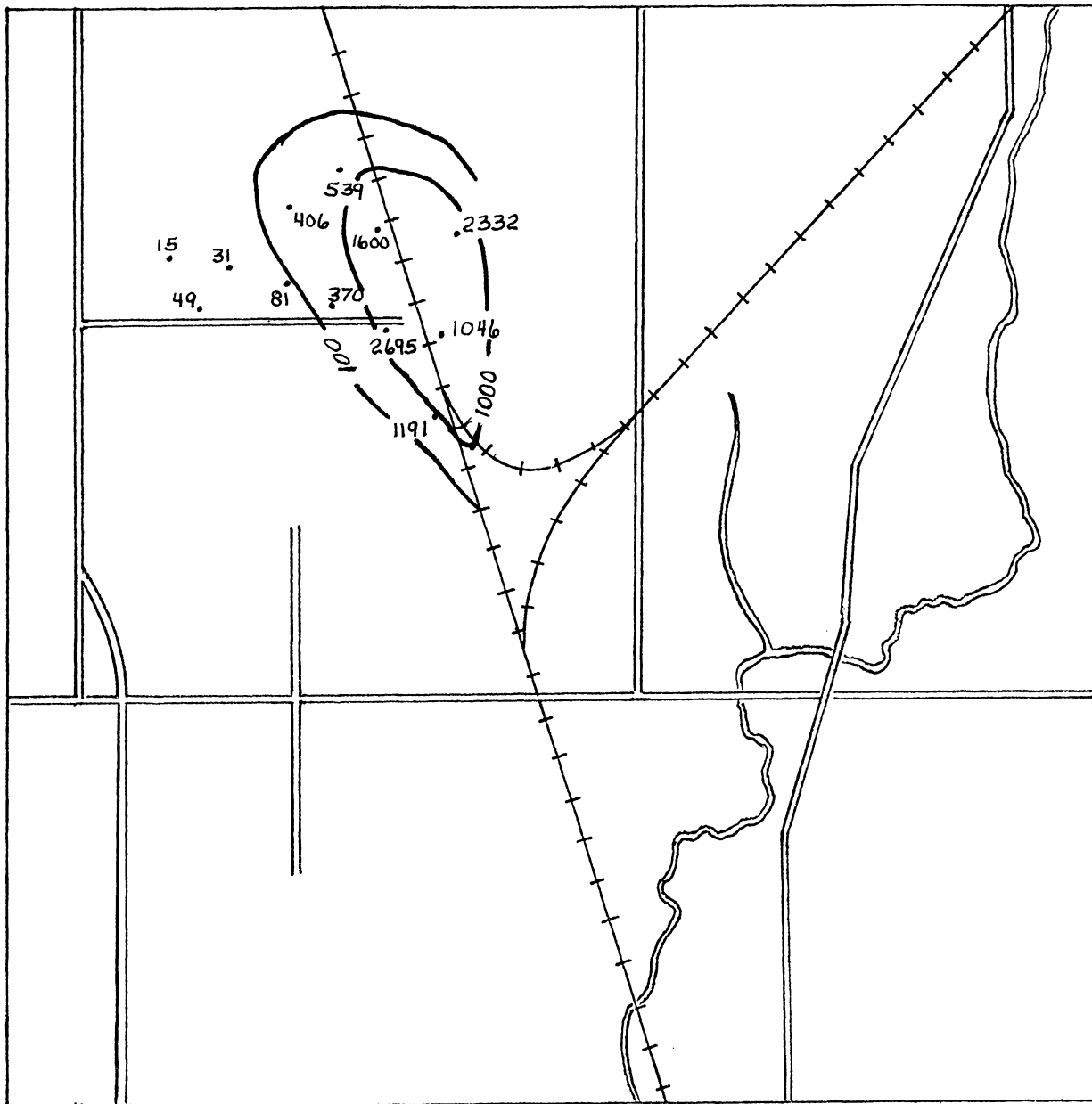


Figure 3. 1971 Chloride Concentrations in Deep Observation Wells. (concentrations in mg/l) from Williams and Works (2).

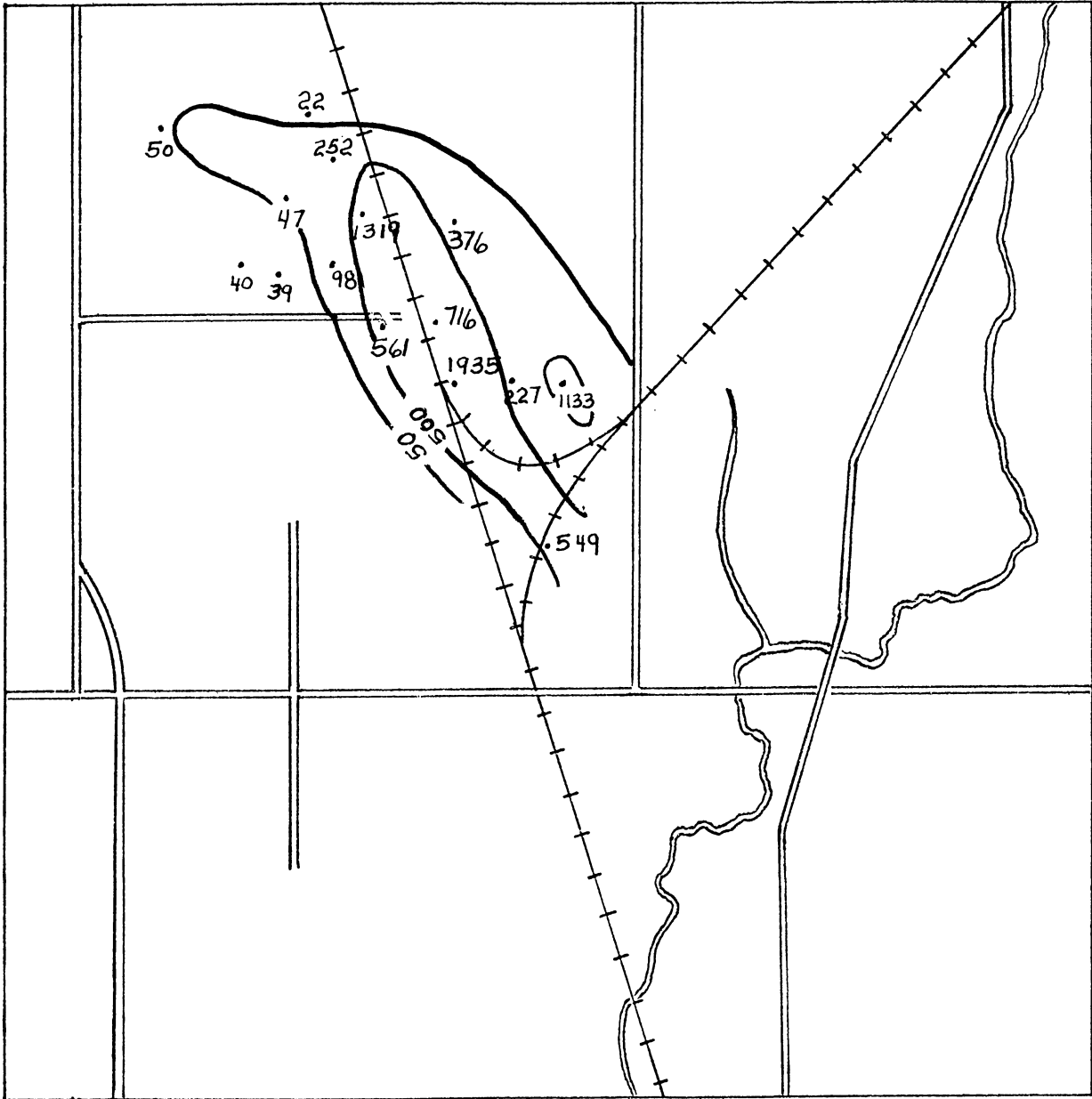


Figure 4. 1974 Chloride Concentrations in Deep Observation Wells. (concentrations in mg/l) from Keck (4).

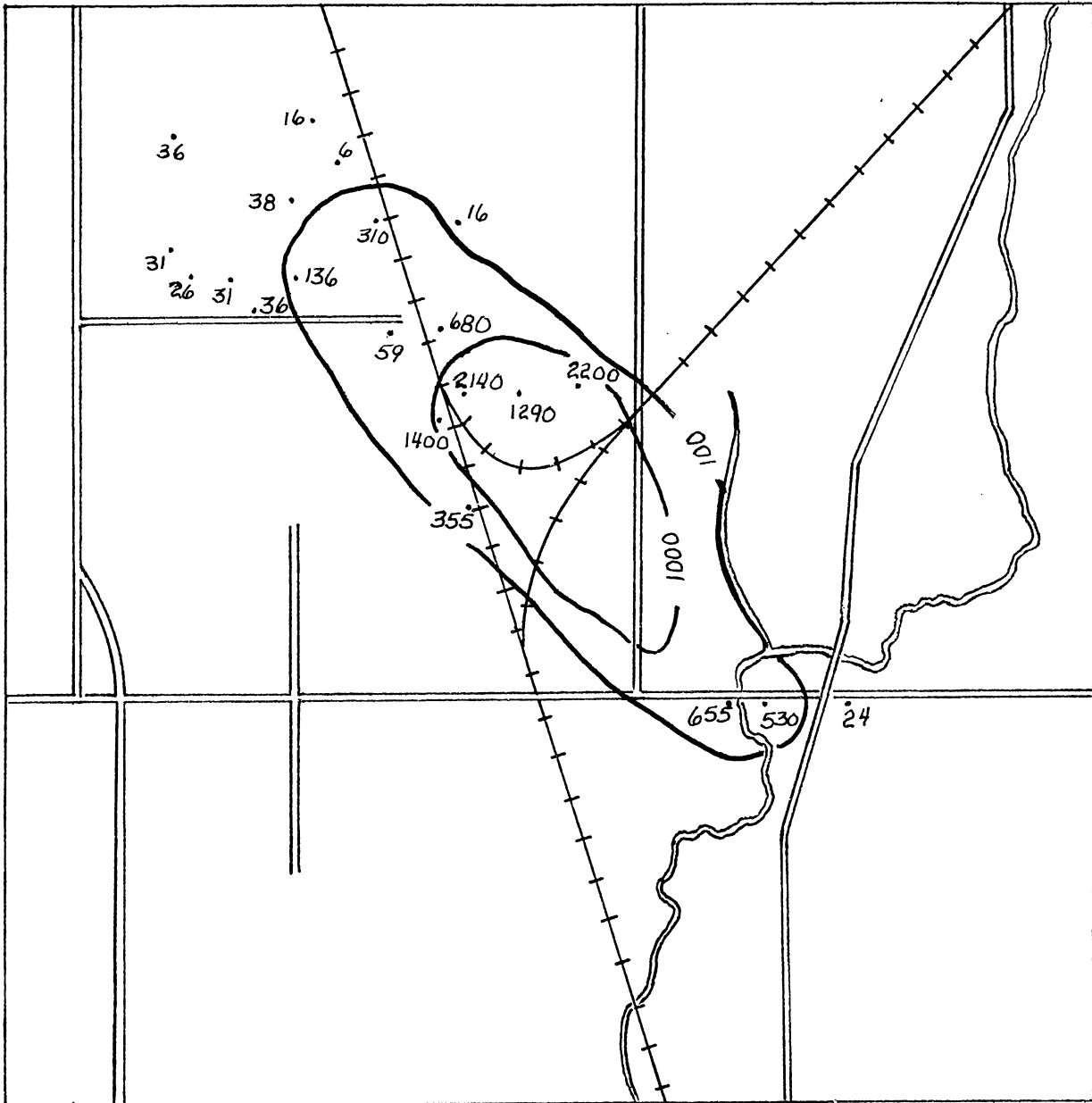


Figure 5. 1977 Chloride Concentrations in Deep Observation Wells. (concentrations in mg/l) from Keck (4).

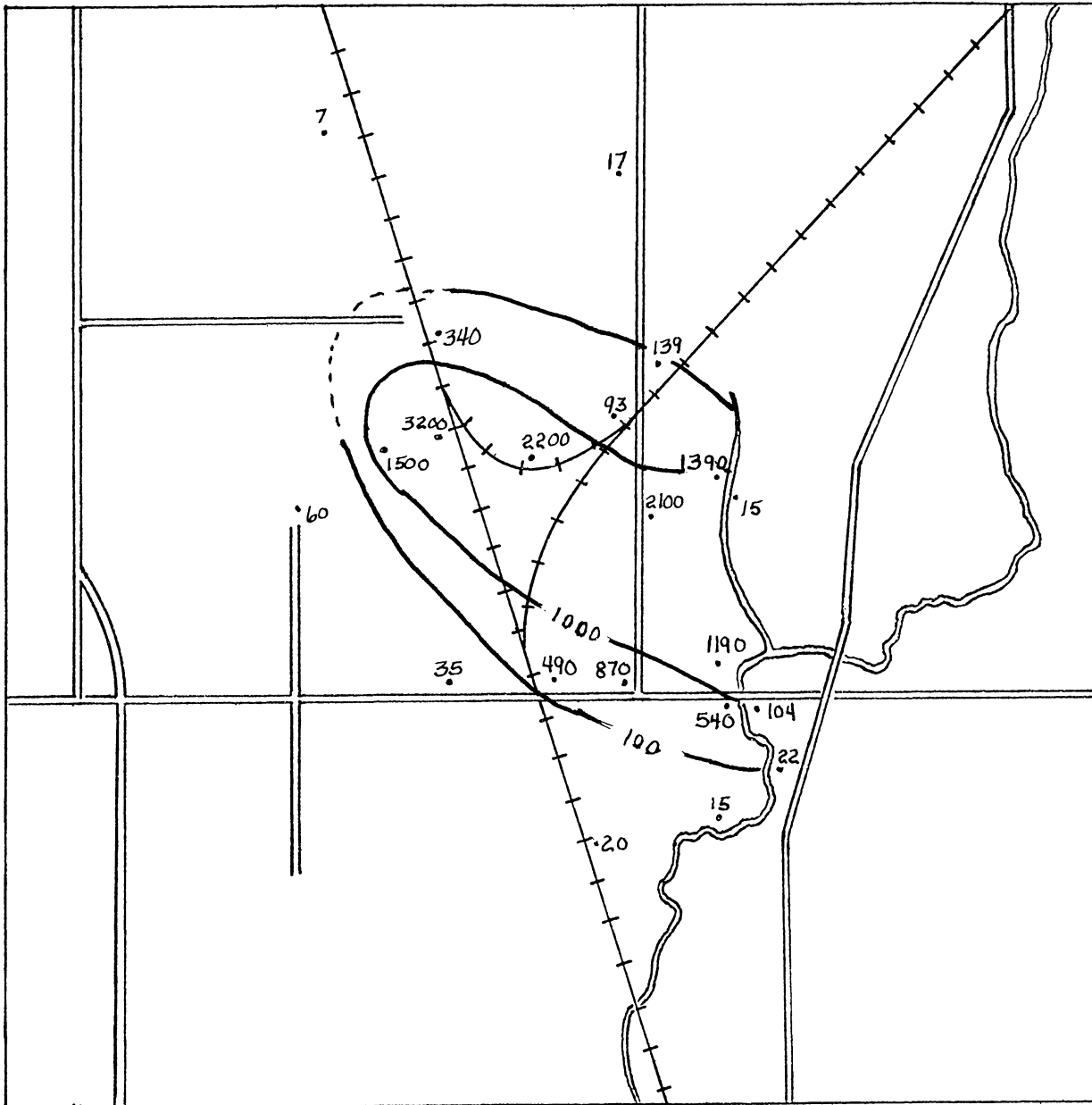


Figure 6. 1978-79 Chloride Concentrations in Deep Observation Wells. (concentrations in mg/l) from DNR (6,7).

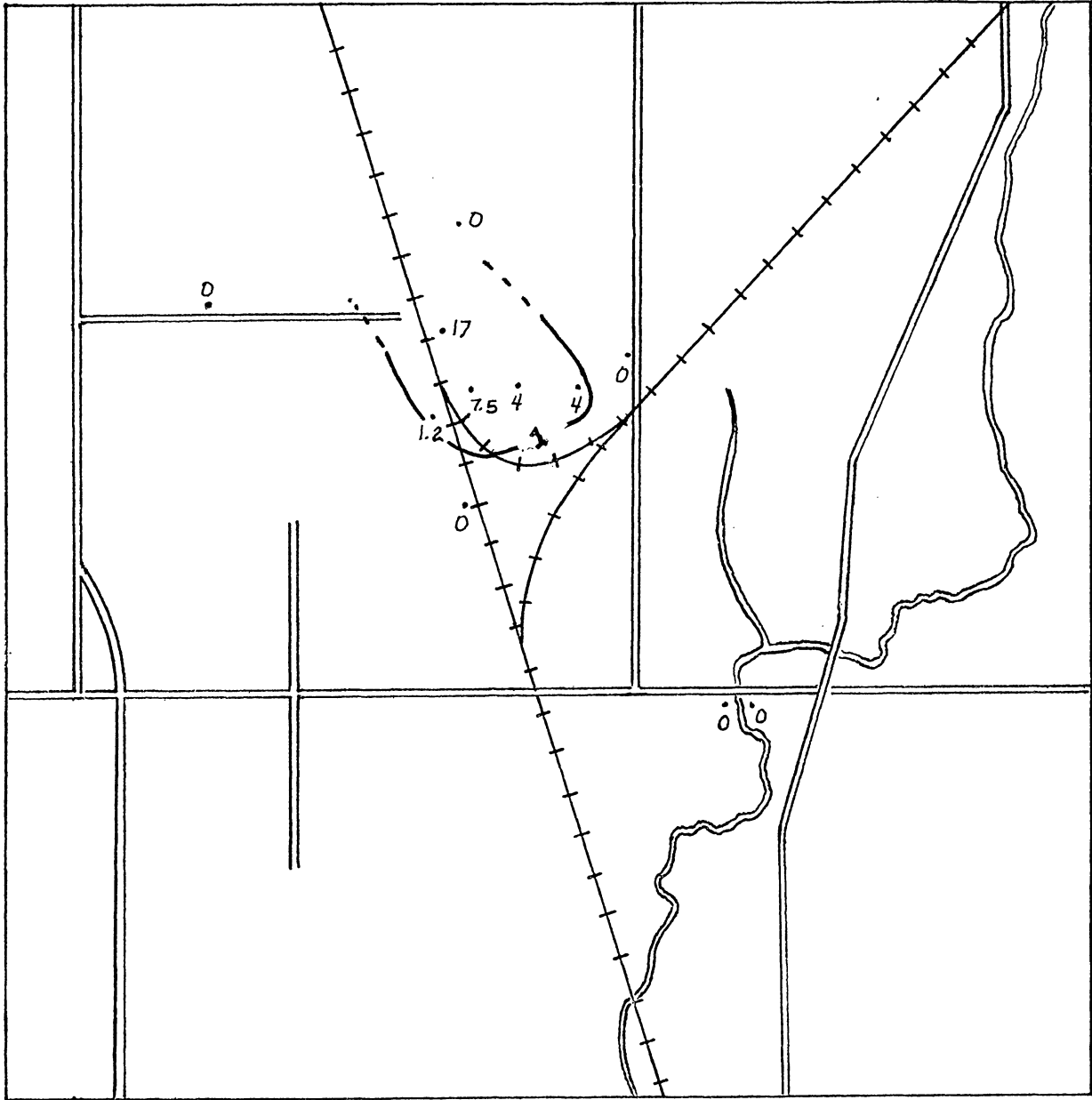


Figure 7. 1975 Phenol Concentrations (mg/l) in Deep Observation Wells (from Williams and Works (2)).

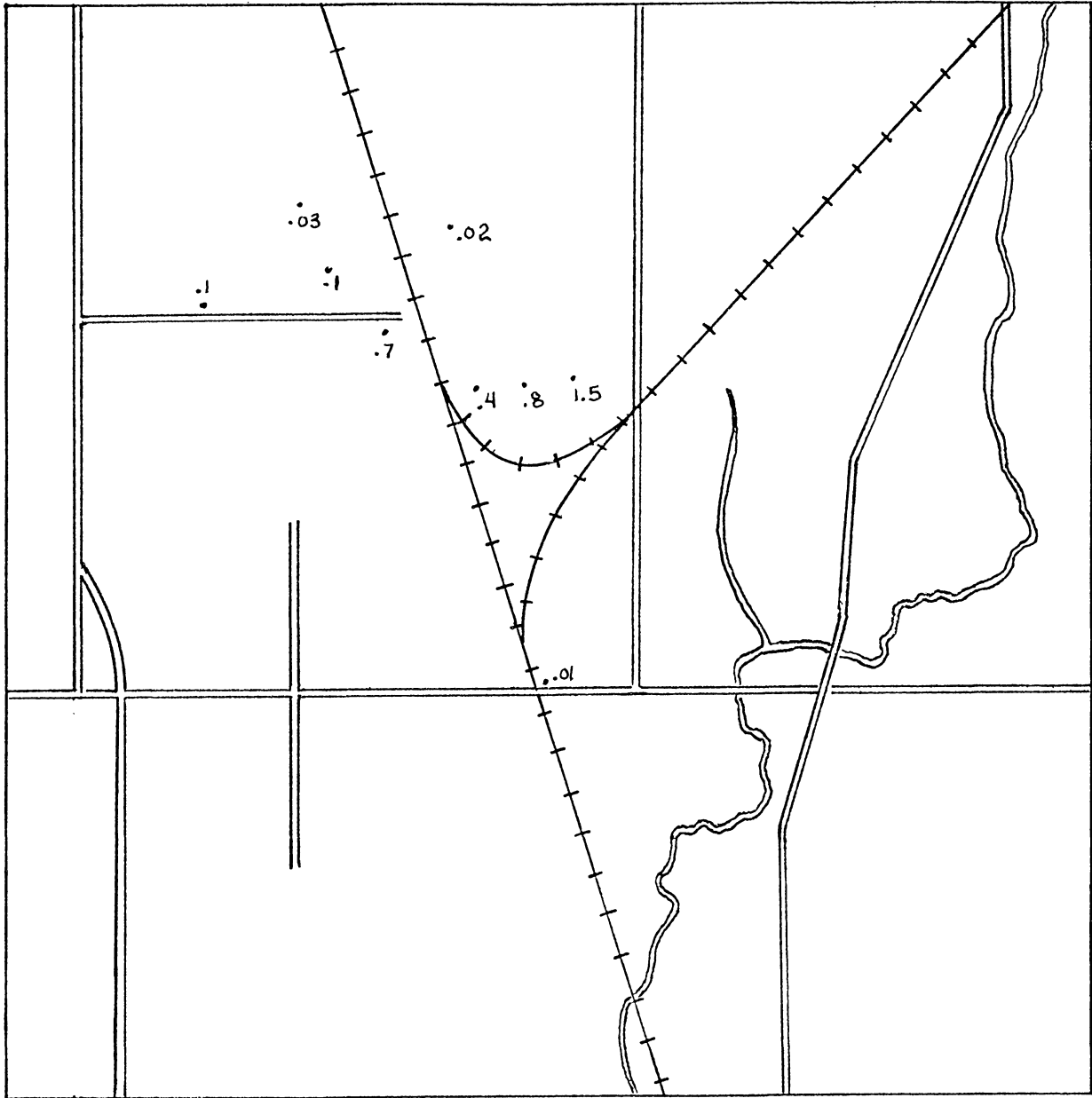


Figure 8. 1977 Phenol Concentrations (mg/l) in Deep Observation Wells (from Muskegon County Health Department (5)).

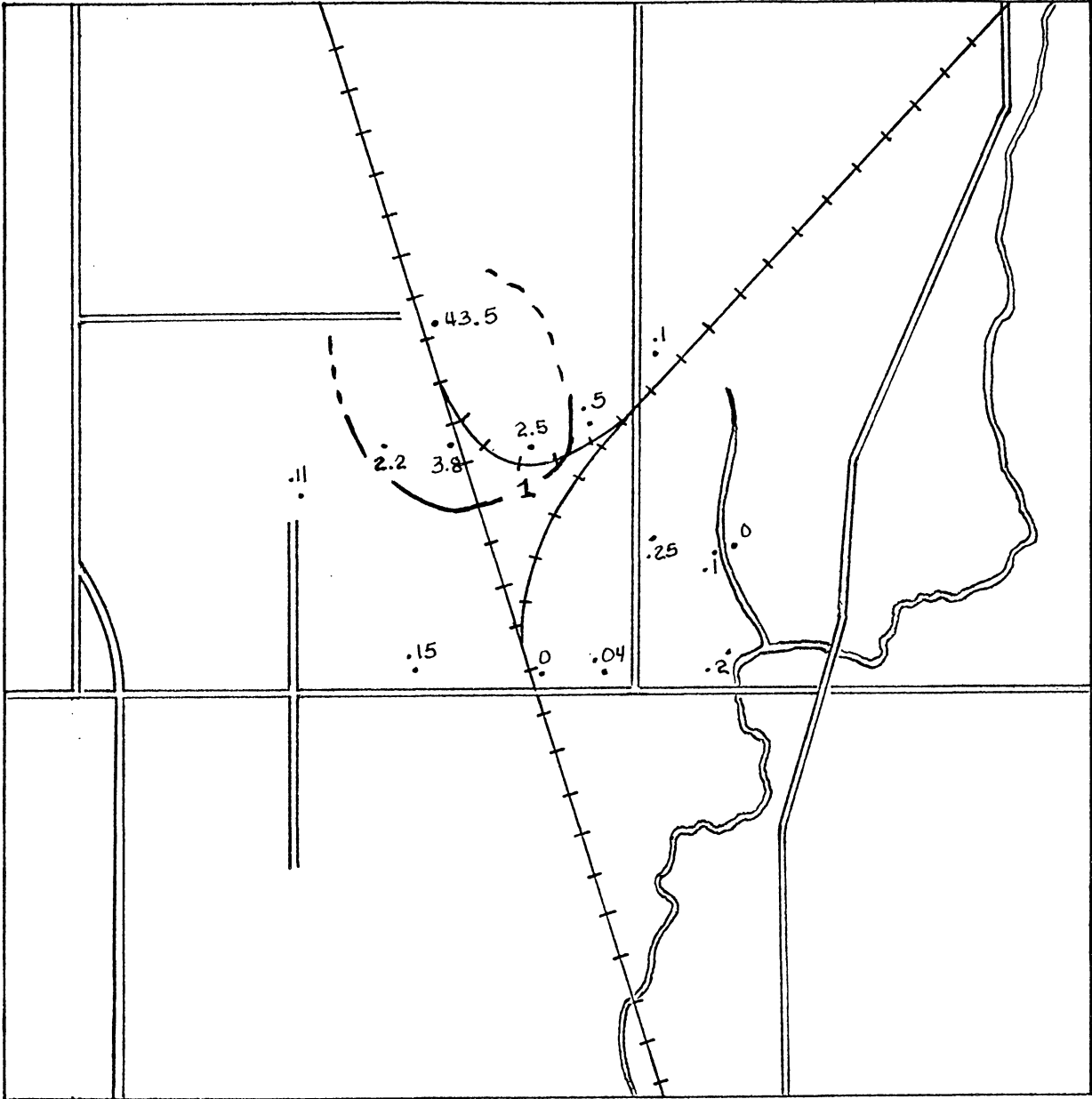


Figure 9. 1978-79 Phenol Concentrations (mg/l) in Deep Observation Wells (from DNR (6,7)).

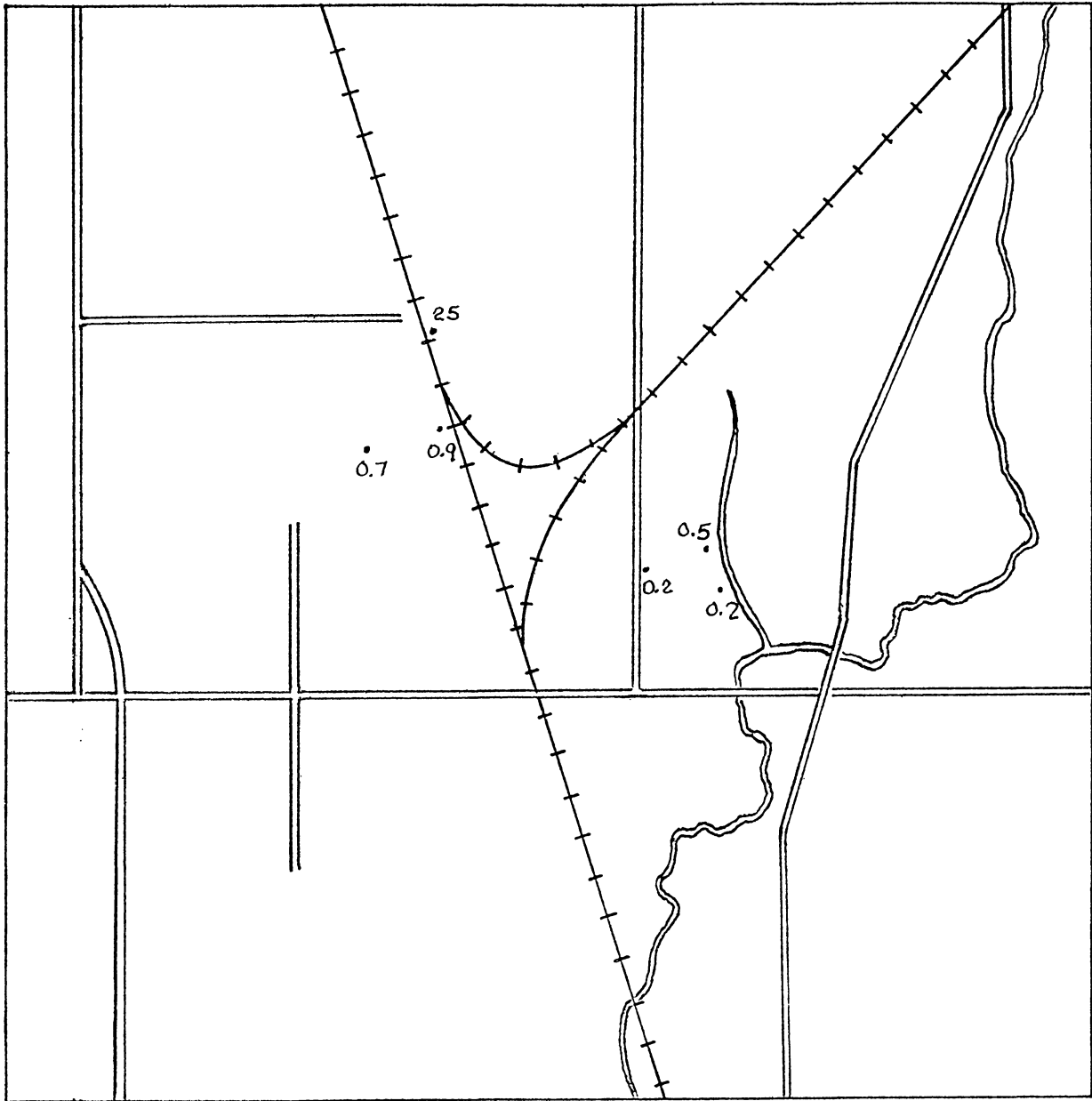


Figure 10. 1978-79 Benzene Concentrations (mg/l) in Deep Observation Wells from DNP (6,7).

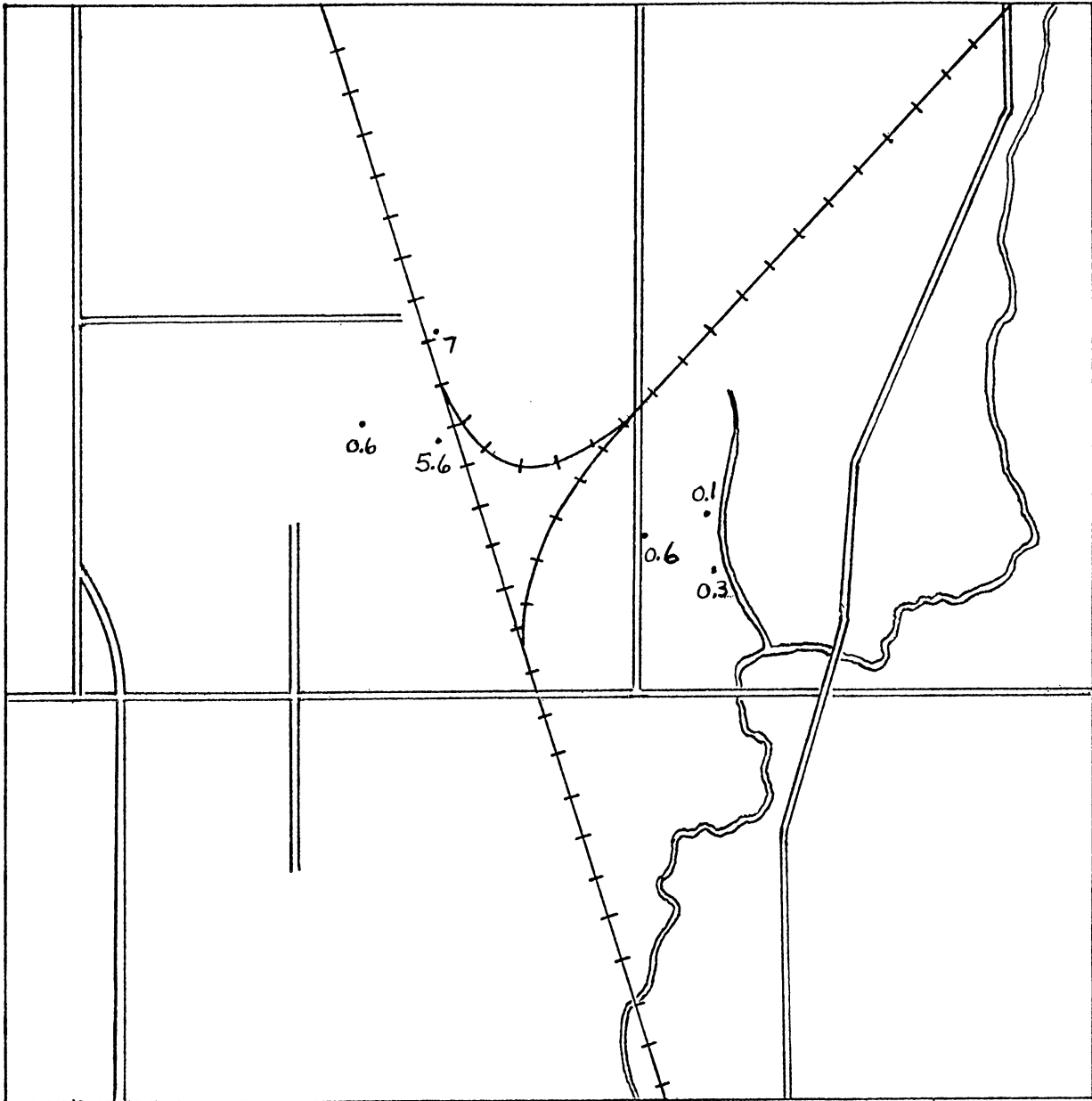


Figure 11. 1978-79 Toluene Concentrations (mg/l) in Deep Observation Wells From DNR (6,7).

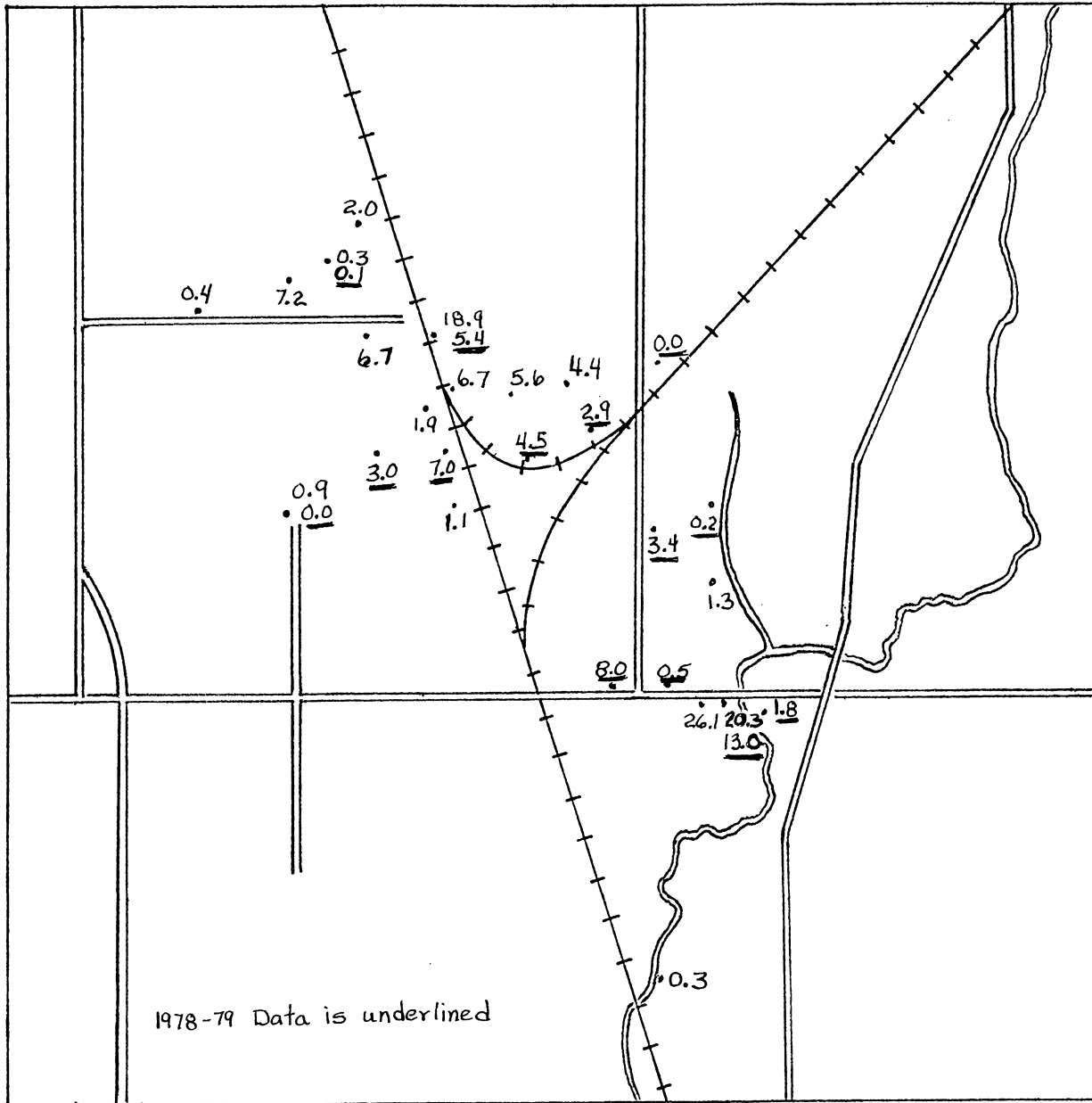


Figure 12. 1977-79 Aromatic Amines Concentrations (mg/l) in Deep Observation Wells from DNR (6,7).

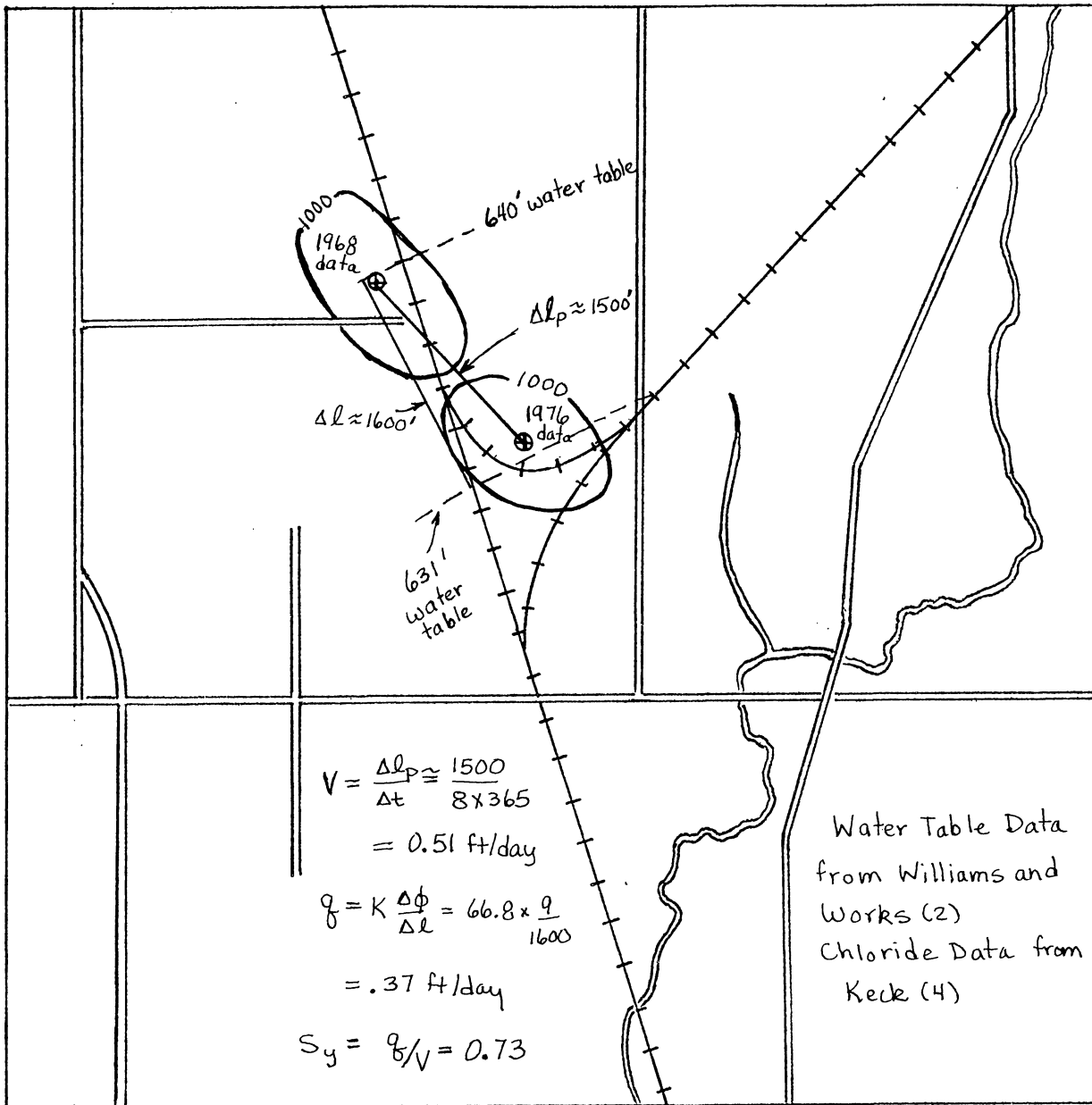


Figure 13. Example Calculation of Specific Yield.

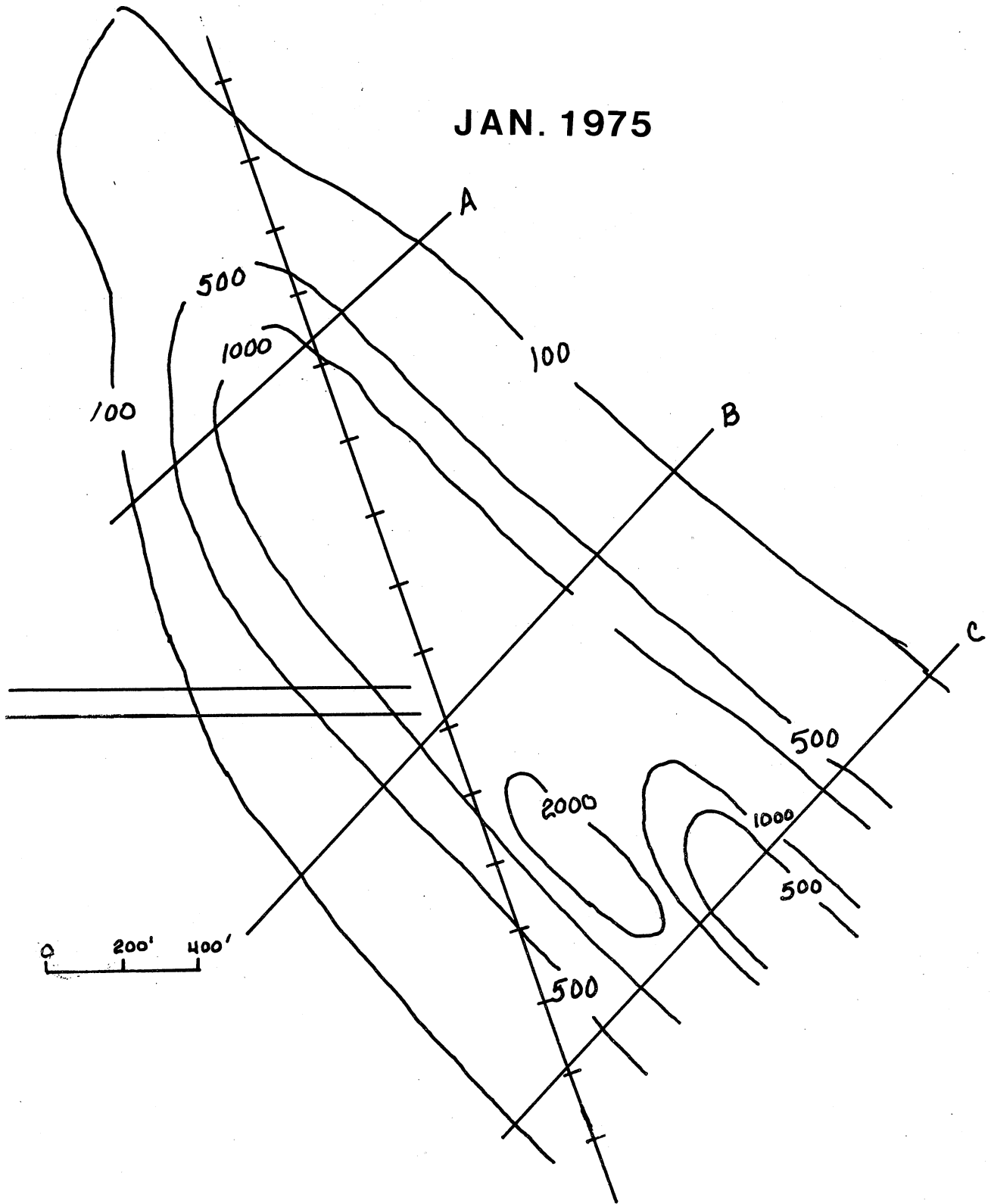


Figure 14. Chloride Plume Detail for Computation of Lateral Dispersivity (from Williams and Works (2)).

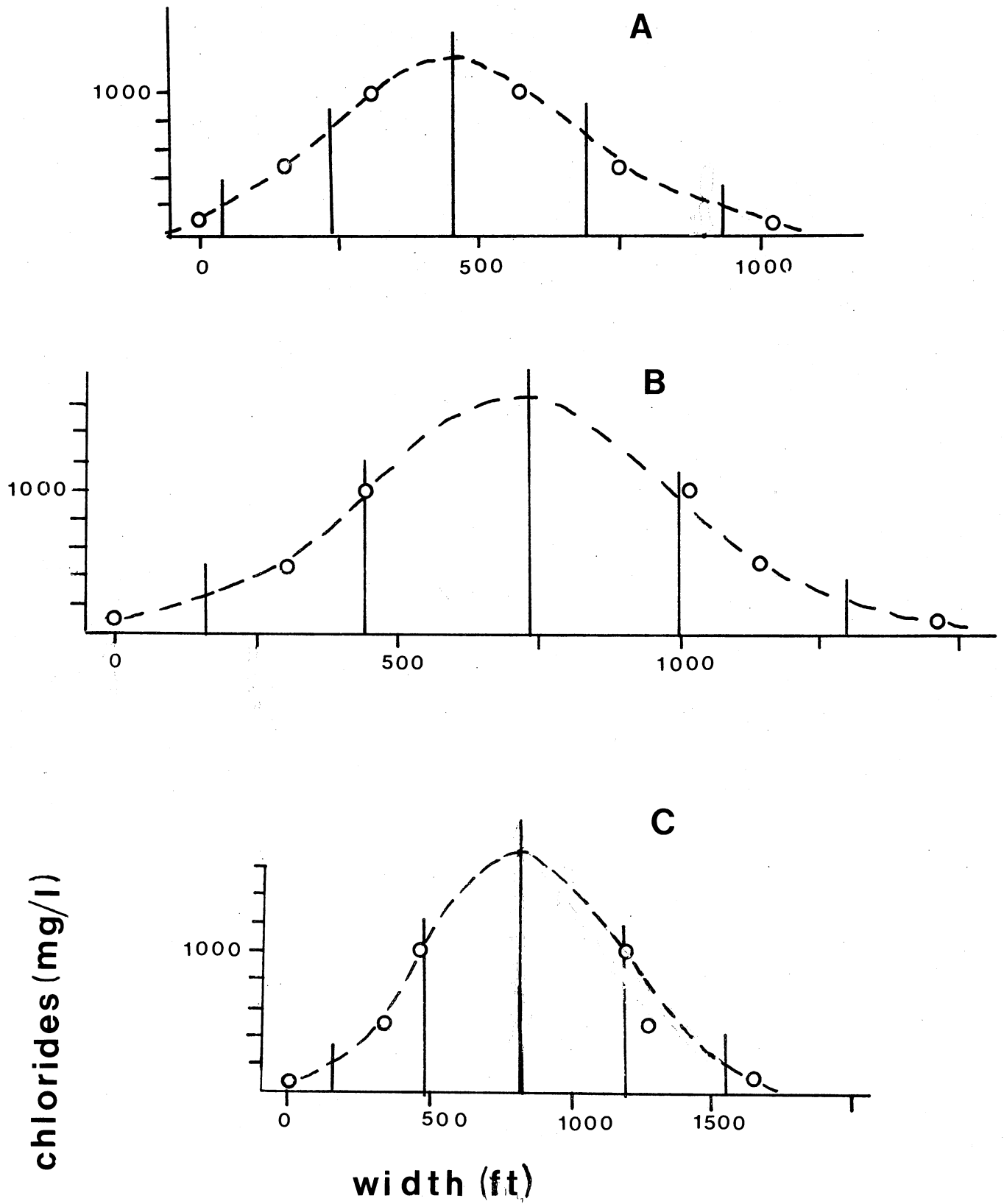


Figure 15. Cross-Sectional Concentration Profiles, Jan. 1975 (from Williams and Works (2)).

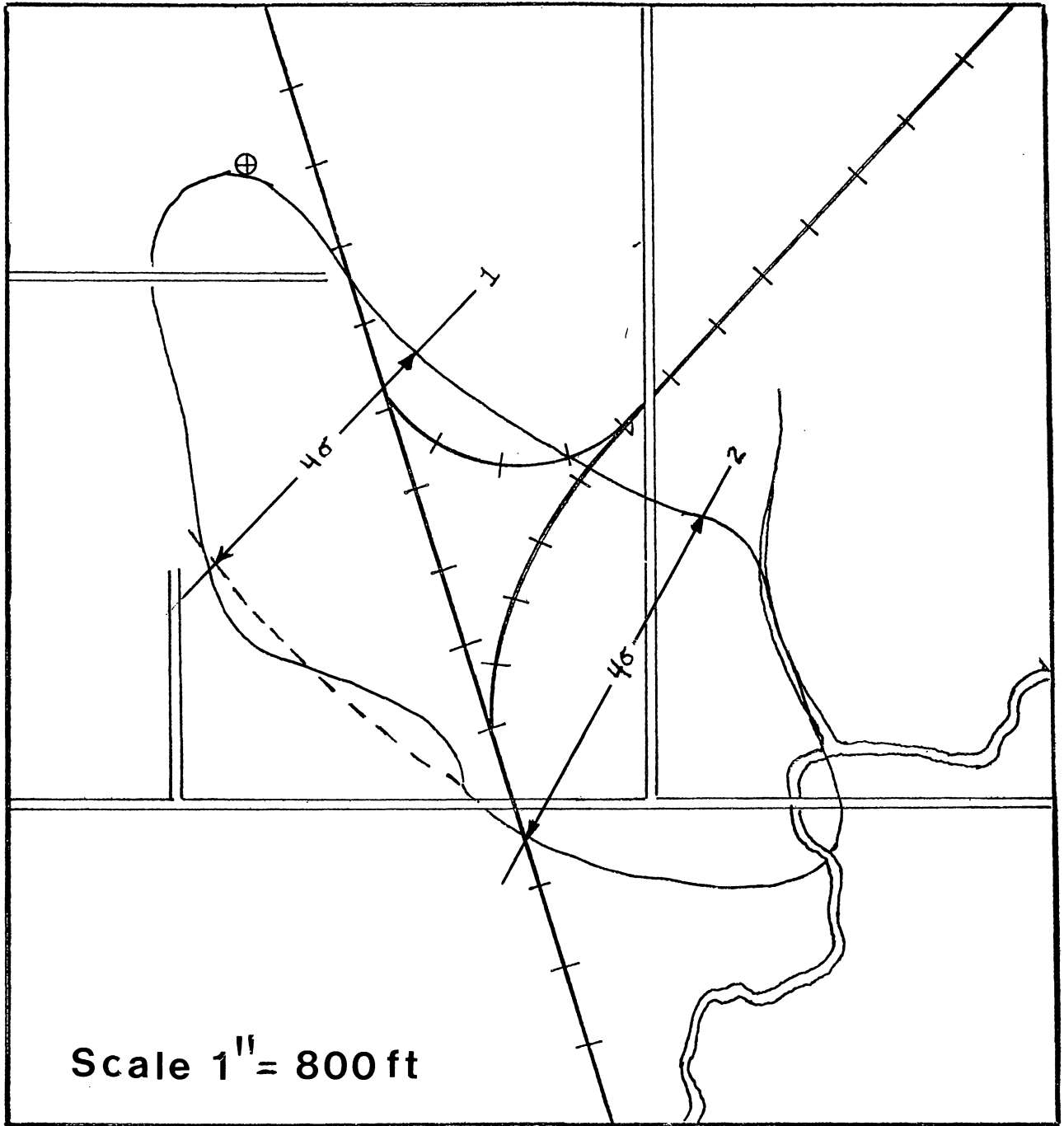


Figure 16. 1979 Plume Extent Estimated by Keck (9) used for Computation of Lateral Dispersion.

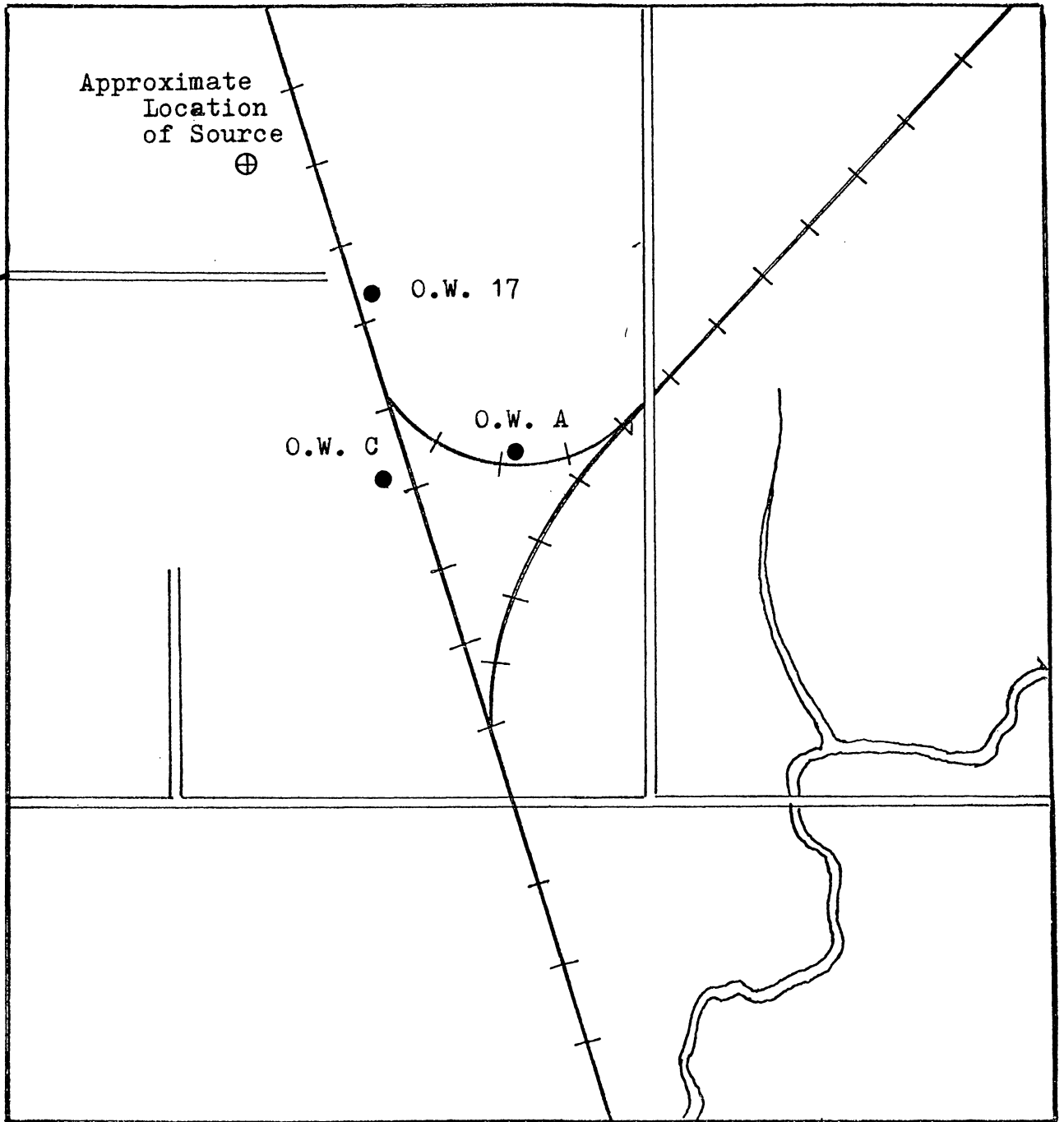


Figure 17. Source and Observation Well Locations.

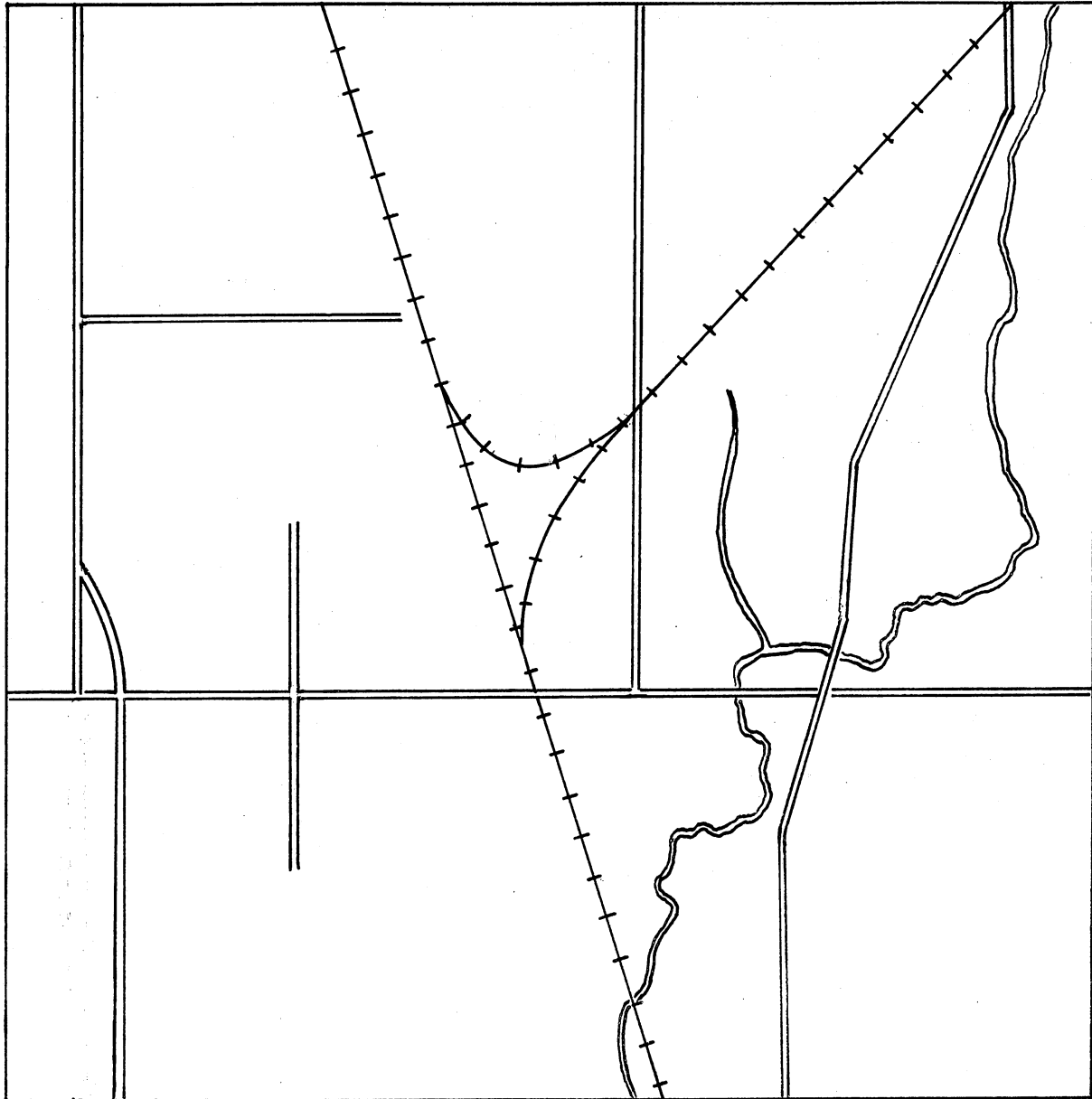
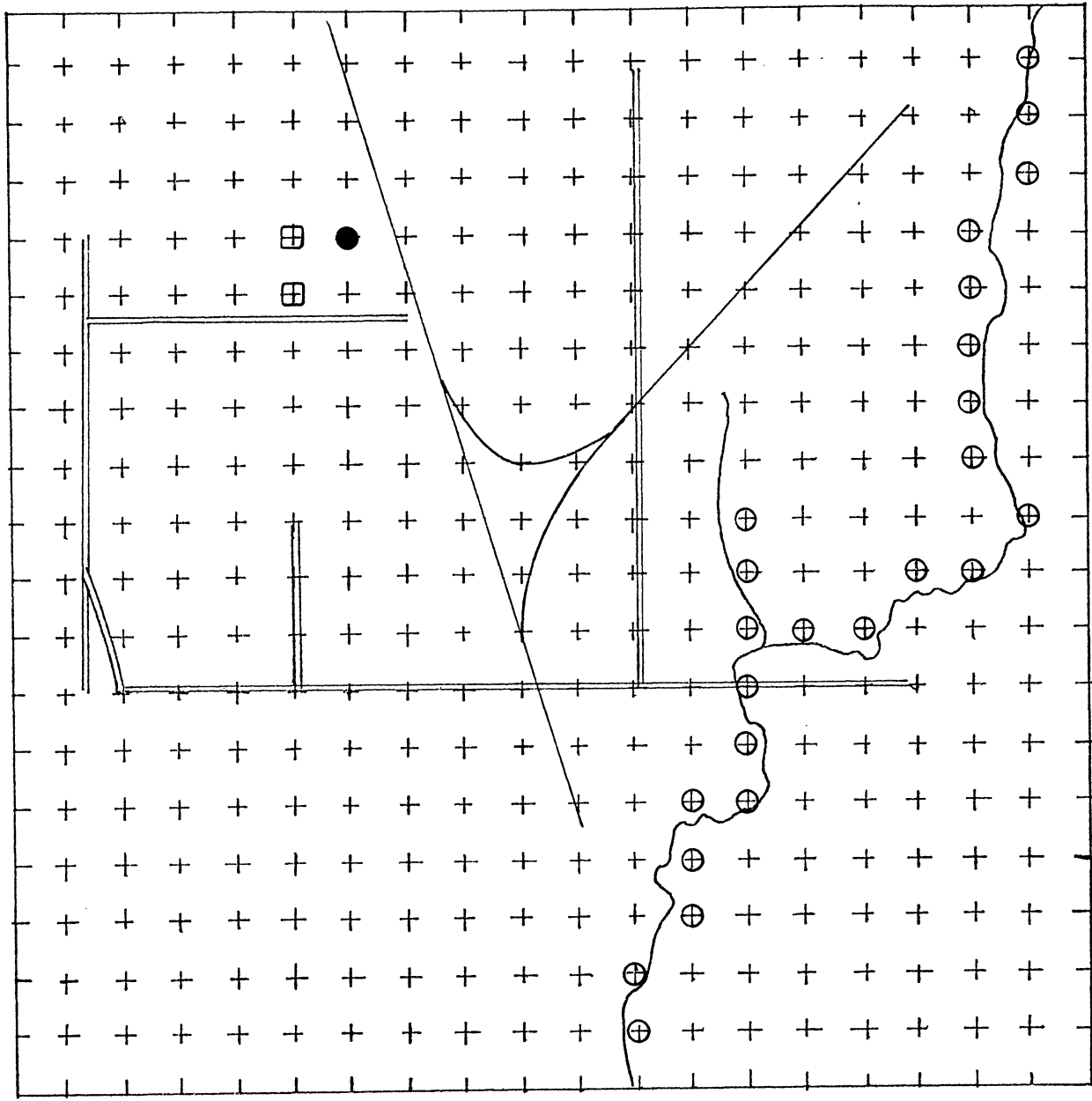


Figure 18. Area Covered by Numerical Model.



- ⊕ Pumping Nodes with Specified Heads
- ⊕ Creek Nodes with Specified Heads
- Contaminant Source Node

Figure 19. Grid Detail for Numerical Model.

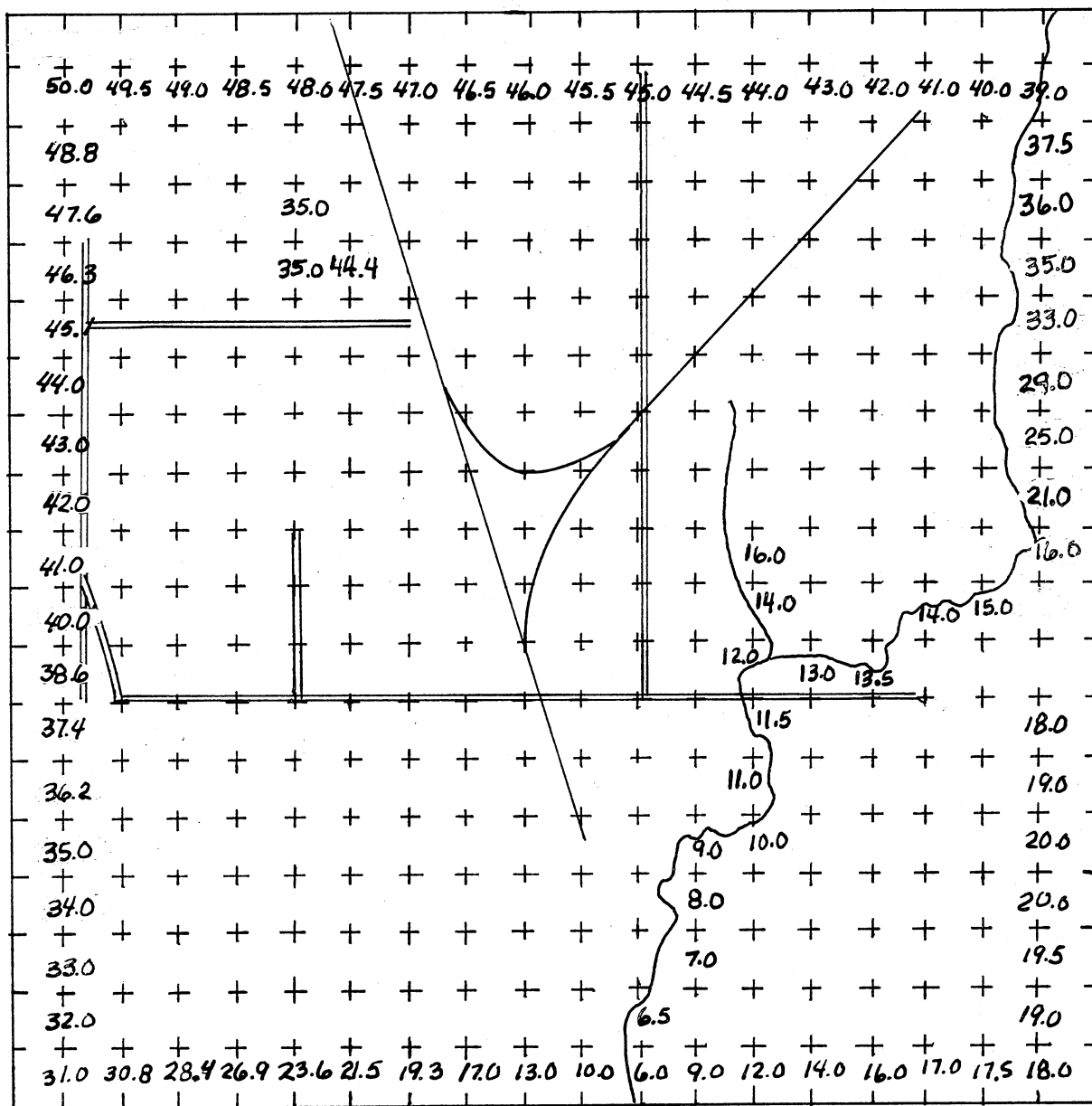


Figure 20. Specified Heads used in Final Numerical Simulation.

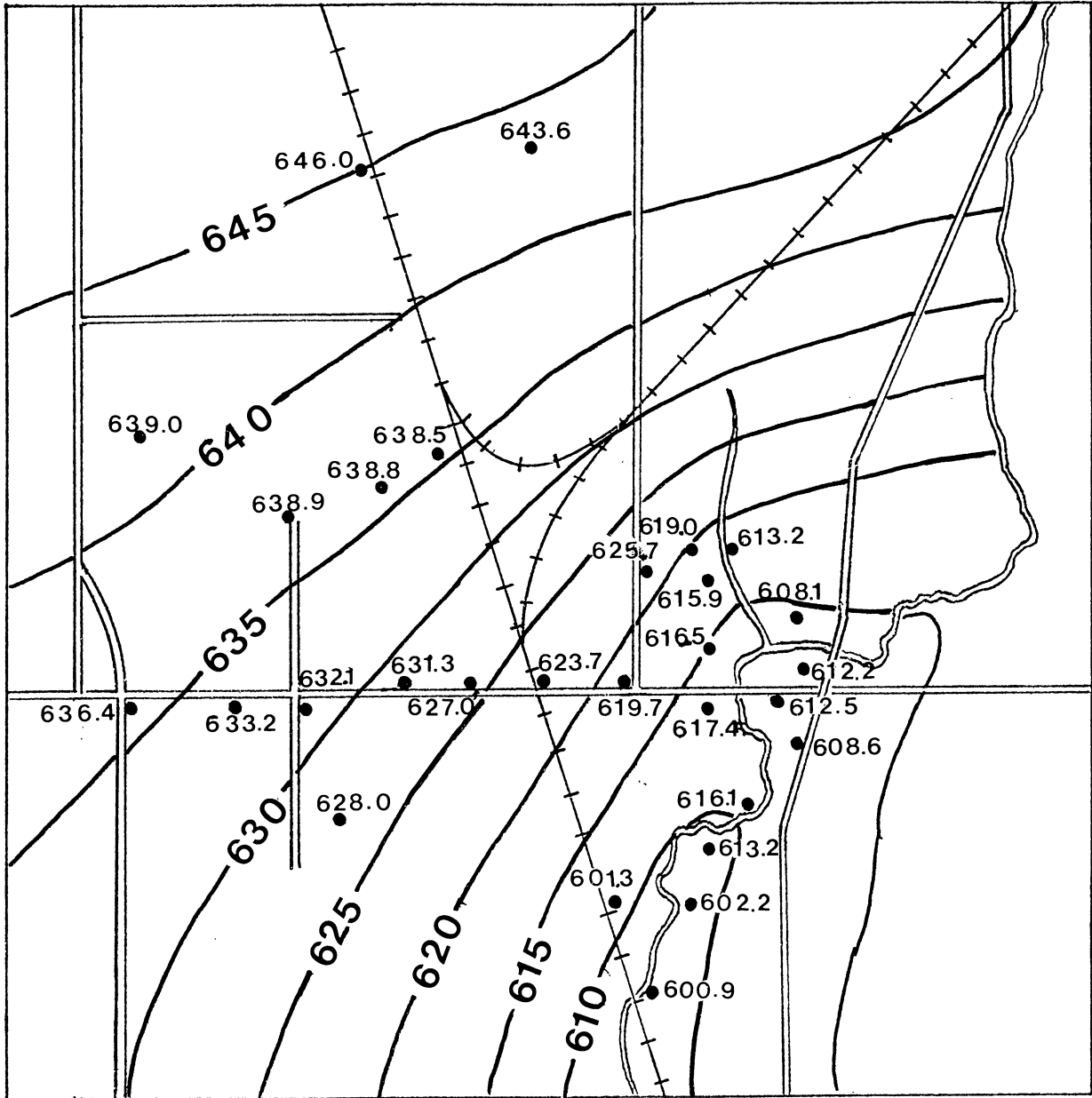


Figure 21. Final Water Table Simulation and Comparison of Water Table Data from Keck (8).

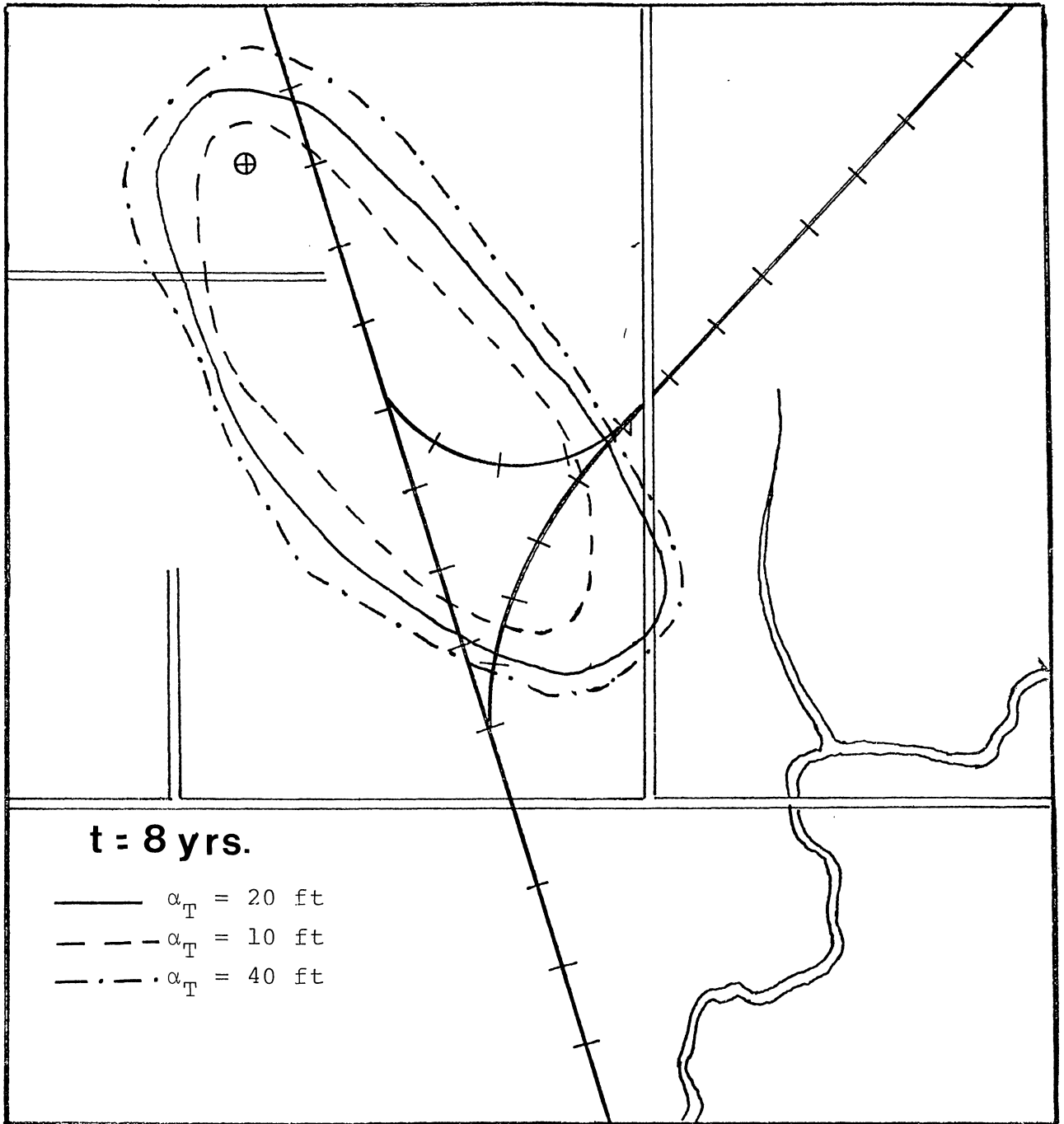


Figure 22. Sensitivity of Plume Extent to Variations in α_T .

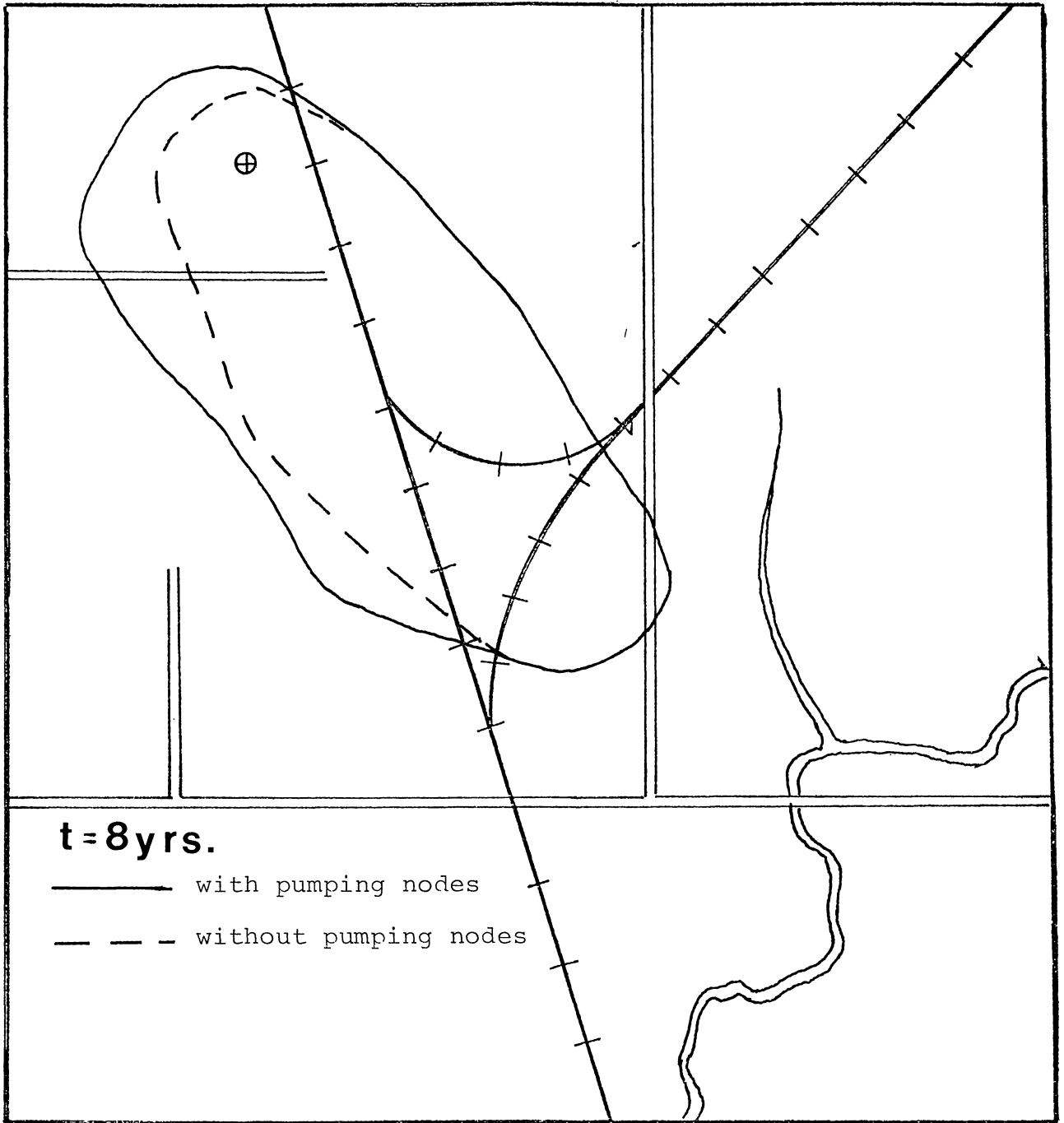


Figure 23. Comparison of Effect of Pumping Nodes on Chloride Plume Extent.

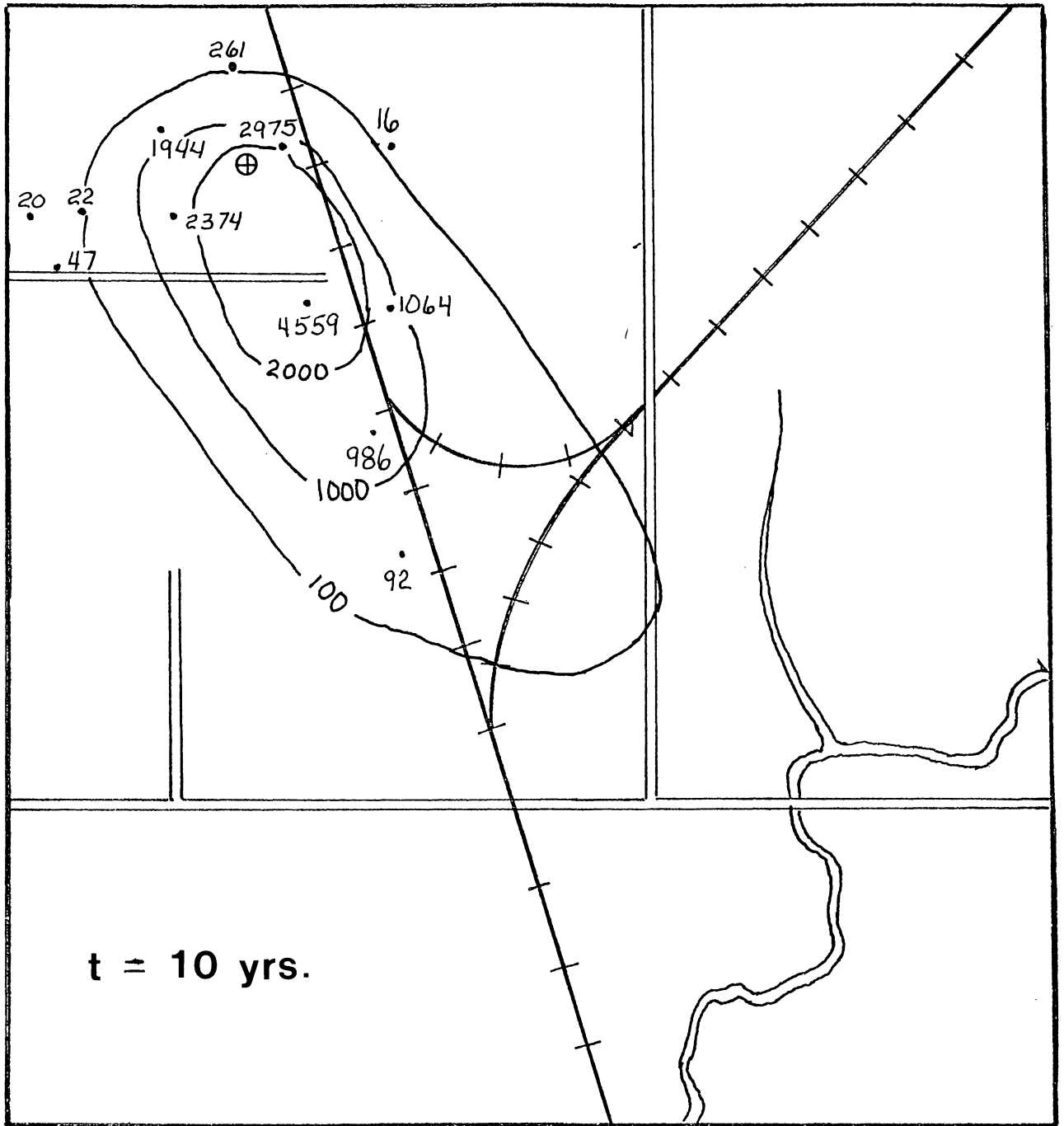


Figure 24. Comparison of 10 Year Numerical Simulation with 1968 Chloride Data (concentration mg/l).

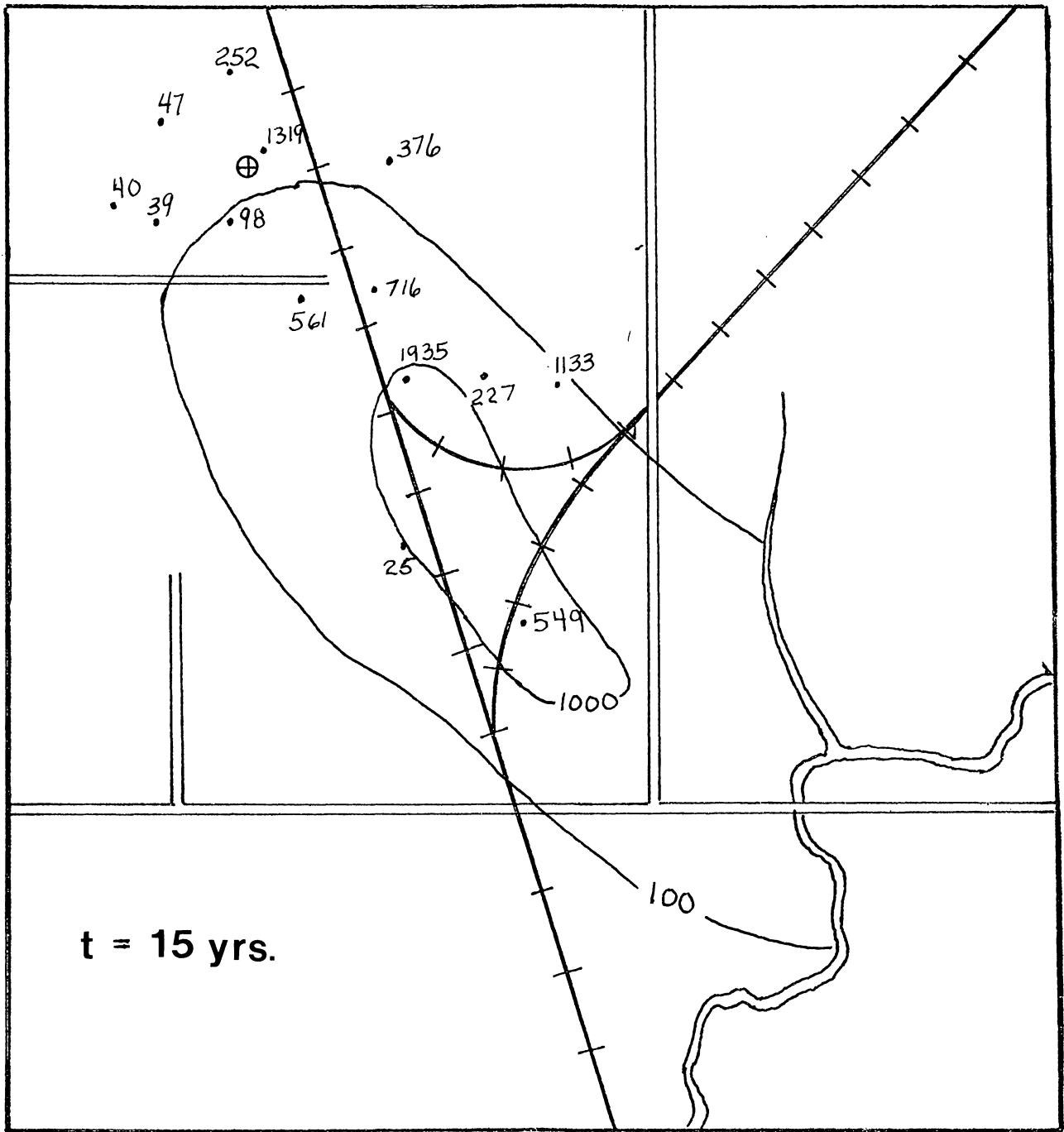


Figure 25. Comparison of 15 Year Numerical Simulation with 1974 Chloride Data (concentration in mg/l).

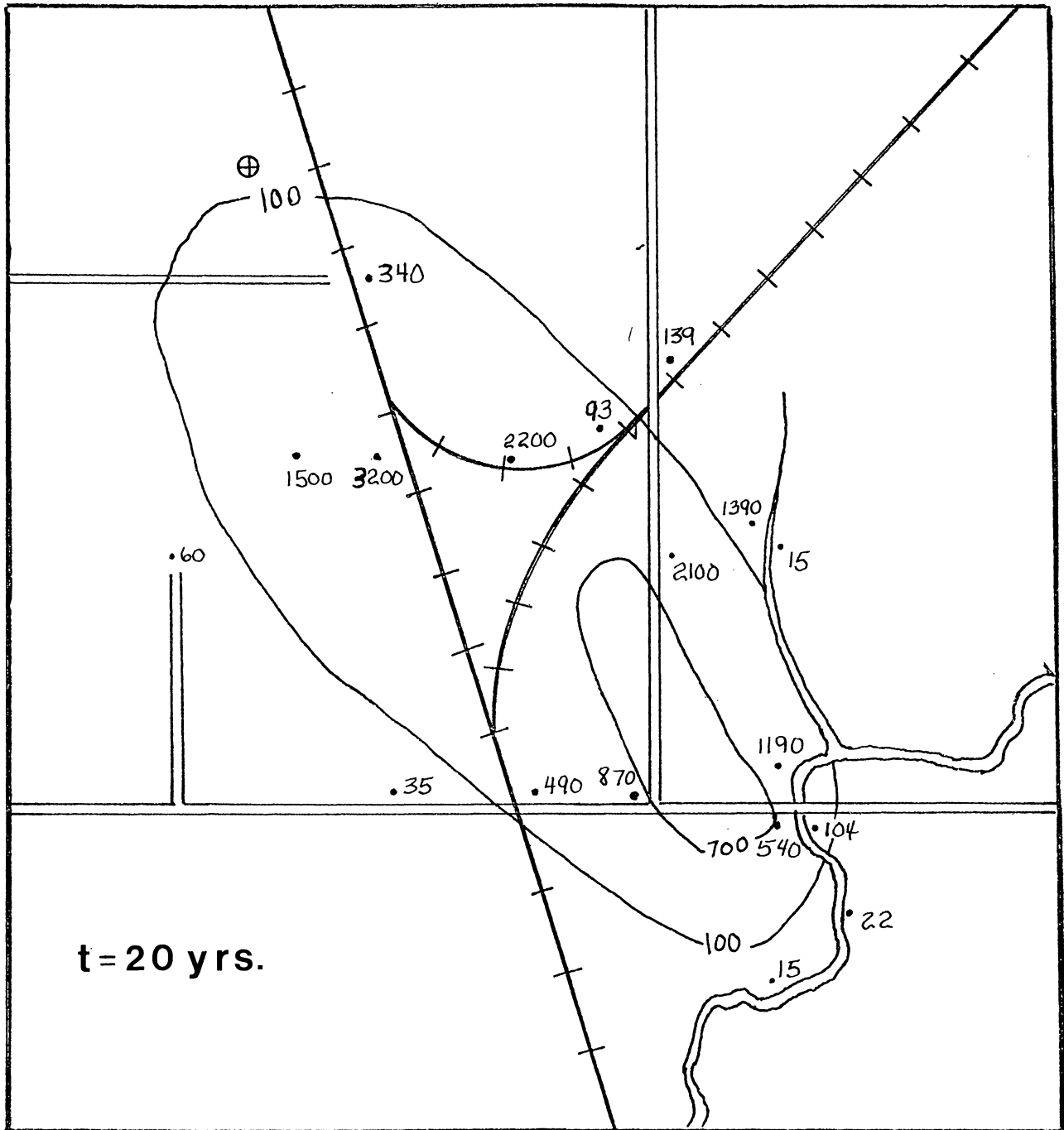


Figure 26. Comparison of 20 Year Numerical Simulation with 1978-79 Chloride Data (concentration in mg/l).

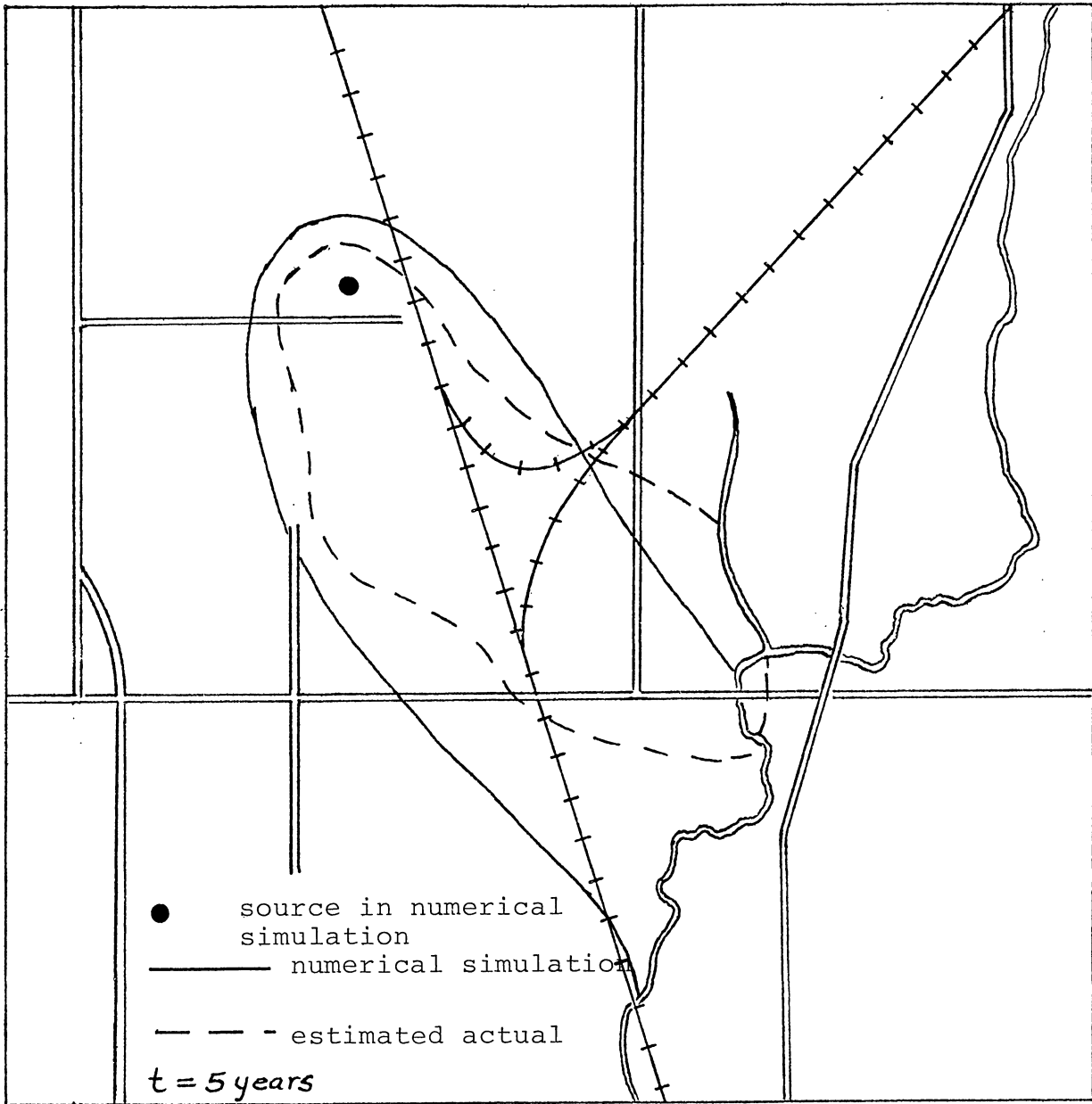


Figure 27. Comparison of Simulated Plume Extent with Aquifer Parameters Estimated by Keck (8) and Chloride Plume in 1978-79.

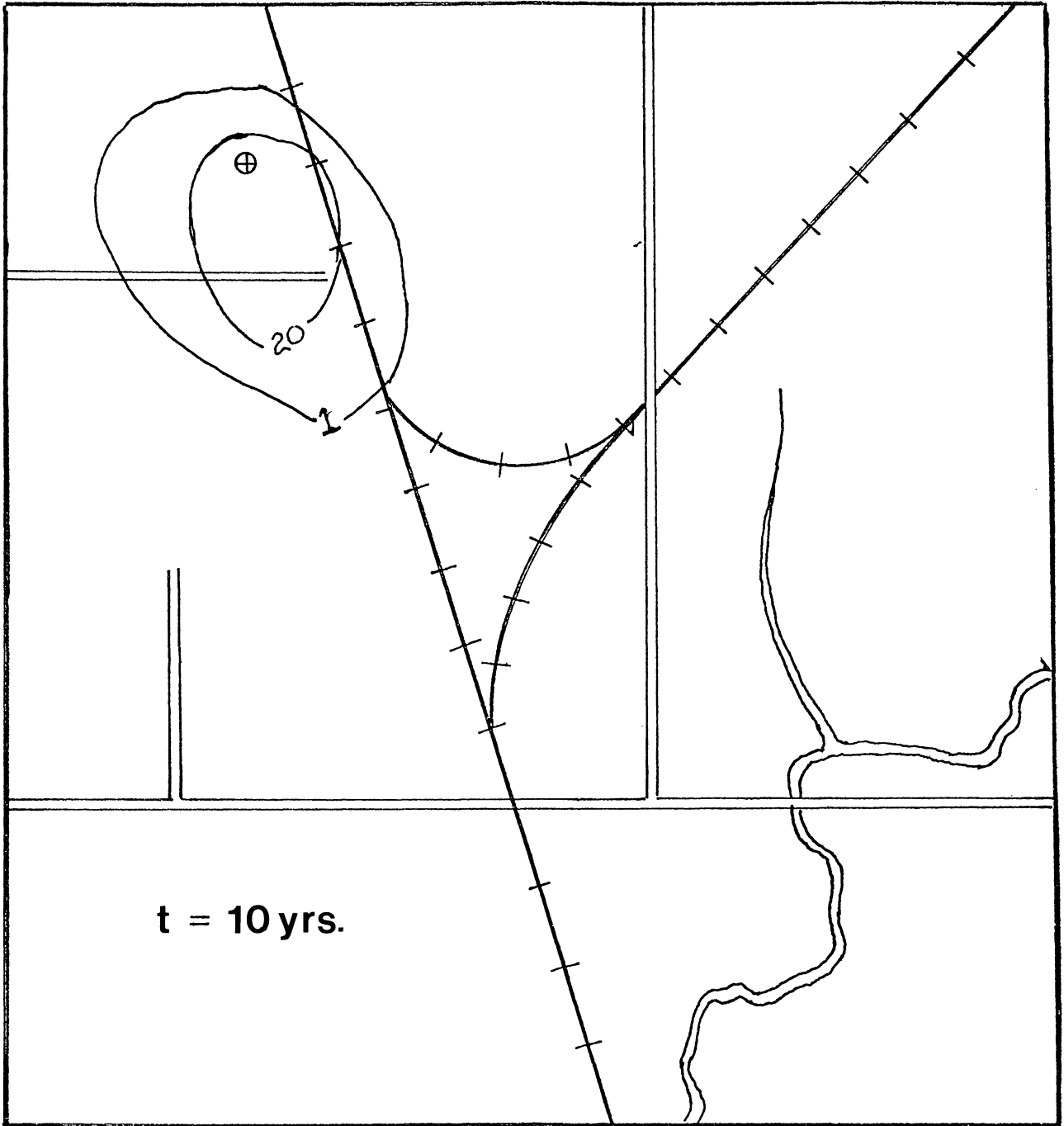


Figure 28. Concentration (mg/l) profile for Phenol after 10 Years. Retardation Factor of 3.

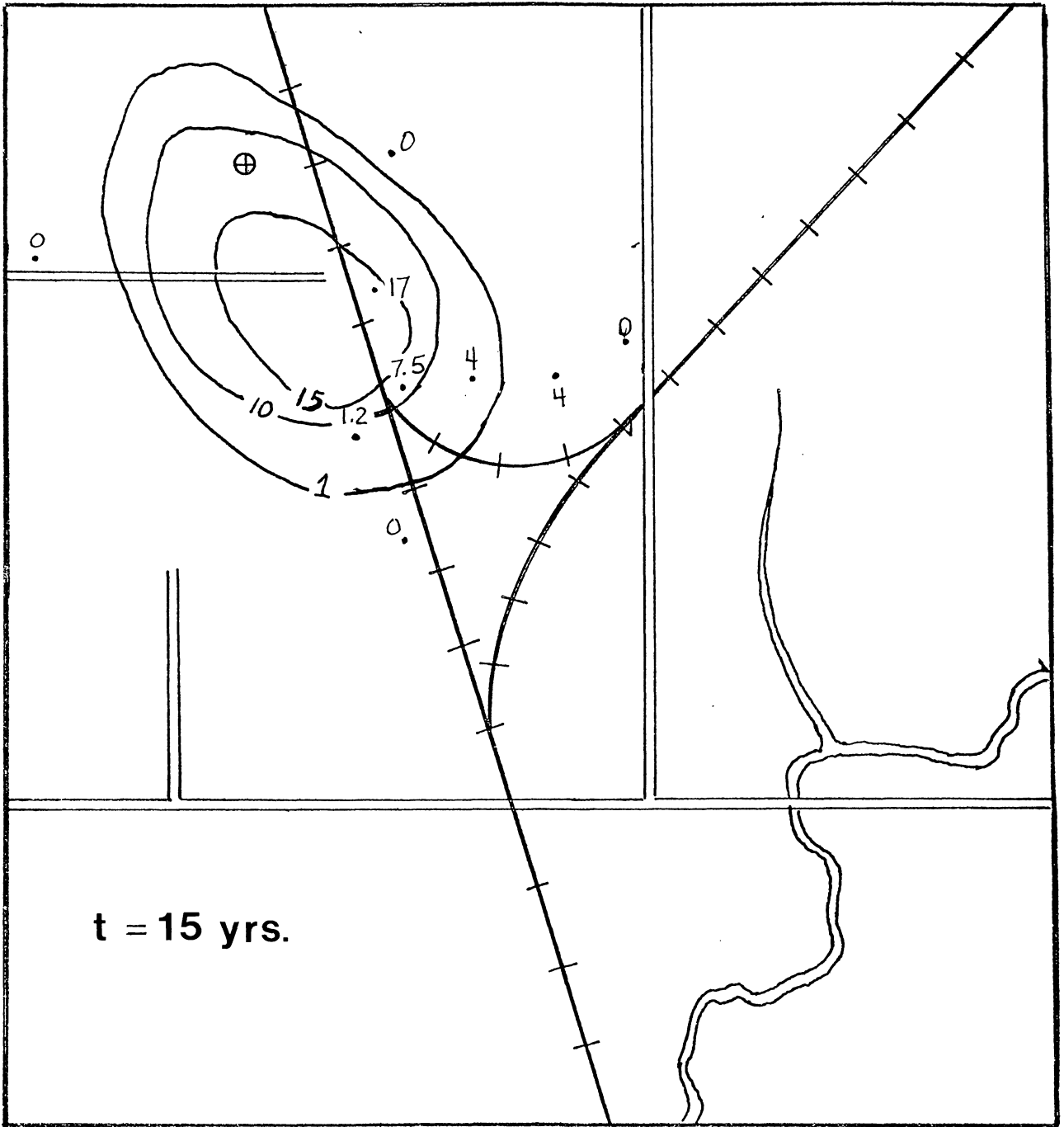


Figure 29. Comparison of 15 Year Numerical Simulation with 1975 Phenol Concentrations (mg/l) Retardation Factor of 3.

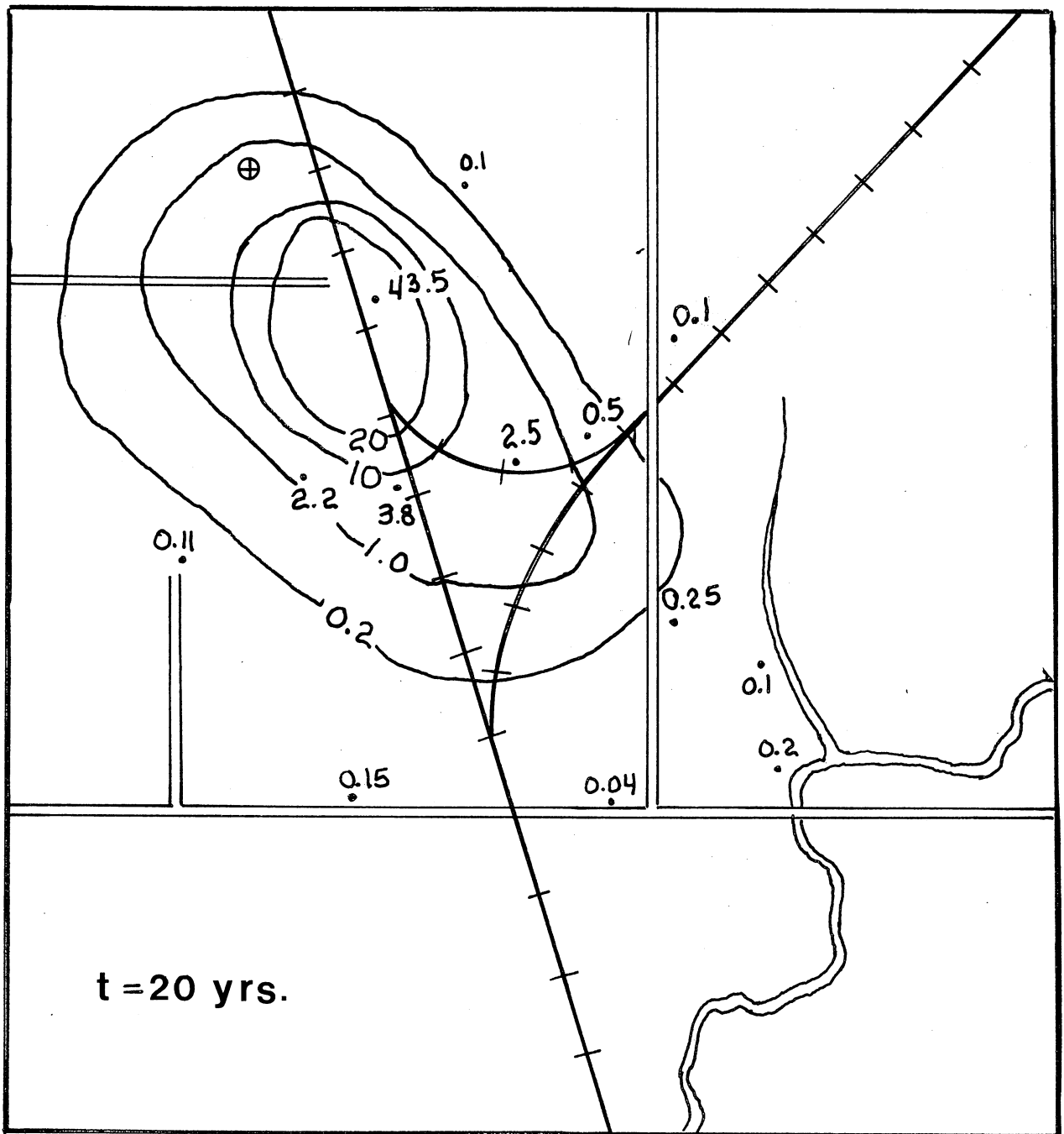


Figure 30. Comparison of 20 Year Numerical Simulation with 1978-79 Phenol Concentrations (mg/l). Retardation Factor 3.

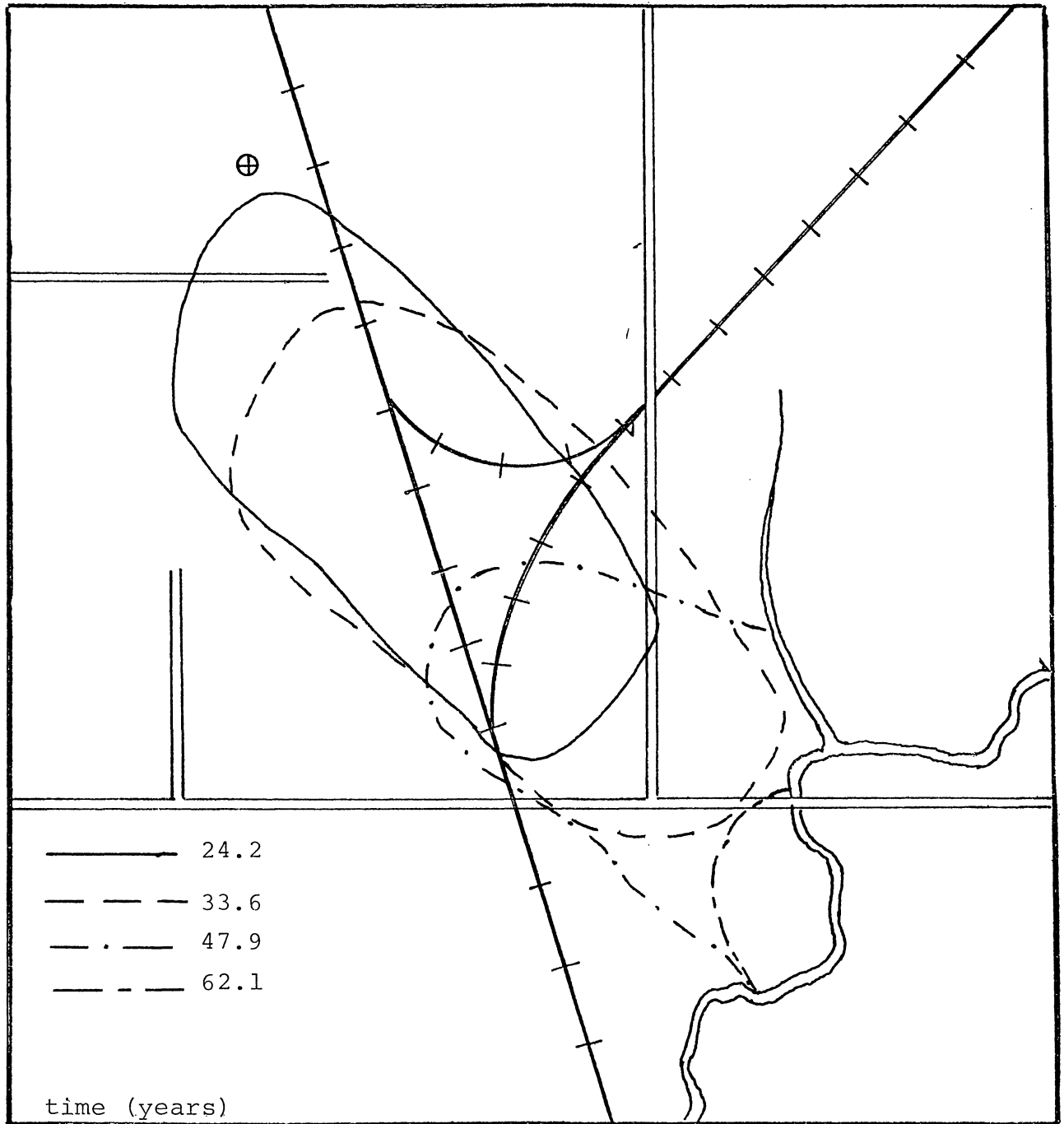


Figure 31. Development of Simulated Phenol Plume with Time.

March 20, 1982

ADDENDUM TO REPORT OF July 1, 1981:
INVESTIGATION OF CONTAMINANT TRANSPORT PARAMETERS IN MICHIGAN
AQUIFERS

This addendum contains the results of additional investigations related to the original work at the Ott-Story Chemical site near Muskegon, Michigan. These additional considerations arose after the discussion with DNR personnel in which the results of the original report were presented in July, 1981. Additional questions arose with respect to the phenol simulations discussed in the original report, specifically related to (1) The sensitivity to the values of the longitudinal dispersivity and (2) Magnitudes of previously reported values for the retardation factor R_d . Additional simulations were prepared to address the first question. During the course of this work, an error was found in the original work such that the dispersivities for the results presented were actually $a_L = 20.0$ ft and $a_T = 6.67$ ft or a factor of three less than reported. Results for $a_L = 60.0$ ft and $a_T = 20.0$ ft have been obtained and are presented in Figs. 32 and 33 and replace Figs. 29 and 30 in the original report. All other conditions in the simulation are exactly as presented in the original report. An additional run was made with $a_L = 200.0$ ft and $a_T = 20.0$ ft to determine the

sensitivity of the results to the assumed value of the longitudinal dispersivity. These results are provided for ease in comparison in Figs. 34 and 35. One of the original questions which resulted in these simulations is in part no longer valid because the longitudinal extent of the plume increases with the correct dispersivities and 1978-1979 observations are more in line with the predicted plume location. Inspection of Figs. 32 - 35 leave some room for interpretation. Apparently the plume location is a little too far to the south relative to the field measurements, a conclusion that may also be obtained from the previous results. Fig. 33 implies an estimated 10 mg/l contour that has moved downgradient further than implied by the data. On the other hand, the 0.25 mg/l contour location is not unreasonable. This more than likely implies that the source strength was not constant, but in fact was increasing with time. It is possible to conclude that Fig. 35 fits the observed data better than Fig. 33; it really depends upon the interpretation of the available data. Presumably the 1978-79 data are better than the 1975 data and should be used for comparison if for no other reason than the fact that more data is available.

An effort was made to determine reasonable values for the values of retardation factors for phenolics in sandy aquifers. Since this consideration is outside of the author's area of expertise, Dr. Walter Weber of the University of Michigan Water Resources Engineering Program was contacted. The result of a personal communication gave an estimate for a distribution

coefficient K_d of approximately 0.91 cm /sm. Since the porosity of the aquifer is necessary to compute the retardation factor through the relation

$$R_d = (1-n)/n \cdot \rho_s \cdot K_d$$

it is only possible to make an estimate of a value for R_d . Table 2 summarizes the computations for a range of realistic values for the porosity. Assuming the distribution coefficient to be approximately correct, these values of R_d are only slightly larger than that estimated from the data in the present study and well within the uncertainty of the estimate. To provide a basis for the interpretation of results, Henry and Force (Dispersion Models in Time and Two Dimensions, J. of the Environmental Engineering Division ASCE, Dec. 1979, pp. 1131-1147) states that values of the retardation factor of 27.8 are typical for aquifers. This number is not qualified by aquifer media type and little basis is available for interpretation. Clay media will exhibit stronger adsorption affinity for most organics and it is possible to expect retardation factors to vary considerably for different media types. In view of this discussion, it is still felt that the retardation factor of three is a realistic estimate to within the uncertainties of the other parameters (hydraulic conductivity and the effective porosity) of the Ott-Story aquifer system.

Table 2. Estimated Range of Retardation Factors
for Phenols ($K_d = 9.1 \times 10^{-7} \text{ m}^3/\text{gm}$)

Porosity	Bulk Density (gm/cm^3)	Retardation Factor
0.2	2.1	10.6
0.3	1.86	5.7
0.4	1.59	4.6
0.5	1.33	3.4

NOTE: This assumes specific gravity of 2.65 for media

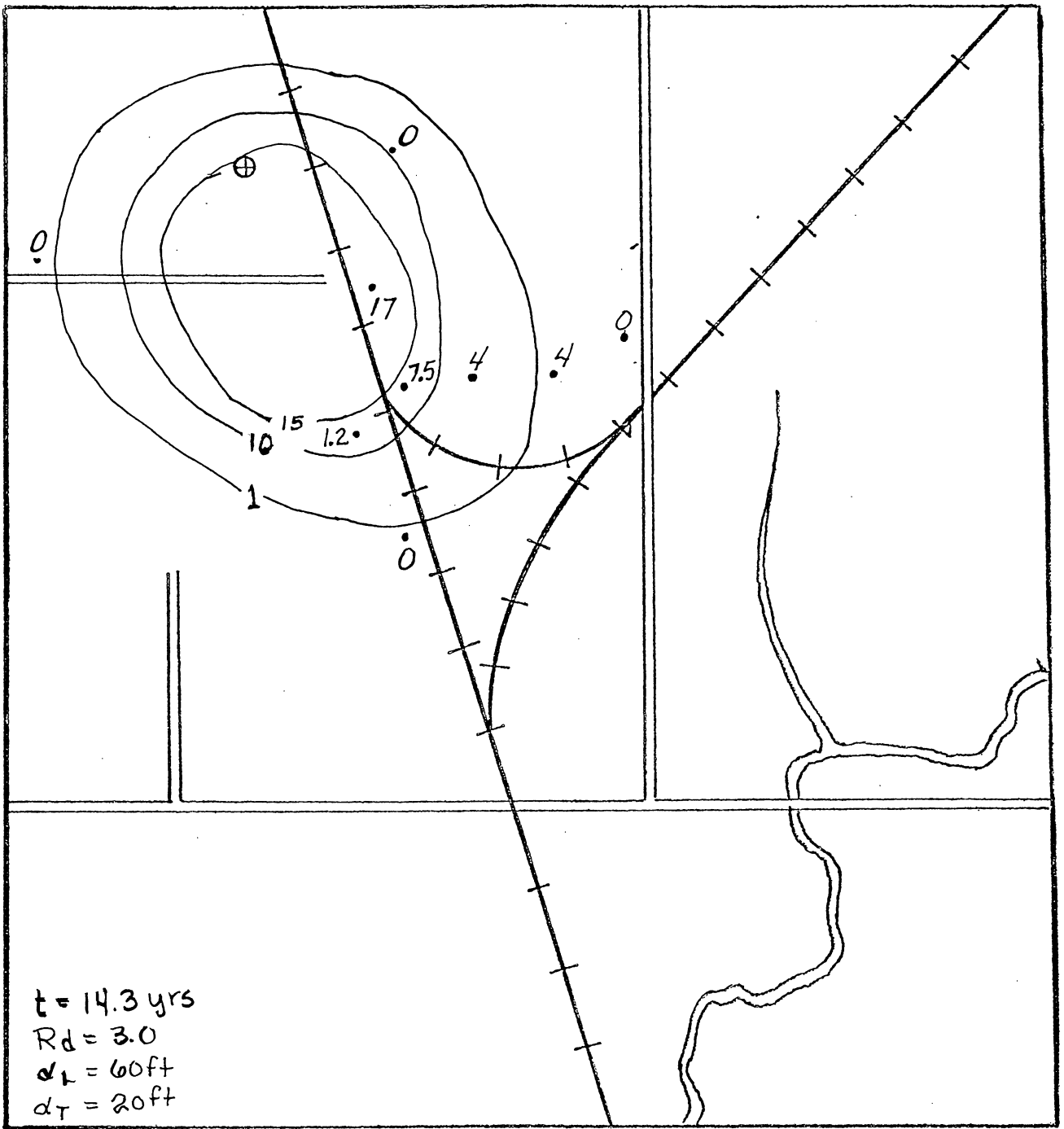


Fig. 32 Comparison of 14.3 year numerical simulation with 1975 Phenol Concentrations (mg/l) ($a_L=60 \text{ ft}$)

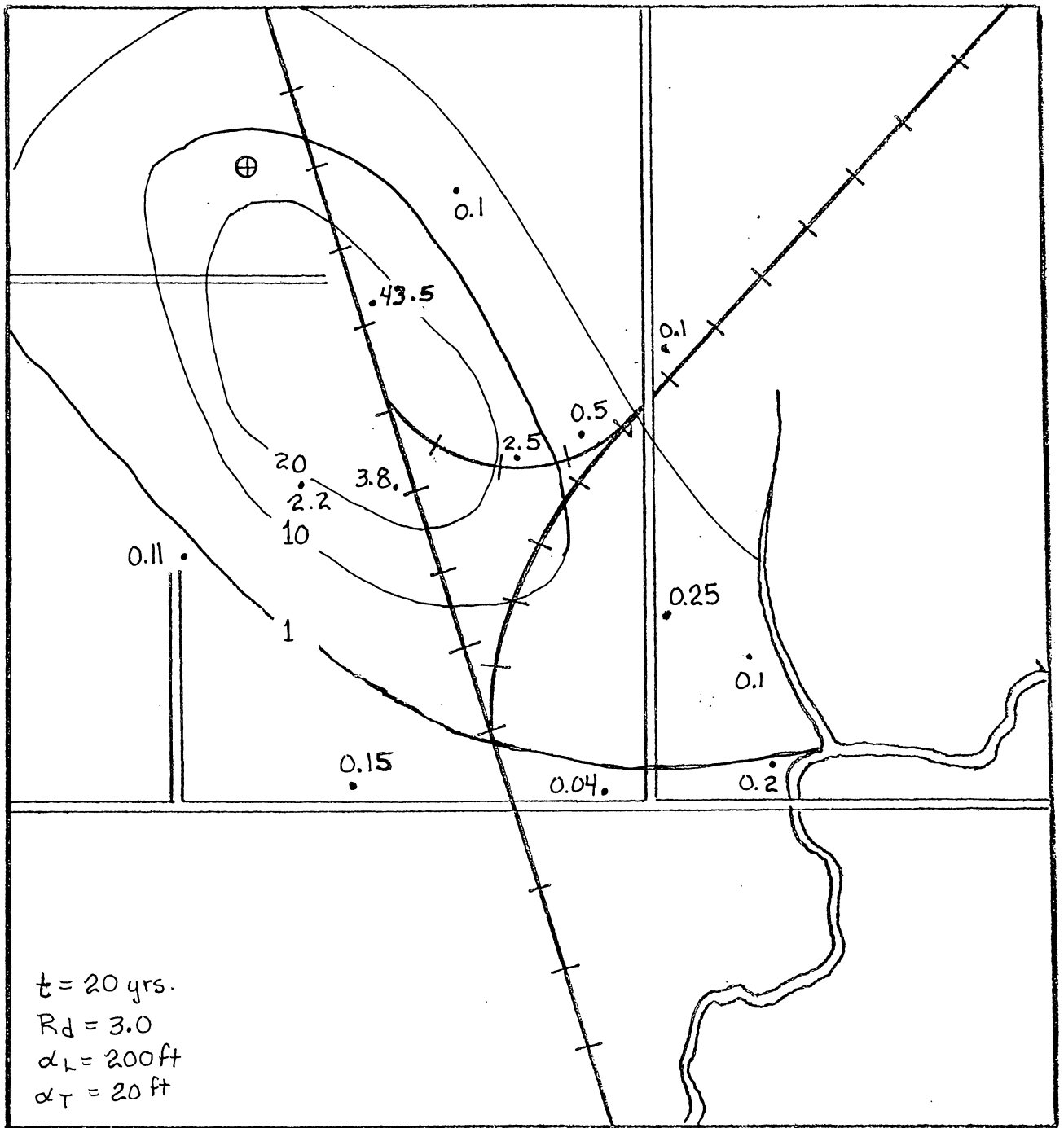


Fig. 33 Comparison of 20 year numerical simulation with 1978-79 Phenol Concentrations (mg/l) ($a_L = 60 \text{ ft}$)

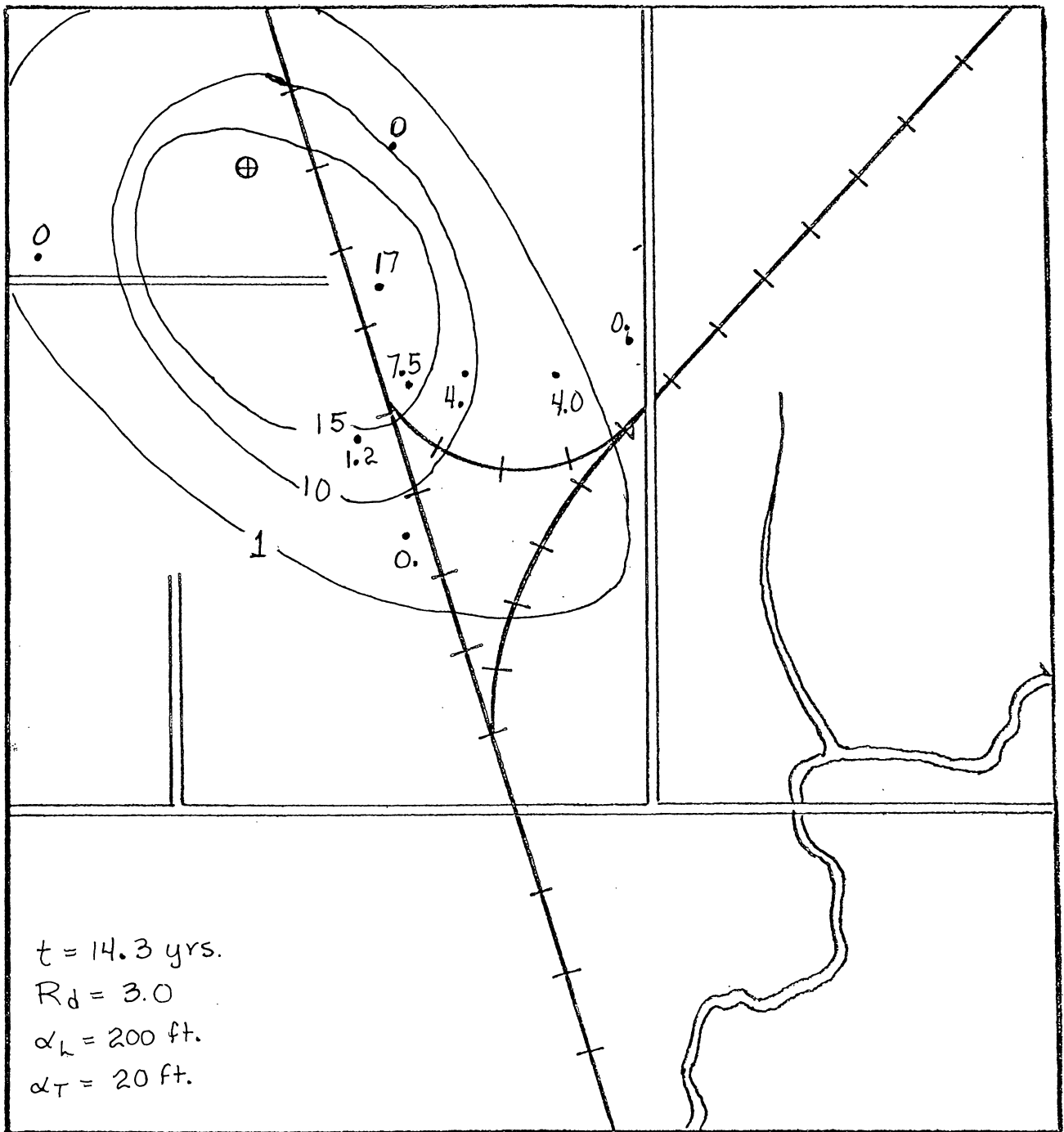


Fig. 34 Comparison of 14.3 year numerical simulation with 1975 Phenol Concentrations (mg/l) ($a_L=200 \text{ ft}$)

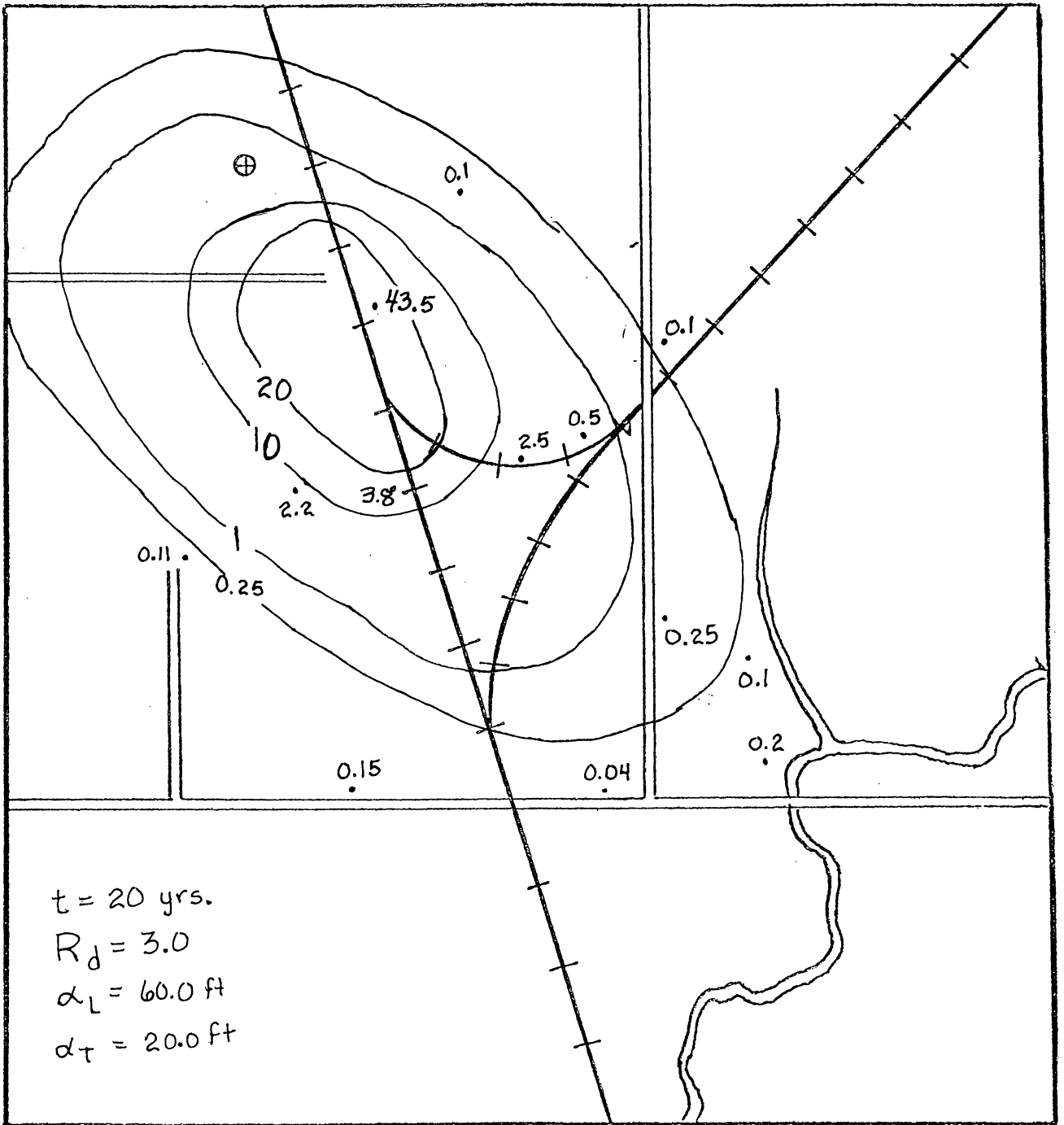


Fig. 35 Comparison of 20 year numerical simulation with 1978-79 Phenol Concentrations (mg/l) ($a_L = 200 \text{ ft}$)

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Greek and Math Symbols

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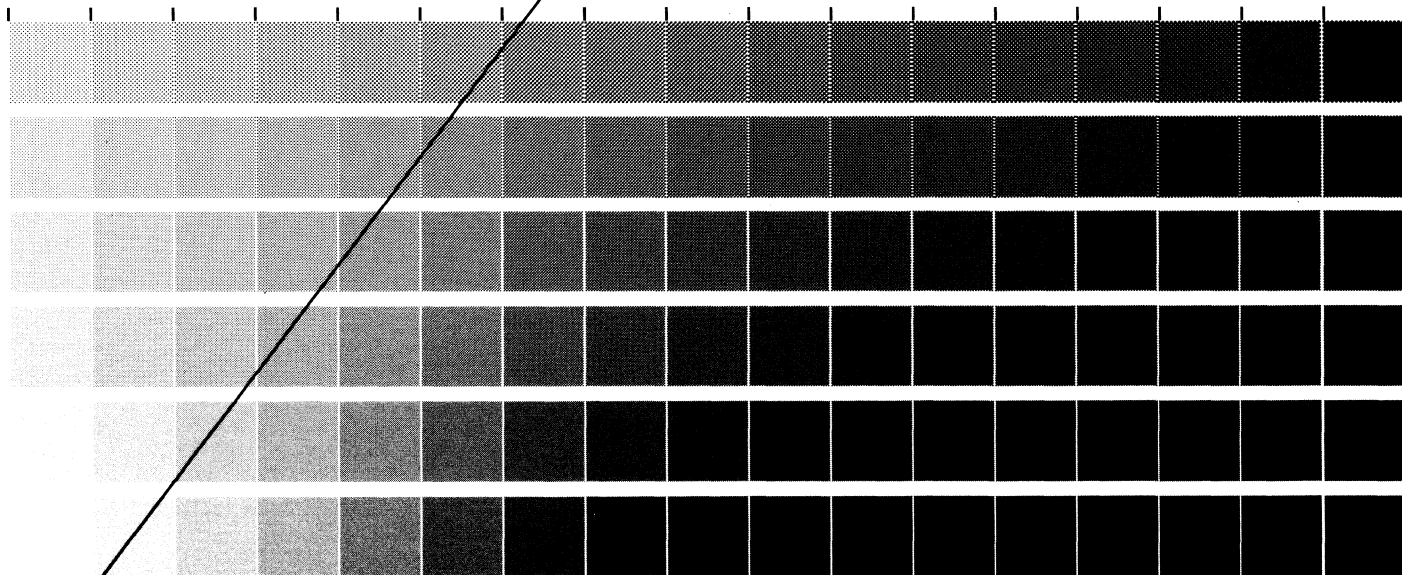
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RIT ALPHANUMERIC RESOLUTION TEST OBJECT, RT-171

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