

THESIS

NUMERICAL MODELING OF GROUNDWATER CONTAMINATION

Submitted by

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ABSTRACT OF THESIS

NUMERICAL MODELING OF GROUNDWATER CONTAMINATION

The effectiveness of numerical models in simulating flow and behavior of contaminants in porous media has not previously been tested for complex boundary conditions encountered in most field problems. This study was undertaken to determine the effectiveness of a model describing movement of contaminants in a shallow, unconfined aquifer. The aquifer selected for use in this study is located in the Denver Basin.

The numerical model used in this study consists of a finite difference form of the two dimensional flow equation and a solution of the convective dispersion equation by the method of characteristics. The equations were solved using the CDC 6400 computer at Colorado State University.

The study established that this numerical model is effective in an application to a field problem with certain limitations. These limitations, their effects on the validity of the solution, and the behavior of the flow situation in the field as interpreted from model results are discussed.

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TABLE OF CONTENTS

	Page
Abstract	iii
INTRODUCTION	1
Location and Description of Study Area.	2
NUMERICAL MODEL - DESCRIPTION AND ASSUMPTIONS . .	5
Description of Numerical Model	6
Equations Used in the Model	6
Adaptation of Data for Modeling.	12
DATA USED	16
Water Table Elevations	16
Bedrock Elevations	18
Permeability and Porosity	18
Concentration	21
RESULTS.	23
Comparison of Results with Analytical Solution	23
Comparison of Results with Field Data.	26
Discussion of Influence of the Solution Technique on Results	33
CONCLUSIONS AND RECOMMENDATIONS.	46
BIBLIOGRAPHY	48
APPENDIX A : DATA USED IN NUMERICAL MODEL	51
APPENDIX B : PROCEDURE FOR OBTAINING PERMEABILITIES	56
APPENDIX C : DESCRIPTION OF COMPUTER PROGRAM . .	63

LIST OF TABLES

<u>Table</u>		<u>Page</u>
A-1	Input Data	52

LIST OF FIGURES

<u>Figure</u>	<u>Page</u>
1-1 Map of Study Area	4
2-1 Map of Study Area with Grid System Superimposed. . .	7
2-2 Representative Grid Showing Velocity Components . . .	8
2-3 Representative Grid Showing Point Relocation Scheme	11
3-1 Water Table Contour Map	17
3-2 Bedrock Contour Map	19
3-3 Measured Chloride Concentration Distribution for June 1956	22
4-1 Comparison of Analytic Solution for One-Dimensional Flow Situation with Solution Obtained from Model .	24
4-2 Computed Distribution of Relative Chloride Concentration for 1955	28
4-3 Chloride Concentrations and Relative Chloride Concentrations	30
4-4 Computed Distribution of Relative Chloride Concentration for 1983	34
4-5a Effect of Unequal Point Spacing in X and Y Directions .	39
4-5b Effects of Elongated Versus Square Grid	39
4-6 Vertical Movement of Contaminants Below Waste Disposal Pond.	42
A-1 Measured Chloride Concentrations for September- October 1955	53

<u>Figure</u>		<u>Page</u>
A-2	Measured Chloride Concentrations for November 1955	54
A-3	Measured Chloride Concentrations for March 1956. .	55
B-1	Representative "Rectangle" from Flownet Showing Parameters Used in Computations	57
B-2	Flownet.	58
B-3	Graphically Determined Permeabilities.	61

LIST OF SYMBOLS

<u>Symbol</u>	<u>Definition</u>	<u>Units</u>
b	distance between streamlines on flownet	L
C	chloride ion concentration	----
C_o	chloride ion concentration at contaminant source	----
D	coefficient of dispersion and molecular diffusion	L^2/T
h	water table elevation	L
i	vectoral direction indicator	----
j	vectoral direction indicator	----
k	permeability	L^2
l	vectoral direction indicator	----
m	saturated thickness of aquifer	L
n	symbol for denoting a specific element	----
Q	discharge	L^3/T
T	transmissibility	L^2/T
t	time	T
v	velocity	L/T
x	distance along horizontal axis of cartesian coordinate system	L
y	distance along vertical axis of cartesian coordinate system	L
γ	specific weight of water	F/L^3
μ_x	dynamic viscosity of water	FT/L^2

INTRODUCTION

In recent years groundwater has become recognized as an important natural resource. Rapid expansion of population and industry in many areas has led to extensive use of groundwater as a source of water supply. At the same time, improper disposal of pollutants has resulted in numerous incidences of groundwater contamination. Conflicts arising among users of groundwater for different purposes have brought about a need for a reliable means of modeling the behavior of contaminants in groundwater aquifers.

The partial differential equation governing flow in porous media is fairly simple, as is the equation describing the behavior of contaminants in groundwater flow. However, the solution techniques for each of these equations are quite complex, making it possible to obtain analytical solutions only for idealized flow situations with simplified boundary conditions, which are inadequate for describing the complicated conditions encountered in the field.

At present the most effective means of describing flow and behavior of contaminants in porous media for complex boundary conditions is through the use of numerical models, solved with the aid of the digital computer. The purpose of this study was to determine the effectiveness of one model in tracing the movement of a contaminant miscible with the native groundwater in a shallow,

unconfined aquifer. The model used in this study is obtained by applying the finite difference technique to the flow equation and the method of characteristics to the dispersion equation.

Location and Description of Study Area

The study area is located northeast of Denver, Colorado, as shown in Figure 1-1. The area is underlain by valley fill deposits ranging from zero to sixty feet in saturated thickness. Groundwater from these deposits is used for irrigation and domestic purposes.

From 1943 to September 1955 wastes from chemical processes were discharged into reservoir A as shown in Figure 1-1. Contaminants known to have been present in the wastewater included chlorides, chlorates, 2,4-D (a herbicide), salts of phosphoric acid, fluorides and arsenic. The bed of the reservoir was permeable and the wastewater percolated readily into the shallow aquifer. In the spring of 1954 crop damage was reported near Derby. Similar complaints from other nearby areas followed¹. Use of the unlined waste disposal pond was reportedly discontinued in 1955. Since that time all industrial wastes have been discharged into Reservoir

¹Petri, L. R., "The Movement of Saline Ground Water in the Vicinity of Derby, Colorado", Proceedings of the 1961 Symposium on Ground Water Contamination, Technical Report W61-5, Robert A. Taft Sanitary Engineering Center, United States Department of Health, Education, and Welfare, April 5-7, 1969, page 120.

F as shown in Figure 1-1. Reservoir F was lined with asphalt in 1955 to prevent leakage of contaminants into the groundwater reservoir².

In 1955 and 1956 a study was conducted by Petri and Smith (4) to identify the manner in which the body of contaminated water moved throughout the area. Hydrogeologic data from Petri and Smith's study along with data taken from Smith, Schneider and Petri (7) was used as input to the finite difference model. Results of Petri and Smith's study included maps of chloride concentration which provided a comparison for results obtained with the finite difference model.

²Walton, Graham, "Public Health Aspects of the Contamination of Ground Water in the Vicinity of Derby, Colorado", Proceedings of the 1961 Symposium on Ground Water Contamination, Technical Report W61-5, Robert A. Taft Sanitary Engineering Center, United States Department of Health, Education, and Welfare, April 5-7, 1969, page 121.

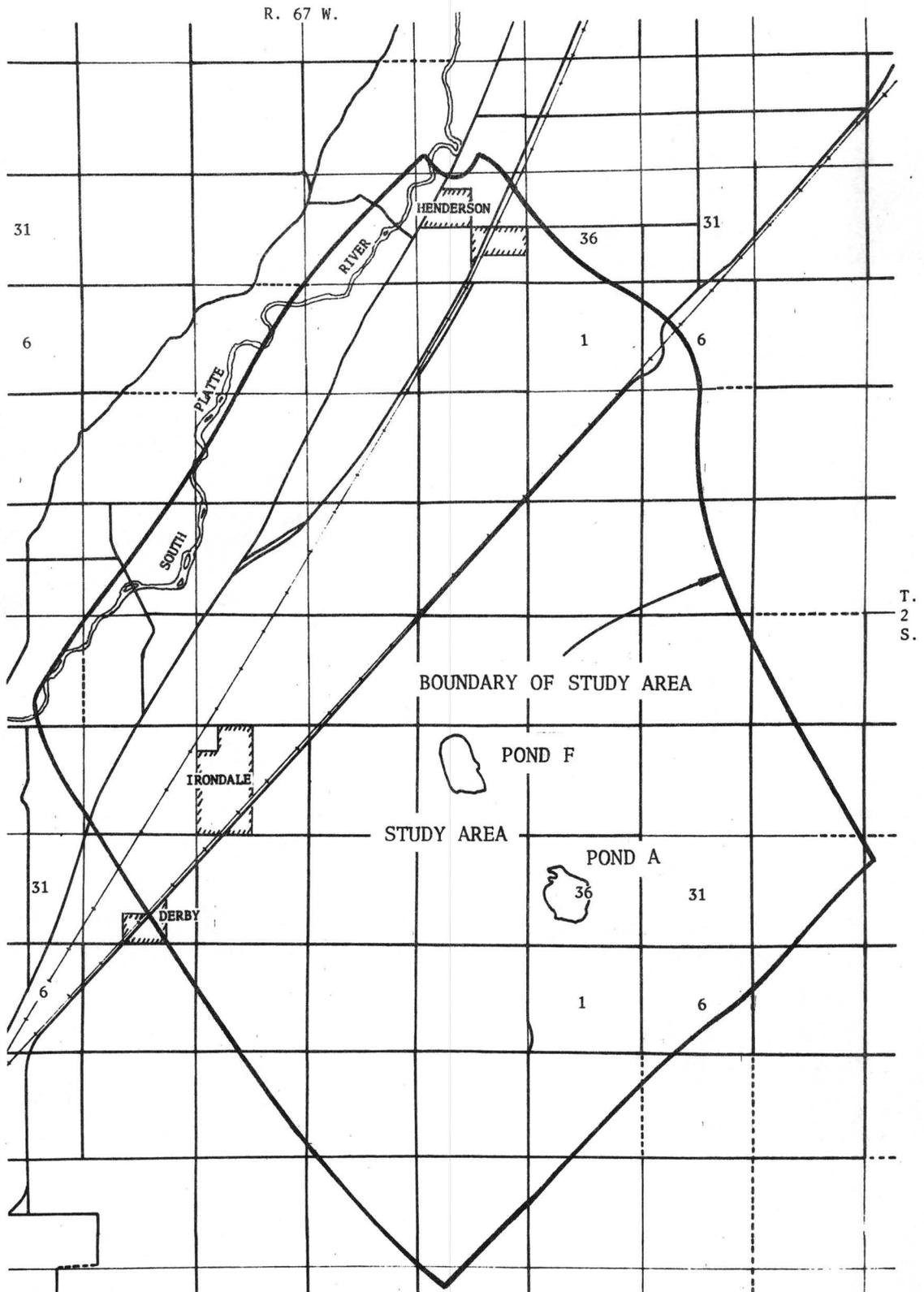


Figure 1-1. Map of study area

NUMERICAL MODEL - DESCRIPTION AND ASSUMPTIONS

A computer simulator was developed by Reddell in 1968 to model the behavior of two miscible fluids under transient flow conditions in a confined aquifer (6). The model was written to accommodate two-dimensional flow in a vertical plane. An implicit, centered-in-space finite difference scheme was used to represent the equations describing the flow phenomena. The method of characteristics was used to model the movement of the contaminants. This simulator was applied to several problems for which analytical solutions exist. Boundary conditions for these problems included uniform porosities and permeabilities, uniform saturated thicknesses, and linear boundaries. Solutions obtained from the model compared well with analytical results, indicating that the method used was a valid means of modeling groundwater flow situations, at least for simple cases.

Pinder and Cooper (5) used the method of characteristics to solve the solute transport equation and the alternating direction iterative procedure to solve the groundwater flow equation. This approach was applied to one-dimensional and two-dimensional transient flow problems, including a saltwater intrusion problem in a coastal aquifer. Results obtained using this approach agreed well with analytical solutions, indicating that it could be used as a valid method for simulating movements of contaminants in groundwater flow problems.

Description of Numerical Model

The study area was represented by a system of two hundred forty square grids, each having an area of 0.25 square miles. Theoretically, a larger number of smaller grids would have yielded more definitive results. However, the grid size used was determined to be appropriate for the amount of the available data. The location of the grid system superimposed on the study area is shown in Figure 2-1. A flowchart and a listing of the computer program used in this study are presented in Appendix C.

Equations Used in the Model

Velocity Equation. The equation for determining flow velocity in groundwater for steady-state conditions is given in tensor notation as:

$$V_l = k_l \frac{\gamma}{\mu} \frac{\partial h}{\partial x_l} \quad (2-1)$$

where

k = permeability

γ = specific weight of water

μ = dynamic viscosity of water

h = water table elevation

x = spatial distance

V = Darcy's velocity

l = direction indicator .

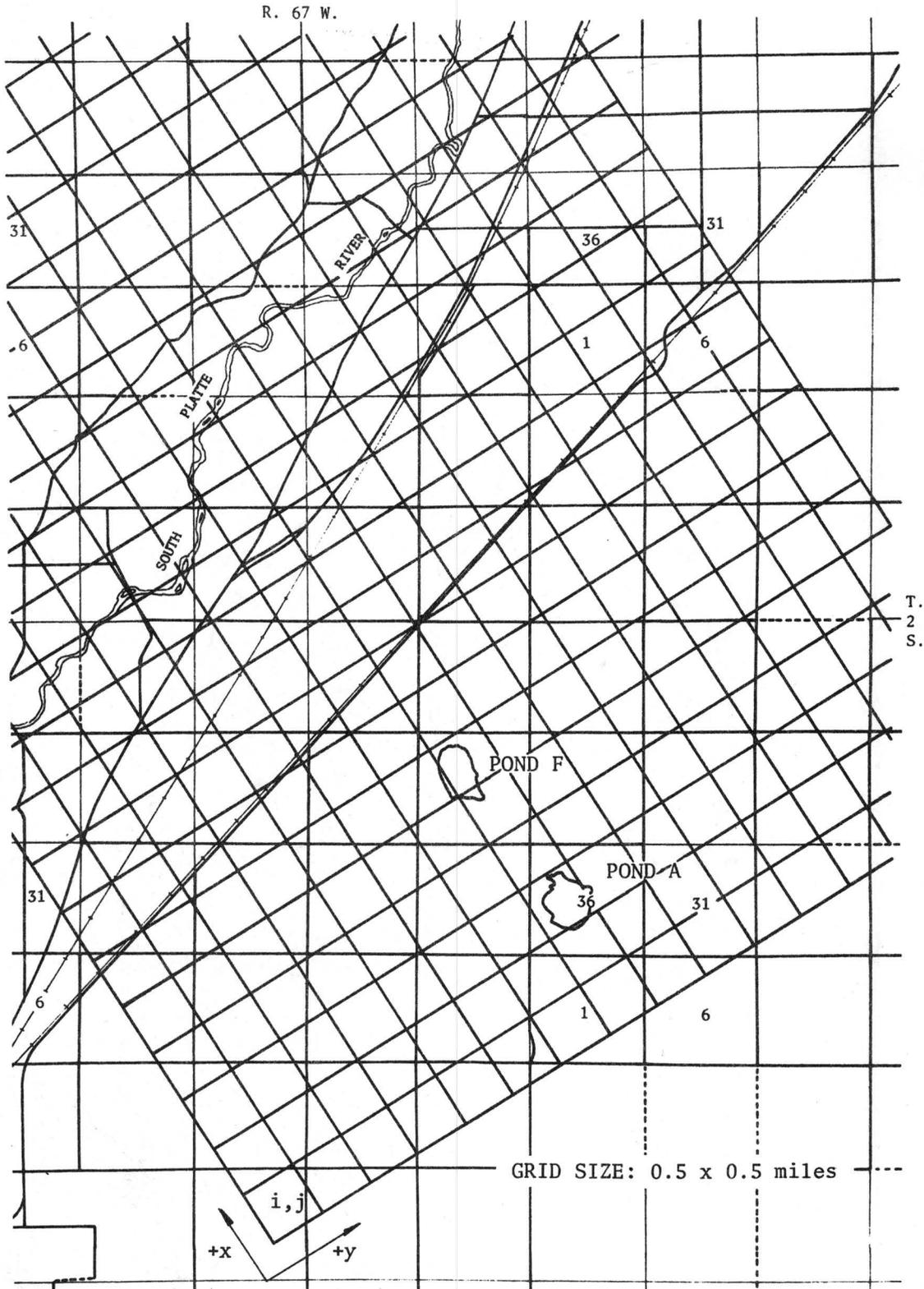


Figure 2-1. Map of study area with grid system superimposed

The two horizontal components of velocity were determined for each grid in the model using a finite difference form of equation 2-1. The grid system was oriented in such manner that the principal directions of flow in the area were in the same direction as the positive X and Y axes of the grid system. The reason for this was to make the technique used to obtain velocity components in each grid as consistent as possible throughout the model.

A typical grid and its four adjacent grids are shown in Figure 2-2. The velocity components for grid (i, j) are not located at the grid center but at the interface of the grid with the one immediately upgradient in each direction as shown.

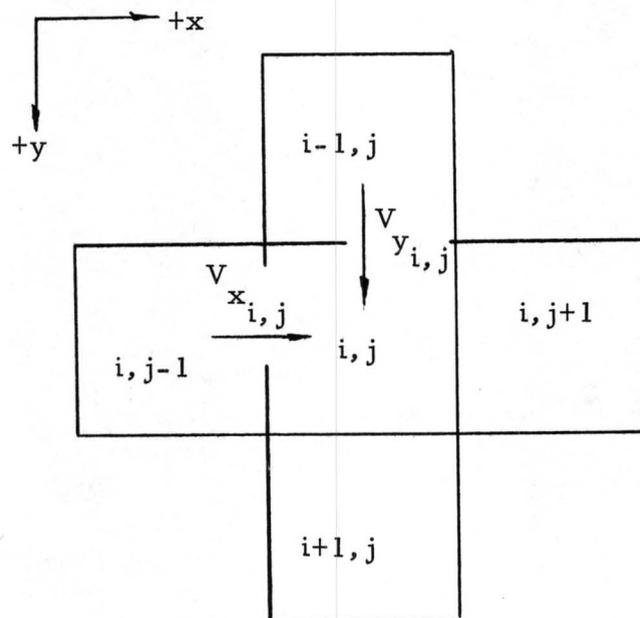


Figure 2-2. Representative grid showing velocity components

The finite difference equations for determining the velocity components in grid (i, j) are

$$V_{x_{i,j}} = \frac{2k_{i,j} k_{i,j-1}}{k_{i,j} + k_{i,j-1}} \frac{\gamma}{\mu} \frac{h_{i,j-1} - h_{i,j}}{\Delta x} \quad (2-2a)$$

$$V_{y_{i,j}} = \frac{2k_{i,j} k_{i-1,j}}{k_{i,j} + k_{i-1,j}} \frac{\gamma}{\mu} \frac{h_{i-1,j} - h_{i,j}}{\Delta x} \quad (2-2b)$$

Equation for Concentration. The equation describing the movement of contaminants is given in tensor notation as:

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x_i} \left(D_{i,j} \frac{\partial C}{\partial x_j} \right) - V_i \frac{\partial C}{\partial x_i} \quad (2-3)$$

where

C = concentration

t = time

D = coefficient of dispersion and molecular diffusion.

The first term on the right hand side of equation 2-3 describes the movement of a contaminant due to dispersion and molecular diffusion. The second term on the right hand side of the equation describes contaminant movement due to velocity convection. Initially both terms were taken into account. However, results of pilot runs showed that, for the flow situation being considered in this study, the velocity convection term was several orders of magnitude larger

than the dispersion and molecular diffusion term. The first term of equation 2-3 was therefore dropped, resulting in:

$$\frac{\partial C}{\partial t} + V_i \frac{\partial C}{\partial x_i} = 0 \quad . \quad (2-4)$$

The solution of this equation by conventional finite difference methods has proven difficult, resulting in either artificial dispersion from the numerical process or an unstable solution. Since Reddell (6) successfully used the method of characteristics in obtaining a solution to equation 2-4, it was used in this study.

The characteristic curves for equation 2-4 are:

$$X_1 = X_1(t), \quad X_2 = X_2(t), \quad C = C(t) \quad . \quad (2-5)$$

These curves are the solutions to the ordinary differential equations

$$\frac{dx_1}{dt} = V_1, \quad \frac{dx_2}{dt} = V_2, \quad \frac{dc}{dt} = f(x_1, x_2, t) \quad . \quad (2-6)$$

The basis of the method of characteristics is that given solutions to equation 2-6, a solution for equation 2-4 may be obtained by following the characteristic curves. This requirement was achieved by assigning a set of moving points to the grid system. Four equally spaced points were placed in each grid and assigned the initial concentration in that grid. Based on its position within a grid, each point was also assigned velocity components obtained by linear

interpolation between the velocity components at the grid interface. Using these velocity components the point was then relocated to its position at the next time level using the finite difference forms:

$$\begin{aligned} X_n^{t+1} &= X_n^t + \Delta t V_{xn} \\ Y_n^{t+1} &= Y_n^t + \Delta t V_{yn} \end{aligned} \quad (2-7)$$

where

n denotes the n th point of the array

t old time level

$t+1$ new time level

Δt time increment

V_x, V_y point velocity components.

Several typical grids, showing points in their original positions with vectors to their locations at the next time level are illustrated in Figure 2-3.

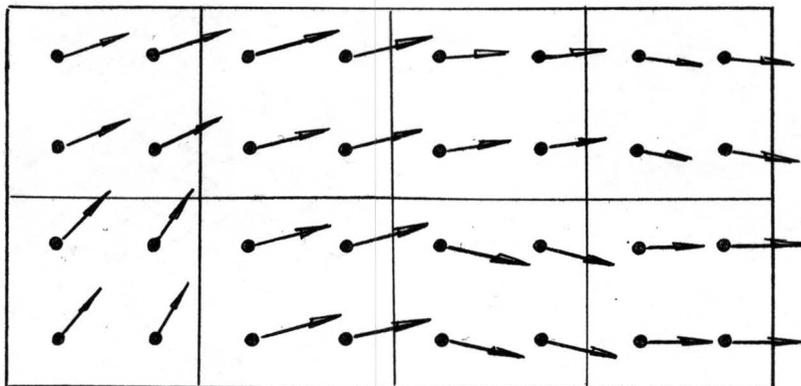


Figure 2-3. Representative grid showing point relocation scheme

After the points had been relocated, new concentrations were calculated for each grid as the average of the point concentrations within its boundaries at the new time level. The points were then assigned the new grid concentration and new velocity components and were again relocated. By repeating this process over a number of time steps, concentration distributions were obtained for various times after initial conditions were specified. In order to alleviate the problem of depleting the supply of points at the inflow boundary of the model and at locations of divergence in the flownet, points were reset at their original locations after each ninth time step. This did not affect the grid concentrations, since they were held constant while the points were reinitialized.

The numerical model described above consisted of a computer program written in Fortran IV for use with the CDC 6400 computer at Colorado State University. A description of the program and its subroutines is given in Appendix C along with a flowchart and a program listing.

Adaptation of Data for Modeling

The following assumptions and simplifications were made for the purpose of presenting the data describing the characteristics of the study area in a form suitable for use with the finite difference model.

RESULTS

The validity of the model was confirmed by obtaining a concentration distribution for an ideal flow situation using the model, and comparing this distribution to the analytical solution for that flow situation. The model was then applied to the field situation described in previous chapters, and the model results were compared to field measurements. After obtaining the concentration distribution which most closely resembled the distribution obtained from field measurements, an analysis was made of the discrepancies between model results and field measurements. This required an analysis of errors.

Comparison of Results with Analytical Solution

The validity of the model was verified using a one-dimensional, steady-state flow situation with constant input of contaminants along a line source at the inflow boundary of the model. Permeability was uniform throughout the model. The water table elevations were assigned to give a constant gradient in the X-direction and zero gradient in the Y-direction. The resulting flow situation was one-dimensional in the X-direction with constant velocity throughout. The analytical solution of equation 2-3 for this flow situation is given by:

Based on available data, the flow of groundwater in the study area was assumed to be in a steady state. This assumption proved to be extremely advantageous. Since the water table is the result of effects of all contributions or depletions to the groundwater supply, a steady state water table indicates that all sources and sinks, evapotranspiration, precipitation and possible interflow with another formation were in equilibrium. While the behavior of any one of these influences was not known, the total effect of all of them on the behavior of the groundwater reservoir was accounted for in the water table map. Thus, knowledge of the amount of precipitation, pumping from wells, evapotranspiration, and contribution from surface water, including the amount of water introduced through the waste disposal pond was not necessary. Hence the waste disposal pond was treated as a source of chloride concentration, but not as a source of water to the groundwater reservoir.

Permeabilities were obtained using the flownet as described in Appendix B. The grid system for the model was oriented so that two sides of the model lay nearly parallel to the primary direction of flow. In order to simplify the process of monitoring the flow across the boundaries of the model, it was decided to eliminate all flow across the two side boundaries. This was easily accomplished by interpreting two streamlines near the side boundaries as impermeable barriers. Since mathematically streamlines and impermeable

barriers are treated identically, this interpretation was valid and did not alter the behavior of the model. Grids through which these two streamlines passed and all grids exterior to these were assigned permeability values of zero.

The model used in this study was developed for two-dimensional flow in the horizontal plane, although velocity components in the vertical direction were known to exist. The reason for using a two-dimensional model versus a three-dimensional model was to reduce computer time required to obtain solutions. The effects of vertical velocity components on the accuracy of the solution obtained from a two-dimensional horizontal model become significant only in the vicinity of wells and in locations where either the bedrock surfaces or the water table slopes are very steep. The flow from wells in this study area are relatively small, so that areas surrounding the well where vertical velocities become significant are too small to be accounted for by the system of grids used in this study. Both the water table and bedrock contours are smooth and well-behaved. The value of the slopes in all locations of the study area are small, so that the errors introduced by neglecting vertical velocities are small. It was therefore concluded that all vertical velocity components could be neglected and the flow field be considered as two-dimensional without significant decrease in the validity of the model.

Due primarily to insufficient data, density and viscosity of the groundwater were taken as constants throughout the study area.

Since the composition and concentration of the contaminated water were unknown, its properties could not be accurately determined. Petri and Smith (4) gave adequate information only on chloride concentration distributions, for which most of the concentrations did not exceed 3000 parts per million. The assumption was made that chlorides accounted for the major part of the contaminants and that the effects on density and viscosity of the other constituents could be neglected. The relatively low salt concentrations being dealt with were not sufficient to change the properties of fresh water appreciably. Hence values of density and viscosity for fresh water were used throughout the area. Effects of seasonal temperature fluctuations on the properties of the groundwater were neglected. In most locations the water table is a sufficient distance below the ground surface to be insulated from the influence of atmospheric temperature fluctuations and the freezing of the ground in winter.

DATA USED

For each grid a single value of each of the following parameters was read in as input data: permeability, porosity, water table elevation, and bedrock elevation. Values for chloride concentration in each grid were also used, not as input to the model, but as a basis of comparison with results obtained with the model.

Water Table Elevations

Elevations of the water table at locations throughout the study area were measured by Petri and Smith (4) at various times during their study in 1955 and 1956. Fluctuations in the water table were found to be insignificant for this period throughout the study area, indicating near-steady-state flow conditions. Water table elevations measured in 1964 were obtained from Smith, Schneider, and Petri (7). These values compared well with Petri and Smith's data, further indicating steady-state flow conditions. Using both sets of data, water table contours were constructed for the study area. A map of these water table contours is shown in Figure 3-1. The water table elevation for each grid was taken as the average value from the contour map within the boundaries of the grid. These values are tabulated in Appendix A in the form in which they served as input data to the model.

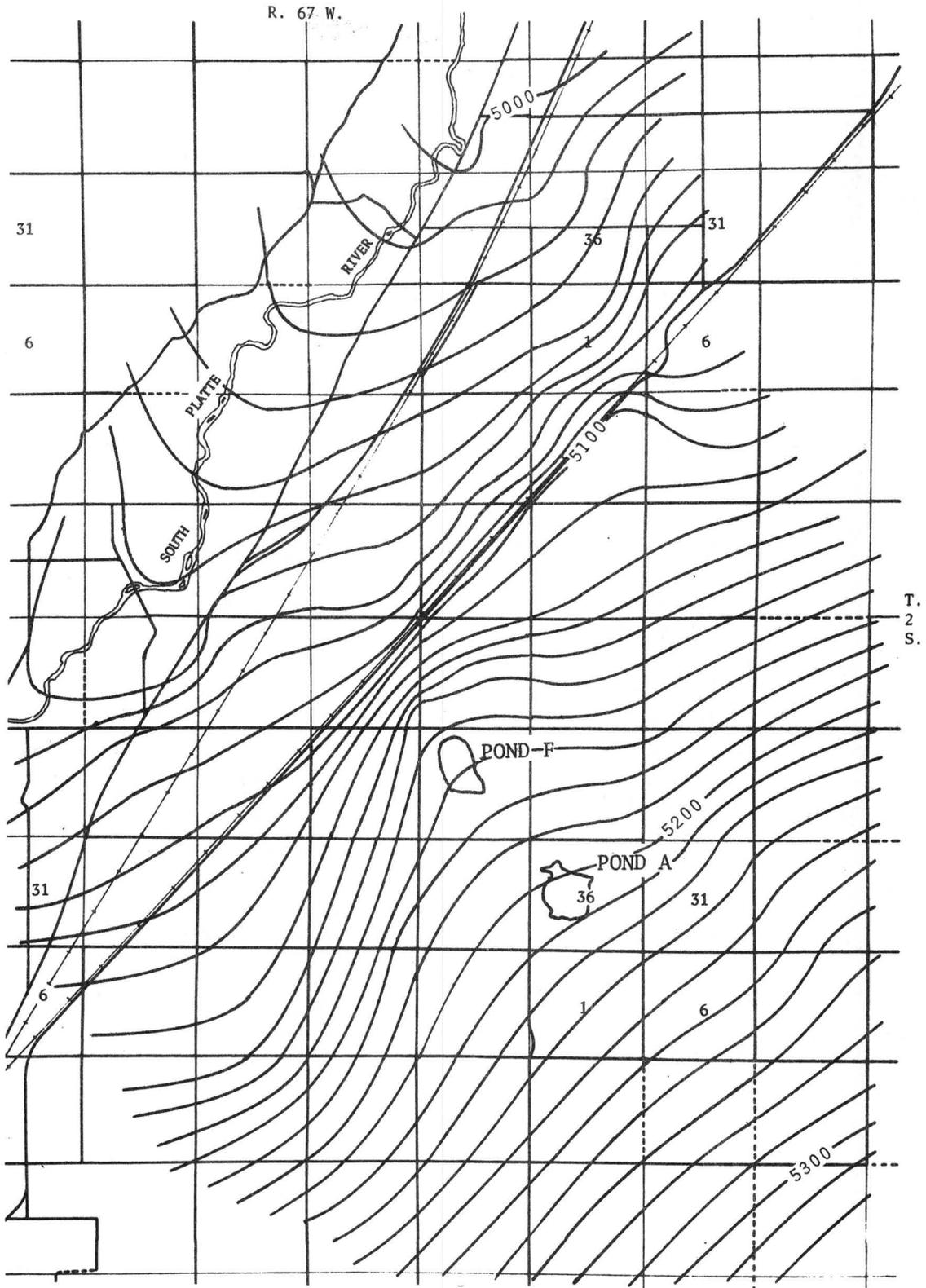


Figure 3-1. Water table contour map (10 foot contour intervals)

Bedrock Elevations

Using data from Petri and Smith's study (4) and Smith, Schneider and Petri (7), a contour map of bedrock elevations was constructed in a manner similar to the construction of the water table contour map. This map is shown in Figure 3-2. The average value from the contour map for the area within each grid was taken as the bedrock elevation for that grid. Values for bedrock elevation are given in the form of input data for the model in Appendix A. For the purposes of this study it was assumed that there was no interflow between bedrock and alluvium.

Permeability and Porosity

Information on both these parameters was inadequate. Velocity at any location is directly proportional to permeability and inversely proportional to porosity. If a valid representation of the flow situation in the study area is to be obtained, accurate values of permeability and porosity should be defined for each grid.

Relative transmissibilities were obtained using a graphical procedure applied to a flownet constructed from the water table contour map. A detailed description of this procedure and the resulting map of relative transmissibilities are given in Appendix B. Relative transmissibilities for each grid were converted to absolute permeabilities using density and viscosity of the water, saturated thickness in each grid, and a conversion factor relating a measured value of

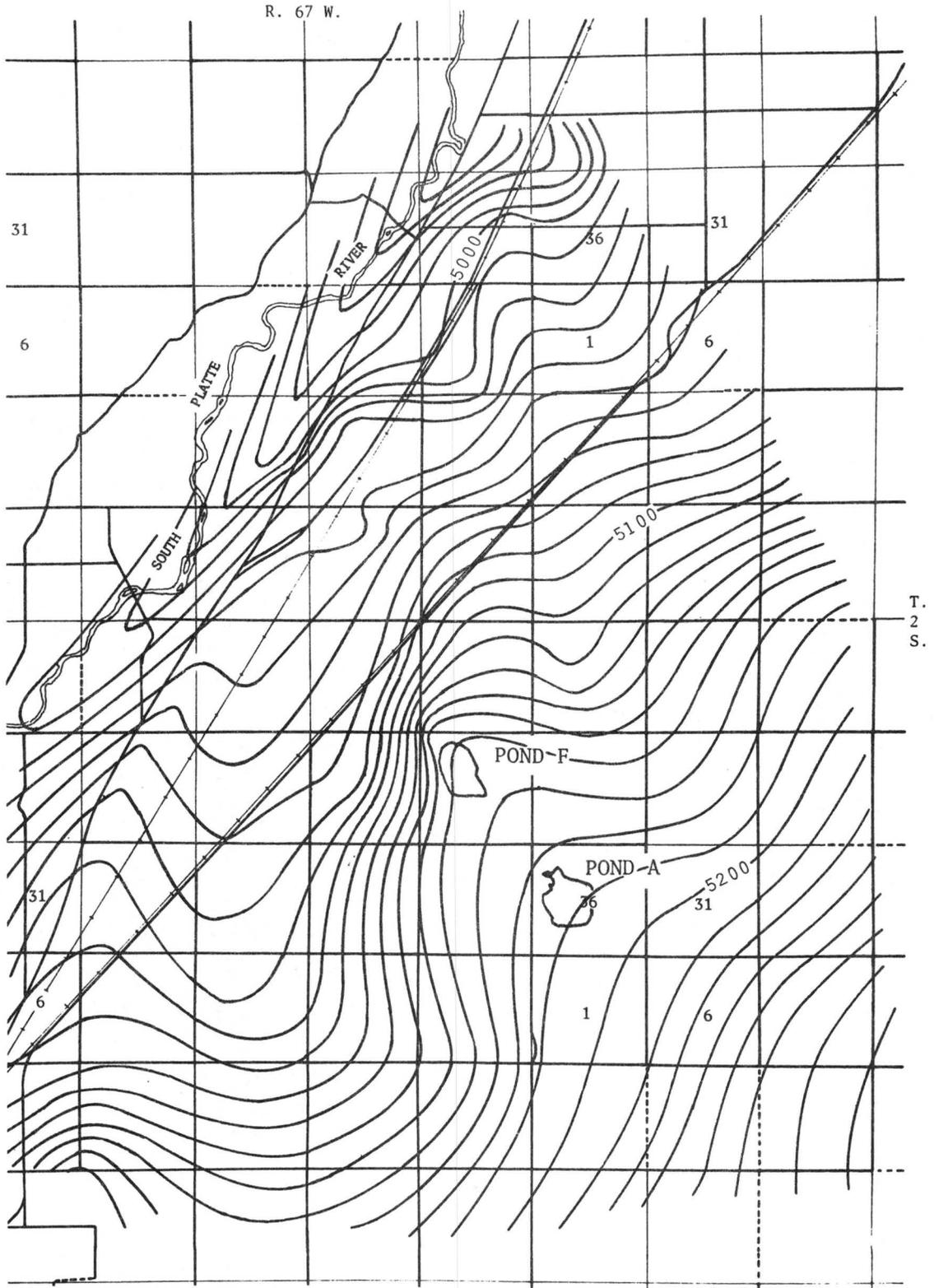


Figure 3-2. Bedrock contour map (10 foot contour intervals)

hydraulic conductivity to the relative transmissibility in one grid. Permeability values for each grid are tabulated in the form of input data for the model in Appendix A.

No method was available for obtaining porosities throughout the area. Therefore, porosity was assumed constant for all grids. This assumption is not too critical, since the porosity for the alluvial material being considered ordinarily does not vary greatly with location.

Both the porosity and the reference hydraulic conductivity used in the conversion of transmissibilities to permeabilities are constants which are used in the same manner for every grid in the model. Hence the adjustment of either or both these constants does not alter the velocity pattern predicted by the model but acts as a time scaling mechanism for the model as a whole. By adjusting either the reference hydraulic conductivity, the porosity, or both, model time could be made to correspond to real time. After several trial runs with the numerical model, a hydraulic conductivity of 8500 gpd/ft^2 in Section 22 and a porosity of 23% in Section 16 of the study area were selected for use in final runs. For comparison, Petri and Smith (4) obtained a permeability of 8500 gpd/ft^2 in Section 22, and a porosity of 32% in Section 16.

Concentration

The following information regarding the nature and behavior of the contaminants was obtained from Petri and Smith (4) and Petri (3). The source of the contamination was determined to be a waste disposal pond located near the center of Section 36 of the study area. The pond was reportedly used from 1943 to September 1955. Although the exact composition and concentration of the wastes discharged into this pond is not known, it has been determined that the waste water contained substantial amounts of chlorides. Chloride ion concentration distributions were measured and presented in the form of contour maps for September-October 1955, November 1955, March 1956, and June, 1956. The map for June 1956 is shown in Figure 3-3. The remaining three maps are given in Appendix A. These maps were useful for comparison with concentration distributions obtained from the finite difference model. It was indicated that the background concentration in most locations throughout the area was less than 100 ppm.

Data from unpublished anonymous sources (1), (2) were available for chloride concentrations at various locations throughout the area from 1960 to 1970. These data were not extensive enough to be used for constructing concentration distribution maps. However, they were useful for gaining knowledge of the behavior of concentration with time for comparison with results obtained from the model.

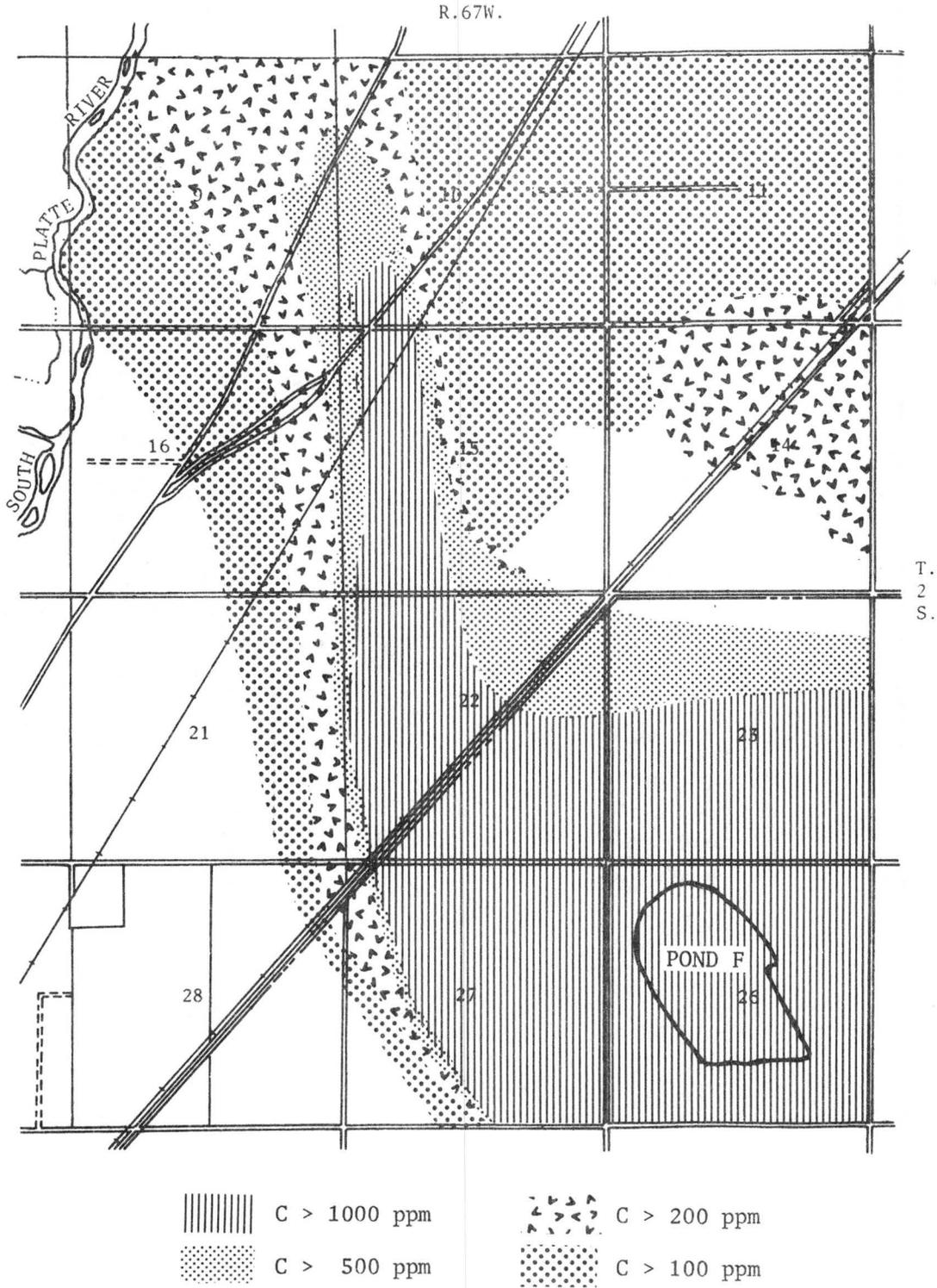


Figure 3-3. Measured chloride concentration distribution for June 1956
(After Petri and Smith (4))

$$\frac{C}{C_o} = \frac{1}{2} \operatorname{erfc} \frac{x-vt}{2\sqrt{D_l t}} + \frac{1}{2} \exp\left(\frac{vx}{D_l}\right) \operatorname{erfc} \frac{x+vt}{2\sqrt{D_l t}} \quad (4-1)$$

where

C = concentration at any location

C_o = concentration at source

x = distance in direction of flow

v = flow velocity in X-direction

t = time

D_l = longitudinal dispersion coefficient.

Using the model, a concentration distribution was obtained at $t = 4.32 \times 10^6$ seconds, with $v = 8.219 \times 10^{-4}$ ft/sec, and $D = 2.062 \times 10^{-6}$ ft²/sec. Using the same values for t , v , and D_l , equation 4-1 was solved for several values of x . Plots of C/C_o versus x for both the numerical solution and the analytical solution are shown in Figure 4-1.

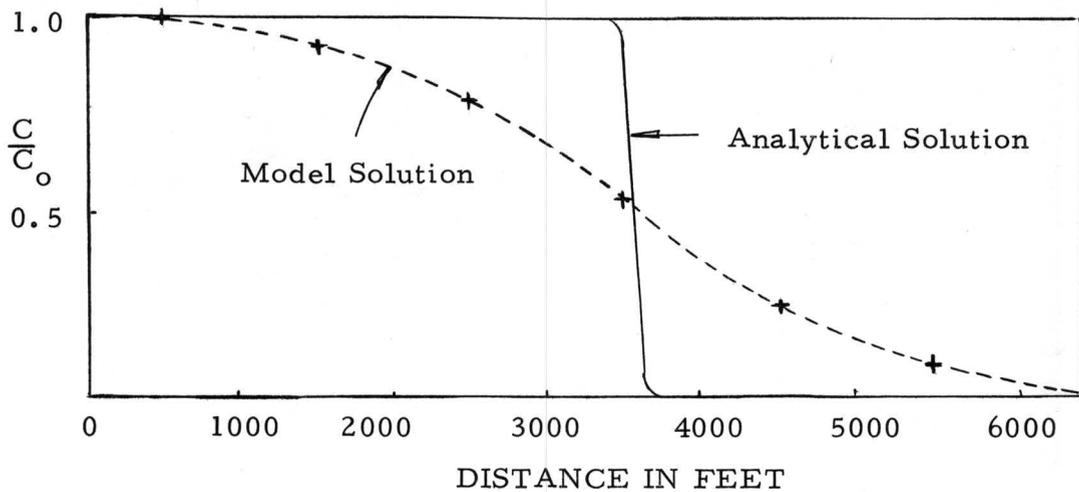


Figure 4-1. Comparison of analytical solution for one-dimensional flow situation with solution from model.

Analysis of the results shown in Figure 4-1 determined that the procedure for relocating concentration points is valid. The analytical solution indicates that the location at which C/C_0 is 0.5 is at all times a distance from the contaminant source equal to the product of the velocity and the elapsed time. The numerical solution satisfies this condition as indicated by its intersection with the analytical solution at a C/C_0 value of approximately 0.5. This was found to be true not only at the particular time for which the concentration distribution is shown in Figure 4-1, but at all times throughout the run.

The numerical model yielded relative concentration values which decreased gradually with increasing distance from the contaminant source, while the analytical solution produced a much more abrupt decrease in relative concentration values over a comparatively short distance. This discrepancy was caused by the artificial dispersion inherent in the method of characteristics. Reddell (6) performed a comparison of an analytical solution to a numerical solution similar to this one and obtained results which matched closely. The grids used in Reddell's model were only a few centimeters in length, so that the distances over which artificial dispersion took place were of the same order of magnitude as the distances over which physical dispersion occurred. Hence the effects of artificial dispersion were partially absorbed by physical dispersion and the

solution was not significantly affected. In this study, however, the grids used were one thousand feet in length, so that the range of distances affected by artificial dispersion was several orders of magnitude larger than the range over which physical dispersion occurred. Since artificial dispersion could not be absorbed by physical dispersion, its effect on the numerically obtained concentration distribution was significant. Thus, for cases in which relatively large grid sizes are used, the effects of artificial dispersion present a serious shortcoming in the use of the method of characteristics in this application. However, it has been observed that these effects are somewhat damped out in cases where changes in the flow patterns are gradual or flow is steady-state, and runs are made over a large number of time increments. Since the flow pattern in the field problem being considered in this study is assumed to be steady-state, it was concluded that the model is capable of producing a valid representation of this field situation.

Comparison of Results with Field Data

For all computer runs, initial conditions were set to correspond to field conditions in 1943 when the use of the waste disposal pond began. Since the chloride concentration in the pond was unknown, the basis for comparison of model results with field data was not absolute concentration, but rather the overall pattern of the concentration distribution and its behavior with time.

It was assumed that from 1943 to 1955 the pond was in constant use. A run was made for a model time of twelve years with a constant concentration of 1.0 in the grid containing the pond. Results of this run should have been similar to the concentration distributions measured by Petri and Smith (4) for 1955-1956. The concentration distribution map from this run is given in Figure 4-2. Comparison indicated that the model results were quite similar to the measured distributions. Of particular interest was the behavior of the contaminants in a narrow band extending northward along the borders of Sections 15 and 16 and Sections 9 and 10 of the study area. Petri and Smith's measurements (4) indicated rapid movement of highly contaminated water through this band. Results from the model also showed high concentrations in this area. Another region of interest was the area in Section 14 where concentrations were unusually low. Although the position of this region was shifted slightly in results from the model, its size, shape, and relatively low concentration were quite similar to the field situation.

Discrepancies may have been caused by discretizing and linear averaging between grid centers for the construction of the contour map, or lack of reliable data, particularly for permeabilities. However, the similarities between the distribution obtained from the model and the distribution from field measurements indicated that the model was effective in simulating this particular flow situation.

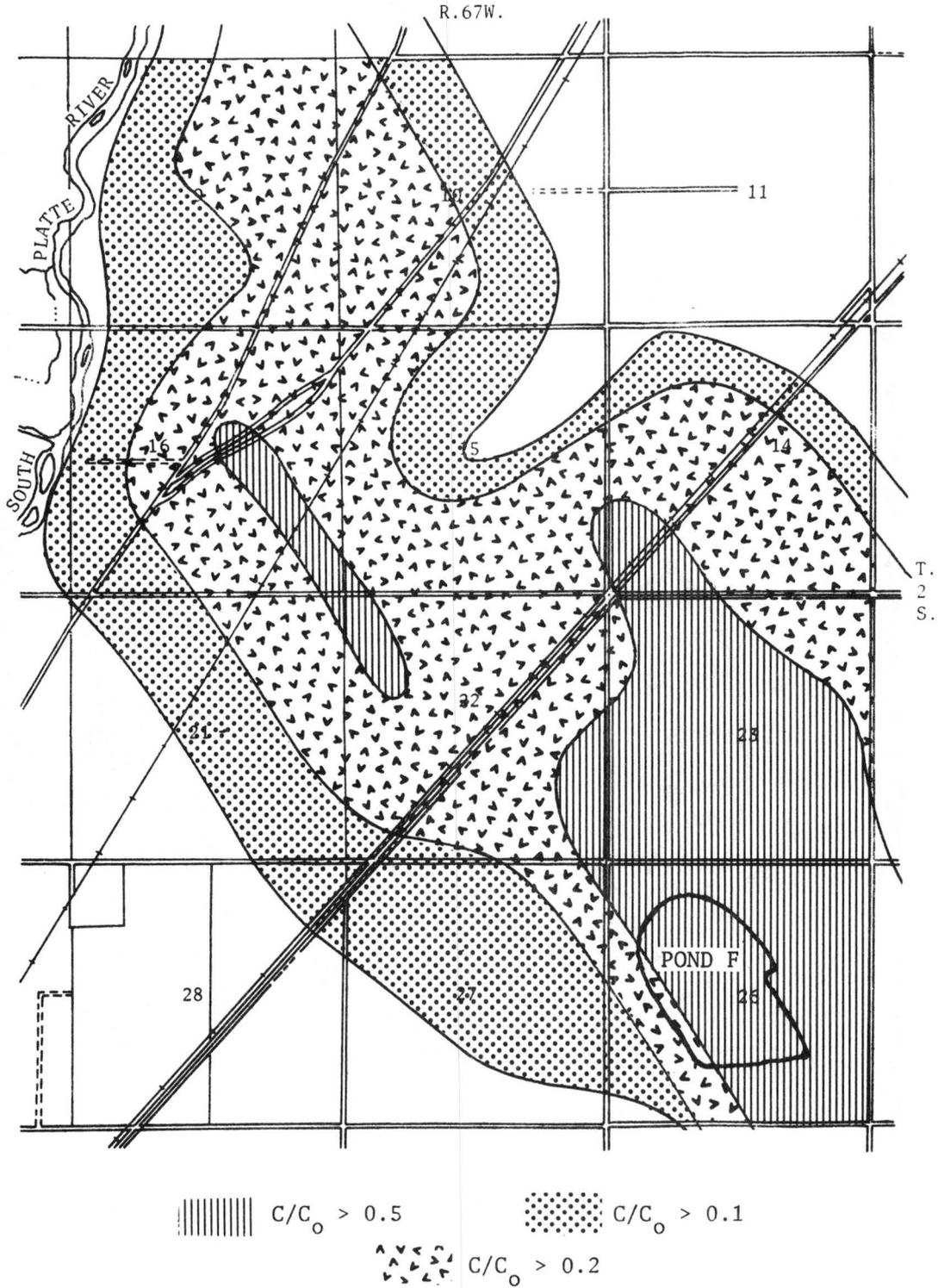


Figure 4-2. Computed distribution of relative chloride concentration for 1955.

Comparisons of concentration distributions obtained from the model for times after 1956 were difficult to evaluate since information regarding the behavior of the waste disposal pond was unavailable, and concentration data were inadequate. However, it was possible to determine the effectiveness of the model as well as to deduce information concerning the behavior of the contaminant source by comparing concentrations over a period of time in one grid of the model with measured concentrations from a well in the corresponding location of the study area. The well selected for the purpose was located at 2-67-9 daac (U.S. Bureau of Land Management notation). The grid in the model corresponding to the location of this well was (8, 12). Well measurements on concentration were made from 1960 to 1970 by anonymous (1).

Three runs were made to obtain concentration distributions after 1955. The first twelve years of each of these runs was identical to the initial run which was described above. At the twelve-year point, the concentration of the grid containing the pond was assigned a new value and the run continued using this new source concentration. Results of these three runs are given in Figure 4-3 along with measured concentrations from the well.

For the first run, the concentration of the source was assigned a value of zero at twelve years. Had the asphalt lining in pond F been completely effective in preventing contamination of the groundwater, and had pond A ceased to contaminate the aquifer as soon as

its use was discontinued, this run should have correctly modeled the observed behavior. Results of this run for grid (8, 12), shown in Figure 4-3, indicated that all contaminants from the waste disposal ponds should have left the study area by 1960. Field measurements show a considerable amount of chloride concentration remaining in the area after 1960, indicating that contamination from the ponds did not cease in 1955. There are several possible reasons for this.

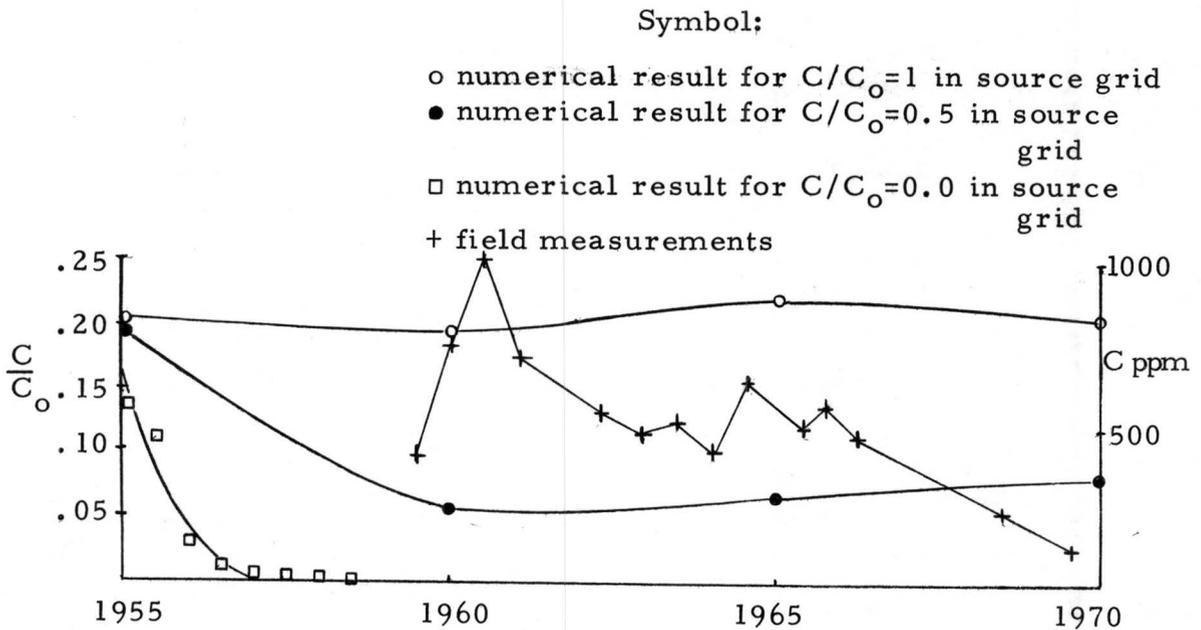


Figure 4-3. Chloride concentrations and relative chloride concentrations for grid (8, 12)

A large amount of contaminated water may have remained in and below the pond, above the water table, after the use of the pond was discontinued. The continued leaching of this body of water into

the ground water reservoir would have continued to cause contamination after 1955. Another possible reason for the continued contamination is that the concentration of salts in and near Pond A may have been high enough so that some of the salts precipitated out of solution and remained stored in the soil for as long as the concentration remained high enough to maintain a saturated solution. After use of the pond was discontinued, fresh water from precipitation or some other source of surface recharge redissolved these salts and transported them into the groundwater reservoir where they continued to cause contamination.

A break in the asphalt liner of Pond F caused by aging, faulty placement or chemical action of some of the wastes in the pond, may have caused the pond to leak, thus continuing the contamination of the groundwater.

In order to model a possible source of contamination from one of the causes mentioned above, a run was made with the source concentration set at 0.5 after 12 years. Results for grid (8, 12) for this run are given in Figure 4-3. After 1955 the concentration declined until about 1965, at which time it approached a quasi-steady-state condition, due to the fact that when the concentration in the permeable zone near the river reached a certain level, the river carried off as much contaminant as the waste disposal pond supplied. Field measurements indicated a yearly decline in the concentration after 1965, indicating that the model was incorrect. Rather than

remaining constant as was modeled, the source was becoming less concentrated as time passed. The field data also indicated an irregular nature in the source of contamination, by the fluctuations in the field data. This may have been caused by irregular surface recharge such as precipitation, dumping of waste water, or seepage from a nearby ditch, which percolated through zones of contaminated soil and carried dissolved salts into the groundwater reservoir. Other possible sources of contamination, such as creeks and ditches in the area which carry effluents of sewage plants, may have contributed to these fluctuations as well³.

Finally a run was made in which the concentration of the source remained at 1.0 throughout the run of forty years. The purpose of this run was to determine the long term effects of having continued disposal of wastes into the unlined pond as was being done prior to 1955. Results of this run for grid (8, 12) are shown in Figure 4-3.

Results indicated that the concentration throughout the area would have become constant in 1956, under the conditions stated above. This quasi-steady-state condition would have been reached when the amount of contaminants carried out of the area by the river became equal to the amount supplied by the pond. The concentration

³Walton, Graham, Public Health Aspects of the Contamination of Groundwater in South Platte River Basin in Vicinity of Henderson, Colorado, August, 1959, United States Department of Health, Education and Welfare, November 2, 1959, page 7.

distribution obtained for 1983 from this run is shown in Figure 4-4. This distribution is very similar to the distribution for 1955 shown in Figure 4-2, since the quasi-steady-state condition was reached soon after 1955.

Comparison of field measurements with model results indicated that contamination of the groundwater from waste disposal ponds did not cease in 1955, but was substantially reduced. A gradual decrease in measured concentrations indicated a possible depletion of the contaminant source. Irregularities in the measured concentration indicated the effects of intermittent surface recharge.

Discussion of Influences of the Solution Technique on Results

In addition to difficulties encountered in obtaining an accurate solution caused by inaccurate or inadequate data, discrepancies between model results and field measurements also occurred because of certain inherent characteristics of the solution technique. A numerical model is, at best, a simplified mathematical representation of a physical process. The assumptions and simplifications which are made to facilitate the use of the model may have significant effects on the form of the results. Several of the more important of these factors which were encountered in this study are discussed here.

Representation by Discrete Elements. The flow of contaminants in a groundwater reservoir is a continuous process in space and

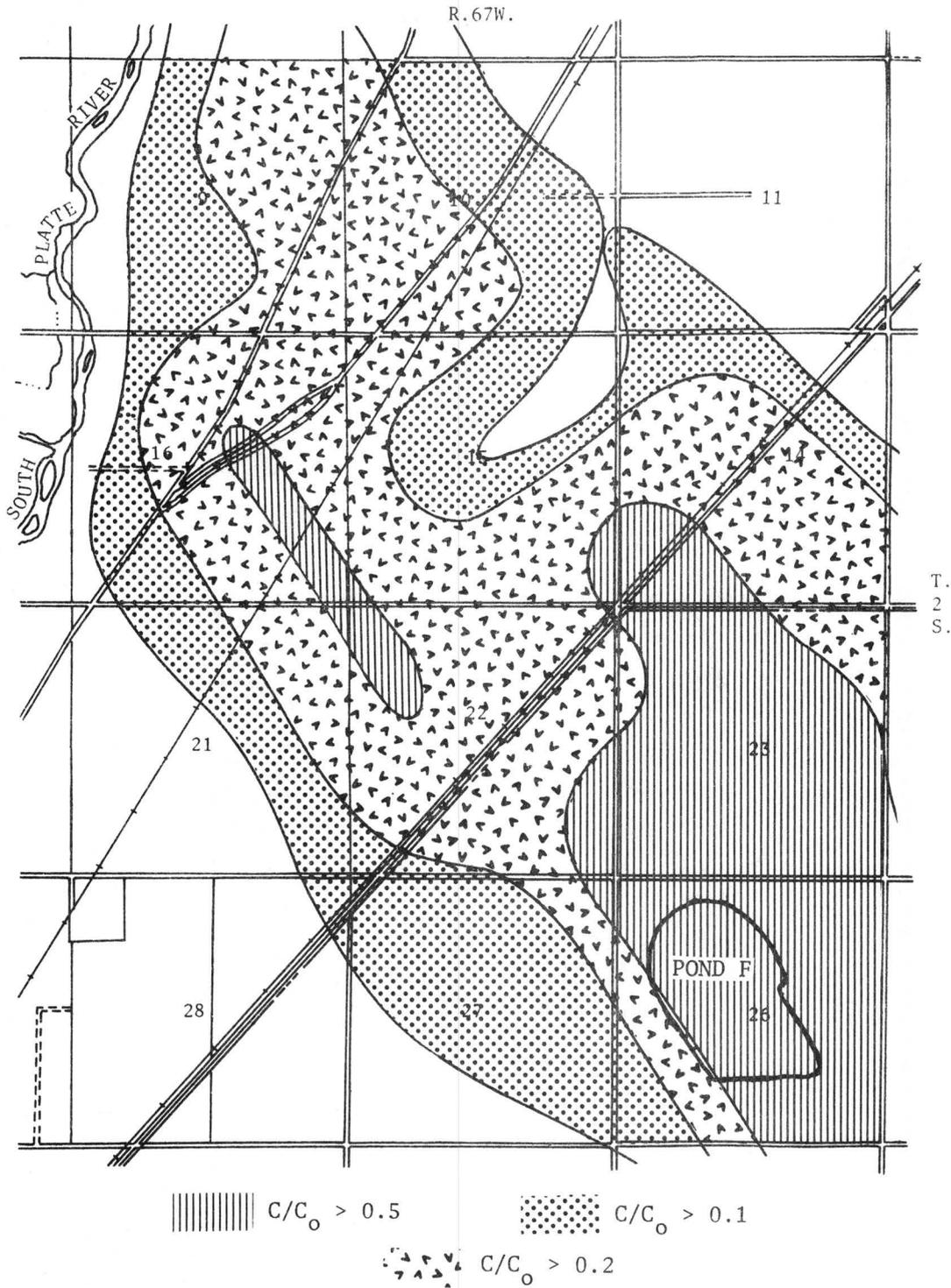


Figure 4-4. Computed distribution of relative chloride concentration for 1983

time. The increments of both distance and time over which conditions remain constant is very small. In a numerical model it is seldom possible to choose increments small enough so that the use of discrete elements does not introduce error, particularly for as large an area as was being considered in this study. However, if the sizes of time and distance increments are chosen appropriately for the existing conditions, error can be minimized without reducing the size of the increments unnecessarily. For this case, fairly large grids of 0.5 miles square were used, since the flow pattern for most of the study area was well-behaved. Since flow in porous media is generally quite slow, and changes are gradual, large time increments of from one week to one month were used in this study. It was determined that the adverse effects of representing the field situation by discrete elements were not serious enough to significantly reduce the validity of the model.

Length of Time Increment. Although the range of appropriate values for the time increment was known, determining the particular value which would yield correct results proved difficult. It was determined from intermediate runs that results were very sensitive to the length of the time increment. A change of as little as two days (15%) caused the resulting concentration distribution to be completely dissimilar to results of runs made with different time increments. The reasons for this sensitivity and the manner in which an appropriate time increment was selected are explained below.

Concentration points were "moved" through each time increment by relocating each of them a distance equal to the vector sum of the velocity components at the point multiplied by the time increment. The ideal choice for a time increment would be one which would move a point a great enough distance to minimize required computer time, but small enough to minimize error.

The use of too large a time increment would cause points to pass through more than one grid per time increment. The result would be a distribution composed of slugs of high concentration surrounded by areas of zero concentration, rather than the smooth, gradual spread which is known to take place in physical reality. A run was made using a time increment of 26.6 days. The resulting distribution showed some gradual spread and a pattern somewhat similar to the measured distribution. However, because points were being moved through the model in a few long steps, they made too few steps to impart enough concentration to the model. As a result, concentrations remained low, spread of contaminants was restricted, and the overall distribution was irregular.

Points were relocated to their original positions after every ninth step to prevent the depletion of points at the inflow boundary and at locations of divergence in the flownet. For this reason it was necessary to choose a time increment large enough so that all points would pass through at least one grid in nine time steps. The

use of too small an increment of time would have had the effect of "trapping" concentration points in grids with low velocities. Concentration is spread by points moving across grid boundaries and imparting their concentrations to other grids. If points move too short a distance to pass out of their original grid before they are re-located at their initial positions, the concentration cannot move into the next grid. A run was made using a time increment of 10 days. The resulting concentration distribution was quite dissimilar to the measured distribution due to the trapping of points in several grids which prevented the spread of concentration from being modeled correctly.

Since velocities throughout the model varied by as much as two orders of magnitude it was impossible to choose a time increment which was appropriate for all locations throughout the model. Due to the large number of points in the model and the wide variation of velocities moving these points, predicting the accuracy of results obtained using any particular time increment was difficult. Therefore, a trial-and-error process was used to obtain the time increment which produced a concentration distribution most closely resembling the distribution obtained from field measurements. This time increment, which was 13.3 days, was used for all final runs. It was assumed that as long as the flow pattern remained unchanged, results from runs using this time increment would be valid. This

assumption gave some reliability to the results of runs made for predicting future contamination of the area, for which no measured concentration distributions were available for comparison.

Although the range of velocities in this case was two orders of magnitude, the computed results obtained indicated that the time increment used was appropriate for most of the points in the model. If trapping of points with low velocities or grid skipping by points with high velocities occurred, the resulting effects were not serious enough to cause appreciable error.

Method of Characteristics. The number and configuration of concentration points in each grid, as well as the shape of the grids were found to have significant effects on the results. Theoretically the larger the number of points, the more accurate and definitive the results. However, investigation by Reddell (6) showed that this was not necessarily true, and that for some cases the accuracy of results decreased as larger numbers of points were used. The reason for this is that the accuracy of results depends, not on a single factor, but on the time increment, flow pattern, and concentration points all behaving in the correct manner simultaneously. Thus various combinations of numbers of points and time increments act together to produce good results while others do not. An increase in the number of points while holding the time increment constant may or may not improve results, depending on

whether a favorable combination is formed. Runs were made using four points per grid and nine points per grid. Although the nine point run required almost twice the computer time used by the four point run the results did not improve significantly and the concentration distribution obtained was dissimilar to the measured distribution in some areas. The four point configuration was used for final runs.

The initial configuration of points and the shape of the finite difference grids had significant effects on the validity of the results. No runs were made using either distorted grids or a configuration of points for which the spacing in the X direction was different from the spacing in the Y direction. However, hand calculations indicated that both conditions would produce distorted concentration distributions as illustrated in Figure 4-5.

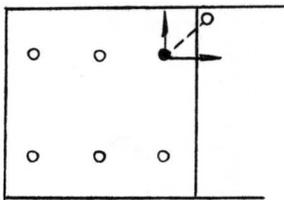


Figure 4-5a. Effect of unequal point spacing in X and Y directions

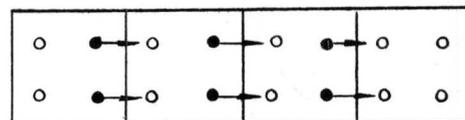
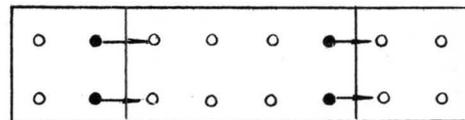


Figure 4-5b. Effects of elongated versus square grid

In Figure 4-5a there are three points per grid in the X direction, but only two in the Y direction. The velocity components are of equal magnitude. The point has been moved through one time increment. Because of the unequal spacing, the point has crossed the grid boundary in the X direction but not in the Y direction. Thus the concentration travels more quickly through the model in the X direction than in the Y direction.

A similar effect is caused by the distorted grid in Figure 4-5b. Points moving into the left end of the elongated grid impart their concentration to the entire grid, so that at the next time increment, some concentration moves into the last grid. By comparison, in the set of four square grids it takes three time increments for a concentration to arrive at the same location, instead of just two. Thus the concentration moves more quickly in the direction of the elongation of the distorted grid. In order to avoid such distortion, a configuration of square grids, each containing four equally spaced points was used in this study.

At locations of divergence in the flownet and relatively high velocities, it was possible for the points to become so arranged that a grid contained no points at a particular time. This occurrence had the effect of setting the concentration in that grid equal to zero. At later time steps points again moved into the grid and the concentration built up accordingly.

Since it was known that in physical reality such events do not occur, an attempt was made to prevent this from happening. When the concentration in any grid dropped to zero, it was reset to a value slightly less than the grid concentration for the previous time step. However, it was observed that this had the effect of creating artificial concentration sources, which did not correctly represent the real situation. Therefore this practice was discontinued.

It was found that averaging the values of concentration in each grid over several time increments, including zero values, produced the correct concentration distribution. Although the occurrence of grid concentrations dropping to zero was somewhat disturbing, re-results indicated that this effect did not decrease the validity of the model, and in fact, this occurrence was a part of the normal operation of the model.

Two Dimensional Representation of Concentration. The use of a two-dimensional model had the effect of making all parameters at any location uniform in the vertical direction, including velocity components, saturated thickness, and concentration. The effects of discretizing these parameters was discussed in a previous section. In the case of concentration, an additional error in this assumption of vertical uniformity was present in the vicinity of the waste disposal pond. The location of the bed of the pond with respect to the water table was unknown. It was almost certain,

however, that the pond bed was some distance above the bedrock in that location. Thus the contaminants from the pond were introduced into the aquifer from above as shown in Figure 4-6.

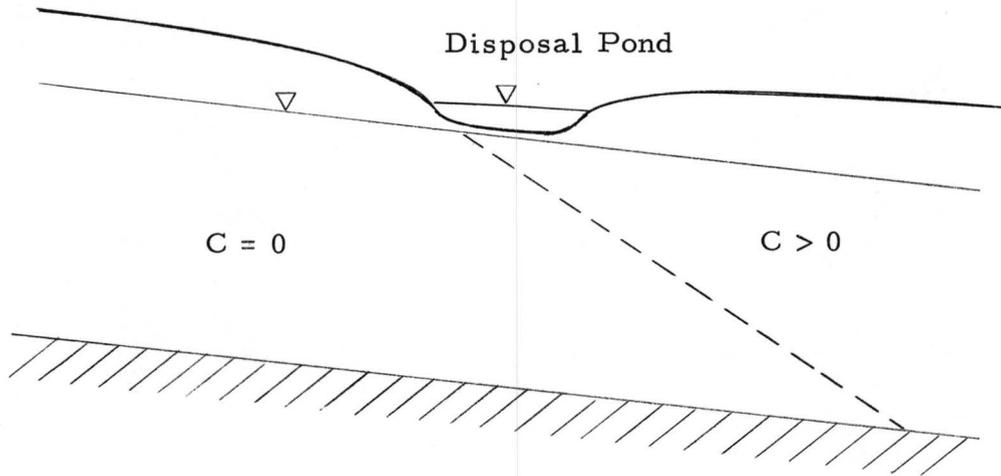


Figure 4-6. Vertical movement of contaminants below waste disposal pond

As soon as the contaminants reached the water table they began mixing with the groundwater. At the same time, however, they were being moved downgradient by the velocity of the groundwater, so that the location at which the concentration became vertically uniform was some distance downgradient from the waste disposal pond. Because of this, the representation of the concentration as uniform in the vertical direction was incorrect in the grid corresponding to the location of the waste disposal pond and possibly some of the adjacent grids downgradient from the pond location.

Since the extent of this effect was not large with respect to the size of the study area, it was assumed that error caused by this misrepresentation was not significant.

Technique for Obtaining Velocities. The method by which grid velocities and point velocities were calculated was based on the premise that flow occurred only in the positive direction of both axes. For this particular flow situation there were a number of locations where flow existed in the negative Y direction. Because of the averaging technique used, which was described in Chapter 3, the Y velocity components in these locations were calculated on the basis of the characteristics of the adjacent downgradient grid, instead of the adjacent upgradient grid as they should have been. Fortunately, most of these negative Y velocity components occurred in locations where gradients were nearly constant and permeabilities were fairly uniform, so that errors caused by the incorrect method of calculation were small. Further refinement of the techniques for calculating velocities, so that the use of the upgradient grid for averaging would always be assured, would be desirable for this case, and would be essential in order to obtain correct solutions in more complex flow situations. Such a refinement was not pursued in this study.

Mass Balance. Values for water table elevation, saturated thickness, and permeability were defined as input data to each grid.

The flow situation was defined for this case as steady state. This implied that net inflow to every grid in the system was zero, and that the continuity equation for any grid could be written as:

$$\begin{aligned}
 & 2 \frac{k_{i-1,j} k_{i,j}}{k_{i-1,j} + k_{i,j}} \frac{(m_{i,j} + m_{i-1,j})}{2} \Delta x \frac{(h_{i-1,j} - h_{i,j})}{\Delta x} \\
 & + 2 \frac{k_{i,j-1} k_{i,j}}{k_{i,j-1} + k_{i,j}} \frac{(m_{i,j} + m_{i,j-1})}{2} \Delta x \frac{(h_{i,j-1} - h_{i,j})}{\Delta x} \\
 & + 2 \frac{k_{i+1,j} k_{i,j}}{k_{i+1,j} + k_{i,j}} \frac{(m_{i,j} + m_{i+1,j})}{2} \Delta x \frac{(h_{i+1,j} - h_{i,j})}{\Delta x} \\
 & + 2 \frac{k_{i,j+1} k_{i,j}}{k_{i,j+1} + k_{i,j}} \frac{(m_{i,j} + m_{i,j+1})}{2} \Delta x \frac{(h_{i,j+1} - h_{i,j})}{\Delta x} = 0. \quad (4-2)
 \end{aligned}$$

Since the right hand side of the equation was defined as zero by definition of steady-state conditions, and since all parameters on the left hand side of the equation were given as input data, equation 4-2 was overdetermined. It was found that for most grids this equation could not be completely satisfied, nor could continuity be satisfied for the model as a whole. The error in mass balance was determined to be approximately thirteen percent of the inflow to the study area.

The failure of the flow situation to exactly satisfy continuity indicated inaccuracy in one or more of the measured parameters. However, it was impossible to determine by what amount each of the

parameters was in error and in what location in the model. Water table elevations and bedrock elevations were both subject to errors in measurement of approximately ten percent. Permeability data was subject both to errors in measurement of the water table and errors in the graphical solution technique. Errors in permeability were estimated to be approximately 25 percent. In spite of these errors, all three parameters were physically reasonable and reliable within certain limits of accuracy. By using these parameters in their original form, the solution obtained could be assigned some measure of reliability. If any of these parameters had been adjusted for the sake of satisfying continuity, their reliability, hence the reliability of the solution, would have been lost. While it would have been desirable for the flow situation to have satisfied continuity, forcing it to do so at the expense of the accuracy of the input parameters would have been self-defeating.

CONCLUSIONS AND RECOMMENDATIONS

From the results of this study it was concluded that, although use of the unlined waste disposal pond was discontinued in 1955, contamination of the groundwater by wastes from this pond has continued in significant amounts since that time.

Despite various difficulties encountered in the operation of the numerical model used in this study, it was concluded that this model could provide an effective means of simulating the behavior of contaminants in many types of two-dimensional flow situations in unconfined aquifers.

The following recommendations for further investigation in this area of interest are given.

1. A study should be undertaken to determine in more detail, the effects of using distorted grids and uneven point configurations, possibly with the intention of discovering a means of using these advantageously.
2. The method of obtaining velocity components should be refined to give a better representation of physical reality.
3. The sensitivity of the results to the choice of time increment and point configuration should be investigated

for the purpose of finding a means of predicting what combination of time increments and point configurations yield valid results.

BIBLIOGRAPHY

1. _____, Group of Graphs of Chloride Concentration from 1960 to 1970, Unpublished, 1970.
2. _____, Group of Tables of Chloride Concentration from 1960 to 1970, Unpublished, 1970.
3. Petrie, L. R., "The Movement of Saline Ground Water in the Vicinity of Derby, Colorado", Proceedings of the 1961 Symposium on Ground Water Contamination, Technical Report W61-5, Robert A. Taft Sanitary Engineering Center, United States Department of Health, Education, and Welfare, April 5-7, 1969.
4. Petri, Lester R., and Smith, Rex O., Investigation of the Quality of Ground Water in the Vicinity of Derby, Colorado, United States Department of the Interior, Geological Survey, Water Resources Division, 1956.
5. Pinder, George F., Cooper, Hilton, H. Jr., "A Numerical Technique for Calculating the Transient Position of the Salt-water Front", Journal of Water Resources Research, Vol. 6, No. 3, June, 1970.
6. Reddell, Donald L., Dispersion in Groundwater Flow Systems, Ph.D. Dissertation, Colorado State University, December, 1969.
7. Smith, Rex O., Schneider, Paul A., and Petri, Lester R., Groundwater Resources of the South Platte River Basin in Western Adams and Southwestern Weld Counties, Colorado, Geological Survey Water Supply Paper 1658, United States Government Printing Office, Washington, D. C., 1964.
8. Todd, David K., Ground Water Hydrology, John Wiley & Sons, Inc., 1959.
9. Walton, Graham, Public Health Aspects of the Contamination of Groundwater in South Platte River Basin in Vicinity of Henderson, Colorado, August 1959, United States Department of Health, Education, and Welfare, November 2, 1959.

10. Walton, Graham, "Public Health Aspects of the Contamination of Ground Water in the Vicinity of Derby, Colorado", Proceedings of the 1961 Symposium on Ground Water Contamination, Technical Report W61-5, Robert A. Taft Sanitary Engineering Center, United States Department of Health, Education, and Welfare, April 1-7, 1969.

APPENDICES

APPENDIX A

DATA USED IN NUMERICAL MODEL

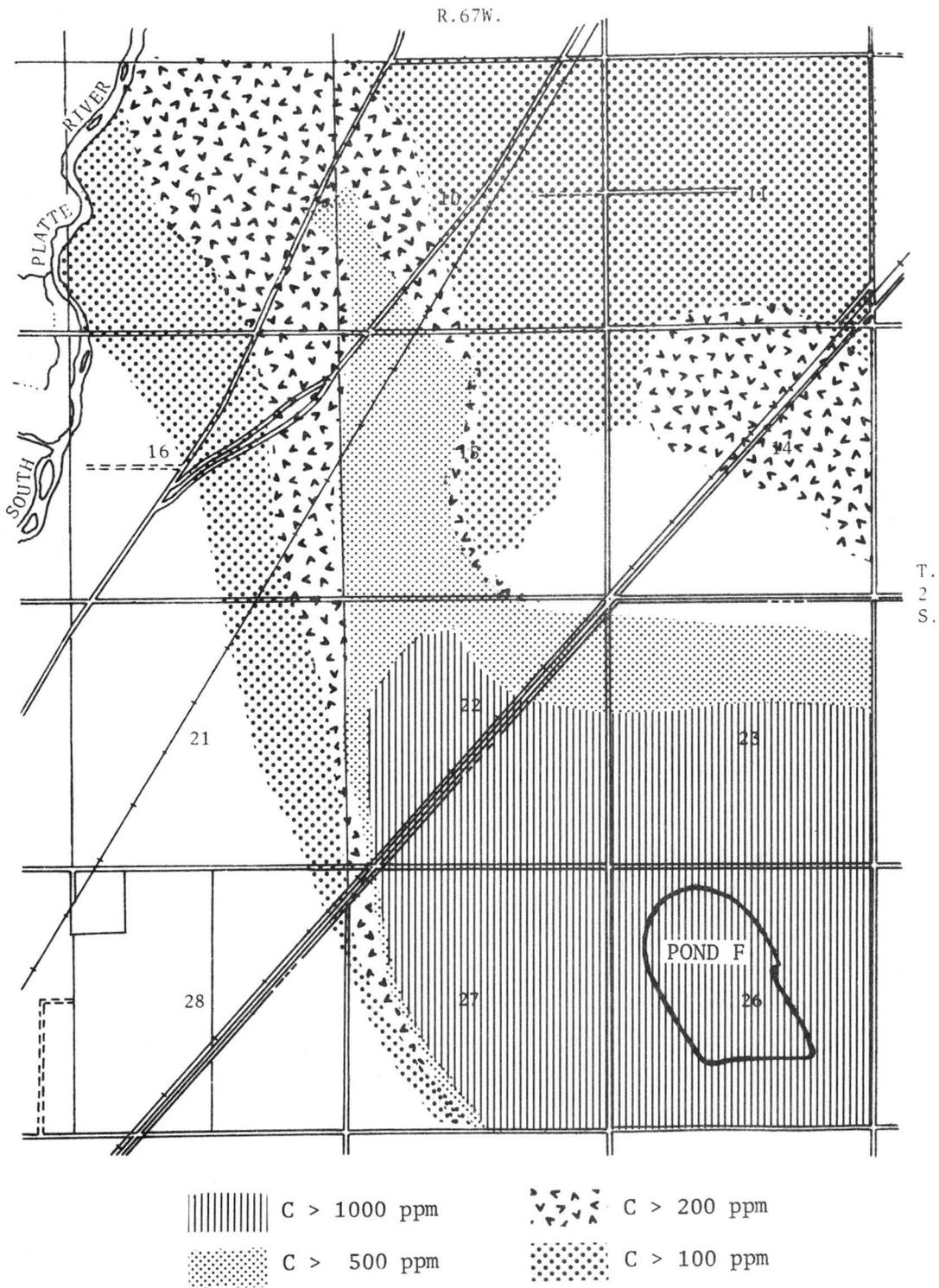


Figure A-1. Measured chloride concentrations for September-October 1955
 (After Petri and Smith (4))

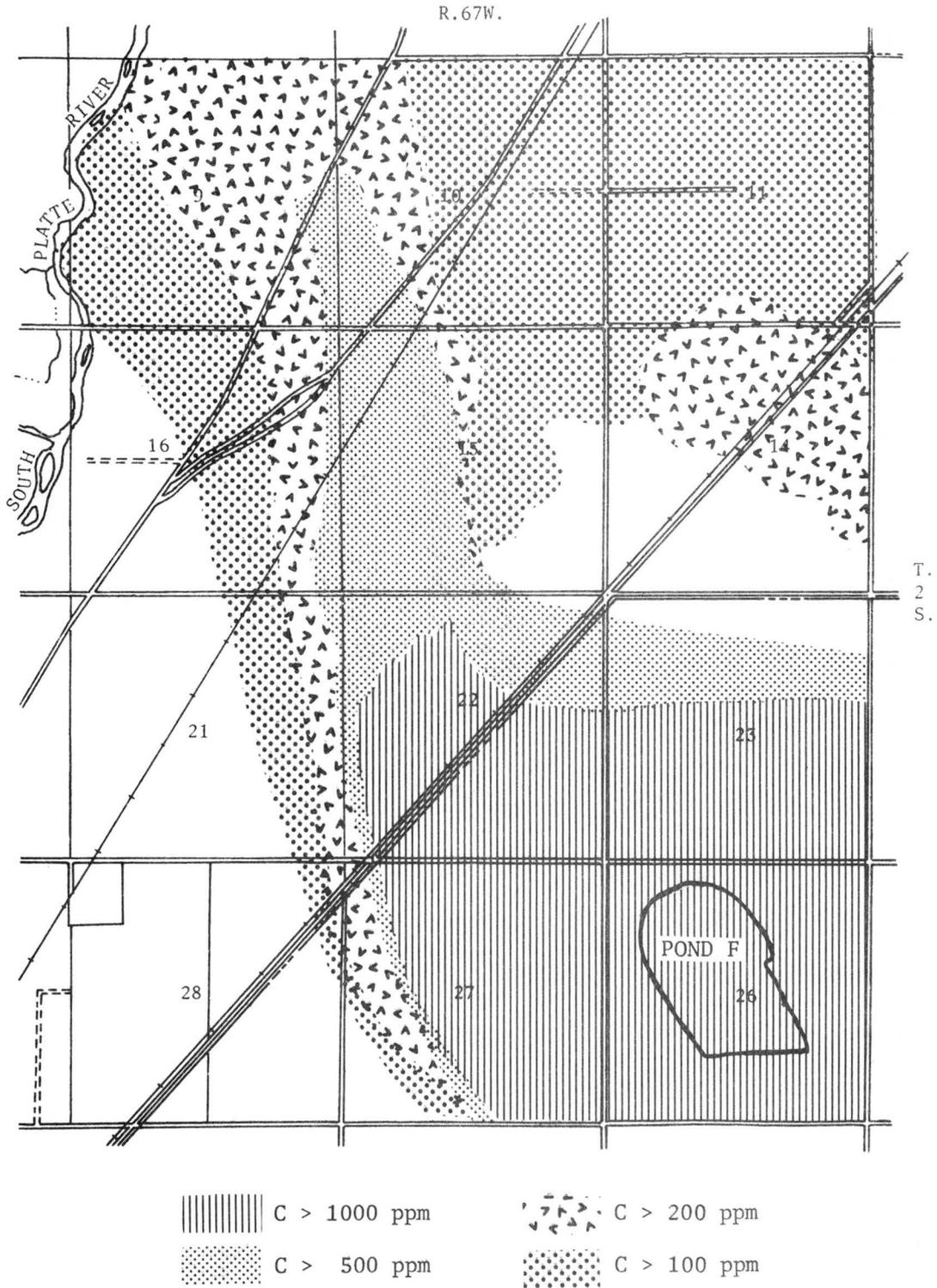


Figure A-2. Measured chloride concentrations for November 1955
 (After Petri and Smith (4))

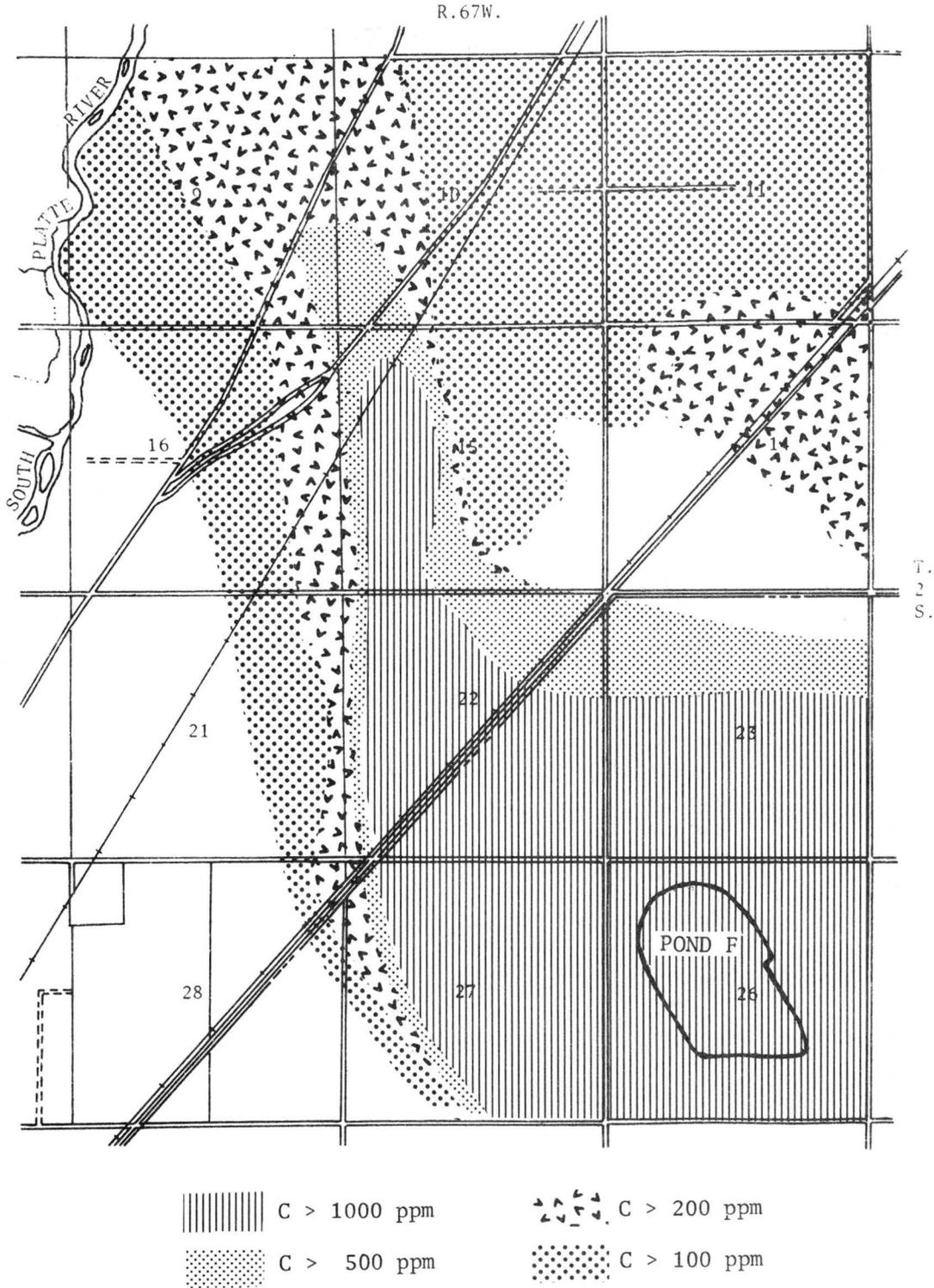


Figure A-3. Measured chloride concentrations for March 1956

(After Petri and Smith (4))

APPENDIX B

PROCEDURE FOR OBTAINING PERMEABILITIES

APPENDIX B

PROCEDURE FOR OBTAINING PERMEABILITIES

The graphical procedure by which values for permeabilities in each grid of the model were obtained employs Darcy's law and the principle of continuity. This procedure is presented by Todd (8). In order for the use of this graphical procedure to be valid flow conditions must be steady-state.

Using the water table contour map, shown in Figure 2-1, a flownet was constructed. Since the permeability in the study area was nonuniform, each two consecutive streamlines and each two consecutive equipotential lines formed "rectangles" instead of the "squares" formed in conventional flownets for homogeneous material. The flownet is shown in Figure B-2.

A portion of the flownet is shown in Figure B-1 with the following parameters defined:

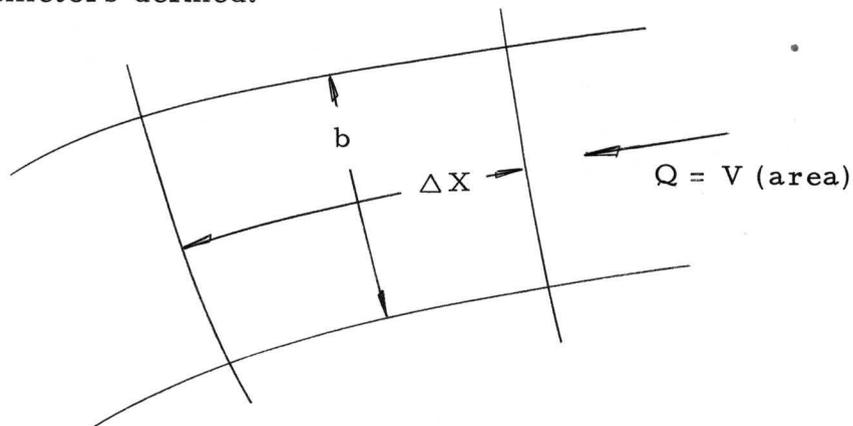


Figure B-1. Representative "rectangle" from flownet showing parameters

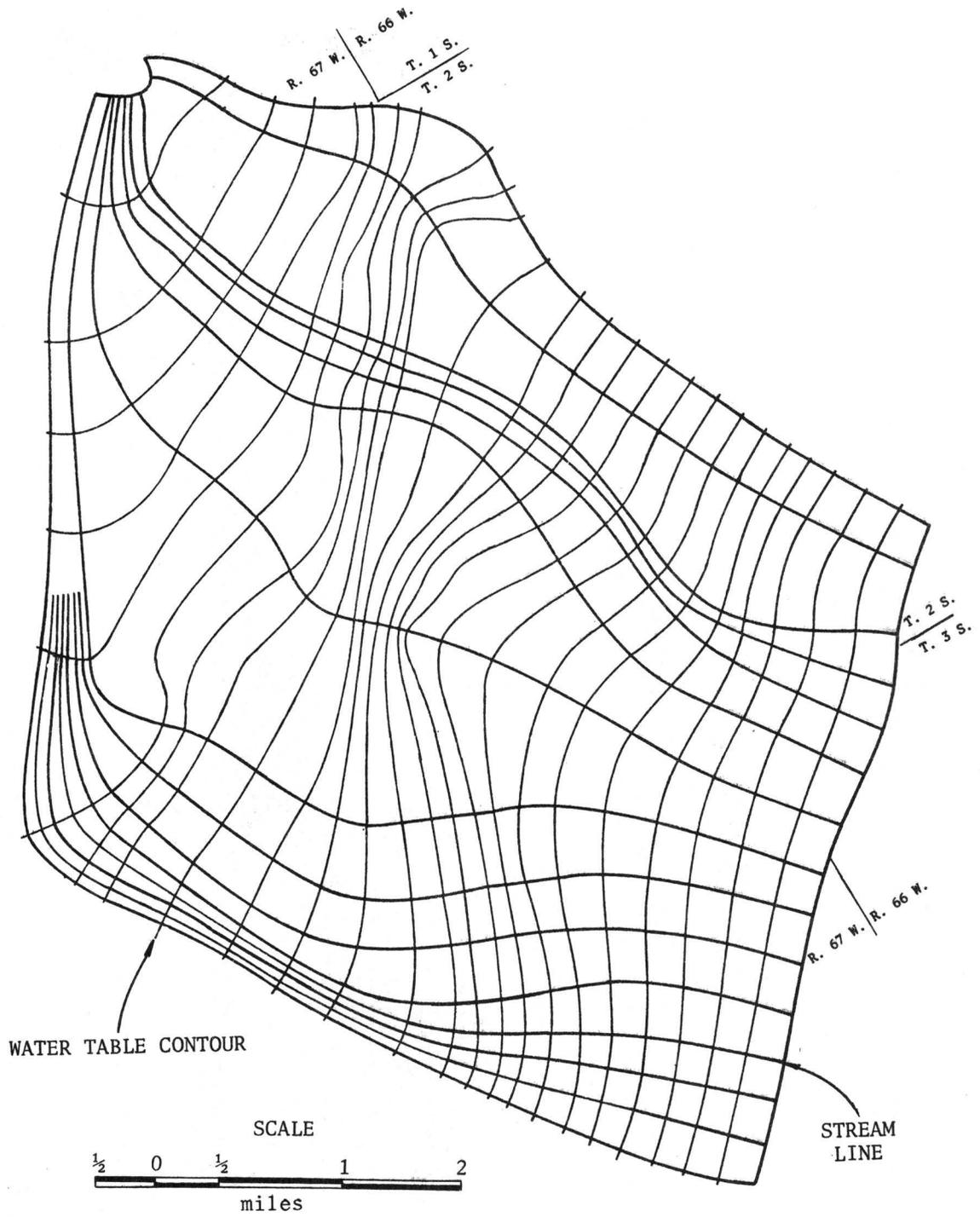


Figure B-2. Flownet

Q = discharge between each two consecutive streamlines. Since by definition, no flow crosses a streamline, Q is constant between each two streamlines for the length of the stream tube. The flownet was constructed so that discharge is everywhere constant.

b = perpendicular distance between two consecutive streamlines at any location.

Δx = perpendicular distance between two consecutive equipotential lines at any location.

V = velocity at any location.

Within each "rectangle" constant values were assumed for gradient and permeability. Average values for b and Δx for each "rectangle" were taken as the width and length. The expression for the discharge in each "rectangle" given these assumptions, is:

$$Q = Tb \frac{\Delta h}{\Delta x} = \text{constant} \quad (\text{B-1})$$

where

T = transmissibility

Δh = equipotential drop across each "rectangle". For all "rectangles" Δh is a constant, equal to the contour interval of the water table elevation map.

Solving for T , equation B-1 becomes:

$$T = \frac{Q}{\Delta h} \frac{\Delta x}{b} \quad (\text{B-2})$$

Since Q and Δh are everywhere constant, equation B-2 may be expressed as:

$$T = (\text{constant}) \left(\frac{\Delta x}{b} \right) \quad . \quad (\text{B-3})$$

The constant in equation B-3 is a conversion factor relating the ratio of the dimensions of some "rectangle" in the flownet to a measured value of transmissibility in the corresponding location of the study area. The relative transmissibility is defined at any location as the value, which when multiplied by the conversion factor, yields the transmissibility. This value is the ratio of the dimensions of the "rectangle" in that location

$$T_{\text{rel}} = \frac{\Delta x}{b} \quad . \quad (\text{B-4})$$

Values of b and Δx are obtained by direct measurement from the flownet. A map of relative transmissibilities in the study area obtained by the method described in this section is given in Figure B-3.

The grid system of the model was superimposed on Figure B-3. The relative transmissibility of each grid was taken as the area-weighted average of the transmissibilities within the grid boundary.

Relative transmissibilities were converted to permeabilities by SUBROUTINE TRANS, using the following procedure. A



Figure B-3. Graphically determined permeabilities

measured hydraulic conductivity in the study area was first converted from units of gpd/ft^2 to units of ft^2 . This value, when divided by the relative permeability of the corresponding grid in the model, served as a dimensionless conversion factor for the entire grid system. Relative transmissibilities were then converted to relative permeabilities by dividing the relative transmissibility in each grid by the saturated thickness of that grid. This conversion, expressed for the $(i, j)^{\text{th}}$ grid is:

$$k_{\text{rel } i, j} = \frac{T_{\text{rel } i, j}}{m_{i, j}} \quad . \quad (\text{B-5})$$

Absolute permeabilities were then obtained by multiplying the relative permeability in each grid by the conversion factor. For grid (i, j) this conversion is expressed as:

$$k_{\text{abs}} = (k_{\text{rel}}) (\text{conv}) \quad . \quad (\text{B-6})$$

These absolute permeability values are tabulated in Appendix A in the form of input data to the model.

APPENDIX C

DESCRIPTION OF COMPUTER PROGRAM

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DESCRIPTION OF COMPUTER PROGRAM

Description of Main Program and Subroutines

SSDISP is the main program. Its function is to read in data, initialize parameters, control the cycling of the time incrementing loop, call subroutines to perform special operations, and control the printing of results.

INICON sets up the array of moving points. It initializes all point locations and concentrations and creates a set of auxiliary points for use at the inflow boundary in case of depletion of regular points.

INIPRT arranges the initial data and supplies headings for printout with the aid of subroutine MATROP.

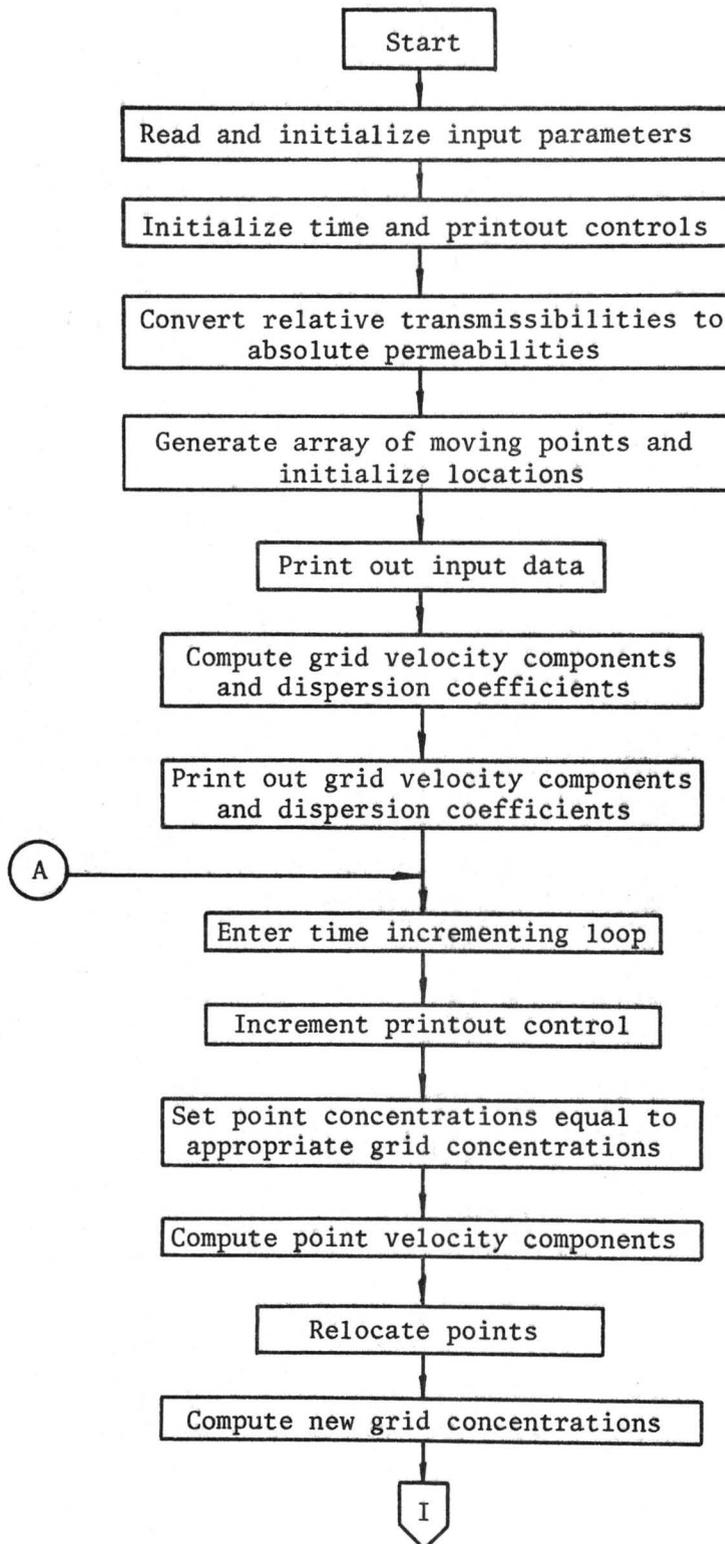
MATROP arranges all two-dimensional arrays in a form suitable for printout, then executes the printout. MATROP is used to print all initial data and final results which are in the form of two-dimensional arrays.

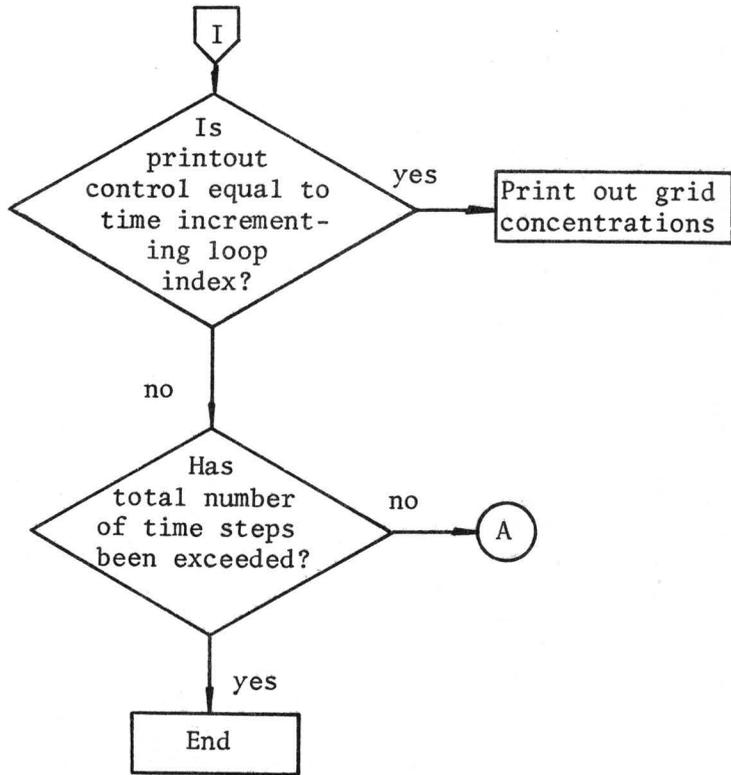
MOVPT executes all calculations pertaining to concentration and movement of contaminants. At each time step this subroutine calculates velocity components for each moving point, relocates all points, computes new grid concentrations, and reassigns these new concentrations to each point.

TRANS converts relative transmissibilities in each grid to absolute permeabilities.

VELOCITY calculates velocity components for each grid interface. When dispersion becomes significant, statements are also available in this subroutine for the calculation of the longitudinal and lateral dispersion coefficients.

FLOWCHART OF PROGRAM SSDISP





```

PROGRAM SSDISP(INPUT,OUTPUT,TAPES=INPUT,TAPE6=OUTPUT)
*****

SSDISP IS THE MAIN PROGRAM. ITS FUNCTIONS ARE TO READ IN DATA, INITIALIZE
PARAMETERS, CONTROL THE CYCLING OF THE TIME INCREMENTING LOOP, CALL
SUBROUTINES TO PERFORM SPECIAL OPERATIONS, AND CONTROL THE PRINTING
OF RESULTS.

*****
      DIMENSION ENDCON(20,30)
      COMMON NR,NC,NPX,NPY,DX,DY,RHO,DELT,ST,FWTOP,G,VIS,NPW,NPL,IR,IC,
1      FK(20,30),H(20,30),POR(20,30),CAVG(20,30),CAVGP(20,30),
2      SUMC(20,30),COUNT(20,30),DFLC(20,30),D11(20,30),D22(20,30),
3      D12(20,30),VX(20,30),VY(20,30),C(2500),X(2500),Y(2500),
4      XIR(100),YIR(100),CIB(100),SL(100),NXPOND,NYPOND,BREV(20,30),
5      XI(2500),YI(2500),NNN,CST
      READ(5,12)NR,NC,NPX,NPY
12  FORMAT(4I5)
      READ(5,112)DX,DY,RHO,DELT,ST,FWTOP,G,VIS
112 FORMAT(8F10.4)
      DELT=40.0/3.0
      READ(5,61) NXPOND,NYPOND
61  FORMAT(2I5)
      DO 7 I=1,NR
      DO 7 J=1,NC
      READ(5,11)NV,NW,FK(I,J),H(I,J),BREV(I,J)
11  FORMAT(2I3,14X,3F20.2)
      POR(I,J)=0.227
      ENDCON(I,J)=0.0
      IF(NV.EQ.I.AND.NW.EQ.J) GO TO 7
      WRITE(6,113)
113 FORMAT(1H0,5X,* DATA CARDS OUT OF ORDER-- CALCULATIONS STOPPED*)
      GO TO 746
7  CONTINUE
      SNAG=0.0
      SLIP=0.0
      LAP=0
      DFCLM=0.0
      CAVGM=0.0
      NPW=NR*NPY
      NPL=NC*NPX
      TIME=0.0
      NNN=0
      CALL TRANS
      CALL INICON
      CALL INIPRT
      ST=ST*86400.0
      DELT=DELT*86400.0
      PCNT=1.0
      IC=NC+1
      IR=NR+1
      CALL VELOCY
      LOOPUL=ST/DELT
      WRITE(6,14)
      CALL MATROP (NR,IC,VX)
      WRITE(6,15)
      CALL MATROP (IR,NC,VY)

```

```

WRITE(6,16)
CALL MATROP (NR,NC,D11)
WRITE(6,17)
CALL MATROP (NR,NC,D22)
WRITE(6,18)
CALL MATROP (NR,NC,D12)
DO 8 ILAST=1,LOOPUL
TIME=TIME+DELT/86400.
LAP=LAP+1
LMAR=LOOPUL-LAP
CALL MOVPT (TIME,DELCM,CAVGM)
IF(LMAR.LT.10.AND.SNAG.LT.0.9) SNAG=1.0
IF(CAVG(8,12).GT.0.5.AND.SLIP.EQ.0.0) SNAG=1.0
IF(SNAG.GE.1.0) GO TO 304
IF(TIME.GT.4310.0.AND.TIME.LT.4330.0) GO TO 65
IF(PCNT.GE.FWTOP.AND.TIME.GT.4600.0) GO TO 65
IF(SNAG.LT.0.9) GO TO 23
304 DO 288 I=1,NR
DO 288 J=1,NC
ENDCON(I,J)=(ENDCON(I,J)*(SNAG-1.0)+CAVC(I,J))/SNAG
288 CONTINUE
IF(SNAG.EQ.10.0.OR.SNAG.EQ.5.0) GO TO 289
GO TO 64
289 IF(SNAG.EQ.5.0) WRITE(6,29) TIME
IF(SNAG.EQ.10.0) WRITE(6,30) TIME
29 FORMAT(1H0,30X,54HCONCENTRATIONS AVERAGED OVER FIVE TIME STEPS AT
2TIME =.F10.2,6H DAYS,1H /)
30 FORMAT(1H0,30X,53HCONCENTRATIONS AVERAGED OVER TEN TIME STEPS AT T
2IME =.F10.2,6H DAYS,1H /)
CALL MATROP(NR,NC,ENDCON)
64 SNAG=SNAG+1.0
IF(SNAG.LE.10.0) GO TO 65
SLIP=1.0
SNAG=0.0
DO 300 I=1,NR
DO 300 J=1,NC
ENDCON(I,J)=0.0
300 CONTINUE
65 WRITE(6,19) TIME
CALL MATROP (NR,NC,CAVGP)
WRITE(6,25) TIME
CALL MATROP (NR,NC,CAVG)
IF(DELCM.EQ.0.0) GO TO 22
WRITE(6,26) TIME
CALL MATROP (NR,NC,DELC)
22 PCNT=0.0
23 CONTINUE
PCNT=PCNT+1.0
8 CONTINUE
9 FORMAT(1H0,10X,9HSTORAGE =.E10.3,10X,14HTRACER STORAGE =.E10.3 )
13 FORMAT(1H ,15F8.3)
14 FORMAT(1H0,60X,* X-VELOCITIES*)
15 FORMAT(1H0,60X,* Y-VELOCITIES*)
16 FORMAT(1H0,60X,* D11 *)
17 FORMAT(1H0,60X,* D22 *)
18 FORMAT(1H0,60X,* D12 *)
19 FORMAT(1H0,52X,15HCAVGP AT TIME =.F10.2,6H DAYS,1H /)
25 FORMAT(1H0,52X,14HCAVG AT TIME =.F10.2,6H DAYS,1H /)
26 FORMAT(1H0,52X,14HDELC AT TIME =.F10.2,6H DAYS,1H /)
746 CALL EXIT
END

```

SUBROUTINE INICON

INICON SETS UP THE ARRAY OF MOVING POINTS. IT INITIALIZES ALL POINT LOCATIONS AND CONCENTRATIONS AND CREATES A SET OF AUXILIARY POINTS FOR USE AT THE INFLOW BOUNDARY IN CASE OF DEPLETION OF REGULAR POINTS.

```

COMMON NR,NC,NPX,NPY,DX,DY,RHO,DELT,ST,FWTOP,G,VIS,NPW,NPL,IR,IC,
1  FK(20,30),H(20,30),POP(20,30),CAVG(20,30),CAVGP(20,30),
2  SUMC(20,30),COUNT(20,30),DELC(20,30),D11(20,30),D22(20,30),
3  D12(20,30),VX(20,30),VY(20,30),C(2500),X(2500),Y(2500),
4  XIR(100),YIR(100),CIB(100),SL(100),NXPOND,NYPOND,BREV(20,30),
5  XI(2500),YI(2500),NNN,CST
  LREG=1-NPW
  LEND=0
  PX=NPX
  PY=NPY
  DO 7 I=1,NR
  DO 7 J=1,NC
  DELC(I,J)=0.0
  CAVG(I,J)=0.0
  IF(I.EQ.NXPOND.AND.J.EQ.NYPOND)CAVG(I,J)=1.00
7  CONTINUE
  DO 17 J=1,NPL
  DSUB=J-1
  XD=(DX/PX)*(0.5+DSUB)
  LREG=LREG+NPW
  LEND=LEND+NPW
  DO 17 I=LREG,LEND
  DSUB=I-LREG
  Y(I)=(DY/PY)*(0.5+DSUB)
  X(I)=XD
  NIR=Y(I)/DY+1.0
  NIC=X(I)/DX+1.0
  C(I)=CAVG(NIR,NIC)
17  CONTINUE
  XD=NC*DX+100.0
  YD=(NR*DY)/2.0
  LREG=NPW*NPL+1.0
  LEND=NPW*NPL+100.0
  DO 27 I=LREG,LEND
  X(I)=XD
  Y(I)=YD
  C(I)=0.0
27  CONTINUE
  NTTL=100+NPW*NPL
  DO 77 I=1,NTTL
  XI(I)=X(I)
  YI(I)=Y(I)
77  CONTINUE
  XD=(DX/PX)*0.5
  DO 37 I=1,NPW
  DSUB=I-1
  YIR(I)=(DY/PY)*(0.5+DSUB)
  XIR(I)=XD
  NIR=YIR(I)/DY+1.0
  CTR(I)=CAVG(NIR,1)
37  CONTINUE
  RETURN
  END

```

SUBROUTINE INTPRT

INTPRT ARRANGES THE INITIAL DATA AND SUPPLIES HEADINGS FOR PRINTOUT,
THEN EXECUTES THE PRINTOUT WITH THE AID OF SUBROUTINE MATROP.

```

COMMON NR,NC,NPX,NPY,DX,DY,RHO,DELT,ST,FWTOP,G,VIS,NPW,NPL,IR,IC
1  FK(20,30),H(20,30),POR(20,30),CAVG(20,30),CAVGP(20,30),
2  SUMC(20,30),COUNT(20,30),DELC(20,30),D11(20,30),D22(20,30),
3  D12(20,30),VX(20,30),VY(20,30),C(2500),X(2500),Y(2500),
4  XIB(100),YIB(100),CIB(100),SL(100),NXPOND,NYPOND,BREV(20,30),
5  XI(2500),YI(2500),NNN,CST
WRITE (6,1)
WRITE(6,2) NR,NC
WRITE (6,3) DELT, ST, FWTOP
WRITE(6,4) DX,DY,G
WRITE (6,7)
CALL MATROP (NR, NC, FK)
WRITE (6,8)
CALL MATROP (NR, NC, POR)
WRITE (6,9)
CALL MATROP (NR, NC, H)
WRITE(6,17)
CALL MATROP(NR,NC,BREV)
WRITE (6,15)
CALL MATROP (NR, NC, CAVG)
WRITE (6,16)
CALL MATROP (NR, NC, DELC)
1 FORMAT (1H1,36X,59H*****TWO-DIMENSIONAL HORIZONTAL FLOW PROBL
1EM***** //)
2 FORMAT(1H0,15HPOW DIMENSION=,I4,10X,18HCOLUMN DIMENSION=,I4)
3 FORMAT (1H0,12HDELTA-TIME =,F10.3,1X,5HDAYS.,10X,16HTOTAL RUN TIME
1 =,F10.3,1X,5HDAYS.,10X,19HPRINT OUT CONTROL =,F10.3)
4 FORMAT(1H0,9HDELTA-X=,F10.3,1X,3HFT.,10X,9HDELTA-Y=,F10.3,1X,3HFT.
1,10X,17HACC. OF GRAVITY=,F10.3)
7 FORMAT (1H0,52X,27HPERMEABILITY MAP (SQ. FT.). //)
8 FORMAT (1H0,58X,13HPOROSITY MAP. //)
9 FORMAT(1H0,52X,32HWATER TABLE ELEVATION MAP (FT.). //)
15 FORMAT (1H0,41X,48HINITIAL CONCENTRATION MAP (SLUG PER CUBIC FOOT)
1. //)
16 FORMAT (1H0,41X,49HCHANGE IN CONCFNTRATION MAP (SLUG PER CUBIC FT.
1). //)
17 FORMAT(1H0,55X,28HBEDROCK ELEVATION MAP(FT.). //)
77 RETURN
END

```

```

SUBROUTINE MATROP (NP, NC, B)
*****
MATROP ARRANGES ALL TWO-DIMENSIONAL ARRAYS IN A FORM SUITABLE FOR PRINTOUT
THEN EXECUTES THE PRINTOUT. MATROP IS USED TO PRINT ALL INITIAL DATA
AND FINAL RESULTS WHICH ARE IN THE FORM OF TWO-DIMENSIONAL ARRAYS.
*****
      DIMENSION B(20,30), A(12)
DIMENSIONS OF B MUST MATCH DIMENSIONS OF VARIABLE CALLED FROM MAIN PROGRAM
      DO 11 I=1,NC,12
      IN=I/12
      DO 9 J=1,NR
      IF((IN+1)*12.LE.NC) 1,3
1 DO 2 JJ=1,12
  JJJ=IN*12+JJ
2 A(JJ)=B(J,JJJ)
  GO TO 6
3 LL=NC-12*IN
  DO 4 JJ=1,LL
  JJJ=IN*12+JJ
4 A(JJ)=B(J,JJJ)
  LL=LL+1
  DO 5 JJ=LL,12
5 A(JJ)=0.0
6 IF (A(1).GT.0.001) GO TO 14
  IF (IN) 7,7,8
7 WRITE (6,12) (A(II),II=1,12),J
  GO TO 9
8 WRITE (6,12) (A(II),II=1,12), IN
  GO TO 9
14 IF(IN) 15,15,16
15 WRITE (6,17) (A(II),II=1,12), J
  GO TO 9
16 WRITE (6,17) (A(II),II=1,12), IN
9 CONTINUE
  IF(NC.LE.(IN+1)*12) 11,10
10 WRITE (6,13)
11 CONTINUE
12 FORMAT (1H ,12E10.3,I4)
13 FORMAT (1H0,/)
17 FORMAT (1H ,12E10.3,I4)
      RETURN
      END

```

SUBROUTINE MOVPT(TIME,DELCM,CAVGM)

MOVPT EXECUTES ALL CALCULATIONS PERTAINING TO CONCENTRATION AND MOVEMENT OF CONTAMINANTS. AT EACH TIME STEP THIS SUBROUTINE CALCULATES VELOCITY COMPONENTS FOR EACH MOVING POINT, RELOCATES ALL POINTS, COMPUTES NEW GRID CONCENTRATIONS, AND REASSIGNS THESE NEW CONCENTRATIONS TO EACH POINT.

```

COMMON NR,NC,NPX,NPY,DX,DY,RHO,DELT,ST,FWTOP,G,VIS,NPW,NPL,IR,IC,
1  FK(20,30),H(20,30),POR(20,30),CAVG(20,30),CAVGP(20,30),
2  SUMC(20,30),COUNT(20,30),DFLC(20,30),D11(20,30),D22(20,30),
3  D12(20,30),VX(20,30),VY(20,30),C(2500),X(2500),Y(2500),
4  XIB(100),YIB(100),CIB(100),SL(100),NXPOND,NYPOND,BREV(20,30),
5  XI(2500),YI(2500),NNN,CST
CST=0.0
DELCM=0.0
CAVGM=0.0
DO 7 I=1,NR
DO 7 J=1,NC
DELC(I,J)=0.0
SUMC(I,J)=0.0
COUNT(I,J)=0.0
CAVGP(I,J)=CAVG(I,J)
7 CONTINUE
NNN=NNN+1
PX=NPX
PY=NPY
ALENX=DX*NC
ALENY=DY*NR
ADISX=DX/PX
ADISY=DY/PY
DO 5 I=1,NPW
NIR=YIB(I)/DY+1.0
NIC=XIB(I)/DX+1.0
IF(NIC.GT.NC) GO TO 99
IF(NIR.LE.0.0) GO TO 99
IF(NIR.GT.NR) GO TO 99
AL=NIR-1
ALL=NIC-1
VXX=VX(NIR,NIC)-(((XIB(I)-(ALL*DX))/DX)*(VX(NIR,NIC)-VX(NIR,NIC+1)
1))
VYY=VY(NIR,NIC)-(((YIB(I)-(AL*DY))/DY)*(VY(NIR,NIC)-VY(NIR+1,NIC))
2)
IF(VXX.GT.0.0)XIR(I)=XIB(I)+(DELT*VXX)
5 CONTINUE
NAP=1
MAD=0
NTTL=NPW*NPL+100
IF(NNN.EQ.8) GO TO 76
GO TO 78
76 NNN=0
DO 77 I=1,NTTL
X(I)=XI(I)
Y(I)=YI(I)
NIR=Y(I)/DY+1.0
NIC=X(I)/DX+1.0

```

```

      C(I)=CAVG(NIR,NIC)
77 CONTINUE
78 DO 20 I=1,NTTL
      NIR=Y(I)/DY+1.0
      NIC=X(I)/DX+1.0
      IF(NIC.GT.NC) GO TO 100
      IF(NIR.LE.0.0) GO TO 100
      IF(NIR.GT.NR) GO TO 100
      AL=NIR-1
      ALL=NIC-1
      C(I)=CAVG(NIR,NIC)
      VXX=VX(NIR,NIC)-(((X(I)-(ALL*DX))/DX)*(VX(NIR,NIC)-VX(NIR,NIC+1)))
      VYY=VY(NIR,NIC)-(((Y(I)-(AL*DY))/DY)*(VY(NIR,NIC)-VY(NIR+1,NIC)))
      IF(VX(NIR,NIC).EQ.0.0.AND.VXX.LT.0.0) GO TO 40
      GO TO 41
40 DISTA=X(I)-(ALL*DX)
      DISTR=ABS(DELT*VXX)
      IF(DISTA.GT.DISTR)VXX=(-DISTA+0.01)/DELT
41 IF(VX(NIR,NIC+1).EQ.0.0.AND.VXX.GT.0.0) GO TO 42
      GO TO 43
42 DISTA=((ALL+1)*DX)-X(I)
      DISTR=ABS(DELT*VXX)
      IF(DISTA.GT.DISTR)VXX=(DISTA-0.01)/DELT
43 IF(VY(NIR,NIC).EQ.0.0.AND.VYY.LT.0.0) GO TO 44
      GO TO 45
44 DISTA=Y(I)-(ALL*DY)
      DISTR=ABS(DELT*VYY)
      IF(DISTA.GT.DISTR)VYY=(-DISTA+0.01)/DELT
45 IF(VY(NIR+1,NIC).EQ.0.0.AND.VYY.GT.0.0) GO TO 46
      GO TO 52
46 DISTA=(ALL+1)*DY-Y(I)
      DISTR=ABS(DELT*VYY)
      IF(DISTA.GT.DISTR)VYY=(DISTA-0.01)/DELT
52 Y(I)=Y(I)+DELT*VYY
      X(I)=X(I)+DELT*VXX
100 IF((X(I).LT.ALENX.AND.Y(I).LT.ALENY).AND.(Y(I).GT.0.0)) GO TO 12
80 IF(MAD.EQ.1) GO TO 12
70 IF(XIB(NAP).GE.ADISX) GO TO 72
      NAP=NAP+1
      IF(NAP.GE.NPW) MAD=1
      IF(NAP.LE.NPW) GO TO 70
      GO TO 12
72 XIB(NAP)=XIB(NAP)-ADISX
      X(I)=XIB(NAP)
      Y(I)=YIB(NAP)
      C(I)=CIB(NAP)
12 NIR=Y(I)/DY+1.0
      NIC=X(I)/DX+1.0
      IF(NIC.GT.NC) GO TO 20
      IF(NIR.GT.NR) GO TO 20
      IF(NIR.LE.0.0) GO TO 20
      SUMC(NIR,NIC)=SUMC(NIR,NIC)+C(I)
      COUNT(NIR,NIC)=COUNT(NIR,NIC)+1.0
20 CONTINUE
      DO 30 I=1,NR
      DO 30 J=1,NC
      CST=0.0
      IF(COUNT(I,J).EQ.0.0) COUNT(I,J)=1.0

```

```

CAVG(I,J)=SUMC(I,J)/COUNT(I,J)
IF(CAVG(I,J).GT.CAVGM) CAVGM=CAVG(I,J)
CST=CAVGP(I,J)-CAVG(I,J)
IF(J.GF.4.AND.CST.GT.0.1) DELC(I,J)=CST
IF(DELC(I,J).GT.DELCM) DELCM=DELC(I,J)
IF(I.EQ.NXPOND.AND.J.EQ.NYPOND)CAVG(I,J)=1.00
IF(TIME.GT.4320.0) CAVG(NXPOND,NYPOND)=0.5
30 CONTINUE
GO TO 470
99 WRITE(6,9A)
98 FORMAT(1H0,* ERROR IN BOUNDARY POINTS- CALCULATIONS STOPPED*)
CST=80.0
470 RETURN
END

```

SUBROUTINE TRANS

```

*****
TRANS CONVERTS RELATIVE TRANSMISSIBILITIES IN EACH GRID TO ABSOLUTE
PERMEABILITIES.

```

```

*****
COMMON NR,NC,NPX,NPY,DX,DY,RHO,DEL,T,ST,FWTOP,G,VIS,NPW,NPL,IR,IC,
1 FK(20,30),H(20,30),POP(20,30),CAVG(20,30),CAVGP(20,30),
2 SUMC(20,30),COUNT(20,30),DELC(20,30),D11(20,30),D22(20,30),
3 D12(20,30),VX(20,30),VY(20,30),C(2500),X(2500),Y(2500),
4 XIB(100),YIB(100),CIB(100),SL(100),NXPOND,NYPOND,BREV(20,30),
5 XI(2500),YI(2500),NNN,CST
NXG=7
NYG=9
CONV=8500.*VIS/(RHO*G*7.48*24.*3600.)
DO 7 I=1,NR
DO 7 J=1,NC
FK(I,J)=FK(I,J)/(H(I,J)-BREV(I,J))
FK(I,J)=FK(I,J)*VIS/(RHO*G)
7 CONTINUE
GODAM=FK(NXG,NYG)
DO 8 I=1,NR
DO 8 J=1,NC
FK(I,J)=FK(I,J)*CONV/GODAM
8 CONTINUE
RETURN
END

```

SUBROUTINE VELOCY

VELOCY CALCULATES VELOCITY COMPONENTS FOR EACH GRID INTERFACE. WHEN DISPERSION BECOMES SIGNIFICANT, STATEMENTS ARE ALSO AVAILABLE IN THIS SUBROUTINE FOR THE CALCULATION OF THE LONGITUDINAL AND LATERAL DISPERSION COEFFICIENTS.

```

COMMON NR,NC,NPX,NPY,DX,DY,RHO,DELT,ST,FWTOP,G,VIS,NPW,NPL,IR,IC,
1  FK(20,30),H(20,30),POR(20,30),CAVG(20,30),CAVGP(20,30),
2  SUMC(20,30),COUNT(20,30),DELC(20,30),D11(20,30),D22(20,30),
3  D12(20,30),VX(20,30),VY(20,30),C(2500),X(2500),Y(2500),
4  XIR(100),YIR(100),CIR(100),SL(100),NXPOND,NYPOND,BREV(20,30),
5  XI(2500),YI(2500),NNN,CST
VISCOSITY, DENSITY, AND REYNOLDS NUMBER FOR EACH GRID ASSUMED CONSTANT
PRESSURES ARE EQUIVALENT TO HEADS, AND DO NOT APPEAR IN EQUATIONS
VXMAX=0.0
DO 10 I=1,NR
DO 9 J=2,NC
IF(FK(I,J).EQ.0.0.OR.FK(I,J-1).EQ.0.0) GO TO 8
DOG=(-2.0)*FK(I,J)*FK(I,J-1)/(DX*VIS*(FK(I,J-1)*POR(I,J)+FK(I,J)
1*POR(I,J-1)))
VX(I,J)=DOG*RHO*G*(H(I,J)-H(I,J-1))
IF(VX(I,J).GT.VXMAX) VXMAX=VX(I,J)
GO TO 9
8 VX(I,J)=0.0
9 CONTINUE
VX(I,1)=VX(I,2)
VX(I,IC)=VX(I,NC)
10 CONTINUE
DO 20 J=1,NC
DO 19 I=2,NR
IF(FK(I,J).EQ.0.0.OR.FK(I-1,J).EQ.0.0) GO TO 18
DOG=(-2.0)*FK(I,J)*FK(I-1,J)/(DY*VIS*(FK(I-1,J)*POR(I,J)+FK(I,J)
1*POR(I-1,J)))
VY(I,J)=DOG*RHO*G*(H(I,J)-H(I-1,J))
GO TO 19
18 VY(I,J)=0.0
19 CONTINUE
VY(1,J)=VY(2,J)
VY(IR,J)=VY(NR,J)
20 CONTINUE
DIFF=0.0
TORT=0.5
DIA=0.00316
DO 30 I=1,NR
DO 30 J=1,NC
VXX=VX(I,J)-0.5*(VX(I,J)-VX(I,J+1))
VYY=VY(I,J)-0.5*(VY(I,J)-VY(I+1,J))
VELX=VXX*VXX
VELY=VYY*VYY
IF(VELX.EQ.0.0.AND.VELY.EQ.0.0) GO TO 21
VEL=SQRT(VELX+VELY)
RE=(VEL*DIA*RHO/VIS)
DL=0.66*(VIS/RHO)*RE**1.2
DT=0.036*(VIS/RHO)*RE**0.7
D11(I,J)=(DL*VXX*VXX)/(VEL*VEL)+(DT*VYY*VYY)/(VEL*VEL)+DIFF*TORT
D22(I,J)=(DT*VXX*VXX)/(VEL*VEL)+(DL*VYY*VYY)/(VEL*VEL)+DIFF*TORT
D12(I,J)=(DL-DT)*VXX*VYY/(VEL*VEL)
GO TO 30
21 D11(I,J)=0.0
D22(I,J)=0.0
D12(I,J)=0.0
30 CONTINUE
460 RETURN
END

```

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