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Single Location Doublet Well to Reduce Salt-Water Encroachment: Phase I – Numerical Simulation

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SINGLE LOCATION DOUBLET WELL TO REDUCE
SALT-WATER ENCROACHMENT: PHASE I - NUMERICAL SIMULATION

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ABSTRACT

Single Location Doublet Well to Reduce
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by

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C.E. Jacob received patents in 1965 for a single location well doublet that would produce fresh water overlying salt-water without upconing of the heavier salt-water and pollution of the fresh water zone. No known evaluation of the concept or development of design criteria has been accomplished. In this study, a finite difference radial flow model was developed to determine groundwater velocities and salt concentration as a function of time and space. This model was verified and is available for evaluating design criteria for Jacob's single location well doublet. Initial runs with the model indicate that the concept has potential, particularly in aquifers with clay lenses in the salt-water zone. Additional runs with the model will be needed to fully establish the design criteria necessary for Jacob's single location well doublet.

ACKNOWLEDGEMENTS

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CHAPTER I

INTRODUCTION

Salt-water encroachment is a problem for groundwater development in many areas of the world. In many coastal areas, fresh groundwater occurs as lenses floating on sea water. As groundwater is developed, the natural flow toward the ocean is reversed and sea-water intrusion occurs. As the salt-water travels inland, the chloride content of wells increases and they become contaminated. Many well fields have been abandoned. Similarly, in many areas of the western United States fresh water aquifers overlie saline-water aquifers. When wells are heavily pumped, salt-water moves upward from the lower saline aquifers, contaminating the well.

A major groundwater problem area in Texas is the El Paso area in the Rio Grande Basin. In particular, the Hueco Bolson Aquifer is being mined, with water level declines of 0.3 to 0.7 meter per year occurring. Surface water in the Rio Grande at El Paso is fully appropriated, and its quality for municipal use is marginal much of the time; exceeding 3000 ppm total dissolved solids many times. The city of El Paso is forced to use available groundwater for their municipal use. Projections by the Texas Department of Water Resources indicate that adequate groundwater is available to meet projected water requirements of El Paso through the year 2030 if saline-water encroachment can be controlled.

The Hueco Bolson Aquifer is underlain by saline-water sands. As the fresh water from the aquifer is mined, the saline-water rises into the overlying fresh water sands and contaminates wells. The Texas Water Development Board (1977) stated that presently and in the future, saline-water encroachment due to mining of the Hueco Bolson Aquifer has and will continue to deteriorate groundwater quality. To reduce the problem, the city of El Paso constructs their new wells so that in-well blending of fresh and slightly saline-water takes place during pumpage. The controlled blending of fresh and slightly saline groundwater will reduce encroachment and extend the useful life of the aquifer. However, no long-term solution has been found.

C.E. Jacob, the noted groundwater hydrologist, received patents in 1965 for a single location well doublet that would produce fresh water overlying salt-water without upconing of the heavier salt-water (Wickersham, 1977). No paper was written by Jacob describing or evaluating his invention prior to his death

in 1970. All written documentation of his concept is included in two patent applications (Jacob 1965a and Jacob 1965b).

Jacob's patents call for a well to penetrate the fresh water zone and extend a substantial distance below the static interface into the salt-water zone. The well bore is divided into lower, intermediate, and upper chambers by the use of two conventional packers spaced along the well bore. The lower packer is set just above the normal static interface. The upper packer is spaced above the lower one and is located in the fresh water zone. Two opposed pumps connected by a common power shaft are simultaneously operated to produce a flow of liquid into and through the three separated well chambers. The upper pump is placed in the top chamber where fresh water is drawn into it and on to the surface for use. The second or lower pump is placed in the intermediate chamber where some saline-water is drawn into it and is discharged into the lower chamber. The saline-water passes through the lower chamber and is injected back into the aquifer several feet below where it was withdrawn. Jacob's idea was to create a "closed cell" of salt-water circulation which would eliminate transfer of the undesired saline-water across a streamline boundary. Thus, fresh water overlying salt-water could be pumped while reducing or eliminating upconing and contamination of the fresh water supply.

No known evaluation of Jacob's patents has been made. This report describes an evaluation of Jacob's single location well doublet. The specific objectives of the study were as follows:

1. Develop a numerical model of Jacob's single location well doublet and evaluate its usefulness with salt-water encroachment problems.

2. Use the numerical model to evaluate design criteria for the construction of Jacob's single location well doublet.

Funding for this project was to have been for a 24-month period. However, because of budgeting problems at the Office of Water Research and Technology during the fall of 1981, money was not actually allocated to the principal investigator until March of 1982. Thus, funding was available for only 18 months, and only Objective 1 above was completed. Objective 2 is not complete and is not included in this report.

CHAPTER II

PREVIOUS WORK

Slichter (1905) injected a salt solution into a well and observed the
time of arrival at a nearby observation well. He observed that the salt did
not arrive at the observation well as a slug, but instead the salt concentration
gradually increased with time to some maximum value. Since Slichter's work,
many investigations have been made on the flow of miscible fluids in porous
media. These investigations are divided into the following four categories
for discussion purposes: (A) theoretical investigations, (B) analytical
investigations, (C) experimental studies, and (D) numerical simulation.

A. Theoretical Investigations

The theoretical investigations have been oriented towards developing a
basic understanding of the dispersion phenomena. These studies attempt to
define the dispersion coefficient in terms of medium properties, fluid proper-
ties, and the fluid velocity.

Dispersion and diffusion may be visualized by the injection of a slug of
dye into a fluid flowing through a porous medium. The center of the slug
will travel along the column axis with the average fluid velocity. As time
increases, the slug will increase in size and mix with the surrounding native
fluid to form concentration profiles. This variation in concentration is
created by both dispersion and diffusion. Diffusion is a direct result of
thermal motion of the individual fluid molecules and takes place under the
influence of a concentration gradient. Dispersion in porous media is a
mechanical or convective mixing process which is the result of individual
fluid particles traveling at variable velocities through irregular shaped pores
and along tortuous microscopic pathlines.

Dispersion results in a variation of concentration similar to that
created by diffusion. However, dispersion is the result of convective mixing
on a microscopic scale; not of a concentration gradient. Because of the
difficulty in describing the boundary conditions for flow through porous media
on a microscopic scale, a macroscopic model is used. When using the macroscopic
model, dispersion is assumed to be proportional to the concentration gradient.
A detailed description of the transition from a microscopic to a macroscopic
model is given by Bear (1979).

To investigate the dispersion process, many porous media models have been used. Perhaps one of the simplest models is a bundle of capillaries. Taylor (1953, 1954) investigated the displacement of a fluid from a straight capillary tube of radius, r, by another fluid miscible with the first. His results indicated that the tracer was dispersed relative to a plane moving with velocity, V, exactly as in a Fickian diffusion process, but with a diffusion coefficient,

$$D = \frac{r^2 V^2}{48 D_d} \tag{1}$$

where D_d is the molecular diffusion coefficient. Aris (1956) generalized Taylor's results by considering a bundle of capillary tubes and obtained an effective diffusion coefficient,

$$D = D_d + \tau \frac{r^2 V^2}{D_d} \tag{2}$$

where τ is a coefficient depending on the shape of the capillary tube's cross-section. Ananthakrishnan et. al. (1965) investigated the range of applicability of Equation 2.

Another theoretical approach is to develop a statistical model of the microscopic motion of marked fluid particles and to average these motions to obtain a macroscopic description of dispersion. Scheidegger (1954) neglected molecular diffusion and used the theory of a random walk extended to three dimensions. However, he assumed that the probability for a particle to move a given distance was the same for all directions. This leads to a dispersion coefficient that has the same value in all directions, and has subsequently been proven wrong.

De Josselin de Jong (1958) also used a statistical approach and was probably the first to develop a model which defined the dispersion coefficient as an anisotropic quantity. His model was constructed of interconnected straight channels oriented at random but uniformly distributed in all directions. The final result was a concentration profile described by a three-dimensional normal distribution in which longitudinal dispersion was greater than transverse dispersion. The concept of longitudinal and transverse dispersion has been verified experimentally (de Josselin de Jong (1958); Bear (1961b)).

Saffman (1959, 1960) used a statistical approach similar to de Josselin de Jong (1958). However, Saffman introduced molecular diffusion into his model

and studied the relationship between mechanical dispersion and molecular diffusion. Saffman's first model (1959) assumed dispersion was large compared to molecular diffusion. Saffman's second model (1960) was for the case where molecular diffusion and dispersion are of the same order of magnitude.

Other statistical models have been investigated by Danckwerts (1953), Beran (1955), Rifai et. al. (1956), and Day (1956). Scheidegger (1957) developed two theoretical models which yielded,

$$D \sim V \tag{3}$$

for one model, and

$$D \sim V^2 \tag{4}$$

for the other model. Equation 4 represents a model where enough residence time exists in each flow channel for molecular sideways diffusion to cause complete mixing between invading and original fluids. Equation 3 represents a model in which no mass is allowed to be transferred from one streamline to another by molecular diffusion. As shall be seen, experimental evidence indicates that Equation 3 comes closer to physical reality. Scheidegger (1960) summarized much of the statistical work done prior to 1960.

Using the results of de Josselin de Jong's work (1958), Bear (1961a) developed an expression for the dispersivity tensor in terms of the average distance traveled by the tracer in the medium. Bear implied that the dispersion coefficient, D_{ij}, was a second rank tensor linear in the components of the velocity. Scheidegger (1961) suggested by induction that:

$$D_{ij} = \epsilon_{ijmn} \frac{V_m V_n}{V} \tag{5}$$

where ϵ_{ijmn} is the coefficient of dispersivity, which is a porous medium property, and $V_m V_n / V$ is a tensor which represents the linear influence of velocity. Scheidegger concluded that the coefficient of dispersivity was a fourth rank tensor with 81 components; but due to certain symmetry properties, contains only 36 independent components in the general case of an anisotropic medium. In isotropic media, there are only two dispersivity constrants.

Work by Poreh (1965) showed from physical and dimensional reasoning that the tensor form of the coefficient of dispersion is,

$$\frac{D_{ij}}{D_d} = F_1 S_{ij} + F_2 \left(\frac{d}{D_d}\right)^2 V_i V_j \tag{6}$$

where d = pore size parameter, S_{ij} = kronecker delta, $V_i V_j$ is a tensor representing the linear influence of velocity, and F_1 and F_2 are even functions of Vd/D_d and Vd/v, the Peclet and Reynolds numbers, respectively. Bear and Bachmat (1967) also showed the dispersion coefficient, D_{ij}, to be a function of the Peclet number.

Several investigators, including Scheidegger (1961) and de Josselin de Jong and Bossen (1961), have suggested that the dispersion of a tracer in fluid flow through saturated homogeneous porous media can be described by the differential equation,

$$\frac{\partial c}{\partial t} = \frac{\partial}{\partial X_i} [D_{ij} \frac{\partial c}{\partial X_j} - V_i C] \tag{7}$$

where C is the tracer concentration, t is time, V_i is the component of the velocity vector in a cartesian coordinate system, and X_i (i=1,2,3) is the cartesian space coordinates. The double summation convention of tensor notation is implied in the use of Equation 7. Bachmat and Bear (1964) gave the dispersion equation in curvilinear coordinates consisting of streamlines and equipotentials ($\Phi-\Psi$ coordinates). Bear and Bachmat (1967) used basic fluid flow equations which are averaged over a representative volume element of porous media to yield the equation of motion and the equation of dispersion.

Perkins and Johnston (1963) gave a good summary of diffusion and dispersion in porous media. A more detailed summary of the theory of dispersion in porous media was given by Bear et. al. (1968, Chapter 11).

B. Analytical Solutions

Most dispersion problems have a direct analogy with heat flow. For this reason, a good reference for analytical solutions is Carslaw and Jaeger (1959) or Crank (1956). Some of the more important analytical solutions are discussed below.

Longitudinal Dispersion -- A semi-infinite column ($X_3 > 0$) of homogeneous and isotropic porous media with a plane source maintained at $X_3 = 0$ is maintained at a constant specific discharge, q, in the X_3-direction. For an isotropic media, the axes of the dispersivity tensor is assumed to coincide with the velocity vector. Thus, Equation 7 reduces to

$$\frac{\partial c}{\partial t} = D_L \frac{\partial^2 C}{\partial X_3^2} - V_3 \frac{\partial c}{\partial X_3} \tag{8}$$

where D_L is the longitudinal dispersion coefficient. Initial and boundary conditions are given by,

$$C(0,t) = C_0 \quad ; \quad t \geq 0$$
$$C(X_3,0) = 0 \quad ; \quad X_3 \geq 0 \tag{9}$$
$$C(\infty,t) = 0 \quad ; \quad t \geq 0$$

Ogata and Banks (1961) used Laplace Transforms to obtain the solution,

$$\frac{C}{C_0} = \frac{1}{2}[\text{erfc}(\frac{X_3 - V_3 t}{2\sqrt{D_L t}}) + \exp(\frac{V_3 X_3}{D_L}) \ \text{erfc}(\frac{X_3 + V_3 t}{2\sqrt{D_L t}})] \tag{10}$$

where erfc(u) = 1 - erf(u). Ogata and Banks showed that the second term in Equation 10 may be neglected in most cases. For instance, if $D_L < 0.002 \ V_3 \ X_3$ a maximum error of less than three percent is introduced by neglecting the second term. Therefore, unless the region close to the source is considered, an approximate solution to Equations 8 and 9 is

$$\frac{C}{C_0} = \frac{1}{2}[\text{erfc}(\frac{X_3 - V_3 t}{2\sqrt{D_L t}})] \tag{11}$$

Ogata (1961, 1964a) gave a solution in integral form to the problem where a slug of radius "a" is injected at $X_3=0$. This problem must consider both longitudinal dispersion and transverse dispersion. Using his solutions, Ogata (1964a) developed experimental procedures for determining both D_L and D_T.

In many physical problems, the tracer being used may react with the solid matrix of the porous medium. Depending on the reaction, the tracer may be adsorbed to the matrix or additional tracer may be produced. To handle such cases, a production term dependent on the concentration is added to Equation 8. Using varying functional relationships for the production term, solutions to this problem have been obtained by Ogata (1964b), Banks and Jerasate (1962), Banks and Ali (1964), and Lapidus and Amundson (1952). A closely related problem is that of radioactive decay of a tracer. Bear et. al. (1968, p. 347) gave the solution to Equations 8 and 9 where the tracer continuously undergoes radioactive decay. Coats and Smith (1964) investigated the effects of dead-end pore volume on dispersion and gave several solutions to the simple diffusion model characterized by Equation 8.

Longitudinal and Lateral Dispersion -- If a rectangular column ($0 \leq X_3 \leq l_3$, $0 \leq X_2 \leq l_2$) is used and a tracer source is maintained over a portion of the input

area $(0 \leq X_2 \leq b)$, then both longitudinal and lateral dispersion will occur. Assuming a homogeneous and isotropic medium with unidirectional flow in the X_3-direction and $\partial c / \partial X_1 = 0$, Equation 7 becomes,

$$\frac{\partial c}{\partial t} = D_L \frac{\partial^2 c}{\partial X_3^2} + D_T \frac{\partial^2 c}{\partial X_2^2} - V_3 \frac{\partial c}{\partial X_3} \tag{12}$$

The initial and boundary conditions are given by:

$$C(X_2, 0, t) = C_0 \; ; \; 0 \leq X_2 \leq b \; ; \; t \geq 0$$
$$C(X_2, 0, t) = 0 \; ; \; b < X_2 < l_2 \; ; \; t \geq 0$$
$$\frac{\partial c(0, X_3, t)}{\partial X_2} = 0 \; ; \; t > 0$$
$$\frac{\partial c(l_2, X_3, t)}{\partial X_2} = 0 \; ; \; t > 0$$
$$C(X_2, \infty, t) = \text{Bounded}$$
$$C(X_2, X_3, 0) = 0 \; ; \; 0 \leq X_2 \leq l_2 \; ; \; X_3 > 0 \tag{13}$$

A series solution to Equations 12 and 13 was given by Bruch and Street (1967). Harleman and Rumer (1963) gave the following approximate steady state solution to Equations 12 and 13,

$$\frac{C}{C_0} = \frac{1}{2} \, \text{erfc} \, [\frac{X_2 - b}{2\sqrt{D_T \, X_3/V_3}}] \tag{14}$$

In their work on waste-water recharge and dispersion, Hoopes and Harleman (1965, 1967a, 1967b) have developed several approximate solutions to the radial dispersion problem. Raimondi et. al. (1959) also gave an approximate solution to the radial dispersion problem. Esmail and Kimbler (1967) gave a solution which allows for alternate injection and production.

Dagan (1967) gave an analytical solution for dispersion in a nonhomogeneous porous column. Using the Laplace Transform, Shamir and Harleman (1966, 1967) developed analytical solutions for longitudinal and lateral dispersion in layered porous media. Bear and Todd (1960, pp. 27-33) gave some analysis of the unsteady flow problem. Banks and Jerasate (1962) allowed the coefficient of dispersion to vary with time, and solved the problem by introducing a different time scale.

C. Experimental Results

Much of the experimental work has attempted to establish relationships so that the dispersion coefficients may be calculated from media and fluid properties. As was pointed out earlier, theoretical models indicate that the dispersion coefficient is a second rank tensor. Experiments of de Josselin de Jong (1958), Bear (1961b) and Bear and Todd (1960) confirm this concept. Scheidegger's work (1961) indicated that for homogeneous and isotropic media. the dispersion tensor reduces to two independent terms; (1) the longitudinal dispersion coefficient, D_L, and (2) the lateral dispersion coefficient, D_T.

Most of the experimental determinations of the longitudinal dispersion coefficient used Equations 10 or 11 as a basis for analysis. Ebach and White (1958) performed experiments on a wide range of particle sizes, shapes, and Reynolds numbers. They empirically postulated that for Reynolds numbers, $R < 100$,

$$\frac{D_L}{\nu} = \alpha_1 \left(\frac{Vd}{\nu}\right)^{\beta_1} \tag{15}$$

where V = fluid velocity, d = particle size of the porous media, and ν = kinematic viscosity. The experimentally determined coefficient α_1 is strongly dependent on the porous medium while β_1 is dependent on flow regime. However, evidence exists (Adam, 1966) that β_1 is also dependent on medium properties. Experimenters have found a large variation in the values of α_1 and β_1. A large percentage of this variation may be attributed to experimental techniques; especially the different methods for measuring concentration.

Harleman and Rumer (1963) found $\alpha_1=0.66$ and $\beta_1=1.2$ while Hoopes and Harleman (1965) found $\alpha_1=1.70$ and $\beta_1=1.2$. Ebach and White (1958) found $\alpha_1=1.92$ and $\beta_1=1.06$. Experimental results for longitudinal dispersion were given by Banks and Ali (1964); Blackwell (1962), Cairns and Prausnitz (1960), Carberry and Bretton (1958), Simpson (1969), and many others.

Equation 15 prompted investigators of lateral dispersion to fit their experimental data to the form,

$$\frac{D_T}{\nu} = \alpha_2 \left(\frac{Vd}{\nu}\right)^{\beta_2} \tag{16}$$

Harleman and Rumer (1963) found $\alpha_2=0.036$ and $\beta_2=0.7$. Hoopes and Harleman (1965) found $\alpha_2=0.11$ and $\beta_2=0.7$. Lateral dispersion has been investigated by Simpson (1962), Blackwell (1962), Grane and Gardner (1961), van der Poel (1962), and Li and Lai (1966).

Harleman et. al. (1963) were able to correlate the longitudinal dispersion coefficient with permeability,

$$\frac{D_L}{\nu} = \alpha_3 (\frac{V\sqrt{k}}{\nu})^{\beta_3} \tag{17}$$

where k is the permeability with units of L^2. Harleman et. al. found $\alpha_3=54$ for spheres and 88 for sand with $\beta_3=1.2$ for both media. Hoopes and Harleman (1965) found results similar to Equation 17, with α_3 dependent upon the media. Rumer (1962) investigated longitudinal dispersion and the effects of unsteady flow on the dispersion coefficient. Simpson (1969) investigated the effects of turbulent flow on the longitudinal dispersion coefficient, and Hoopes and Harleman (1967a) showed the dispersion coefficient along streamlines to be the same for both uniform and nonuniform flow at the same velocity.

The effects of molecular diffusion on the above Reynolds number type relationships has been debated in the literature. Relationships such as Equations 15, 16, and 17 would appear to be invalid for all ranges of Reynolds numbers. Biggar and Nielsen (1960) gave a very lucid account of the effects of molecular diffusion on dispersion. They proved that molecular diffusion is very important at small flow velocities, when the medium consists of a natural soil skeleton instead of washed sands or glass beads, and for unsaturated flow. They hypothesized that the presence of dead-end pores (a characteristic of the soil) is highly important in determining the effects of molecular diffusion on the total dispersion process. Coats and Smith (1964) also treated the dead-end pore problem. Bear et. al. (1968, pp. 332-335) stated that the dispersion co-efficient depends on the flow pattern (e.g. velocity), Peclet number (Vd/D_d), and on some fundamental medium characteristics. A plot of D_L/D_d vs. Vd/D_d is broken up into five regions and characteristics of each region are discussed by Bear.

Adam (1966) used dimensional analysis and experimental results to determine the effects of anisotropic porous media on the dispersion tensor. Adam argued that experimental evidence indicating the dispersion coefficient is nonlinear in the velocity (i.e., exponent of velocity is different than one) is incompatable

with Equation 3 proposed by Scheidegger (1961) and Bear (1961a). However, List and Brooks (1967) analyzed numerous experimental results and were critical of the velocity power law relationships.

From these various investigations the conclusion is reached that the dispersion coefficient is indeed a tensor of rank two; but an adequate relationship has not been developed for describing the phenomenon over a large range of flow parameters. Much more theoretical work is needed in this area.

A study of dispersion using the concept of similitude has been done by very few people. Raats and Scotter (1968) considered geometrically similar media and sought the conditions for dynamic similarity. Bachmat (1967) investigated the criteria for similitude of the dispersion phenomena in homogeneous and isotropic porous media. Heller (1963) also presented a good discussion on scaling of flows in porous mediums.

Few results from field experiments are available. Harpaz and Bear (1964) presented results of laboratory and field tests on underground storage operations with a single recharging well and with two wells, one recharging and one pumping. Lau et. al. (1957) performed some field tests to evaluate various tracers, and found the chloride ion to be the best. Field oriented laboratory experiments have been conducted by Hoopes and Harleman (1965, 1967b) on wastewater recharge and by Rumer and Harleman (1963) on salt-water intrusion along coastal aquifers. Esmail and Kimbler (1967) investigated the effects of gravity segregation and dispersion on the problem of storing fresh water in saline aquifers.

D.   Numerical Solutions

Because of the difficulty in obtaining analytical solutions to groundwater flow problems, many investigators are now using numerical solutions. Numerical solutions of immiscible flow problems have met with more success than miscible flow problems. Much work remains to be done on developing satisfactory numerical techniques for the dispersion problem.

Many of the reservoir simulation techniques involving immiscible fluids have been developed in the petroleum industry. Douglas, Peaceman, and Rachford (1959) employed an alternating-direction-implicit procedure (ADIP) to solve a two-dimensional, two-phase, incompressible flow model. Blair and Peaceman (1963) extended this to include the effects of compressibility. Larkin (1964) used the alternating-direction-explicit-procedure (ADEP). Quon et. al. (1965, 1966) also used ADEP in a reservoir simulator. Coats and Terhune (1966) and Carter (1967)

compared the ADIP and ADEP techniques. Bjordammen and Coats (1967) compared alternating direction and successive overrelaxation techniques for the simulation of two- and three-dimensional, two-phase flow reservoirs. Other reservoir simulators have been described by Dougherty and Mitchell (1964), Fagin and Stewart (1966), and Breitenbach, Thurnau, and van Poollen (1968a, b, and c).

Digital computer simulators in the groundwater field have not been as widely developed as in the petroleum industry. Bittinger et. al. (1967), Tyson and Weber (1964), and Chun, Weber, and Mido (1964) have presented information on reservoir simulation in the groundwater industry. The above mentioned works are just a few of the ones which have been developed in the last few years on reservoir simulation using numerical analysis and digital computers.

The problem of miscible flow has not been treated as extensively numerically as the immiscible flow problem. Peaceman and Rachford (1962) presented a centered-in-time and centered-in-distance equation combined with a "transfer of overshoot" procedure which was demonstrated to work well in one dimension. However, subsequent testing has shown that for multidimensional displacement their method involved a numerical dispersion of the same order of magnitude as the physical dispersion.

Garder, Peaceman and Pozzi (1964) used the method of characteristics to improve the numerical solution to the miscible flow problem, but did not consider the dispersion coefficient as a tensor. Stone and Brian (1963) made a thorough analysis of a numerical scheme to solve the one-dimensional dispersion equation. They used three adjacent grids at two time levels, and assigned arbitrary weighting coefficients to the convective and time terms. They then proposed an iterative scheme with three cycles per time step to improve the solution. No consideration was given to the effects of changes in viscosity or density.

Hoopes and Harleman (1965) used an explicit finite difference scheme to obtain a solution for the problem of radial flow from a well. By neglecting lateral dispersion, they also obtained a solution to a two-well problem. The size of the grid spacing and time increment were restricted for the explicit scheme because of a stability criterion. This presented some problems because of large amounts of required computer time.

Shamir and Harleman (1966) used a very ingenious concept in their numerical technique. First they wrote the dispersion equation in terms of the stream function and potential function (i.e., in terms of Φ and Ψ coordinates). They noted that the velocity is everywhere tangential to the streamlines, and thus

their equation was one dimensional in the convective term. They then used the Stone and Brian (1963) numerical technique for one-dimensional flow and handled the lateral dispersion with an ADIP technique. If the major axis of the dispersion tensor coincides with the velocity vector, then Shamir and Harleman's technique will consider the dispersion coefficient as a tensor. However, their scheme does not consider the effects of density or viscosity changes; nor does it consider unsteady flow except in the few cases where the streamlines do not change position with time.

Nelson (1965) described a computer program for predicting waste transport in groundwater. The program generated permeability information and stream functions using a potential map with a small amount of permeability information. However, he considered a "piston type" flow and neglected dispersion entirely.

Summary -- In summary, the following results are important to the present study:

   (1)   The dispersion coefficient is an anisotropic quantity and must be treated as a second rank tensor.

   (2)   The dispersion coefficient is linearly related to the components of velocity as given by Equation 5.

   (3)   The analytical solution to the longitudinal dispersion problem is given by Equation 10.

   (4)   An approximate steady state solution to the longitudinal and lateral dispersion problem is given by Equation 14.

   (5)   The longitudinal and lateral dispersion coefficients can be obtained from the empirical relationships given by Equations 15, 16, and 17.

   (6)   Numerical solutions to the problem of miscible displacement in porous media have proven to be difficult. The numerical techniques of Stone and Brian (1963), Garder et. al. (1964), and Shamir and Harleman (1966) appear to be the most successful.

CHAPTER III

MATHEMATICAL MODEL

An analysis of Jacob's single location well doublet involves two miscible fluids: (1) fresh water and (2) saline water. These fluids have two different densities and are separated by a transition zone. Dispersion is a predominate characteristic of the simultaneous flow of two miscible fluids. The solution of Jacob's single location well doublet requires the simultaneous solution of a set of coupled equations: (1) the equation governing fluid flow and (2) the equation governing the convective-dispersion transport of a tracer. We will consider the tracer to be a conservative fluid (no adsorption or decay).

Fluid Flow Equation

A flow equation for the mixture of two miscible fluids is derived by combining the conservation of mass equation for the mixture, Darcy's law, and an equation of state describing the pressure-volume-temperature-concentration relationship. The result is an equation involving two dependent variables, fluid pressure and tracer concentration. Assuming radial symmetry, i.e. $\frac{\partial (\ )}{\partial \theta} = 0$, the final equation in cylindrical coordinates is:

$$\frac{1}{r} \frac{\partial}{\partial r} \left[\frac{\rho r k_r}{\mu} \left(\frac{\partial P}{\partial r} + \rho g \frac{\partial h}{\partial r} \right) \right] + \frac{\partial}{\partial z} \left[\frac{\rho k_z}{\mu} \left(\frac{\partial P}{\partial z} + \rho g \frac{\partial h}{\partial z} \right) \right]$$

$$= \rho_o \phi_o (\beta + C_F) \frac{\partial P}{\partial t} + \alpha \phi_o \frac{\partial C}{\partial t} + \rho_p Q \tag{18}$$

where: $\Delta r, \Delta z$ = dimensions of volume element (L),

r, z = cylindrical coordinate system (L),

ρ = fluid density (ML^{-3}),

ρ_o = reference fluid density (ML^{-3}),

k_r, k_z = Permeability in r and z directions, respectively (L^2),

μ = fluid viscosity (FTL^{-2}),

P = fluid pressure (FL^{-2}),

g = acceleration of gravity (LT^{-2}),

h = elevation of volume element above datum (L),

ϕ_o = reference value of porosity ($\cdot$),

β = fluid compressibility ($L^2 F^{-1}$),

C_F = formation compressibility factor ($L^2 F^{-1}$),

α = proportionality factor relating concentration and density ($\cdot$),

C = mass concentration of tracer (ML^{-3}),

ρ_p = density of produced or injected fluid (ML^{-3}),

Q = rate of fluid production or injection (L^3T^{-1}),

t = time (T).

To obtain Equation 18, the following assumptions were made: (1) Darcy's law is applicable, (2) single phase flow, (3) isothermal flow, (4) a linear relationship between change in porosity and change in pressure, (5) size of volume element does not vary with time, and (6) a linear relationship between density, pressure, and concentration.

The flow of groundwater through an aquifer is used in this study, and the validity of Darcy's law presents no serious obstacles. For problems in the nonlinear flow regime, additional terms involving the gradient of pressure raised to some power would be needed in Equation 18. Should a multiphase problem be considered, then equations of the form of Equation 18 would need to be developed for each phase and the saturation, S, would be different than one. The assumption of isothermal flow eliminates having to consider the density in Equation 18 as a function of temperature, and considering the size of the volume element invariant with time permits the elimination of rdrdθdz from each term in Equation 18. The use of a linear relationship between "change in porosity" - "change in pressure" and density-pressure-concentration is discussed below.

Dispersion Equation

A convective-dispersion equation may be obtained by combining the conservation of mass equation for the tracer, Fick's law, and an equation of state. The general dispersion equation is given by:

$$\frac{\partial c}{\partial t} = \frac{1}{r} \left\{ \frac{\partial}{\partial r} \left[r \, D_{rr}^{*} \frac{\partial c}{\partial r} + r \, D_{rz}^{*} \frac{\partial c}{\partial z} \right] + \frac{\partial}{\partial z} \left[r \, D_{zr}^{*} \frac{\partial c}{\partial r} + r \, D_{zz}^{*} \frac{\partial c}{\partial z} \right] \right\}$$

$$- V_r \frac{\partial c}{\partial r} - V_z \frac{\partial c}{\partial z} - C_p \, Q \qquad (19)$$

where: D_{rr}^{*}, D_{rz}^{*}, D_{zr}^{*}, D_{zz}^{*} = hydrodynamic dispersion coefficient which is a second rank tensor (L^2T^{-1}),

V_r, V_z = fluid seepage velocity in r and z directions, respectively, (LT^{-1}),

C_p = concentration of tracer in produced or injection fluid (ML^{-3}), and

all other terms are as previously described.

Assumptions necessary to obtain Equation 19 are: (1) diffusion is described by Fick's law, (2) the convective mixing called dispersion is proportional to the concentration gradient, and (3) single-phase flow exists.

The use of Fick's law to describe diffusion means that a dilute solution is being used. In addition, any diffusion due to temperature gradients or velocity gradients is disregarded. Assuming that dispersion is proportional to a concentration gradient is discussed by Bear (1979).

Auxiliary Equations

Because of the interrelationship among several of the parameters in Equations 18 and 19, the following auxiliary equations are needed in the mathematical model. The components of the seepage velocity for the fluid mixture may be obtained from Darcy's law, and are given by:

$$V_i = -\frac{k_i}{\phi\mu} \left[\frac{\partial P}{\partial X_i} + \rho g \frac{\partial h}{\partial X_i}\right] \; ; \; i = r, z \tag{20}$$

The relationship between the porosity of the porous medium and the fluid pressure is assumed to be,

$$\phi = \phi_o \left[1 + C_F (P - P_o)\right] \tag{21}$$

where: ϕ_o = original porosity (dimensionless), and

P_o = original fluid pressure (FL^{-2}).

The density of the fluid mixture is assumed to be a linear function of the fluid pressure and tracer concentration,

$$\rho = \rho_o + \beta\rho_o (P - P_o) + \alpha (C - C_o) \tag{22}$$

where: ρ_o = original fluid density (ML^{-3}), and

C_o = original tracer concentration (ML^{-3}).

Also, the viscosity is assumed to be a linear function of the concentration,

$$\mu = \mu_o + \lambda(C - C_o) \tag{23}$$

where: μ_o = original viscosity (FTL^{-2}), and

λ = proportionality factor relating concentration and viscosity (dimensionless).

The use of Equations 21, 22, and 23 are assumptions. Equation 21 has been used in the petroleum industry with success (Breitenbach et. al, 1968b). Depending upon the fluids used, relationships other than those given by Equations 22

and 23 may be desirable. In this study, salt water and fresh water are used as the two fluids, and the linear relationships of Equations 22 and 23 are believed to be adequate.

Dispersion Coefficients

Equation 19 is developed in a general way so that any value may be used for the four components of the dispersion tensor. However, the use of a functional relationship is desirable which will give the values of all four components in a systematic manner.

Assuming an isotropic porous medium, the "tortuosity" tensor, T_{ij}, is given by:

$$T_{ij} = TS_{ij} \tag{24}$$

where: T = tortuosity factor (dimensionless), and

S_{ij} = kronecker delta.

Thus, the four components of the diffusion tensor are:

$$D_d \, T_{rr} = D_d \, T_{zz} = D_d \, T \tag{25a}$$

and

$$D_d \, T_{zr} = D_d \, T_{rz} = 0 \tag{25b}$$

Scheidegger (1961) gave the relationship,

$$D_{ij} = \varepsilon_{ijmn} \frac{V_m V_n}{V} \tag{26}$$

where: ε_{ijmn} = the dispersivity of the medium, a fourth rank tensor (L),

V_m, V_n = the components of velocity in the m and n directions, respectively (LT^{-1}), and

V = magnitude of the velocity (LT^{-1}).

For an isotropic media, Scheidegger shows that the dispersivities reduce to only two terms, ε_1 and ε_2, with

$$\varepsilon_{\alpha\alpha\alpha\alpha} = \varepsilon_1$$
$$\varepsilon_{\alpha\alpha\beta\beta} = \varepsilon_2$$
$$\varepsilon_{\alpha\beta\alpha\beta} = \tfrac{1}{2} (\varepsilon_1 - \varepsilon_2)$$
$$\varepsilon_{\alpha\beta\beta\alpha} = \tfrac{1}{2} (\varepsilon_1 - \varepsilon_2)$$

all other $\varepsilon\text{'s} = 0$ \hfill (27)

The longitudinal and transverse dispersion coefficients are related to the dispersivities by:

$$D_L = \varepsilon_1 V \tag{28a}$$

and

$$D_T = \varepsilon_2 V \tag{28b}$$

Expanding Equation 26, introducing Equations 27 and 28, and adding the diffusion tensor given by Equation 25, the following functional relationship for the four components of the hydrodynamic dispersion coefficient are obtained:

$$D_{rr}^* = D_L \frac{V_r V_r}{V^2} + D_T \frac{V_z V_z}{V^2} + D_d T \quad ,$$

$$D_{zz}^* = D_T \frac{V_r V_r}{V^2} + D_L \frac{V_z V_z}{V^2} + D_d T \quad ,$$

$$D_{rz}^* = D_{zr}^* = (D_L - D_T) \frac{V_r V_z}{V^2} \quad , \tag{29}$$

Other functional relationships for obtaining the components of the hydrodynamic dispersion tensor are given by Bear et. al. (1968), Poreh (1965), and List and Brooks (1967).

CHAPTER IV

DEVELOPMENT OF COMPUTER SIMULATOR

The computer simulation of the miscible displacement problem will be developed by writing the finite difference form for each of the equations given in Chapter III. The computer simulator is developed for a two-dimensional vertical flow problem.

Finite Difference Form of Two-Dimensional Flow Equation

An implicit, centered-in-space finite difference scheme is used to approximate the time and space derivatives of Equation 18. The two-dimensional finite difference equation has the form:

$$\rho_r^+ N_r^+ P_{i+1,k}^{t+1} + \rho_r^- N_r^- P_{i-1,k}^{t+1} + \rho_z^+ N_z^+ P_{i,k+1}^{t+1} + \rho_z^- N_z^- P_{i,k-1}^{t+1}$$

$$- [\rho_r^+ N_r^+ + \rho_r^- N_r^- + \rho_z^+ N_z^+ + \rho_z^- N_z^- + \rho_{i,k} (C_{F_{i,k}} + \beta_{i,k})/\Delta t] P_{i,k}^{t+1}$$

$$= - \frac{\rho_{i,k} (C_{F_{i,k}} + \beta_{i,k})}{\Delta t} P_{i,k}^t + \frac{\alpha_{i,k} (C_{i,k}^t - C_{i,k}^{t-1})}{\Delta t_o} + (\frac{\rho_P Q}{\phi \Delta r \Delta z})_{i,k}$$

$$- [(\rho_r^+)^2 N_r^+ g \Delta h_r^+ + (\rho_r^-)^2 N_r^- g \Delta h_r^- + (\rho_z^+)^2 N_z^+ g \Delta h_z^+ + (\rho_z^-)^2 N_z^- g \Delta h_z^-] \qquad (30)$$

Here i and k indicate the grid row and grid column respectively, and t indicates time level.

A cylindrical grid system is superimposed onto the region of interest, and Equation 30 written for each grid. The dimensions of the grids, Δr, and Δz, are assumed to be variable over the entire region. The coefficients, $\rho_{r,z}^\pm$ and $N_{r,z}^\pm$, are held constant during each time step. Approximation of the original non-linear equation is obtained by adjusting the values of $\rho_{r,z}^\pm$ and $N_{r,z}^\pm$ after each computation. If the change in $\rho_{r,z}^\pm$ and $N_{r,z}^\pm$ is small during each Δt, this procedure will produce acceptable results.

The change in concentration with respect to time on the right hand side of Equation 30 is calculated using the change in concentration from the previous time step, Δt_o. If the change in concentration during each Δt is small, this will also produce acceptable results. If necessary, an iteration between the solution of the flow equation and the dispersion equation can improve this approximation.

If the rectangular grid system has m-rows and n-columns, then there will be mn grids. Since Equation 30 contains unknown pressures from each of the four adjacent grids plus an unknown pressure for the grid in question, the result of writing Equation 30 for all grids is a set of mn simultaneous algebraic equations. This set may be written in matrix form as:

$$[A] \, [P] = [rhs] \qquad (31)$$

where [A] is a mn by mn matrix containing the coefficients of pressure, [P] is a mn column vector containing the unknown pressures, and [rhs] is a mn column vector containing all the factors on the right hand side of Equation 30.

Finite Difference Form of Two-Dimensional Dispersion Equation

The numerical solution of the multi-dimensional dispersion equation (Equation 19) has been a difficult problem. If the convective and production terms are neglected, the equation is a second order partial differential equation of parabolic type (heat flow equation) and is of the same form as Equation 18. A dispersion equation of this type could be solved in the same way as the flow equation given in Equations 30 and 31. This particular type of equation has been successfully solved numerically many times.

Now suppose that the dispersion and production terms of Equation 14 are neglected. Then the resulting equation is a first order partial differential equation of hyperbolic type and has been treated numerically with some success in one dimension. However, extension to two or more dimensions has proven diffi-cult. Usually one of two things happens: (1) the numerical solution develops oscillations or (2) it becomes smeared by "artificial dispersion" resulting from the numerical process. Thus, when convection and dispersion are considered simultaneously, this "artificial dispersion" may dominate the low physical dispersion which characterizes miscible displacement.

In problems of miscible displacement, the amount of dispersion is usually very small, and this makes the convective-dispersion equation almost of the hyperbolic type. Garder et. al. (1964) recognized this and developed a numerical technique for solving the convective-dispersion equation based on the method of characteristics.

The basis of the method of characteristics is the introduction of a set of moving points into each grid. Each of the moving points is assigned a concen-tration, which varies with time. At each time interval, the moving points in a two-dimensional system are relocated using a finite difference form given by,

$$X_{r\ell}^{t+1} = X_{r\ell}^{t} + \Delta t \ V_{r\ell}^{t+1} \tag{32}$$

and

$$X_{z\ell}^{t+1} = X_{z\ell}^{t} + \Delta t \ V_{z\ell}^{t+1} \tag{33}$$

where t+1 is the new time level, t is the old time level, Δt is the time increment, $X_{r\ell}$ and $X_{z\ell}$ are the coordinates of the ℓth moving point, while $V_{r\ell}$ and $V_{z\ell}$ are the velocities of the ℓth moving point in the r- and z-directions.

Each cell in the grid system is assigned a concentration equal to the average of the concentrations of the moving points located inside the cell at time t+1. The concentration of the cell and each moving point inside the cell is then modified for dispersion by solving $dc/dt = f(X_1, X_2, X_3, t)$ using an explicit, centered-in-space finite difference equation. The two-dimensional form of this equation is:

$$
\begin{aligned}
C_{i,k}^{t+1} = \ & C_{i,k}^{t+\Delta} + E_{rr}^{+} \ (C_{i+1,k}^{t+\Delta} - C_{i,k}^{t+\Delta}) - E_{rr}^{-} \ (C_{i,k}^{t+\Delta} - C_{i-1,k}^{t+\Delta}) \\[4pt]
& + E_{zz}^{+} \ (C_{i,k+1}^{t+\Delta} - C_{i,k}^{t+\Delta}) - E_{zz}^{-} \ (C_{i,k}^{t+\Delta} - C_{i,k-1}^{t+\Delta}) \\[4pt]
& + G_{rz}^{+} \ (C_{i,k+1}^{t+\Delta} + C_{i+1,k+1}^{t+\Delta} - C_{i,k-1}^{t+\Delta} - C_{i+1,k-1}^{t+\Delta}) \\[4pt]
& - G_{r,z}^{-} \ (C_{i-1,k+1}^{t+\Delta} + C_{i,k+1}^{t+\Delta} - C_{i,k-1}^{t+\Delta} - C_{i-1,k-1}^{t+\Delta}) \\[4pt]
& + G_{zr}^{+} \ (C_{i+1,k+1}^{t+\Delta} + C_{i+1,k}^{t+\Delta} - C_{i-1,k+1}^{t+\Delta} - C_{i-1,k}^{t+\Delta}) \\[4pt]
& - G_{zr}^{-} \ (C_{i+1,k}^{t+\Delta} + C_{i+1,k=1}^{t+\Delta} - C_{i-1,k}^{t+\Delta} - C_{i-1,k-1}^{t+\Delta}).
\end{aligned}
\tag{34}
$$

Here i and k indicate grid rows and grid columns respectively, t+1 is the new time level and t+Δ is a time level somewhere between t and t+1.

Finite Difference Form of Velocity Equation

In the method of characteristics described above, a determination of the seepage velocity is necessary for relocating the moving points during each time step. This is accomplished with the following procedure. The flow equation (Equation 18) is solved for the pressures at time level t+1. These pressures are assigned to the centers of each of the grids. Using these pressures and Darcy's law, a value for the seepage velocity at the contact between two

adjacent grids may be calculated. A seepage velocity is assigned to each moving point within a grid based on the value of the seepage velocities at the interfaces. A linear interpolation is used in making this assignment.

Boundary Conditions

Appropriate boundary conditions due to geologic and hydrologic influences must be used to obtain a solution. These conditions take the form of (a) no-flow boundaries, (b) hydraulic boundaries at ground surfaces, (c) groundwater underflow boundaries, and (d) known tracer concentrations maintained at certain boundaries.

No-flow boundaries are simulated by assigning a permeability of zero, a longitudinal dispersion coefficient of zero, and a transverse dispersion coefficient of zero to the grids located along the boundary. Hydraulic boundaries at the ground surface are most commonly encountered in the form of a direct connection between a groundwater aquifer and a river or lake, and are simulated by programming a time-varying or constant water pressure in the appropriate grids. Groundwater underflow boundaries occur when only a portion of an aquifer is being studied. This boundary condition may be simulated in many ways, but perhaps the simplest is to project the pressure gradient and concentration gradient across the boundary and calculate the rate of underflow using these projected gradients. Boundary conditions for known tracer concentrations must be specified also. These conditions are handled in this simulation by the moving points. As fluid leaves the model, moving points with their corresponding concentration values are removed from the system. As fluid enters the model, moving points with the appropriate boundary concentrations are added to the system.

Description of the Computer Program

The computer simulation was programmed in Fortran IV using vector processing and ran on the Cyber 205 Computer at Colorado State University.

The MAIN program accepts the input data and governs the sequence of operations to be performed. Subroutine INICON assigns a uniform distribution of "moving" points to each grid along with the initial value of concentration assigned to each point. Subroutine READIN reads in or assigns appropriate values to all physical quantities such as permeability, porosity, viscosity, etc. All of the initial values are then printed out using subroutine INIPRT and subroutine MATROP.

Subroutine MATSOL sets up the coefficient matrix, [A], and the right hand side column vector, [rhs], for solving the pressure equation. This subroutine, as is presently written, may take care of two types of boundary conditions: (1) a constant pressure boundary, and (2) a no-flow boundary. Other boundary conditions besides these may easily be added to the program. MATSOL checks the boundary conditions and makes the appropriate changes in [A] and [rhs].

To solve the set of equations set up by MATSOL, the solution of a set of simultaneous equations is required. A general numerical solution should offer several solution techniques such as Gauss elimination, successive overrelaxation (SOR), or iterative alternating direction implicit procedure (ADIPIT). For a review of these techniques, the reader is referred to Breitenbach et. al. (1968b).

Gauss elimination is by far the most reliable numerical method one can choose for solving the matrix given by Equation 31. Several codes for use on vector processing machines are available; so we chose Gauss elimination as our matrix solver.

Subroutine VELOCY calculates the velocities at each grid interface. This routine also calculates the longitudinal and lateral dispersion coefficients using a velocity power relationship. With values for the dispersion coefficients and velocity components, Equation 29 is used to calculate the components of the dispersion tensor.

Subroutine MOVPT uses the velocities calculated in VELOCY to obtain the velocity components of each moving point. Each point is then moved to a new location by use of Equations 32 and 33. A section of this subroutine determines which of the points has moved out of the model. These points are tagged and introduced at an inflow boundary with the appropriate boundary concentration. Of all the subroutines developed for this simulator, MOVPT is probably the least general. At the present time, minor changes in the program must be made when boundary conditions are changed to allow for the proper removal and re-introduction of the moving points. After each point has been moved to a new location, the average concentration of each grid is calculated by arithmetically averaging the concentrations of the "moving points" located in the grid.

With the average concentrations of each grid determined, subroutine DISP uses Equation 34 to determine the change in concentration due to dispersion. The end result is the concentration of each grid at time $t+\Delta t$. To conclude a time step, a mass balance of the system is calculated and appropriate changes in density, viscosity, and porosity are made using Equations 21, 22, and 23. A test

for print out is made and the program returns to subroutine MATSOL where the pressure equation is resolved and the entire process repeated for the nest time step.

CHAPTER V

RESULTS AND DISCUSSION

Because of the difficulty in obtaining theoretical criteria for the validity of the numerical simulator, experience with actual problems is a necessity. The numerical solution of the pressure equation has been done successfully many times. However, the solution of the dispersion equation by the "method of characteristics" (MOC) has not been so widely studied.

Verification

Unfortunately, there is little field data available from operating saline aquifer systems. Therefore, verification of the model was done by numerical checks and comparison with analytical solutions for simplified systems.

The model was numerically checked by performing a water and tracer mass balance at the end of each time step. The ratio:

$$MB = \frac{(Input-Output)}{Change\ in\ Storage} \tag{35}$$

was unity to a minimum of seven significant digits for both the water mass and tracer mass for all time steps. This indicates that all water mass and tracer mass was conserved in the system.

Due to the coupling of the two transport mechanisms, it was undesirable to completely isolate one from the other. However, tracer and water mass fluxes were used which allowed this complicated flow system to approach simpler systems for which analytical solutions are available.

For example, by making the tracer concentration in the injected water equal to the tracer concentration of the groundwater, the system should respond as if there were water mass flow only. Comparison of values of water pressure from a representative plane of the simulation with those calculated from the popular Theis (1935) solution is shown in Figure 1. This pressure profile was for a confined aquifer with a transmissivity of 0.13 m^2 s^{-1} and a storage coefficient of 1.4 x 10^{-5} after water had been injected at 0.63 m^3 s^{-1} for 5000 sec. The model predicts a slightly lower water table than the theis solution due to the constant head boundary at 10^4 m. as opposed to the infinite radius assumed in the Theis (1935) solution.
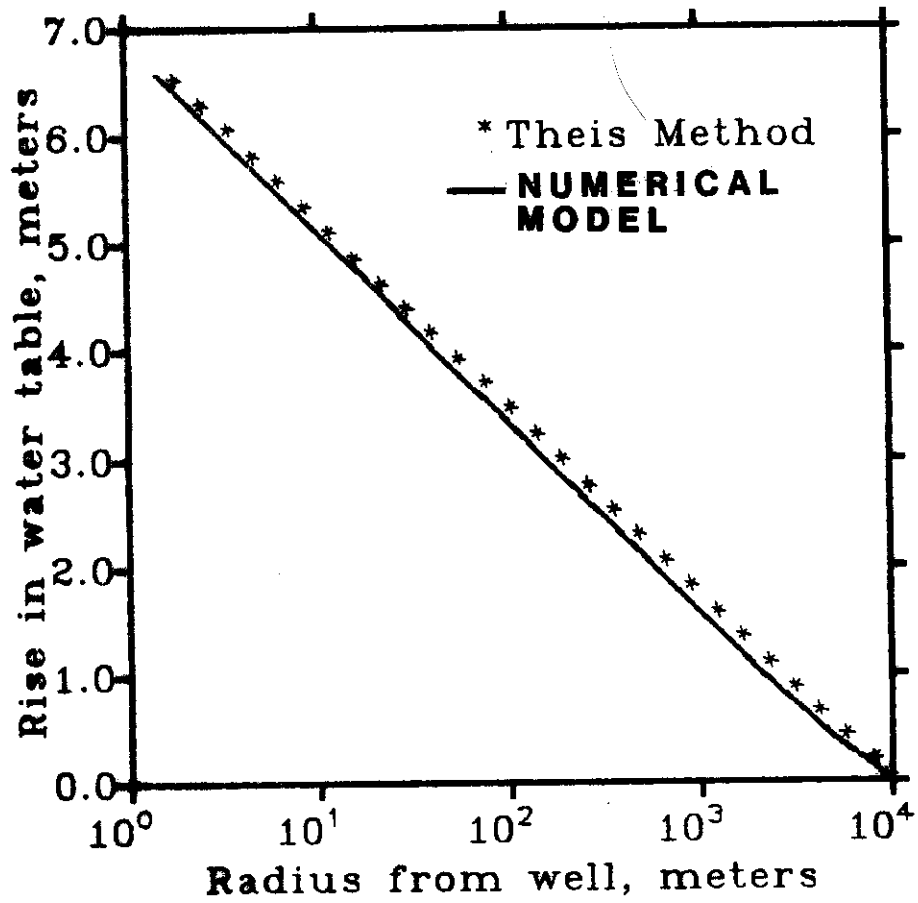
Figure 1. Comparison of computer model and Theis
solution for water level rise.

A constant water and tracer mass injection rate and a negligible fluid and media compressibility reduces the system to nearly the one solved analytically by Hoopes and Harleman (1967a). Values of concentration from a representative plane of the simulation are compared to the analytical solution of Hoopes and Harleman in Figure 2. This concentration profile was for a 50 m thick aquifer with confining layers on the top and bottom. Water with a concentration of 100 percent was injected at 0.063 m^3 s^{-1} into the well for 7.0 x 10^4 sec. The coarse grid spacing accounts for some of the disagreement at the concentration front between 2.34 and 11.8 m. The models' concentration front leads slightly due to some numerical dispersion in the model.

Verification of the Method of Characteristics

If the results of known analytical solutions can be reproduced, a great deal of confidence in the numerical solution can be gained. An analytical solution to the one dimensional problem with a step input of the tracer as a boundary condition is available. Garder et. al. (1964) showed that accurate solutions of one-dimensional problems can be obtained by the MOC over a wide range of values of the dispersion coefficient, including zero. They also showed that the moving points do not need to be uniformly spaced, and that increasing the number of moving points beyond two points per grid did not significantly improve the accuracy of the solution. A run was made using the data of Garder et. al. (1964), and excellent results were obtained.

An analysis of the slightly more difficult problem of two dimensional dispersion is the next logical step. A rectangular region, $0 \leq X_3 \leq \ell_3$ and $0 \leq X_2 \leq \ell_2$ is considered in which the flow is along the X_3-axis with a steady, uniform seepage velocity, V_3. A fluid of concentration, C_o, is injected over a portion of the input boundary ($0 \leq X_2 \leq b$), while the remaining portion of the boundary ($b \leq X_2 \leq \ell_2$) is injected with a fluid of zero concentration. A schematic of this particular problem is shown in the upper right hand corner of Figure 3.

When the input concentration at $X_3 = 0$ is maintained for a long time, the concentration distribution will approach a steady state. Harleman and Rumer (1963) neglected the longitudinal dispersion term in the differential equation and solved the steady state problem. Neglecting the lognitudinal dispersion is valid because $\partial^2 C / \partial X_3^2$ is very small at steady state. Their approximate solution for the steady state case was:

$$\frac{C}{C_o} = \frac{1}{2} \text{ erfc } [\frac{X_2 - b}{2\sqrt{D_T \, X_3/V_3}}] \qquad (36)$$
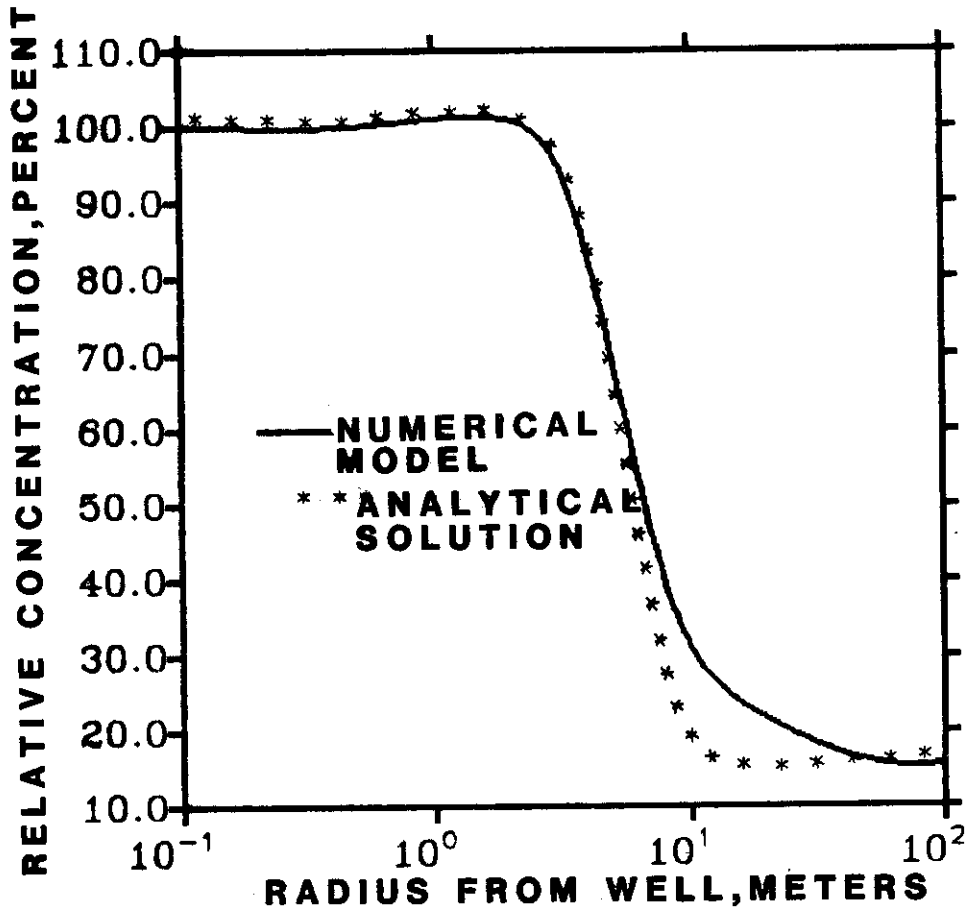
Figure 2. Comparison of computer model and
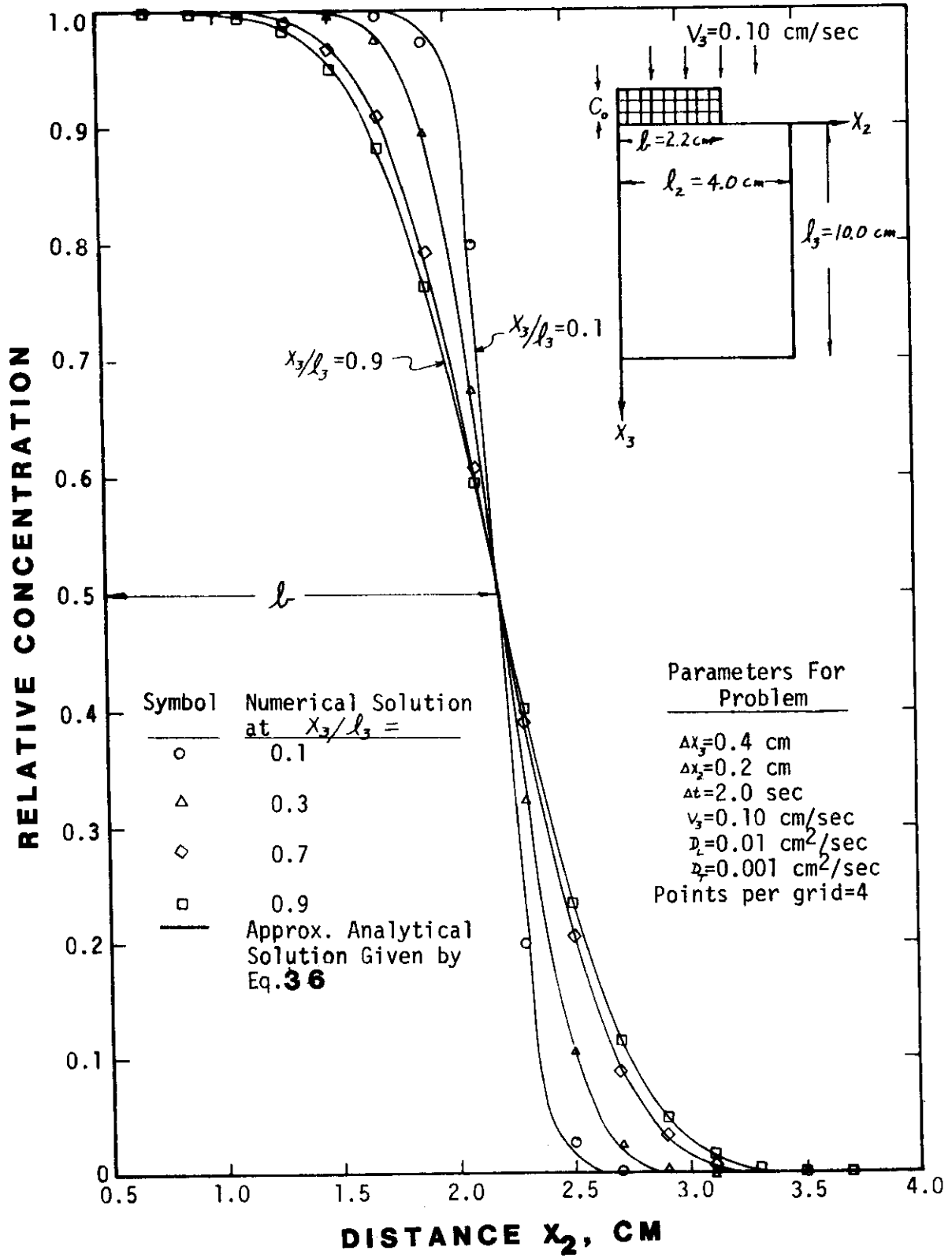analytical solution for concentration
profile.

Figure 3. Comparison of MOC model and analytical solution for two-dimensional dispersion.

The numerical solution of this problem using the MOC was compared with the solution given by Equation 36. Data for this run are: 25 x 20 grids on $0 \leq X_3 \leq 10$ cm and $0 \leq X_2 \leq 4$ cm, $V_3 = 0.10$ cm/sec, $D_L = 0.01$ cm^2/sec, $D_T = 0.001$ cm^2/sec, points per grid = 4, $\Delta X_3 = 0.4$ cm, $\Delta X_2 = 0.2$ cm, b = 2.2 cm, and $\Delta t = 2.0$ sec. As was done for the one dimensional problem, the computer program bypassed the solutions of the pressure equation and velocity equation. Steady state conditions were achieved at about 200 seconds, or after about 100 time steps. The computer time required to solve the dispersion equation for this problem was about 0.55 secs/time step. The step input of concentration was handled numerically by letting $C/C_o = 1.0$ for $X_2 < b$, $C/C_o = 0.5$ for $X_2 = b$, and $C/C_o = 0.0$ for $X_2 > b$.

The numerical solution provided the transient concentration distribution, but no check of its accuracy was made since Equation 36 is for steady state. The numerical results at steady state (t=200 secs) are compared with the approximate analytical solution (Equation 36) in Figure 3. The accuracy of the results appear to be quite good except for the area close to $X_3=0$. This should be expected since the assumption of $\partial^2 C/\partial X_3^2 = 0$ in the analytical solution is not valid in this area. Some of this discrepancy may also be the result of the very steep concentration profile in the X_2-direction for the area close to $X_3=0$. Although not tried, smaller grid dimensions in the X_2-direction might improve the results.

The MOC appears to be capable of solving problems of longitudinal and lateral dispersion with as much ease as it did longitudinal dispersion alone. No problems with "overshoot" occurred and no numerical smearing was noticed.

Dispersion Along Equilibrium Salt-Water Wedge

In the above section, the numerical simulation of the dispersion equation and the water flow equation were compared with known analytical solutions. However, the total simulator using both the dispersion equation and the flow equation have not been used. A problem which seems favorable to this type of analysis is the salt-water intrusion problem. Rumer and Harleman (1963) used a laboratory model of a two-dimensional confined aquifer to investigate convection and dispersion along a salt-water wedge. Columbus (1965) used a Hele-Shaw model to investigate sea-water intrusion in an unconfined model neglecting dispersion. Because Rumer and Harleman's (1963) data contained information on the value of the coefficients, a computer run was made using the data from one of their laboratory runs.

The equilibrium salt-water wedge, when subjected to the steady flow of fresh water to the ocean, will develop a transition zone. Using Darcy's law and the Dupuit-Forchheimer approximation, the specific discharge of fresh water per unit width of ocean front, $\tilde{q}$, can be written as

$$\tilde{q} = K \; y \; \frac{dh^*}{dX_1} \tag{37}$$

in which K = hydraulic conductivity, y is the distance between the top of the aquifer and the wedge interface, and h^* is the piezometric head (Figure 4). The medium is assumed to be homogeneous, isotropic, and no mixing occurs at the interface.

The condition of equal pressures in the salt-water and the fresh water at each point along the interface yields

$$y = \frac{\rho_f}{\Delta\rho} \; h^* - \frac{\rho_s}{\Delta\rho} \; \xi \tag{38}$$

where ρ_f and ρ_s are the densities of fresh and salt-water, respectively, and $\Delta\rho = \rho_s - \rho_f$. Substituting Equation 38 into Equation 37, integrating and solving for h^8, Rumer and Harleman (1963) found an equation for the interface of the following form:

$$y = \frac{2\tilde{q}}{K \; \Delta\rho/\rho_f} \; X_1 + \left(\frac{0.741 \; \tilde{q}}{K \; \Delta\rho/\rho_f}\right)^2 \tag{39}$$

Although the static interface between fresh and salt-water will be subjected to dispersion, Rumer and Harleman (1963) showed that the position of the mean isoclor (C=0.5) is adequately predicted by Equation 39.

Rumer and Harleman (1963) gave the following information for their Run No. N-2: $\tilde{q}=0.0733$ cm^2/sec, $\Delta\rho/\rho_f=0.006$, K=0.835 cm/sec, porous medium = plastic spheres, and median grain diameter = 0.965 mm. A computer run was made using Rumer and Harleman's information, plus some additional data required by the numerical simulator. The data used in the computer run are: $\Delta X_1=6.0$ cm, $\Delta X_2=6.0$ cm, $\Delta t=500$ sec, $k=9.885 \times 10^{-6}$cm^2, $\phi=0.39$, $\rho_f=1.000$, $\rho_s=1.006$, $\Delta\rho=0.006$, $\mu=.0116$ poise, fluid compressibility = 0.0, rock compressibility = 0.0, $\lambda=0.0$, $\alpha=0.006$, grid dimensions = 12 x 27, depth of aquifer = 60 cm, length of aquifer = 156 cm, $\xi=33$ cm, $\tilde{q}=0.0736$ cm^2/sec, moving points per grid = 2, and the acceleration of gravity = 980 cm/sec^2. In addition to these data, the dispersion coefficients were assumed to be given by:

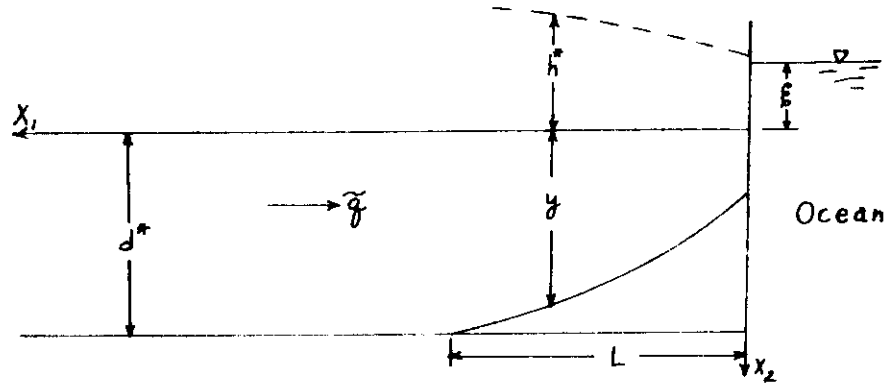Figure 4. Equilibrium wedge in a confined aquifer.

$$\frac{D_L \, \rho}{\mu} = 0.66 \, (\frac{V \, d_{50} \, \rho}{\mu})^{1.2} \tag{40}$$

and

$$\frac{D_T \, \rho}{\mu} = 0.036 \, (\frac{V \, d_{50} \rho}{\mu})^{0.7} \tag{41}$$

The reason for using Equations 40 and 41 is that Harleman and Rumer (1963) determined these relationships for the same medium (plastic spheres) used by Rumer and Harleman (1963) in their study of sea water intrusion.

The computer run was made for 60 time steps or about 8.33 hours. Whether this was long enough for the wedge to reach equilibrium is unknown. The concentrations were not changing very rapidly, and the toe of the wedge was moving very slowly. Therefore, the wedge was assumed to be in equilibrium. The computer time required for solving both the flow equation and dispersion equation for this 12 x 27 grid network was about 3.4 sec per time step.

A comparison of the fresh water head calculated numerically and by Equation 39 is shown in Figure 5. The comparison shows that the numerical results and those by Equation 39 are very close except for the region close to the ocean front. This would be the region affected most by the use of the Dupuit-Forchheimer assumptions.

Figure 6 shows a comparison of the mean concentration line (C/C_o=0.50) calculated numerically and the interface location obtained from Equation 39. These results are good except in the vicinity of the wedge toe. Several factors may be contributing to this error. First, the numerical results may not be completely at a steady state. Another factor which proved a limitation on this problem is the extremely steep concentration profiles. In fact, the profile is so steep that the grid concentrations obtained from the computer were generally either C/C_o=1.0 or C/C_o=0.0. Very few grids had a value for C/C_o between these two extremes. Thus, a large amount of interpolation was required to determine the line C/C_o=0.5. To alleviate this problem, smaller spatial dimensions are needed. Last, it must be remembered that Equation 39 is only an approximation itself.
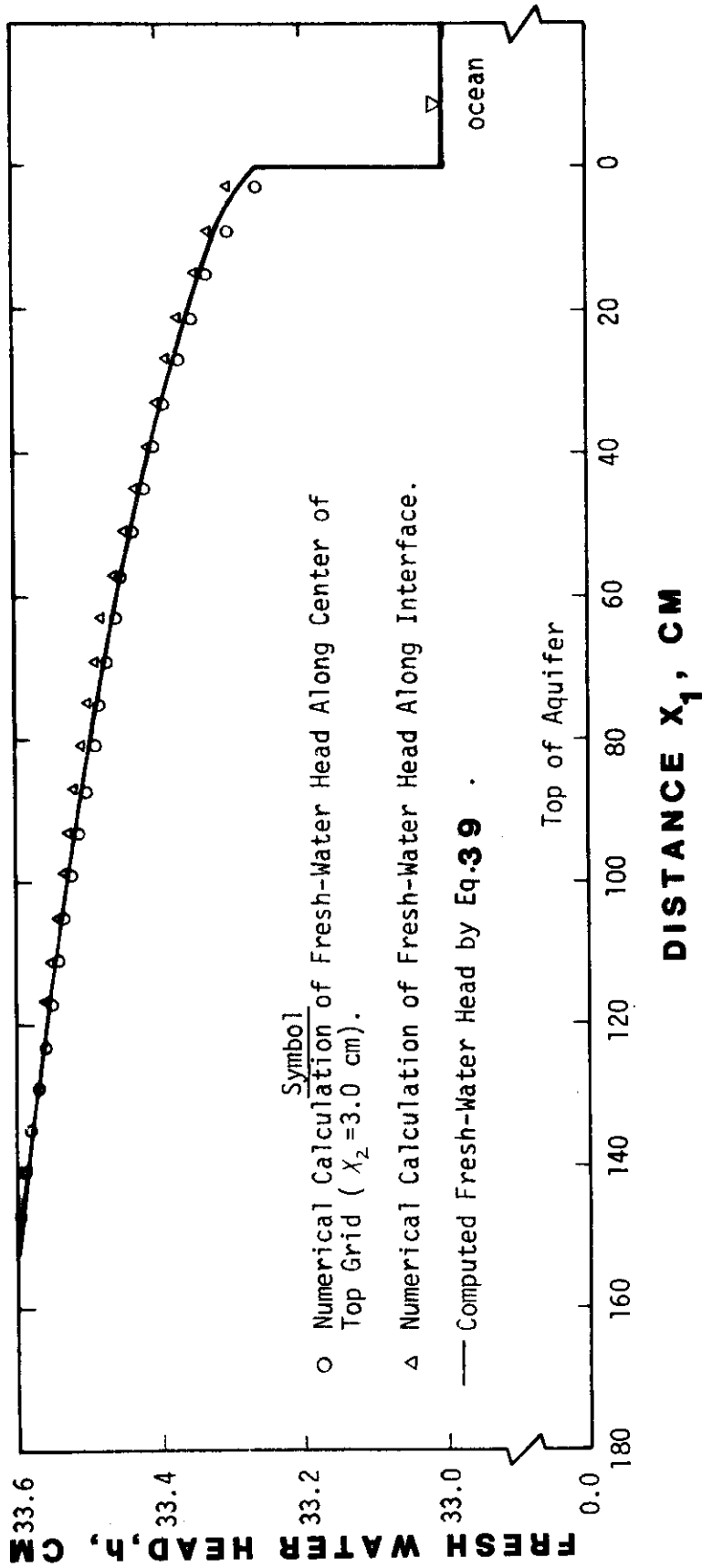
Figure 5. Comparison of fresh water head computed numerically and analytically for the salt-water intrusion problem.
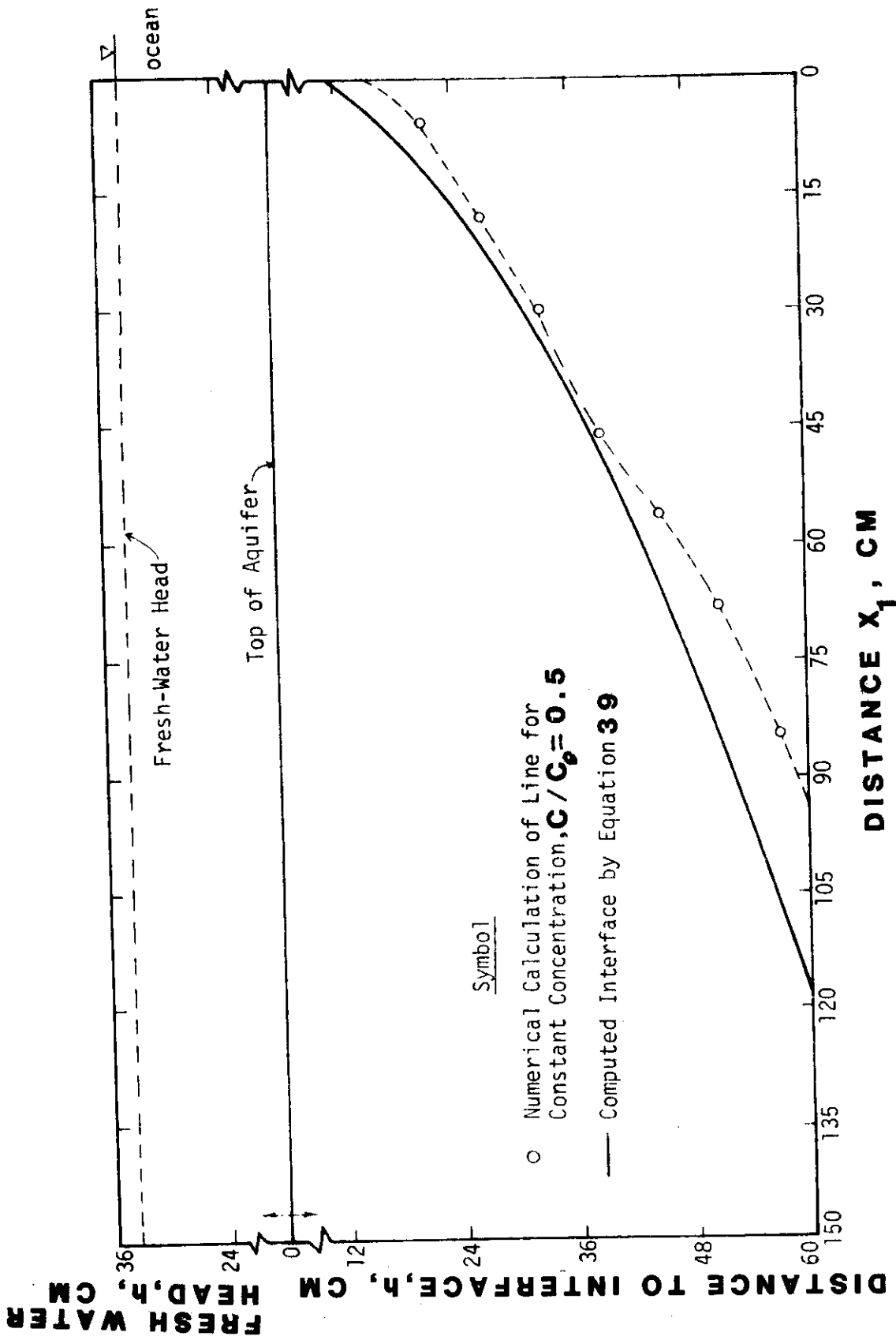
Figure 6. Comparison of salt-water interface location calculated with the numerical model and analytically.

CHAPTER VI

SUMMARY AND CONCLUSIONS

A two-dimensional radial flow model for a mixture of miscible fluids (fresh water and salt-water) was derived. Also, a two-dimensional radial convective-dispersion equation describing the movement of a tracer miscible with groundwater was derived. Finite difference forms of these two equations were developed.

The model was verified for a radial flow problem in which salt-water is injected into a fresh water zone. The model was then built to simulate Jacob's single location well doublet for controlling salt-water intrusion. The method appears to be promising, particularly in aquifers with clay lenses. The model was developed for running on a vector processing computer such as the Cyber 205 or Cray. Copies of the model are available upon request.

While an evaluation of design parameters for the single location well doublet was a second goal of this research, funding for the project was terminated after one year, and design parameters have not been evaluated. Through a grant from the CDC Corporation, Cyber 205 computer time has been made available to us and we will complete the evaluation of design parameters for the single location well doublet.

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