Simulation of Bromide Transport in a Layered Aquifer Using Two-Dimensional and Three-Dimensional Computer Models

Kathleen Michelle Hewitt
Western Michigan University

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SIMULATION OF BROMIDE TRANSPORT IN A LAYERED AQUIFER USING TWO-DIMENSIONAL AND THREE-DIMENSIONAL COMPUTER MODELS

by

Kathleen Michelle Hewitt

A Thesis
Submitted to the Faculty of The Graduate College in partial fulfillment of the requirements for the Degree of Master of Science Department of Geology

Western Michigan University Kalamazoo, Michigan June 1990
Simulation of a two-well tracer test at a site near Mobile, Alabama was performed and compared with the experimental breakthrough curve. The models used to simulate the test results were the three-dimensional USGS code HST3D and the two-dimensional USGS code MOC. The results of the three-dimensional model were also compared with the results of the two-dimensional model.

The three-dimensional model HST3D predicted the measured breakthrough curve accurately with the exception of early arrival times of the tracer in the withdrawal well. The two-dimensional model MOC did not accurately predict the bromide concentration in the withdrawal well during the two-well test. When the dispersivity was increased forty-fold, the MOC results approximated the measured breakthrough curve.
ACKNOWLEDGEMENTS

I would like to thank my advisors in the Department of Geology, Academic Computer Services, Stan Williams from the International Groundwater Modeling Center, Ken Kipp from the United States Geological Survey, and my family for all their help and support in the course of this research.

Kathleen Michelle Hewitt
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Simulation of bromide transport in a layered aquifer using two-dimensional and three-dimensional computer models

Hewitt, Kathleen Michelle, M.S.

Western Michigan University, 1990
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CHAPTER I

INTRODUCTION AND STATEMENT OF THE PROBLEM

Introduction

The need to accurately predict the flow of contaminants in groundwater has become increasingly important as the number of contaminated groundwater sites has increased dramatically in past years. Many numerical groundwater contaminant transport models have become available in an attempt to meet this need, and their ability to accurately predict the location of contaminants in time and space has become an important issue.

The following investigation was undertaken with the purpose of determining the validity of studies which utilize these numeric computer models. The investigation involved applying two general numerical models to a published data set. The published data set comes from a bromide tracer test performed at a site near Mobile, Alabama, in an aquifer consisting of a Quaternary fluvial terrace deposit (Molz, Guven, Melville, Crocker, & Matteson, 1986). This tracer test was used to predict the tracer movement based on the vertical distribution of horizontal hydraulic conductivity inferred from independent
tracer tests. In the experiment by Molz et al., 1986, two separate wells were used. A tracer solution was injected in one well and produced at a second well at the same constant rate, 0.9464 m³/min (Figure 1). The results of this two-well test were then simulated by two independent models. The first of these was a three-dimensional finite element model which was developed to simulate two-well tests (Huyakorn, Andersen, Molz, Guven, & Melville, 1986). The model employs fully three-dimensional dispersion and a curvilinear coordinate system which conforms to the curved groundwater flowlines created by the two-well pumping pattern. The second model was also developed specifically to fit the flowline geometry for two-well tests, but it is based solely on advection (Guven, Falta, Molz, & Melville, 1986). The results of both simulations predicted quite accurately the recovery concentrations of the two-well test without any prior calibration or knowledge of the test results. The Mobile data set, when utilized with these models, appears to contain enough data to accurately predict the location of contaminants in time and space and was therefore selected for use in the current investigation.

The objective of this study was to determine whether general contaminant transport models which are often applied to predict the plume movement at sites can successfully predict chemical movement at this nearly
Figure 1. Two-Well Test Configuration and Flow Pattern in a Perfectly Stratified Aquifer.

Source: Molz et al., 1986, p 1032.
homogeneous site. These general transport models use rectangular grids which cannot conform to all the groundwater flowlines created by the two-well pumping pattern as did the two models cited above. The following models were applied to the Mobile data set: the three-dimensional United States Geological Survey code HST3D (Kipp, 1987) and the widely used two-dimensional USGS code MOC, version 2.5 (Konikow & Bredehoeft, 1978). Conclusions regarding the validity of studies utilizing HST3D and MOC can be drawn by applying these models to the published data set and comparing their results with the measured concentration versus time curve. If these models cannot predict the measured breakthrough curve at this site for this relatively small and simple test, the chances of their correctly predicting contaminant plume movement based on a similar data set at a larger and more heterogeneous site are quite small.

This investigation used both two-dimensional and three-dimensional computer models and compared their results. Molz, Guven, & Melville (1983) determined in an examination of scale-dependent dispersion coefficients that the vertical distribution of horizontal conductivity and the local vertical transverse dispersion coefficient play key roles in the dispersion process. They concluded that the spreading of a solute near the source is primarily due to different advection rates at different aquifer
elevations and that this spreading is not adequately represented by a scale-dependent dispersion coefficient. Scaling up the dispersivity value in a computer model is necessary when the dimensionality of a calibrated model does not match the dimensionality of the system which is being modeled. Therefore, using a two-dimensional areal model to simulate a three-dimensional physical system will require a dispersivity value which is orders of magnitude larger than the actual value because the three-dimensional nature of the dispersion process is not represented. In a three-dimensional model the vertical distribution of horizontal hydraulic conductivity and the transverse dispersivity can be utilized to represent this dispersion process (Domenico & Robbins, 1984).

The Mobile Site

Background

The Mobile site refers to a portion of the Barry Steam Plant which is located approximately 32 km north of Mobile, Alabama. Auburn University began experimental study of aquifer thermal energy storage at the site in the summer of 1976 (Parr, Molz, & Melville, 1983). The surficial deposits at the site consist of a Quaternary terrace deposit comprised of interbedded sand and clay units deposited along the western edge of the Mobile River.
These deposits extend down to the Tertiary-Quaternary contact located at a depth of approximately 61 m. Miocene deposits are found below this depth and consist of undifferentiated sands, silty clays, and thin-bedded limestones which extend to a depth of approximately 305 m. The sand formation extending from approximately 30 m to 61 m below the land surface constitutes the confined aquifer used for the thermal energy storage experiment. It is composed of medium sand containing a variable but maximum content of 15% silt and clay by weight.

Various pumping tests were performed at the Mobile site during the Auburn study including an anisotropy pump test, a leaky aquifer pump test, and standard pump tests. Parr et al. (1983), established the following: a regional gradient of 3.3 E-4, a porosity of 0.33, a longitudinal dispersivity value of 9.1 cm, a hydraulic conductivity of 53.6 m/day, a storage coefficient ranging from values of 0.00049 to 0.00069, a transmissivity ranging from values of 1,130 m²/day to 1,140 m²/day, and a ratio of horizontal permeability to vertical permeability equal to 6.71.

Further research was begun at the site in the spring of 1984 when a series of single-well tracer tests and a two-well tracer test were performed in the 21.6 m thick confined sand aquifer (Molz et al., 1986).
Single-Well Test

Single-well tracer tests were performed with the purpose of inferring the vertical distribution of horizontal hydraulic conductivity distribution between an injection well and a multilevel observation well. In the tests a conservative tracer solution was injected into the aquifer for a period of time and then withdrawn through the same well. Throughout the test duration the concentration of the injected/withdrawn water was recorded as a function of time at the injection/withdrawal well and at one or more nearby multilevel observation wells which were also used to infer tracer travel times for different aquifer depths. The inferred vertical distribution of horizontal hydraulic conductivity shown in Figure 2 is a composite result of these single-well tests.

Two-Well Test

The test consisted of injecting a bromide tracer solution of variable but known concentration into a fully-screened injection well at a constant rate of 0.9464 m³/min (Figure 3). A fully-screened pumping well located 38.28 m from the injection well was simultaneously withdrawing the solution at the same constant rate (Figure 1). The two-well tracer test was performed in the nonrecirculating mode, which refers to disposal of the withdrawn water at a
Figure 2. Inferred Normalized Hydraulic Conductivity Distribution Based on the Results of a Single-Well Test.

Source: Molz et al., 1986, p 1032.
Figure 3. Injection Well Bromide Tracer Concentration Versus Time During the First 80 Hours of the Two-Well Test.

Source: Molz et al., 1986, p 1032.
safe distance from the test area. The tracer was injected for 3.19 days followed by pure water injection, while the total duration of the entire two-well test was 32.5 days. Throughout this period the concentration of the withdrawn water was recorded as a function of time at the pumping well (Figure 4) and at a multilevel observation well. The observation well contained seven 0.9-m-long sampling zones which were kept continuously mixed using peristaltic sampling pumps. This test was used to determine whether the hydraulic conductivity distribution established by the single-well tests was applicable over the longer distances involved in the two-well test.

Two-Well Test Simulation

Prior to this study, the two-well test was simulated using two separate and independent computer models. The data supplied for the simulations is presented in Table 1.

The first model, developed under contract to Auburn University by GeoTrans, Inc., Herndon, Virginia, is a three-dimensional advection-dispersion model. The numerical formulation of the model is performed in three-dimensional curvilinear coordinates developed specifically for the simulation of two-well tracer tests conducted in perfectly stratified aquifers (Huyakorn et al., 1986). For the simulation of the Mobile two-well test, stratified and steady horizontal flow within each homogeneous, isotropic
Figure 4. Measured Bromide Concentration Versus Time in the Withdrawal Well During the Two-Well Test.

Source: Molz et al., 1986, p 1033.
<table>
<thead>
<tr>
<th>Layer (i)</th>
<th>Layer Center ($z_i$), m</th>
<th>Layer Thickness, m</th>
<th>Normalized Conductivity $K(z_i)K_{max}$</th>
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<tr>
<td>Transverse (vertical) dispersivity</td>
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<td>Tracer injection time</td>
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<td>Total injection time</td>
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<td>Porosity</td>
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<tr>
<td>Aquifer thickness</td>
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<tr>
<td>Molecular diffusion coefficient</td>
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<td>Screen location (injection well)</td>
<td>fully penetrating</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Screen location (withdrawal well)</td>
<td>fully penetrating</td>
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<tr>
<td>E3 observation well coordinates</td>
<td>(x=13.56 m, y=0)</td>
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Source: Molz et al., 1986, p 1034.
layer was assumed. The model evaluates the Darcy velocity distribution based on the advection pattern for the flow between an injection and production well and uses it to solve the advection-dispersion equation written in three-dimensional curvilinear coordinates.

The second model used to simulate the two-well test results was developed at Auburn University (Guven et al., 1986). The Two-Well Advection Model (TWAM) assumes that the aquifer is horizontal, confined, of constant thickness and porosity, and perfectly stratified in the vicinity of the two wells. The model is based solely on the stratified velocity field obtained from a steady-state analytical solution, ignoring completely any local hydrodynamic dispersion.

Both simulations did a remarkable job of predicting the bromide concentration in the withdrawal well during the two-well test (Figure 5). These results were obtained with no prior calibration or knowledge of the test results shown in Figure 5 and are based on the information in Table 1. The information in this table comes directly from field measurements or calculations derived from field measurements with the exception of the dispersivity and porosity. The dispersivity values were chosen to be small finite values similar in scale to those determined by Parr et al. (1983). A porosity of 0.41 was measured in the laboratory on Shelby tube samples which were moderately
Figure 5. Comparison of Measured and Predicted Bromide Tracer Concentration Versus Time in the Withdrawal Well Based on the Normalized Hydraulic Conductivity Distribution Shown in Figure 1.

Source: Molz et al., 1986, p 1034.
disturbed. Because this value is probably higher than the porosity of an undisturbed sample, a smaller value of 0.35 was chosen.

The similarity between the two separate simulation results indicates that hydrodynamic dispersion has a negligible effect on the tracer concentration at the withdrawal well. The results of the two-well tracer test and these simulations suggest that the spreading of the tracer slug over the distances involved in the two-well test depended largely on velocity variations that were controlled by the permeability distribution shown in Figure 2 (Molz et al., 1986).
CHAPTER II

MOBILE DATA APPLICATION TO GENERAL MODELS

HST3D

Introduction

The first model used in this investigation was HST3D: A Computer Code for Simulation of Heat and Solute Transport in Three-Dimensional Ground-Water Flow Systems. The HST3D computer code by Kenneth L. Kipp Jr., 1987, is a descendent of the Survey Waste Injection Program (SWIP) which was developed for the U.S. Geological Survey in 1976 and revised in 1979. HST3D may be used to simulate groundwater flow and associated heat and/or solute transport in saturated, three-dimensional flow systems with variable density and viscosity. It is a finite difference model which allows the option of three-dimensional cartesian or axisymmetric, cylindrical coordinate systems. The program has a length of approximately 12,000 lines of code and the capability to simulate a wide variety of physical systems.

The current investigation, which utilized HST3D to simulate the two-well test results at the Mobile site, did not require its more complex capabilities such as variable density and viscosity. HST3D was chosen to be the three-
dimensional (3-D) model used in this investigation primarily because it was easy to acquire, and was expected to become the standard 3-D model due to USGS support.

**HST3D Simulation Results**

The information presented in Table 1 was input into the model along with values of vertical permeability based on the ratio of horizontal permeability to vertical permeability determined from the anisotropy pump test. The model was run on the Floating Point System (FPS) computer at Western Michigan University, Kalamazoo, due to HST3D's large computational and memory requirements. Simulations on the FPS lasted approximately 40 minutes.

Figure 6 illustrates the simulated breakthrough curves for the first two runs, one which utilized the horizontal transverse dispersivity, and the other which utilized the vertical transverse dispersivity. Because Table 1 contains two values of transverse dispersivity and HST3D requires the input of only one value for this parameter, two simulations were run to determine which value was the most appropriate. The resulting curves are nearly identical; therefore, the transverse dispersivity chosen in the simulation of the two-well test results appears to be irrelevant. The measured breakthrough curve is also shown in Figure 6 for comparison with the simulated curves. The overall character of the curves is quite similar, but the
Figure 6. Comparison of Measured and Predicted Bromide Concentration Versus Time Using HST3D with the Data Found in Table 1.
simulation curves have significantly early arrival times and have broader peaks than the measured curve.

The longitudinal and transverse dispersivity values were altered by varying orders of magnitude to obtain a better fit between the curves. Figure 7 illustrates the simulation results when the dispersivities were increased by one and two orders of magnitude. Increasing the dispersivities by one order of magnitude had very little effect on the first arrival time of the bromide, but the overall concentration values were lowered. When the dispersivities were increased by two orders of magnitude the arrival times of the bromide were even earlier than with the original data set and the curve had a much lower peak concentration than the measured curve. The curve shifted very little when the dispersivities were decreased by one order of magnitude, with the only visible effect being a slight increase in peak concentration values (Figure 8). The simulation was run one time with only the transverse dispersivity increased to determine if it affected the first arrival times. The effect on the simulated curve was slightly later arrival times and a lower peak concentration (Figure 9).

Other input parameters were varied in an attempt to obtain a better match between the simulated and the measured breakthrough curves. The other options which were varied to determine the effect on the breakthrough curve
Figure 7. Comparison of Measured and Predicted Bromide Concentration Versus Time Using HST3D with Increased Dispersivities.
Figure 8. Comparison of Measured and Predicted Bromide Concentration Versus Time Using HST3D with Decreased Dispersivities.
Figure 9. Comparison of Measured and Predicted Bromide Concentration Versus Time Using HST3D with Increased Transverse Dispersivity.
included the spatial discretization, the temporal discretization, and the hydraulic conductivity in the most conductive layer.

The spatial discretization was changed from upstream differencing (backwards in space) to centered in space. In the upstream finite difference approximation the derivative for the change in head with respect to \( x \) is replaced by differences between the nodes \( i \) and \( i-1 \). The centered approximation refers to replacing the derivative by differences between the nodes \( i+1 \) and \( i-1 \). Figure 10 illustrates the resulting effects on the simulated breakthrough curve. The concentration values increased, and the first arrival of the bromide in the withdrawal well was slightly later. This breakthrough curve did a very good job of approximating the measured breakthrough curve except for the slight increase in peak concentration.

The temporal discretization was varied from implicit (backwards in time) to centered in time with similar results (Figure 11). This simulated breakthrough curve also closely approximated the measured breakthrough curve. Implicit time discretization refers to the evaluation of the spatial derivatives between the current time step, \( n \) and the next time step, \( n+1 \). When the spatial derivatives are evaluated at \( n+1/2 \) this is referred to as centered in time. Centered spatial and temporal discretization yielded the best match between the simulated and measured curves at
Figure 10. Comparison of Measured and Predicted Bromide Concentration Versus Time Using HST3D with Varying Spatial Discretization.
Figure 11. Comparison of Measured and Predicted Bromide Concentration Versus Time Using HST3D with Varying Temporal Discretization.
early times, but the peak concentration values were much too high (Figure 11).

To study the sensitivity of the solution to hydraulic conductivity, the hydraulic conductivity of the most conductive layer was decreased from 119.1 m/day to 100 m/day. The effect on the original simulation curve was negligible as shown in Figure 12.

The twelve layers of the aquifer with different hydraulic conductivities were reassigned the average value described by Parr et al. (1983) in an attempt to determine the effect of a diminished data set on the simulation results. The result, as shown in Figure 13, is a curve with a slower arrival time which at early times approximated the measured curve more closely than any of the previous runs with twelve layers of varying hydraulic conductivity. However, in the peak and declining limb of the curve the concentration values were not as close to the measured values as those resulting from the original data set.

Because HST3D solves the transient flow equation and the previous simulations assumed steady-state conditions, simulations were also run with equilibration periods prior to transport of the bromide tracer. During these equilibration periods only water was injected into the aquifer, and then the two-well test was simulated. Figure 14 illustrates the measured curve, the simulation curve
Figure 12. Comparison of Measured and Predicted Bromide Concentration Versus Time Using HST3D with the Hydraulic Conductivity in the Most Conductive Layer Increased.
CONCENTRATION (MG/L) VS. TIME (HRS) AT THE MOBILE SITE USING HST3D (VER 1.1) AVERAGE K VALUE

Figure 13. Comparison of Measured and Predicted Bromide Concentration Versus Time Using HST3D with an Average Hydraulic Conductivity Value.
Figure 14. Comparison of Measured and Predicted Bromide Concentration Versus Time Using HST3D with a One-Week Equilibration Period.
from the original data set, and the resulting curve when the original data set was run with an equilibration period of one week. The two simulation curves were identical. An equilibration period of one month was simulated to determine if a longer period of time was necessary for steady-state conditions to be achieved. The only variation in the original simulation curve was a slight increase in the peak concentration values (Figure 15).

The last parameter which was varied in the data file was the grid spacing. Delta x and delta y were increased by a factor of four. Figure 16 illustrates the resulting simulation curve with an equilibration period of one week. The result was an even earlier arrival of the bromide in the withdrawal well and decreased concentration values.

**HST3D Discussion**

The simulation curves obtained using HST3D were quite similar to the measured curve except for the early arrival of the bromide tracer in the withdrawal well. These early arrival times in the simulation results could not be eliminated. A possible explanation for these early arrival times could be artificial dispersion resulting from the numerical method utilized by the model, not the dispersion terms in the data set. This artificial dispersion occurs when the grid spacing is not sufficiently small and when upstream spatial differencing or implicit time differencing
Figure 15. Comparison of Measured and Predicted Bromide Concentration Versus Time Using HST3D with a One-Month Equilibration Period.
Figure 16. Comparison of Measured and Predicted Bromide Concentration Versus Time Using HST3D with Delta X and Y Increased by a Factor of Four.
are selected. Another related source of numerical dispersion occurs when the rectangular finite difference grid cuts across the arcing flowlines. Each time a flowline obliquely enters a new grid block, the tracer front is artificially dispersed. This is related to the other numerical dispersion because the dispersion is greater in larger grid blocks.

The criterion suggested to limit numerical dispersion is: \( \frac{\Delta x}{2} \ll \text{longitudinal dispersivity} \) (Kipp, 1987). The \( \Delta x \) and \( \Delta y \) values used in the simulations were 5 m. Therefore \( \frac{\Delta x}{2} = 2.5 \text{ m} \), which is not \( \ll 0.15 \text{ m} \). More than 384 nodes in the \( x \) direction would be necessary to meet this criterion. The \( \Delta x \) and \( \Delta y \) values of 5 m were the smallest possible values which allowed the required area to be modeled and kept the number of nodes within the computer storage available.

Determining the effect of decreasing the \( \Delta x \) and \( \Delta y \) values on the simulation results was desired but impossible due to these storage requirements. Therefore, the effect of cell size on the simulation results was illustrated by increasing \( \Delta x \) and \( \Delta y \) by a factor of four, from 5 m to 20 m (Figure 16). Decreased concentration values and even earlier arrival times were the result suggesting that increased numerical dispersion was occurring.

The simulation curves obtained using the hydraulic
conductivity distribution with depth and an average hydraulic conductivity were compared in Figure 13. The average hydraulic conductivity curve more closely approximated the measured curve during early simulation times, while the varying hydraulic conductivity curve more closely matched the peak and declining limb of the measured curve. This was not the expected result with a diminished data set. Results with less predictive capability would be anticipated when less information is available concerning the three-dimensional system which is being modeled. The fact that the average hydraulic conductivity simulated breakthrough curve approximated the measured breakthrough curve as well as the varying hydraulic conductivity simulated curve may be attributed to the lack of major heterogeneities in the aquifer. The hydraulic conductivity distribution inferred from the single-well tracer tests varies by a factor of 4, while in many aquifers this distribution may vary by a factor of 10 or 100.
MOC

Introduction

The second model used in this investigation was MOC: Method-of-Characteristics Model for Solute Transport by L. F. Konikow and J. D. Bredehoeft, 1978. MOC is a two-dimensional finite-difference model which simulates solute transport and dispersion in groundwater. The model uses an alternating-direction implicit procedure to solve the groundwater flow equation, and the method of characteristics to solve the solute-transport equation. The method of characteristics uses a particle-tracking procedure to represent advective transport and a two-step explicit procedure to solve a finite-difference equation which represents hydrodynamic dispersion, fluid sources and sinks, and divergence of velocity (Konikow & Bredehoeft, 1978). MOC was chosen to be used in this investigation because it is a two-dimensional computer model which is commonly used in groundwater modeling studies. Because it is two-dimensional it is more simplified and requires less input data and computer memory and storage than a three-dimensional model. In this investigation MOC was run on a portable 286 microcomputer with simulations lasting approximately 70 minutes.
MOC Simulation Results

The initial data was input into MOC with an average hydraulic conductivity along with suggested values for model parameters such as CELDIS, the cell distance a particle is permitted to move in one particle move, and NPTPND, the number of particles per node. The boundary conditions were no-flow along the entire margin of the grid, and the maximum number of time steps was allowed in each pumping period.

The results of the first simulation demonstrated that the cumulative mass balance and the chemical mass balance were unacceptable. It was determined after consultation with the International Groundwater Modeling Center that the solution to the flow equation was not converging in the first pumping period because the time steps were too small. Therefore, one time step was allowed in the first pumping period and the cumulative mass balance was then corrected.

The high chemical mass balance errors were more difficult to correct. Different parameters were varied in an attempt to lower these errors. First, the boundary conditions were changed from impermeable to constant-head boundaries which generated a flat water table. The next parameter which was varied was the width of the finite difference cell, XDEL and YDEL, used in the simulation. Various values for XDEL and YDEL were input ranging from 15
feet to 50 feet. A value of 40 feet yielded the smallest percent error and was used in subsequent simulations. The number of time steps allowed in a pumping period was also varied to determine the effect on the mass balance error, and the best values were then used in each pumping period. The third parameter to be varied was CELDIS. Values ranging from 0.05 to 0.5 were input and the resulting percent chemical mass balance error noted. The value which yielded the lowest mass balance errors was 0.05.

The model was then run with the above parameters at their values determined to produce the minimum chemical mass balance percent error along with the original data. The resulting breakthrough curve is shown in comparison with the measured curve in Figure 17. The simulated concentration values are much higher than the measured values. Therefore, the dispersivity value was varied in an attempt to obtain a closer match between the simulated and measured breakthrough curve.

The longitudinal dispersivity value was increased by one order of magnitude from 0.492 feet to 4.92 feet. The resulting curve is shown along with the measured curve and the original simulated curve in Figure 18. The resulting simulation curve had a lower peak concentration value and in general came closer to approximating the experimental data curve than the original simulated curve. The bromide tracer showed up earlier and for a longer period of time in
Figure 17. Comparison of Measured and Predicted Bromide Concentration Versus Time Using MOC with the Data Found in Table 1.
Figure 18. Comparison of Measured and Predicted Bromide Concentration Versus Time Using MOC with the Longitudinal Dispersivity Increased by One Order of Magnitude.
the withdrawal well. This is to be expected when the
dispersivity value is increased. The chemical mass balance
error also decreased with an increase in longitudinal
dispersivity. This pattern is illustrated to an even
greater extent when the dispersivity was increased two
orders of magnitude to 49.2 feet (Figure 19). The measured
breakthrough curve lies somewhere between the simulated
curves resulting from a dispersivity value increased by one
order of magnitude and two orders of magnitude.

The dispersivity value was varied between 4.92 feet
and 49.2 feet, and the value which yielded the best match
between the simulated and measured breakthrough curves was
determined by trial and error. The closest match to the
measured curve was obtained with a longitudinal
dispersivity value which was 40 times the actual value of
0.492 feet. The simulated breakthrough curve shown in
Figure 20 resulted from a dispersivity value of 19.68 feet.
This simulation curve approximates the experimental peak
concentration value and the late portion of the measured
breakthrough curve very accurately. However, the simulated
curve resulting from a dispersivity value of 19.68 feet
does not represent a predictive breakthrough curve. It is
the result of adjusting the input data to match a known
experimental breakthrough curve.

A simulation was also run with the dispersivity
decreased by one order of magnitude to a value of 0.0492
Figure 19. Comparison of Measured and Predicted Bromide Concentration Versus Time Using MOC with the Longitudinal Dispersivity Increased by Two Orders of Magnitude.
Figure 20. Comparison of Measured and Predicted Bromide Concentration Versus Time Using MOC with the Longitudinal Dispersivity Increased by a Factor of 40.
feet. Figure 21 illustrates the resulting breakthrough curve and demonstrates that the original simulation curve was altered very little.

**MOC Discussion**

Determining the appropriate values for various model input parameters was necessary to achieve low chemical mass balance errors. CELDIS, NPTPND, the number of time steps allowed in a pumping period, and the longitudinal dispersivity all affected the chemical mass balance errors and concentration values obtained in the simulation results.

The measured breakthrough curve and the simulated breakthrough curve using the data in Table 1 were significantly different. The peak concentration values in the original simulation curve were more than twice the measured values. The closest approximation to the experimental data curve using MOC was obtained when the longitudinal dispersivity value was increased by a factor of 40. This increase in dispersivity was necessary to compensate for the loss of the vertical dimension when using a two-dimensional areal model and a vertically averaged hydraulic conductivity to simulate contaminant transport in the stratified aquifer at the Mobile site.
CONCENTRATION (MG/L) VS TIME (HRS) AT THE MOBILE SITE
USING MOC (VER 2.5) DISPERSIVITY DECREASED

Figure 21. Comparison of Measured and Predicted Bromide Concentration Versus Time Using MOC with the Longitudinal Dispersivity Decreased by One Order of Magnitude.
CHAPTER III

CONCLUSIONS

Figure 22 illustrates the original HST3D simulated, the best fit MOC simulated, and the measured breakthrough curves. The same information is shown in Figure 23, except the HST3D breakthrough curve was obtained with the average hydraulic conductivity value. The HST3D and MOC simulation results are shown in comparison with the measured breakthrough curve and the GeoTrans and TWAM simulation results in Figure 24. The HST3D simulated curve resulted from the original data found in Table 1, and the MOC simulated curve resulted from the dispersivity increased by a factor of 40.

The results of this investigation seem to imply that the general three-dimensional model HST3D was capable of predicting the bromide concentration values in the withdrawal well at the Mobile site during the two-well test. The HST3D simulation results were not as accurate as the results of the GeoTrans, Inc. model or the TWAM. However, these models are site-specific because their grids are specifically designed to follow the flowlines resulting from two-well tests.

The early arrival times of the HST3D simulation
CONCENTRATION (MG/L) VS. TIME (HRS) AT THE MOBILE SITE

HST3D, MOC, AND MEASURED BREAKTHROUGH CURVES

Figure 22. Comparison of Measured and Predicted Bromide Concentration Versus Time Using HST3D with the Original Data and MOC with the Dispersivity Increased by a Factor of 40.
Figure 23. Comparison of Measured and Predicted Bromide Concentration Versus Time Using HST3D with an Average Hydraulic Conductivity and MOC with the Dispersivity Increased by a Factor of 40.
Figure 24. Comparison of Measured and Predicted Bromide Concentration Versus Time Using GeoTrans, TWAM, HST3D with Original Data, and MOC with Dispersivity Increased by a Factor of 40.

Source: Molz et al., 1986, p 1034.
results were the most severe limitation in the model's ability to predict the tracer concentration during the test. With a smaller grid spacing these early arrival times probably could be eliminated, but this may be impractical when modeling a site which covers a large area. The area being modeled in this investigation was approximately 115 meters by 60 meters in an areal view and 21.6 meters in the vertical. Even when modeling this small area it was necessary to run the simulations on the biggest, fastest mainframe computer (the FPS) at Western Michigan University and to limit the grid spacing.

The similarity between the simulation results using an average hydraulic conductivity and twelve layers of hydraulic conductivity was unexpected. The use of twelve layers in the simulation seems to provide the predictive capability of the model, not whether the horizontal hydraulic conductivity variation in the vertical is identified. This is probably due to the fact that the hydraulic conductivity distribution in the aquifer at the Mobile site varies by a factor of 4 and therefore, is not extremely heterogeneous.

The simulation results obtained in this investigation demonstrated that the two-dimensional model MOC was unable to predict the recovery concentrations of the tracer throughout the two-well test using the previously mentioned model input parameters and the data contained in Table 1.
With prior knowledge of the experimental data curve the data could be manipulated to achieve a close match between the measured and simulated breakthrough curves. The loss of the vertical dimension when using the two-dimensional areal model was compensated for by increasing the longitudinal dispersivity by a factor of 40 times the original value.

The results of this investigation indicate that the three-dimensional model HST3D was able to be used in a predictive manner when using the data in Table 1 to simulate the results of the two-well test at the Mobile site. The two-dimensional model MOC, however, was unable to predict the concentration of bromide in the withdrawal well at the Mobile site. With regard to modeling studies using these general numeric contaminant transport models, the three-dimensionality of HST3D seemed to lend itself to achieving valid results while MOC needs calibration to achieve results which are consistent with experimental field data. To calibrate MOC to one particular set of field data at one site and subsequently attempt to use it in a predictive sense at a future date may not yield valid results. The size of the plume being modeled could be different and therefore, the scale of the problem would be different. In an areal model such as MOC this change in scale would necessitate an increase in the dispersivity value used in the simulation.
The above conclusions are based solely on the comparison of simulation results of two models using the data from one field experiment. Further comparison between different three-dimensional and two-dimensional models when simulating a variety of field experiments would be necessary to generalize these conclusions. They are valid only for the above models using the data from Table 1 and the anisotropy value of 6.71 to simulate the results of the two-well test at the Mobile site.
BIBLIOGRAPHY


