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by

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A THESIS SUBMITTED
IN PARTIAL FULFILLMENT OF THE
REQUIREMENTS FOR THE DEGREE
Master of Science

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November, 1995
ABSTRACT


by

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FLOTRAN, a code written by a Rice faculty member, is designed to solve the advection-dispersion-reaction equation for contaminant transport in three dimensions. In this thesis, FLOTRAN is tested in several different scenarios to determine the accuracy of the code and to eliminate programming errors. The testing scenarios utilized include testing in radially dominated flow conditions, testing against analytical solutions, and testing against a three dimensional model of the Borden Landfill site. Overall, the testing was successful. In the tests with analytical solutions, FLOTRAN matches the analytical solutions, generally within a few percent, and often within one percent, as measured by the average absolute error. In the testing against the Borden Landfill model, FLOTRAN performed well, demonstrating the usefulness of its variable grid thickness option. As a final test, and as an exercise in itself, FLOTRAN is also used to model trichloroethylene (TCE) contamination at a site in Arizona. TCE was discovered in two City of Phoenix water wells in late 1981, a discovery which led to placing the area on the National Priorities List, and extensive study of the area. The emphasis of the modeling is to determine conditions in the subsurface before the discovery of TCE in the water wells. Of the several possible sources of contamination in the area, modeling suggests that one in particular is responsible for the contamination in the city water wells prior to 1981.
Acknowledgments

I would like to thank my advisor, Philip Bedient, for all his help in locating troublespots and theoretical mishaps. I would also like to thank the author of FLOTTRAN, Clint Dawson, for his patience in reading my electronic mail about my difficulties, and for fixing the (very few) errors I found. Thanks also to Katherine Ensor, for agreeing to join my committee at the last minute. And to Mason Tomson for his comments on my thesis. I would like to thank the National Science Foundation for supporting my work through a NSF Graduate Traineeship in Computational Environmental Science and Engineering (Grant # GER9355087).

I am very much indebted to my colleagues Maged, Manar, Gary, Howard, Karen, Kevin, Mark, Paul, and Shawn for their comments on my work throughout, and to Naoko, for her help with many things.

I would also like to thank my parents, Jack and Peggy for instilling in me the desire to achieve my best, and my alternate parents, Charles and Brookie for continually asking how the work was progressing.

Last of all, I would like to thank my wife, Angela, and my daughter, Rachel, for their love and support. Without them, this would never have been possible.
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Chapter 1. Introduction.

1.1. Importance of Numerical Models to Ground Water Flow and Transport Applications.

In the 1850s, Henry Darcy built a physical model for ground water flow (Fetter, 1993). Through his experiments with this soil column, he was able to deduce a mathematical relationship between head differences and the rate of flow of water through his model. Similar mathematical relationships have been derived to describe the transport of constituents dissolved in the ground water. In their more general forms, these mathematical relationships are differential equations which can be solved explicitly only in certain geometrically and geophysically simple cases. When the geophysical conditions which are in question approach any realistic complexity, the differential equations cannot be solved analytically, and there is a need for more complex approximations. In some cases, one can assume the site is similar to one of the cases for which the equations have been solved analytically, and one can apply the analytical solution to determine the rate and amount of contaminant transport. More often, however, the situation is sufficiently complex to invalidate any assumptions which could allow the use of simple analytical solutions. In these cases, one must turn to numerical models.

1.2. Importance of Validation of Numerical Models.

Numerical ground water models are widely used to predict outcomes such as effectiveness of remediation schemes, extent of ground water contamination by a release of chemicals, saltwater intrusion, and capture zones around water supply wells (to determine areas in which to restrict activities in order to reduce contamination risk). The results of these modeling efforts can be used for legislative/regulatory purposes or in
litigation to determine responsibility for ground water contamination. Because use of these models can have tremendous financial consequences, it is important for the user to be sure that the model correctly solves the intended equations, and does so with minimal error.

Most numerical methods introduce some error in the solution of a differential equation. (In some simple cases, the error is mathematically zero because of the formulation of the approximation. The equations governing ground water flow and contaminant transport are much too complicated for this to happen.) One purpose of validating a numerical model is to determine if the level of error is acceptable and, of course, to eliminate programming errors that may be made in large computer codes.

Computer models have been written for purposes ranging from predicting the weather to predicting the rate of heat flow through an iron bar. Unfortunately, improper use of computer models has led to skepticism about the accuracy of models. The formulation of any numerical model involves making assumptions about the system being modeled. In the case of meteorological modeling, there are many assumptions which must be made, since the system being modeled is so large and complex. Therefore, a weather prediction model must be used with extreme caution. Heat transfer through an iron bar, on the other hand is a fairly simple problem. The assumptions in this type of problem can be negligible, resulting in a model with a high degree of accuracy which can be used with confidence.

In order to avoid errors in the use of the model, the user must know the effects of these assumptions, and determine whether, including the assumptions, the model can be applied to the situation at hand. Proper testing of a model can indicate situations in which the model should not be applied.
1.3. Objectives.

During the early 1990's, Clint Dawson, then a faculty member at Rice University, developed a numerical model for ground water flow and contaminant transport in porous media. The model, called FLOTRAN, solves the equations for ground water flow in three dimensions, and incorporates advection, dispersion, linear sorption, and biodegradation in its solution of the contaminant transport equations. Dawson (personal communication) states (a) that the code includes "cell-by-cell and global mass conservation," and (b) that "strongly advective flow can be modeled with minimal oscillation and numerical diffusion." These and other features of FLOTRAN make it a very attractive model, however, before using FLOTRAN to model an actual field site, it needs to be tested.

The testing and validation of FLOTRAN discussed herein is performed with certain objectives in mind. The work behind this thesis is an attempt to show that FLOTRAN can:

1. correctly model hydrologically simple scenarios,
2. properly account for advection, dispersion, sorption and biodegradation when these processes are present,
3. account for aquifer heterogeneity, and
4. model a complex field site with many extraction wells, variable hydraulic conductivity, variable thickness, and recharge.

In addition, the author attempts to determine the types of situations for which FLOTRAN is inappropriate.
Chapter 2. Literature Survey.

2.1. Ground Water Modeling.

The explanation of ground water flow mechanics occurred when Henry Darcy built his first sand column and used it to develop Darcy’s Law. Darcy’s Law provided hydrologists with a reliable method for estimating the velocity which ground water, and its contaminants, would move in an aquifer. (Fetter, 1993) Other processes that affect the transport of contaminants in an aquifer include diffusion along concentration gradients, mechanical dispersion through mixing, sorption/desorption of contaminants onto soil particles, and reactions of contaminants, including biodegradation. In order to estimate the actual flow and transport of a contaminant, one must have mathematical descriptions of these processes. A review of these processes and descriptions follows.

2.1.1. Transport Processes and Mathematical Descriptions.

Darcy’s sand-filled pipe experiment in 1856 was the first physical model of ground water flow (Fetter, 1993). Darcy used his experiment to determine a mathematical relationship between the change in head and the flow rate in the pipe. This relationship can be written for one-dimensional flow as

\[ v_D = -K \frac{dh}{dl}, \]

Eq. 2.1

where \( v_D \) is called the Darcy velocity, \( K \) is the hydraulic conductivity, a measure of the permeability of the porous medium, and \( \frac{dh}{dl} \) is the hydraulic gradient, where \( dh \) is the change in hydraulic head, and \( dl \) is the horizontal distance between measurement points. The Darcy velocity describes the actual volume of water flowing in a system, and if multiplied by a vertical cross sectional area perpendicular to the direction of flow will give the volume flux of water passing through that plane. Since ground water is passing through a porous medium, the effect of that medium on the ground water velocity should
be accounted for. The seepage velocity, \( v_x = \nu D / \theta \), which is the Darcy velocity divided by the porosity of the medium, \( \theta \), describes the actual travel velocity of a packet of water through the medium.

For one dimensional flow, Darcy’s Law, given as Equation 2.1, is adequate. When one extrapolates to three dimensional flow, however, the concept of anisotropy must be considered. In an isotropic system, such as a uniform sand, the hydraulic conductivity is the same in all directions, however, most systems are anisotropic, meaning that the hydraulic conductivity is different in different directions. Generally, anisotropy can be oriented along any three independent directions, called the major axes of anisotropy. For convenience, the major axes of anisotropy are usually chosen to be the axes of the model grid. Thus the conductivity in the \( x \)-direction, \( K_{xx} \), is not the same as \( K_{yy} \), the conductivity in the \( y \)-direction.

Freeze and Cherry (1979) discuss the effects of anisotropy on Darcy’s Law. In the case where the coordinate system is oriented along the major axes of anisotropy, the three dimensional form of Darcy’s Law is written

\[
\begin{align*}
v_x &= K_{xx} \frac{\partial h}{\partial x}, \\
v_y &= K_{yy} \frac{\partial h}{\partial y}, \\
v_z &= K_{zz} \frac{\partial h}{\partial z},
\end{align*}
\]

Eq. 2.2

where \( v_x \) is the Darcy velocity in the \( x \) direction, \( K_{xx} \) is the hydraulic conductivity in the \( x \) direction, and \( \frac{\partial h}{\partial x} \) is the hydraulic gradient in the \( x \) direction. The \( y \) and \( z \) directions are similar to the \( x \) direction.

If there is a solute in the ground water, based on Darcy’s Law, it should flow along with the ground water. Fetter (1993) shows the derivation of the equation which describes this ‘advective’ transport. It is
\[ \frac{\partial C}{\partial t} = -v_x \frac{\partial C}{\partial x}, \]  
Eq. 2.3

where \( C \) is the concentration of solute and \( v_x \) is the seepage velocity.

In a similar manner, hydrologists and other scientists have used physical models to determine mathematical relationships among various transport parameters. Ogata (1970) traces the development of the mathematical description of dispersion from its discovery in the early 1900s by Slichter. Slichter was investigating the use of salt as a tracer in ground water flow and noticed that the salt concentration in his experiments increased gradually at the measurement point, instead of abruptly, as would be predicted by Equation 2.3. According to Ogata, Slichter explained that this behavior was a result of the different velocities of water in different capillary tubes in the porous medium. Slichter's explanation of this phenomenon is still used to describe mechanical dispersion. The mathematical description of dispersion is assumed to take the same form as Fick's law of diffusion.

Fick's first law describes the process of mass flowing from an area of high concentration toward an area of lower concentration. It takes the form

\[ F = -D_d \frac{dC}{dx}, \]  
Eq. 2.4

where \( F \) is a mass flux of solute (\( M/L^2/T \)), \( D_d \) is the molecular diffusion coefficient (\( L^2/T \)), \( C \) is the solute concentration (\( M/L^3 \)), and \( dC/dx \) is the concentration gradient (\( M/L^3/L \)). (Fetter, 1993)

Fick's second law describes the diffusion along a concentration gradient when the concentrations are changing with time. In one dimension, it is

\[ \frac{\partial C}{Dt} = D_d \frac{\partial^2 C}{\partial x^2}, \]  
Eq. 2.5

where \( \partial C/\partial t \) is the change in concentration with time (\( M/L^3/T \)). Ogata (1970) describes the theoretical and experimental work that confirmed that this assumption is reasonably
accurate. The experimental work suggests that dispersion is a sum of mechanical
dispersion and diffusion. Mathematically, this is written \( D = D_x + D_d \) where \( D_x \)
represents mechanical dispersion, and \( D \) represents total dispersion. Another assumption
that is widely accepted is that the mechanical dispersion is proportional to the velocity.
Putting this all together and assuming isotropic conditions, one gets

\[
D = \alpha v + D_d
\]  
Eq. 2.6

where \( \alpha \) is called the dispersivity and has units of length. Often the molecular diffusion
coefficient is very small compared to mechanical diffusion, and is simply ignored.

(Freeze and Cherry, 1979)

Dispersivity is generally considered to be anisotropic. The major axes of
anisotropy for dispersivity as used in numerical models are: horizontal along the direction
of flow (longitudinal), horizontal perpendicular to the direction of flow (transverse), and
vertical. These dispersivities are multiplied by the magnitude of the velocity vector to
find the dispersion coefficient for the indicated direction.

Freyburg (1986) discusses a field dispersion test performed at the Canadian
Forces Base Borden Landfill. A slug of contaminated water was injected into the aquifer
and allowed to migrate downgradient for over two years. During the course of the two
year study, over 19,900 water samples were analyzed from over 5000 sampling points in
three dimensions. The results of this test indicate that dispersion is anisotropic, and that
in two dimensions, dispersion in the direction of flow (longitudinal) is generally 3 to 10
times higher than dispersion perpendicular to the direction of flow (transverse). (See also
McKay et al., 1986; Roberts et al., 1986; Curtis et al., 1986; Sudicky, 1986)

Adsorption is another transport process which has been described mathematically,
and therefore can be modeled. Adsorption (or sorption) is a process by which some
portion of a solute can become attached to a solid (in this case, the aquifer medium).
Sorption experiments consist of placing a known volume of water containing a known
mass of solute into a container containing a known mass of solid. After allowing the mixture to come to equilibrium, the concentration of solute in the liquid can be used to determine how much solute sorbed to the solid. (Freeze and Cherry, 1979; Kan and Tomson, 1990) After repeating this experiment several times with different concentrations of solute, an isotherm can be plotted. (The name 'isotherm' refers to the fact that all these experiments are performed at the same temperature.) Three functional forms have been postulated to fit the shape of plotted isotherm data, the linear sorption isotherm, the Freundlich sorption isotherm, and the Langmuir sorption isotherm.

The linear sorption isotherm assumes that there is a direct, linear relationship between the equilibrium concentration of solute and the equilibrium amount of solute sorbed onto the solid. The functional form that describes the linear isotherm is

\[ C^* = K_d C, \]  

Eq. 2.7

where \( C^* \) = mass of solute sorbed per dry unit weight of solute (mg/kg), \( C \) = concentration of solute in solution in equilibrium with \( C^* \) (mg/L), \( K_d \) = distribution coefficient (L/kg).

Since the linear isotherm is utilized in FLOTRAN, the other, nonlinear, descriptions of sorption behavior are not discussed in detail. Karickhoff (1984) discusses the Freundlich and Langmuir isotherms. More recent work on modeling sorption is discussed in Weber and Miller (1988).

The combination of advection, dispersion, and a linear isotherm description of sorption leads to this equation for transport of solute in one dimension (Freeze and Cherry, 1979)

\[ \frac{\partial C}{\partial t} \left(1 + \frac{\rho_b K_d}{\theta}\right) = D_L \frac{\partial^2 C}{\partial x^2} - v_x \frac{\partial C}{\partial x}. \]  

Eq. 2.8

where \( D_L \) is the dispersion coefficient analogous to the diffusion coefficient in Equation 2.5. In Equation 2.8, the factor \( 1 + \frac{\rho_b K_d}{\theta} \) is called the retardation factor \( R_t \). This is
because the linear sorption isotherm has the effect of slowing down, or retarding, all of the other transport processes by a factor of $R_F$. (Freeze and Cherry, 1979; Ward et al., 1986; Fetter, 1993)

The biodegradation of organic contaminants in the subsurface has been a much studied topic since the mid-1980's. Biodegradation is the process by which microorganisms utilize a ground water contaminant as a food source. Biodegradable contaminants are organic materials, such as fuel or synthetic organic materials. As the microbe utilizes the contaminant, it also uses an electron acceptor, which can be oxygen (aerobic) or one of several other compounds (anaerobic) such as $SO_4^{2-}$, $NO_3^-$, $CO_2$, or $Fe^{3+}$. In complete aerobic biodegradation, oxygen and hydrocarbon combine to form water, carbon dioxide, and new cell material. (Bedient et al., 1994)

A mathematical formulation describing aerobic biodegradation of hydrocarbons and growth of microbes is given in Borden and Bedient (1986). It is based on a modification of the Monod function, as shown below.

$$\frac{dH}{dt} = -M_t k \left( \frac{H}{K_h + H} \right) \left( \frac{O}{K_o + O} \right)$$

Eq. 2.9

$$\frac{dO}{dt} = -M_t k_F \left( \frac{H}{K_h + H} \right) \left( \frac{O}{K_o + O} \right)$$

Eq. 2.10

$$\frac{dM_t}{dt} = M_t k Y \left( \frac{H}{K_h + H} \right) \left( \frac{O}{K_o + O} \right) + k_c Y C - b M_t$$

Eq. 2.11

where $H = \text{hydrocarbon concentration (mg/l)},$ $O = \text{oxygen concentration (mg/l)},$ $M_t = \text{total microbial population (mg),}$ $k = \text{maximum hydrocarbon utilization rate per unit mass of microbes (mg hydrocarbon / mg microbes / day)},$ $Y = \text{microbial yield coefficient (mg microbes / mg hydrocarbon)},$ $K_o = \text{oxygen half-saturation constant (mg/l)},$ $K_h = \text{hydrocarbon half-saturation constant (mg/l)},$ $k_c = \text{first order decay rate of natural hydrocarbon (/day)},$ $C = \text{natural organic carbon concentration (mg/l)},$ $b = \text{microbial decay rate (/day), and}$ $F = \text{ratio of oxygen to hydrocarbon consumed (mg O_2 / mg hydrocarbon)}.$
Equations 2.9 - 2.11 describe an oxygen limiting environment in which, as the concentration of oxygen is reduced, the rate of biodegradation is also reduced, until there is no biodegradation when there is no oxygen. Similar behavior is seen for the hydrocarbon concentration.

Borden and Bedient (1986) proposed an instantaneous reaction model for biodegradation. The proposed model states that in any model cell, either all of the hydrocarbon or all of the oxygen will be consumed in each time step. The model takes the following form

\[ H_{n+1} = H_n - O_n/F; \quad O_{n+1} = 0, \quad \text{when } H_n > O_n/F, \quad \text{Eq. 2.12} \]

or

\[ O_{n+1} = O_n - H_n/F; \quad H_{n+1} = 0, \quad \text{when } O_n > H_n/F. \quad \text{Eq. 2.13} \]

where \( H_n, H_{n+1}, O_n, \) and \( O_{n+1} \) are the hydrocarbon and oxygen concentrations at time steps \( n \) and \( n+1 \), respectively.

In a one dimensional simulation of contaminant transport and biodegradation, Borden and Bedient (1986) found that the instantaneous reaction results were almost identical to the results obtained using the full Monod formulation. In cases where the ground water velocity is sufficiently slow, the instantaneous reaction model should provide good results.


The advent of the computer allowed for the solution of these mathematical models by various numerical methods. A computer program cannot directly differentiate or integrate the partial differential equations which describe ground water flow and contaminant transport. The programmer must use some approximation to solve them. The finite difference, finite element, and 'method of characteristics' methods are commonly used to form these approximations. (Garder et al., 1964; Pinder, 1984) Using
these approximations, one can convert the differential equation into a system of algebraic
equations which can be solved iteratively.

2.1.2.1 Finite Difference Method.

The simplest of these methods is the finite difference method. The essence of
finite difference approximation is that one can estimate the derivative of a function \( f \) at a
point \( x_0 \) by using the values of \( f \) at \( x_0 \), and at a neighboring point or points. (Hoffmann
and Chiang, 1993)

A derivative of the function \( f(x_0) \) can be approximated by values of \( f \) at \( x_0 \), and at
neighboring points \( (x_0 + \Delta x, x_0 - \Delta x, \text{etc.}) \). Following is an example of an approximation to
the first derivative of \( f \). If \( f \) is an analytical function, \( f(x_0 + \Delta x) \) can be represented by a
Taylor Series expansion

\[
f(x_0 + \Delta x) = f(x_0) + (\Delta x) \frac{df}{dx}
|_{x_0} + \frac{(\Delta x)^2}{2!} \frac{d^2 f}{dx^2}
|_{x_0} + \cdots. \tag{Eq. 2.12}
\]

Solving Equation 2.12 for \( df/dx \), one obtains

\[
\left. \frac{df}{dx} \right|_{x_0} = \frac{f(x_0 + \Delta x) - f(x_0)}{\Delta x} - \frac{\Delta x}{2!} \frac{d^2 f}{dx^2}
|_{x_0} + \cdots, \tag{Eq. 2.13}
\]

or

\[
\left. \frac{df}{dx} \right|_{x_0} = \frac{f(x_0 + \Delta x) - f(x_0)}{\Delta x} + O(\Delta x), \tag{Eq. 2.14}
\]

where \( O((\Delta x)^n) \) is read as 'terms of order \( (\Delta x)^n \),' and represents all the terms which are
multiplied by \( (\Delta x)^m \), where \( m \geq n \). Equation 2.14 represents a first order approximation
of \( df/dx \) at the point \( x_0 \). Using Taylor Series expansions along with other techniques, one
can formulate approximations for any derivative which are of the desired accuracy.

Higher order approximations more closely approximate the derivative for a given \( \Delta x \) than
do lower order approximations. Partial derivatives can be approximated in a similar
manner. (Hoffmann and Chiang, 1993)
2.1.2.2 Finite Element Method.

The finite element method is another method of approximating the differential equations. This method is based on dividing the model area into elements, which can be rectangular, triangular, or even a quadrilateral with curvilinear sides, and estimating the value of a function in the interior of the element from the values of the function at the corners, or nodes, of the element. For a one dimensional, linear finite element which stretches from \( x = 0 \) to \( x = h \), two basis functions are created, \( \phi_1 \) and \( \phi_2 \). These functions are devised such that

\[
C(x) = C(0)\phi_1 + C(h)\phi_2 \quad \text{for} \ 0 \leq x \leq h. \quad \text{Eq. 2.15}
\]

The choice of the basis functions determines the accuracy with which the governing equation is approximated, and thus determines the amount of numerical error.

A detailed explanation of the finite element method can be found in Pinder and Gray (1977). The finite element method is more difficult to program, and usually requires more computation time than finite difference methods, but it is usually more accurate.

2.1.2.1 Method of Characteristics.

The other method commonly used in ground water modeling is the method of characteristics (MOC). (Garder et al., 1964; Konikow and Bredehoef, 1978) The method of characteristics models contaminant transport by means of a particle tracking method. In each model cell, a number of particles are created at the beginning of the simulation. Each particle is assigned a concentration and a regularly spaced location in the model cell. During the simulation, these particles are allowed to flow across the model area. Once the flow velocities at the centers of the model cells have been determined, each particle moves according to the fluid velocity interpolated at its location. After moving the particles as shown in Figure 2.1, the concentration in each model cell is determined by averaging the concentrations of the particles located within it.
(The concentrations associated with the particles are not averaged over the cell during each time step; they only change when the dispersion term is calculated.) Lastly, the change in concentration due to dispersion is calculated cell by cell, and that change in concentration is added to each particle within the cell.

![Particle at Beginning of Time Step.](image1)

![Particle at End of Time Step.](image2)

Figure 2.1: Particles moving along flow lines in the MOC.

One major advantage of this type of transport modeling is that in the cases where the dispersivities are zero, the particle concentrations never change. The model cell concentrations are simply calculated by averaging the concentrations of the particles within the cell. This allows the model to control averaging errors commonly known as numerical dispersion.

2.1.3. Numerical Models.

Numerical models for ground water flow and contaminant transport have been available since at least 1970. (Ogata, 1970; Prickett and Lonnquist, 1971; Trescott et al., 1976; Pinder, 1984) Among the more widely used numerical models are MODFLOW, the USGS Method of Characteristics model (MOC), and BIOPLUME II, which is based on MOC.

The Modular Three-Dimensional Finite Difference Ground-Water Flow Model (MODFLOW) written by McDonald and Harbaugh (1984) was among the first widely accepted ground water flow models, and is still considered one of the most reliable (Bedient et al., 1994). MODFLOW uses finite difference methods to approximate the ground water flow equations. MODFLOW allows the user to specify constant head or no-
flow boundary conditions, confined an unconfined aquifers, injection/extraction wells, rivers, drains, and diffuse recharge. MODFLOW will model ground water flow under either steady state or transient conditions. The user has a choice of three different solution techniques, the strongly implicit procedure (SIP), the slice-successive overrelaxation (SSOR) method, and the preconditioned conjugate-gradient (PCG) method. The SIP and SSOR solution methods are iterative methods.

In SIP, the values of the heads, \( H_n \), at time, \( t_n \), are used to calculate an estimate of the heads \( H_n^i \). These values are then used to calculate a new estimate \( H_n^{i+1} \). This is repeated until the maximum change in heads from estimate \( i \) to estimate \( i+1 \) is less than the required tolerance. This value of heads is then \( H_{n+1} \).

The SSOR method divides the model domain into slices, and iterates over the slices. Head changes in one slice are calculated assuming that the values in the surrounding slices are accurate. Then the head changes are multiplied by an acceleration parameter, \( \omega \), and added to the heads in that slice. When calculating heads in the next slice, the newly calculated values of the first slice are used. This procedure is repeated for all slices, then repeated for the whole domain until the maximum head change in any cell is less than the prescribed tolerance. The SIP and SOR methods are discussed in McDonald and Harbaugh (1984) and in Remson, et al., (1971). The PCG method is discussed in Hill (1990).

The USGS Solute Transport Model (MOC), written by Konikow and Bredehoef (1978), uses the method of characteristics and particle tracking methods to model ground water flow and contaminant transport, including advection, dispersion and sorption processes. The MOC code has been modified (BIOPLUME II) to model hydrocarbon and oxygen transport, and biodegradation using a fast equilibrium model (Rifai et al., 1987; Rifai and Bedient, 1987)

BIOPLUME II allows the user to specify constant head or no-flow boundary conditions, diffuse recharge, and injection/extraction wells. It will model contaminant
transport under steady state or transient flow conditions. The method of characteristics, however can produce high mass balance errors for either hydrocarbon or oxygen. Care must be taken to keep the mass balance errors low (<10%).

2.2. Testing and Validation of Ground Water Models.

As the objective of this work is to test and validate the ground water flow and transport model, FLOTRAN, a search was undertaken for reports on testing ground water models. Also, there has been a search for articles or books citing any other relevant tests for numerical ground water flow and contaminant transport models.


In 1985, van der Heijde presented the International Ground Water Modeling Center’s (IGWMC) “standard ground water model review.” This testing protocol involves three levels of sophistication. Level I testing uses six problems with analytical solutions available. Level II testing uses “two hypothetical field situations with irregular geometry, complex boundary conditions, and heterogeneous and anisotropic system characteristics.” Level III testing involves a simulation of ground water contamination at the Borden Landfill site. (Cherry, 1983) The situations used for testing by van der Heijde are set out in Table 2.1 (after van der Heijde, 1985, Table I.). The actual testing protocol was laid out by Huyakorn (1984).
Table 2.1. Level I test problems for ground water flow and transport models.

<table>
<thead>
<tr>
<th>Process</th>
<th>Dimension</th>
<th>Boundary Condition(s)</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>I.1 Transport in a semi-infinite column.</td>
<td>1-D</td>
<td>1st-type inlet</td>
<td>Ogata and Banks, 1961</td>
</tr>
<tr>
<td>I.2 Transport in a semi-infinite column; non-conservative species.</td>
<td>1-D</td>
<td>3rd-type inlet</td>
<td>Coats and Smith, 1964</td>
</tr>
<tr>
<td>I.3 Transport from a point source in a uniform ground water flow field.</td>
<td>2-D</td>
<td>2nd-type inlet,</td>
<td>Hunt, 1978</td>
</tr>
<tr>
<td></td>
<td></td>
<td>continuous</td>
<td>Wilson and Miller, 1978</td>
</tr>
<tr>
<td>I.4 Transport of a solute slug in a uniform ground water flow field.</td>
<td>2-D</td>
<td>2nd-type inlet,</td>
<td>Sauty, 1980</td>
</tr>
<tr>
<td></td>
<td></td>
<td>slug</td>
<td></td>
</tr>
<tr>
<td>I.5 Transport in a radial flow field created by an injection well.</td>
<td>radial</td>
<td>1st-type</td>
<td>Hoopes and Harleman, 1966</td>
</tr>
<tr>
<td>I.6 Transport in a nonuniform flow field by a recharging-discharging well pair.</td>
<td>2-D</td>
<td>1st-type inlet</td>
<td>Hoopes and Harleman, 1967</td>
</tr>
</tbody>
</table>

In this work, Problems I.2, the Level II problems, and Problem III.1 are not used for testing as they are not appropriate for use with FLOTRAN. Problem I.2 requires a decaying boundary condition, and the Level II problems and Problem III.1 require triangular finite element meshes. Also, Problem I.6 is not used, as a similar problem is modeled in the comparison with El-Kadi (1988) as follows. More detailed descriptions of the test problems used are in the appropriate chapter and section.

2.2.2. Effects of Large Scale Radial Stressing on Accuracy of Ground Water Models.

El-Kadi (1985) tested the USGS mass transport model (MOC) in three situations where ground water flow is dominated by radial flow toward or away from a well and the model cells are very large. Situations like these are not recommended by the authors of the code, however, El-Kadi finds records of such use in the literature. In his paper, he reports that for a single well injecting, then attempting to recover contaminants, MOC
simulations agree fairly well with an approximate analytical solution derived by Gelhar and Collins (1971). El-Kadi also models a recharge/recovery doublet case. In this case, the numerical simulation accurately matches the semi-analytical model RESSQ (Javandel et al., 1984) until the recovery well begins to pump contaminated water, at which time the numerical solution begins to fluctuate wildly. Finally, El-Kadi reports reasonable behavior for a simulation of “plume capture where the cases involved a single well or two wells.” There is some overestimation of the flow necessary to provide for complete capture, but El-Kadi concludes that the model is reasonable for estimation when there is no analytical solution available. The first two of these testing scenarios are more fully described in Chapter 4.

2.2.3. Grid Orientation Effects.

As a general rule, the orientation of the grid in a modeling effort is used as a convenience. Often the grid will be oriented in a north-south direction, or along the direction of major streets. Warwick and Stoffregen (1991) tested the USGS MOC code for numerical dispersion caused by a grid orientation which is non-orthogonal to the flow direction. Using a grid rotated approximately 25 degrees from the direction of flow and another grid oriented along the direction of flow, they attempted to match observed data on a tracer slug to model output. Warwick and Stoffregen noted that the amount of transverse dispersion in the non-orthogonal case exceeded actual observations, even though a transverse dispersivity of 0.0 ft was used. The orthogonal case required a transverse dispersivity of 0.15 ft to match observed dispersion. Hence all of the transverse dispersion in the non-orthogonal case is attributed to numerical dispersion.

Goode and Konikow (1991) tested a model called MOC3D (which is based on the method of characteristics [as is BIOPLUME II] and is coupled to MODFLOW) on a similar situation. When the direction of flow was along the grid orientation, the results agreed well with an analytical solution, but when the direction of flow was at a diagonal to the
grid orientation, NOC3D produced an hourglass shaped plume. They concluded that whenever possible, the grid should be oriented along the direction of flow.

A numerical ground water flow and contaminant transport model can be useful at ground water contamination sites, but investigators must know that the model has been tested and shown to closely approximate the intended equations. The following chapters describe the theory behind an the application of a flow and transport model called FLOTRAN. Chapter 3 describes the theory behind FLOTRAN and some of the modeling assumptions. Chapter 4 describes the testing and validation of FLOTRAN for simple analytical situations, and in comparison with previous modeling of a more complex ‘field’ site. Chapter 5 details the use of FLOTRAN to model a complex TCE contamination site in Arizona.
Chapter 3. **FLOTTRAN — Theory and Application.**

3.1. Flow and Transport Modeling.

**FLOTTRAN** is a Fortran code which solves the governing equation for fluid flow in one stage, then solves the system of equations for contaminant transport in a second stage. These equations are discussed below. **FLOTTRAN** solves the appropriate partial differential equations using finite differencing techniques.

3.2. Flow Theory in **FLOTTRAN**.

The governing equation for fluid flow in a porous medium is

\[
S_x \frac{\partial h}{\partial t} + \nabla \times \mathbf{u} = q, \quad \text{for } x \in \Omega \subset \mathbb{R}^3, t \in [0, T],
\]

Eq. 3.1

where \( \mathbf{u} = \left( \frac{\partial h}{\partial x}, \frac{\partial h}{\partial y}, \frac{\partial h}{\partial z} \right) \).

Eq. 3.2

In Equation 3.1, \( \mathbf{u} = (u, v, w) \) is the Darcy velocity vector \((L/T)\), \( h \) is the hydraulic head \((L)\), \( K_x, K_y \) and \( K_z \) are hydraulic conductivities \((L/T)\) in the \( x, y \), and \( z \) directions, respectively, and \( S_x \) is the specific storage \((L^3/L)\) of the porous medium. In addition, \( \Omega = [0, L_x] \times [0, L_y] \times [0, L_z], \) with \( L_{x,y,z} \geq 0 \). In Equation 3.1, \( q \) represents the flow rates \((L^3/T)\) at injection and production wells, which are treated as point sources and sinks.

Equations 3.1 and 3.2 are solved with the initial condition \( h(x, 0) = h^0(x) \), and Dirichlet and/or Neumann boundary conditions, which are represented mathematically as follows

\[
h = h_B(x), \quad x \in \Gamma,
\]

Eq. 3.3

\[
\mathbf{u} \cdot \eta = g(x), \quad x \in \partial \Omega - \Gamma,
\]

Eq. 3.4
where \( \eta \) is the outward normal to \( \partial \Omega \), \( \Gamma \) is the portion of the boundary on which Dirichlet boundary conditions are applied, and \( \partial \Omega - \Gamma \) is the remaining boundary. Either a Dirichlet or a Neumann boundary condition is applied at each point of \( \partial \Omega \). The values of \( h_B \) and \( g \) are possibly spatially dependent, and may be mixed on any boundary. The boundary conditions are assumed to be independent of time. (Dawson, 1991; Weiser and Wheeler, 1988)

Dirichlet boundary conditions are also known as constant head boundary conditions. The user specifies a value for the ground water head, and the model forces that value at that location and computes the other heads with that condition. Neumann boundary conditions are also called constant flux boundary conditions. A flux can be specified at the boundary, and the model adds or subtracts the appropriate volume of water from the appropriate cells in each time step. If the specified flux is zero, the boundary is referred to as a no-flow or impermeable boundary.

Currently, transient flow conditions cannot be simulated with FLOTRAN. Steady state flow equations are identical to transient flow equations if the time derivative is removed. (Practically, this is done by setting the specific storage equal to zero.)

Dawson solves Equations 3.1 - 3.4 in the code FLOTRAN by use of a block-centered finite difference procedure which is described in Bell et al. (1988), Dawson (1991), Dawson (1990), Dawson (1993), and Dawson and Wheeler (1992). Figure 3.1 shows the layout of the grid. Heads and concentrations are calculated at the centers of the grid blocks (labeled \( x_{\frac{N_x}{2}}, y_{\frac{N_y}{2}} \) in the figure). The model domain extends from \( x_1 = 0 \) to \( x_{N_x+1} = L_x \) in the \( x \) direction and similarly in the \( y \) and \( z \) directions. \( N_x, N_y, \) and \( N_z \) are the number of grid blocks in the \( x, y, \) and \( z \) directions, respectively.
Figure 3.1: Layout of block-centered grid used by FLOTTRAN.

The model domains used by FLOTTRAN are basically rectangular bricks. Variable cell spacing is allowed by varying the distance between any two consecutive columns (x), rows (y), or layers (z). For example, all the cells in a column must have the same value of Δx, but may have varying Δy and Δz. This method allows for some flexibility in choosing the mesh, but essentially requires that the aquifer be rectangular.

Recently, the code has been modified to allow the user to specify a general geometry. FLOTTRAN maps the nonuniform real domain to a rectangular block domain, as discussed above, then performs all the calculations on the rectangular domain, and maps the results back to the real domain. (Dawson, personal communication) These changes are mostly transparent to the user.

3.3. Transport Theory in FLOTTRAN.

The contaminant transport portion of FLOTTRAN solves the system of transport equations known as the advection-dispersion equation with reaction

\[
\frac{\partial}{\partial t}(\theta c_i + A(c_i)) - \nabla \cdot (D \nabla c_i - u c_i) = q \bar{c}_i + R_i(c_1, \ldots, c_J).
\]  \hspace{1cm} \text{Eq. 3.5}

where \( c_i \) (M/L^3) represents the concentration of component \( i, i = 1, \ldots, J \), and there are \( J \) different contaminants being modeled, \( \theta \) is the porosity, \( A(c_i) \) models adsorption/desorption of the component \( i \) using a linear sorption isotherm, \( D \) is the
hydrodynamic diffusion/dispersion tensor, which includes the effects of molecular
diffusion and transverse and longitudinal dispersion, \( u = (u, v, w) \) is the Darcy velocity, \( R_i \)
models chemical reactions between components (e.g., biodegradation) as discussed later,
\( q \) represents flow rates at production and injection wells and \( \bar{c}_i \) is the concentration in
the cell containing a well. It is specified at injection wells and \( \bar{c}_i = c_i \) at production
wells. Boundary conditions are the same as for the flow equations (Equations. 3.3 and
3.4). The user can also specify a constant or spatially variable initial concentration for
each component. (Dawson, 1992)

The advection-dispersion equation is solved using Godunov-mixed methods
described in Dawson (1993). Advection is solved using an unsplit, higher order Godunov
finite difference approach, while dispersion is modeled using a lower order mixed method
finite element approach, which reduces to a finite difference procedure when applied to
rectangular elements, as in FLOTRAN. The resulting approximation is second order
accurate in space, and first order accurate in time.

The Godunov finite difference approach used for the advection solution is an
'upstream differencing' technique, which uses differences biased in the direction of the
characteristic speed. (Harten et al., 1983) This characteristic speed is the same as is used
to determine particle movement in the method of characteristics model. It is applied
explicitly to the advective transport equation.

Dispersive transport is modeled implicitly via a lower order mixed method.
Mixed methods are finite element methods in which interelement continuity is
determined by a mixture of two basic methods, one involving the imposition of
concentration continuity at the element boundaries, and the other involving continuity of
the gradient of concentration at the boundaries. A more detailed description of mixed
finite element methods is available in Poceski (1992). The mixed method chosen is such
that for a rectangular domain, it reduces to a finite difference method. (Dawson, 1988)
Time steps are chosen based on the following two criteria. The first of these criteria, known as a CFL time constraint, is that

$$\Delta t \leq \frac{\text{CFL}}{h R_f} \max(|u|,|v|,|w|) \Omega,$$

Eq. 3.6

where CFL $\leq 1$ is a user input time constraint. Lowering the value of CFL will reduce the time step size when the user determines that such reduction is necessary. In addition, $h$ is the minimum grid spacing, and $R_f$ is the retardation factor. The second of these criteria is included to limit pumpage to or from a cell to the volume of water in the cell. It is given as

$$\Delta t \leq \min_n \left( \frac{\theta \Delta x \Delta y \Delta z}{|q_n|} \right),$$

Eq. 3.7

where $\Delta x$, $\Delta y$, and $\Delta z$ are the grid spacings in the grid block containing the $n^{th}$ well, and $q_n$ is the flow rate at the $n^{th}$ well. (Dawson, 1993)

3.4. Reactions Between Components.

Reactions are modeled explicitly in a manner similar to that of BIOPLUME II (Rifai and Bedient, 1990). Two components are modeled in a reactive scenario. Component 1 is always oxygen, and component 2 is always the hydrocarbon to be reacted with the oxygen. Advection and diffusion processes are modeled separately for each component, creating two ‘plumes’, one of oxygen, and one of hydrocarbon. The reaction step is performed on the oxygen and hydrocarbon which coexist in a cell after the advection and dispersion subroutines are performed.

To this point, the reaction modeling is essentially the same as in BIOPLUME II. The difference comes in the assumptions about how the oxygen and hydrocarbon plumes react. BIOPLUME II treats the reaction as one which comes to a ‘fast equilibrium,’ using the available oxygen and hydrocarbon until one is totally removed from that model cell. In FLOTTRAN, growth of microbes and removal of oxygen and hydrocarbon from the
subsurface are modeled using a modification of the Monod function described in Borden and Bedient (1986) (see Equations 2.9 - 2.11).

The reaction step is performed using a time-splitting technique. The reaction step is performed every time step after the advection and dispersion routines have been performed. FLOTRAN then splits the time step, \( dt \), into \( N_{\text{small}} \) time steps of size \( dt_r = \frac{dt}{N_{\text{small}}} \), and performs the reaction routine using this smaller time step. The amounts of oxygen and hydrocarbon removed from a cell are limited to what is present in the cell at the beginning of the reaction subroutine and by the stoichiometric balance.

This reaction subroutine can be forced to perform the same 'fast equilibrium' that is performed by BIOPLUME II (Borden and Bedient, 1986a; Rifai and Bedient, 1990) by setting \( N_{\text{small}} = 1 \), setting the half-saturation constants, \( K_h \) and \( K_o \), to be very small (<10^{-5}*(the minimum expected concentration of \( O \) or \( H \))), and by setting the hydrocarbon utilization rate, \( k \), to be very large (>10^5*(the maximum concentration of \( H \))). Setting these values will assure that \( dH/dt \) and \( dO/dt \) are both very large negative numbers, and that all of either the oxygen or hydrocarbon in a cell is used in the reaction.

3.5. Modeling of Sorption Processes.

Sorption is modeled through use of a linear isotherm. The user enters a retardation factor \( R'_f = \frac{\rho_b K_d}{\theta} \), where \( \rho_b \) is the bulk density, \( K_d \) is the distribution coefficient, and \( \theta \) is the porosity of the aquifer. Note that this retardation factor is not the retardation factor generally referred to in ground water modeling. The retardation factor is generally defined as \( R_f = 1 + \frac{\rho_b K_d}{\theta} \). Inspection of the first term in Equation 3.5 explains the difference. Freeze and Cherry (1979) write the one-dimensional advection-diffusion equation with linear adsorption as follows

\[
\frac{\partial C}{\partial t} \left(1 + \frac{\rho_b K_d}{\theta}\right) = D_L \frac{\partial^2 C}{\partial x^2} - v_x \frac{\partial C}{\partial x}.
\]

Eq. 3.8
Comparing Equation 3.8 to Equation 3.5 shows that the difference is that Equation 3.8 has been divided by $\theta$, and considers $A(c_i) = \rho_b K_d c_i$. The formulation given in Equation 3.5 leaves open the option of having a nonlinear adsorption term, which has not been implemented. The current implementation is for a linear isotherm, and is identical to that of Equation 3.8. The presence of a linear adsorption isotherm assumes that all of the contaminant transport and reaction mechanisms are equally slowed by the adsorptive retardation. Essentially, the concentration which would be given by the advection, dispersion and reaction solutions is divided by $R_f$. A similar method of modeling sorption is also used in BIoPLUME II. (Rifai et al., 1987)

### 3.6. Advantages and Limitations of FLOTAN

One of the major advantages of FLOTAN is that it has low mass balance errors. The largest mass balance error reported during this testing is around $10^{-3}$ %. It is also a fairly robust program which can successfully simulate complex situations.

Inputs for FLOTAN include a master input file, including grid size, model domain, porosity, and all the constant input parameters. Any variable input parameters are specified in the input file by giving a filename. The modularity of the input formats makes FLOTAN easy to use, and makes it easy to change spatially varying parameters, such as the hydraulic conductivity. Requiring the spatially varying inputs to be given in a separate file allows the main input file to be concise. Any initial concentrations are read from a file of the same format as a FLOTAN output file, so that a ‘restart’ may be run simply by taking the output from one run, and renaming it as the initial concentration file for the next run.

One of FLOTAN’s limitations is that the user cannot specify changing pumping, boundary conditions, etc. in one input file. In order to run multiple stress periods, the user must create an input file for each, and must rename output files in between runs to avoid having them overwritten by the next run. These difficulties, however, are
outweighed in the author's opinion by the benefits gained from the program's modularity. The method of saving outputs in different files may clutter up the user's directory, but these files are in a form that can be used for either contouring purposes or for a 'restart.' In contrast, all the concentration outputs from BIOPLUME II are written to the same file, and starting concentrations are in the input file, so that if the user needs to do a 'restart,' he must edit the input file and insert part of the previous output file into the proper position.

Also, at present, the program does not echo all of the inputs in an output file. This can make finding an error in the input files very difficult. This will undoubtedly be remedied before the program is distributed widely.

One major limitation of FLOTRAN is that it is not set up to perform transient flow simulations. It is the author's understanding that only minor changes are necessary to implement transient flow calculations, but at present these have not been implemented. Another limitation, which FLOTRAN's author has corrected, was the code's inability to simulate single layer systems. In addition, the author has recently added the capability to simulate systems with a general geometry. This is especially useful in areas with variable aquifer thickness.

One way in which the input to FLOTRAN needs work is on the units of required input variables. At present, the user can specify the units for the grid size (L1), pumpage (L2³/T1), and time step size (T2), dispersivity must be in the same units as the domain length (L1), but the molecular diffusion constant must be in (L1²/s). In addition, conductivities must be given in specific units (cm/s). In the above cases, L1, L2³/T1, and T2 are user specified. The author (of this thesis) modified the input requirements and added the ability to specify these units. It is the author's opinion that flexibility in designating input units is desirable. As long as the conversions are correctly programmed, errors in conversion of input values can be reduced. (For example, MODFLOW requires the user to input all variables in the same units, so that if the user
chooses miles and years for L and T, he must convert hydraulic conductivity to miles/year, which are not common units for conductivity.
Chapter 4. Testing and Validation of FLOTRAN.

4.1. Qualitative Testing.

The initial testing of FLOTRAN was of a qualitative nature meant to answer the question: “If you put in a simple scenario, do the model outputs agree with the expected qualitative results?” Three scenarios were modeled with this intent: (1) a simple test of grid orientation effects, (2) a simple test of retardation by sorption, and (3) a comparison of biodegradation with a BIOPLUME II.

4.1.1. Dispersivity Testing and Grid Orientation Effects.

The first simulation performed is a qualitative test of FLOTRAN’s handling of transport in different directions. It involves the transport of a slug of water containing 10 mg/L of a conservative tracer in a uniform flow field modeled with flow in the x-direction, y-direction, and at a 45 degree angle to each. This simulation was performed on a 41 x 41 grid of 5 ft square cells. A smaller grid is shown in Figure 4.1 for description only.

![Diagram of grid with arrows indicating flow](image)

Figure 4.1: Location of contaminant slugs and direction of flow for dispersivity testing.

In the actual testing grid, the tracer slugs were 5 foot squares located 25 – 30 ft from the left and bottom edges of the grid in the x- and y-direction cases, respectively,
and 25 - 30 ft from each edge in the diagonal case. The tracer slugs were centered and in the same relative positions as the x, y, and d in Figure 4.1.* The grid layout and other simulation parameters are given in Table 4.1.

Table 4.1: Input values for dispersivity testing.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Grid</td>
<td>$41 \times 41 \times 2$</td>
</tr>
<tr>
<td>$\Delta x$</td>
<td>5 ft</td>
</tr>
<tr>
<td>$\Delta y$</td>
<td>5 ft</td>
</tr>
<tr>
<td>$\Delta z$</td>
<td>2.5 ft</td>
</tr>
<tr>
<td>Hydraulic conductivity, $K_x$</td>
<td>$2.82 \times 10^{-2}$ cm/s</td>
</tr>
<tr>
<td>Hydraulic conductivity, $K_y$</td>
<td>$2.82 \times 10^{-2}$ cm/s</td>
</tr>
<tr>
<td>Hydraulic conductivity, $K_z$</td>
<td>$2.82 \times 10^{-4}$ cm/s</td>
</tr>
<tr>
<td>Longitudinal dispersivity, $\alpha_L$</td>
<td>0.6 ft</td>
</tr>
<tr>
<td>Transverse dispersivity, $\alpha_T$</td>
<td>0.06 ft</td>
</tr>
<tr>
<td>Hydraulic gradient, $dh/dl$</td>
<td>$5 \times 10^{-3}$</td>
</tr>
<tr>
<td>Porosity, $\theta$</td>
<td>0.4</td>
</tr>
</tbody>
</table>

A comparison of output for the x- and y-direction cases showed that the water surface and concentration profiles were identical. This shows that FLOTRAN is able to compute the direction of ground water flow and to apply the appropriate dispersion coefficients ($\alpha_L$ for dispersion in the direction of flow, and $\alpha_T$ transverse to the direction of flow). None of these results are shown, as they are trivial. A comparison of the orthogonal flow case (flow in the x-direction) with the diagonal flow case (flow at a 45 degree angle to the grid) shows differences in the shape of the plume due to dispersion. Figure 4.2a shows the dispersion of the slug in the orthogonal case, and Figure 4.2b shows the dispersion in the diagonal case. The concentrations are contoured at equal intervals, starting from 0.0 mg/L. The contour interval is given in the caption of each plot. By inspection, it is obvious that flow on a diagonal causes a substantial amount of

* Due to a programming feature, FLOTRAN could not accept a single layer problem at the time that this simulation was performed. This has been changed. Several of the situations, however, have been simulated with two identical layers. All boundary conditions and initial conditions in such simulations were unvarying in the z-direction, and as expected, the results were identical in the two layers in all cases.
(a) Orthogonal with dispersion, contour lines every 0.5 mg/l.

(b) Diagonal with dispersion, contour lines every 0.1 mg/l.

(c) Orthogonal without dispersion contour lines every 1.0 mg/l.

(d) Diagonal without dispersion contour lines every 0.1 mg/l.

Figure 4.2: Advection and dispersion of a slug of contaminant in a uniform two-dimensional flow field.
numerical dispersion. Some numerical dispersion is expected when the flow is at a 45 degree angle to the grid orientation. (Goode and Konikow, 1991; Warwick and Stoffregen, 1991)

The same simulations were run a second time, with the dispersivities set to zero. The results are similar: the orthogonal case behaves well, with no dispersion, and the diagonal case demonstrates numerical dispersion similar to the case with dispersion. These results are plotted in Figures 4.2c and 4.2d. Table 4.2 shows the effect of the numerical dispersion on the maximum concentration at times of 5, 25, 50, and 70 days.

Mass balance errors calculated for these simulations are on the order of $10^{-9}$ mg/L. A separate check was performed on the total mass of contaminant, and it confirmed that all the mass initially present in the simulation was present at the end. (This check was of lower accuracy than the mass balance computed by the code, because it was performed on model outputs which are saved to the nearest $10^{-7}$ mg/L.)

The marked numerical dispersion in the diagonal case noted here prompted the addition of diagonal flow cases to two of the simulations with analytical solutions. These cases are presented in §4.3.1.1 and §4.3.2.1.

Table 4.2: Maximum concentrations as the slug of contaminant flows down gradient. (Initial concentration = 10 mg/L.)

<table>
<thead>
<tr>
<th>Time</th>
<th>5 days</th>
<th>25 days</th>
<th>50 days</th>
<th>70 days</th>
</tr>
</thead>
<tbody>
<tr>
<td>Orthogonal – Dispersion (mg/L)</td>
<td>7.97</td>
<td>3.94</td>
<td>2.29</td>
<td>1.71</td>
</tr>
<tr>
<td>Diagonal – Dispersion (mg/L)</td>
<td>2.63</td>
<td>0.75</td>
<td>0.39</td>
<td>0.29</td>
</tr>
<tr>
<td>Orthogonal – No Dispersion (mg/L)</td>
<td>9.98</td>
<td>9.91</td>
<td>9.81</td>
<td>9.74</td>
</tr>
<tr>
<td>Diagonal – No Dispersion (mg/L)</td>
<td>3.07</td>
<td>1.02</td>
<td>0.59</td>
<td>0.47</td>
</tr>
</tbody>
</table>
4.1.2. Testing of Sorption Processes.

Sorption processes are simulated by the use of a linear sorption isotherm, which causes all the other processes being simulated to proceed at a reduced rate. This method has been used extensively, and is relatively easy to implement, so a simple test will adequately validate the modeling of these processes. Sorption processes were tested using the same basic situation as the $x$-direction orthogonal case with dispersion in § 4.1.1. (See Table 4.1) The only inputs changed were the retardation factor and the times for printing output.

For this test, a retardation factor of 2 was compared with the 'no retardation' case ($R_f = 1$). Results are plotted at times of 50 and 100 days in Figures 4.3a–d for the 'no retardation' and the 'retardation' cases. Including the retardation factor slows the advection of the tracer slug. Since the 'retardation' case is slowed by a factor of two, the resulting plume at $t = 100$ days should be equivalent to the 'no retardation' case at $t = 50$ days. Figures 4.3a and 4.3d show the corresponding plumes. The shapes of these two plumes are very similar, and their centers of mass are at the same maximum concentration and location, as shown in Table 4.3. Similar results were seen when a 1-dimensional constant concentration simulation was performed. These results are not shown.

<table>
<thead>
<tr>
<th>Case</th>
<th>$C_{\text{max}}$ at 50 days</th>
<th>$C_{\text{max}}$ at 100 days</th>
</tr>
</thead>
<tbody>
<tr>
<td>No Retardation</td>
<td>2.25 mg/L</td>
<td>1.22 mg/L</td>
</tr>
<tr>
<td>Retardation</td>
<td>3.89 mg/L</td>
<td>2.25 mg/L</td>
</tr>
</tbody>
</table>

Table 4.3: Maximum concentrations observed in sorption simulation.
Figure 4.3: Effects of sorption/retardation on the advection and dispersion of a slug of contaminant.
4.1.3. Testing of Biodegradation Subroutines.

As a test of the biodegradation subroutine, a direct comparison with BIOPLU EM II was performed. Identical simulations were set up on FLOTRAN and BIOPLU EM II. As is noted in § 3.4, FLOTRAN inputs can be set such that the biodegradation process is modeled in the same way as BIOPLU EM II.

4.1.3.1. Note on setting up identical simulations with FLOTRAN and BIOPLU EM II.

FLOTRAN and BIOPLU EM II apply boundary conditions in very different ways, so care must be used in setting up simulations that are indeed identical. FLOTRAN applies the boundary conditions at the outside edge of the exterior grid cell, while BIOPLU EM II applies them at the center of the cell specified in a nodeID array. (See Rifai et al., 1987 for BIOPLU EM II input specifications.) Because of this difference, it was necessary to use a non-uniform grid for FLOTRAN and to set \( \Delta x \) and \( \Delta y \) on the exterior cells equal to 2.5 ft. (See Figure 4.4) In addition, BIOPLU EM II requires a buffer layer of grid cells around any constant head boundaries in the model domain.
Figure 4.4: Identical BIOPLUME II and FLOTRAN model grids with boundary conditions.

Shading is used in Figure 4.4 to identify No-Flow and Constant Head boundaries in the BIOPLUME II model setup because these cells exist and are defined as such. The same scheme cannot be used for FLOTRAN, because all cells defined for a FLOTRAN model are active cells. Boundary conditions are applied at the edges of the cells. Drawing them as shaded areas would be misleading, implying that there are actual cells defined as No-Flow cells or Constant Head cells.

This setup gives the closest feasible approximation to identical model areas. It is not perfect, as is evidenced by the fact that in FLOTRAN, there are two more columns of active cells in this setup than there are in BIOPLUME II (along the two no-flow boundaries), however that is the only way to apply the boundary conditions along the same lines. This limitation will apply to any comparison with a no-flow boundary.

For the model area shown in Figure 4.4, the BIOPLUME II model is set up on a 9 \times 10 grid, and the FLOTRAN model is set up on a 9 \times 8 grid. Flow is vertical, from top to bottom. Since BIOPLUME II applies boundary conditions at the center of the specified

9 \times 10 BIOPLUME II model with boundary conditions. Identical 9 \times 8 FLOTRAN model, with appropriate boundary conditions.

\[ \text{No-Flow Boundary} \]

\[ \text{Constant Head Boundary} \]
cells, the distance between the upper and lower constant head boundaries, \( L_y = 6\Delta y + 2\times(\Delta y/2) = 7\Delta y \), where \( \Delta y \) is the height of one model cell. In order to achieve the same \( L_y \) for the FLOTRAN model, while keeping the centers of the cells in the same positions relative to the constant head boundaries, the upper and lower boundaries in the FLOTRAN model must be half the size of the other cells. In addition, since FLOTRAN does not require a no-flow 'boundary layer,' these cells from the BIOPLUME II simulation are omitted. For this reason, the FLOTRAN model requires fewer cells around a constant head boundary.

Setting up the cells this way allows the user to compare calculations directly, for both codes compute concentrations at the center of the cells, which are at the same locations in this setup, and are at the same distances from the boundaries. The only difference is that the concentrations in the boundary cells are calculated at different places, however this is insignificant if the 'action' is taking place sufficiently far from the boundaries.

4.1.3.2. Biodegradation Testing.

Two identical grids were set up—one each on FLOTRAN \((41 \times 41)\) and BIOPLUME II \((43 \times 41)\)—according to the principles in § 4.1.3.1. Biodegradation is tested on a 200 ft \(\times\) 200 ft model area, with an injection well 50 ft. from the left side, and uniform flow from left to right.

The following parameter values were used in both simulations:
\[ \Delta x = \Delta y = 5 \text{ ft}, \]
Porosity, \( \theta = 0.4, \)
Thickness, \( b = 20 \text{ ft}, \)
Contaminant injection rate, \( Q = 1 \text{ gpm}, \)
Contaminant concentration, \( C_0 = 100 \text{ mg/L}, \)
Hydraulic gradient, \( \partial h/\partial l = 0.005, \) and
Hydraulic conductivity, \( K = 80 \text{ ft/day}. \)

The background seepage velocity of the system thus created is 1 ft/day. It is assumed that the hydrocarbon sorbs to the soil with a retardation factor of 2, and that the oxygen does not, and has a retardation factor of 1. Consequently, a bulk density of 1.75 kg/L and a distribution coefficient of 0.274 L/kg were entered in the \textsc{bioplume \II} input. Biodegradation parameters used in the \textsc{bioplume \II} simulation were: the ratio of oxygen consumed to hydrocarbon consumed \( F = 3.0, \) decay half-life \( \lambda = 0.0 \text{ sec}, \) anaerobic decay coefficient = 0.0 /day.

Biodegradation parameters used in the \textsc{flotran} simulation were:

- **Hydrocarbon utilization rate**
  
  per unit mass of microorganisms, \( k = 1.7 \times 10^5 \text{ /day}, \)

- **First order decay rate of natural organic carbon** \( K_c = 2.7 \times 10^{-6} \text{ /day}, \)

- **Natural organic carbon concentration** \( C = 0.0 \text{ mg/L}, \)

- **Ratio of oxygen to hydrocarbon consumed** \( F = 3.0, \)

- **Yield (g cells produced / g hydrocarbon consumed)** \( Y = 0.5, \)

- **Hydrocarbon half-saturation constant** \( K_h = 0.1 \times 10^{-4} \text{ mg/L}, \)

- **Oxygen half-saturation constant** \( K_o = 0.1 \times 10^{-4} \text{ mg/L}, \)

These parameters will produce biodegradation equivalent to the ‘fast equilibrium’ model used by \textsc{bioplume \II}, (Borden and Bedient, 1986) as discussed in \S\ 3.4.

In each simulation, a well is placed 50 feet from the left constant head boundary. This well is injecting water contaminated with 100.0 mg/L of hydrocarbon, and totally devoid of oxygen. The left boundary (upgradient) is introducing water which is oxygenated at 8.0 mg/L. Initially all the water in the aquifer has 8.0 mg/L of dissolved oxygen in it and is free of hydrocarbon contamination. Figure 4.5a shows the
Figure 4.5: Hydrocarbon concentrations downstream of an injection well.
hydrocarbon plumes after 50 days of simulation for the FLOTRAN and BIOPLUME II simulations, while Figure 4.5b shows the difference between the two plumes. Inspection of Figure 4.5 shows reasonable agreement between the plumes generated by FLOTRAN and BIOPLUME II. The hydrocarbon plume from the BIOPLUME II simulation is very compact, with steeper edges than the FLOTRAN simulation, especially transverse to the direction of flow. The maximum concentrations in the hydrocarbon plumes are: 87.83 mg/L for BIOPLUME II and 83.27 mg/L for FLOTRAN. This is consistent with the observation that the BIOPLUME II plume is more compact. One measure of plume length is the location of the point along the center line at which the concentration is half that of the maximum concentration. In this simulation, that is about 40 mg/L for each model. Using this measure, both the modeled hydrocarbon plumes have a ‘length’ of approximately 55 ft after 50 days of simulation. Figure 4.5b shows that the maximum difference between the two simulated plumes is greater than 20 mg/L. This large difference is due to the extreme steepness of the hydrocarbon plumes. A difference of less than 3 ft. in the position of the edge of the plume creates a 20 mg/L difference in concentration values.

Figure 4.6a shows the oxygen depleted areas around the hydrocarbon plume. Since the hydrocarbon plume in the FLOTRAN simulation is slightly larger than that in the BIOPLUME II simulation, the resulting oxygen depleted area is also larger in the FLOTRAN simulation. Oxygen concentrations range from 0.0 mg/L in both simulations to 8.20 mg/L in BIOPLUME II and 8.00 mg/L in FLOTRAN. There is overshoot in the BIOPLUME II simulation, creating oxygen values greater than the physically possible. This is in response to the very sharp front near the edge of the hydrocarbon plume. Inspection of the FLOTRAN output files shows overshoot on the order of 0.0006 mg/L upgradient of the injection well. Figure 4.6b shows the difference in oxygen concentrations between the simulations. Once again, the differences are most pronounced along the sharp fronts. The hydrocarbon plume and the oxygen depleted area
Figure 4.6: Oxygen concentrations downstream of an injection well.
from the FLOTRAN simulation show greater dispersion than those from the BIOPLUME II simulation.

Inspection of the output files indicates that the model cells on the inside edge of the hydrocarbon plume have hydrocarbon present, but no oxygen, and model cells on the outside edge of the hydrocarbon plume have oxygen present, but no hydrocarbon. This behavior is expected, as discussed in §3.4. In addition, a temporary run-time printout of hydrocarbon and oxygen concentrations before and after the biodegradation step indicates that the proper changes in hydrocarbon and oxygen concentrations were being calculated during the trial run.

Maximum mass balance errors for BIOPLUME II were about 2% for hydrocarbon, and about 9% for oxygen, while FLOTRAN gave maximum mass balance errors of approximately $7 \times 10^{-7}$% for hydrocarbon and $2 \times 10^{-5}$% for oxygen.


El-Kadi (1988) simulated three situations in radially convergent or divergent situations with a coarse grid. He states that "the objective of the study is to verify MOC for situations pertinent to remedial actions by recovery wells." Two of these situations are (1) recharge followed by recovery from a single well, and (2) a recharge/recovery doublet.


In this situation, contaminated water is injected into the aquifer for a time $t_1$, then the flow is reversed, and water is removed from the aquifer. Gelhar and Collins (1971) derived an analytical expression which approximates the concentration in the well during this process. The expression reads

$$
\frac{C}{C_0} = \frac{1}{2} \text{erfc}\left(-\sqrt{\frac{16 \alpha}{3R}} \left[2 - \sqrt{V|V|^{1/2}}\right]^{1/2}\right),
$$

Eq. 4.8
where \[ V = \frac{(2t_1 - t)}{t_1} \] Eq. 4.9

and \[ R = \left(\frac{Qt_1}{\pi\theta B}\right)^{1/2}. \] Eq. 4.10

In Equations 4.8 - 4.10, \( t \) is the time since the beginning of the injection cycle and \( t_1 \) is the time at which injection stops and recovery begins. Therefore, \( V \) is not a physical volume, but is a measure of how much of the injected water remains in the subsurface at time \( t \). When \( V = 0 \), \( (t = 2t_1) \), the same amount of water has been removed from the well in the recovery stage as was injected into the well in the injection stage. Other variables are: \( Q \), the flow rate (assumed to be the same in injection and recovery); \( \theta \), the porosity; and \( B \), the (constant) thickness of the aquifer.

Four subcases were simulated in this test case. The parameters which differ between the cases are given in Table 4.4, while the test parameters which are common to all of the subcases are defined in Table 4.5. The four test cases are also simulated with \textsc{bioplume ii}, recreating the work of El-Kadi.

| Table 4.4: Variable parameters for test cases 1.A, 1.B, 1.C, and 1.D. |
|-----------------------------|------------|-------------|----------|
| Case | \( \alpha_L \) (ft) | \( t_1 \) (years) | \( Q \) (cfs) |
| 1.A | 100 | 2.5 | 1.0 |
| 1.B | 100 | 1.0 | 1.0 |
| 1.C | 0.001 | 2.5 | 1.0 |
| 1.D | 100 | 2.5 | 0.5 |
Table 4.5: Common parameters for test cases 1.A, 1.B, 1.C, and 1.D.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Symbol</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hydraulic conductivity</td>
<td>K</td>
<td>0.005 ft/s</td>
</tr>
<tr>
<td>Aquifer thickness</td>
<td>B</td>
<td>20.0 ft</td>
</tr>
<tr>
<td>Porosity</td>
<td>φ</td>
<td>0.30</td>
</tr>
<tr>
<td>Ratio of longitudinal to transverse dispersivity</td>
<td>α_L/α_T</td>
<td>1.0</td>
</tr>
<tr>
<td>Grid size in x direction</td>
<td>Δx</td>
<td>900. ft</td>
</tr>
<tr>
<td>Grid size in y direction</td>
<td>Δy</td>
<td>900. ft</td>
</tr>
<tr>
<td>Number of grid increments in x direction</td>
<td>N_x</td>
<td>9</td>
</tr>
<tr>
<td>Number of grid increments in y direction</td>
<td>N_y</td>
<td>*</td>
</tr>
<tr>
<td>Concentration of injected water</td>
<td>C_0</td>
<td>100.0 %</td>
</tr>
</tbody>
</table>

* MOC requires an extra layer of grid cells outside the constant head boundary. For this reason, there are 11 grid cells in the MOC modeling, but only 9 in the FLOTRAN modeling.

Figure 4.7a - d, illustrates the results of the experiments 1.A to 1.D for the FLOTRAN and BIOPLUME II (MOC) simulations. The results of the BIOPLUME II recreations shown in Figure 4.7 do not agree with those shown in El-Kadi (1988), although all the parameters used are taken directly from his paper. For cases A, B, and D, El-Kadi’s simulations all have concentrations at t = 0.25 years of around 90% of C_0, while in the recreated BIOPLUME II runs, the concentration at t = 0.25 years is consistently around 56% of C_0. The author has triple-checked his BIOPLUME II input file, and finds it totally in agreement with the input parameters given in El-Kadi’s paper. In addition, the analytical solutions calculated by the author do not agree with those shown in El-Kadi’s paper. The author has checked the analytical solution against that presented in the original paper, and found no discrepancies. It is the author’s opinion that although there are several errors in the presentation of this problem by El-Kadi, the technique has merit as a test.

The closeness of fit between the analytical solution and the numerical solution may be measured by the average absolute error. This error is calculated by taking the average of the absolute values of the difference between the two solutions. Using this
Figure 4.7: Estimated time dependence of relative concentration for recharge/recovery from a single well.
measure, the errors for the four runs using FLOTTRAN are 5.6, 1.5, 11.5, and 5.9 mg/L, respectively, and the errors for the BIOPLUME II runs are 5.7, 10.4, 8.3, and 7.4 mg/L. Neither model performs extremely well on this test.

The stresses in this simulation are rather severe, yet the results are on the right order of magnitude, and consistently within 15% of the value given by the analytical solution (except for case 1.C, where the numerical dispersion greatly affects the concentrations). For cases 1.A, 1.C, and 1.D, an estimate of the ‘actual’ dispersivity, which is the input dispersivity plus the dispersivity added by numerical dispersion, is given by attempting to fit the analytical solution to the FLOTTRAN solution using the dispersivity as the fitting parameter. The ‘added dispersivity’ due to numerical dispersion can then be determined by subtracting the dispersivity used in the numerical model from the dispersivity of the best fit with the analytical solution. In each of these three cases, the numerical dispersion added about 70 - 100 ft to the input value of dispersivity.

4.2.2. Case 2 — A Recharge/Recovery Doublet.

The second case tested by El-Kadi (1988) was a recharge/recovery doublet. In this case, on a similar grid there is an injection well 2700 ft (3 cells) from a recovery well pumping at the same flow rate. Javandel et al. (1984) coded a semi-analytical solution to the purely advective transport in this situation. The model, called RESSQ, calculates the velocity field in a domain defined by injection and production wells, and tracks the contaminant front away from the injection well along a fixed number of streamlines emanating from the injection well. The concentration in the recovery well is determined by averaging contaminant concentrations among the streamlines entering the well. When the contaminant front reaches the recovery well along a given streamline the concentration at the well immediately jumps to its new value. The number of streamlines modeled determines the smoothness of the resulting breakthrough curve.
When El-Kadi (1988) modeled this situation with MOC, the concentration in the recovery well fluctuated around 3/4 of the semi-analytical concentrations given by RESSQ. The magnitude of the fluctuations in the MOC solution was about half the average concentration at any given time.

The recharge/recovery doublet was simulated on a $9 \times 10$ MOC grid, and therefore on a $9 \times 8$ FLOTRAN grid, since the extra layer of cells was not required. Figure 4.8 shows the MOC setup for the simulation. The FLOTRAN setup is identical, except as discussed in § 4.1.3.1. Other input parameters are the same as in Table 4.5, except that $Q_{in} = Q_{out} = 1.0$ cfs.

![Aquifer model for the recharge/recovery doublet.](image)

The test case was run on a $9 \times 8$ grid with FLOTRAN, and on a $9 \times 10$ grid with BIOPLUME II, to confirm El-Kadi’s observations. The resulting concentration breakthrough curves are shown in Figure 4.9. Two features are evident from the first runs: 1) The solution given by FLOTRAN does not fluctuate like the MOC/BIOPLUME II solution does, and 2) the FLOTRAN concentrations are also about 3/4 of the RESSQ value.

In the $9 \times 8$ grid runs, neither model reached the concentrations predicted by RESSQ. The reason for this was that the model domain was simply too small. The contaminant was running into the constant head and no-flow boundaries. In order to more accurately model this scenario, the model domain was enlarged. Increasing the
Figure 4.9: Concentrations in the recovery well of a recharge/recovery pair for (a) FLOTRAN vs. RESSQ and (b) BIOPLUME II vs. RESSQ.
model domain to a $14 \times 16$ (or $14 \times 18$) grid and retaining the same grid size ($900 \times 900$ ft) improved the results. In addition, this larger grid was divided up into smaller grid blocks ($225 \times 225$ ft). Runs were made with both FLOTRAN and BIOPLUME II using the larger grids. The results are also shown on Figure 4.9.

Figure 4.9a shows the resulting concentration breakthrough at the recovery well for the FLOTRAN simulations. A significant improvement (from 26.8% error to 12.2%) is observed by simply increasing the size of the model domain, and an additional improvement (to 10.7%), especially near the breakthrough time, is seen with the mesh refinement. A further mesh refinement (not shown) improves the results by about 0.1%. Errors for this simulation are given as percent differences from the RESSQ solution at the last time step.

Figure 4.9b shows the results of the same simulations done with BIOPLUME II. In all three simulations, the concentration in the recovery well fluctuates. In the original simulation, the concentration fluctuates around a curve about 25% below the RESSQ solution, which is where the original FLOTRAN solution lies. Increasing the model domain improves the simulation in that the fluctuations are centered more closely on the RESSQ solution, however the amplitude of the fluctuations is not reduced. Mesh refinement does not improve the results.
4.3. Level I Testing — Problems with Analytical Solutions to the Transport Equations.

Huyakorn et al. (1984) presents several techniques for testing numerical models. The first of these, Level I, involve testing against analytical solutions to the flow and transport equations given in Chapter 3 (Equations 3.4 - 3.9). For several geometrically simple situations, there exist analytical solutions to these equations. Some of these situations were used in the testing of FLOTTRAN, as follows.

4.3.1. Problem I.1 One-Dimensional Transport from a Constant Concentration Boundary.

Problem I.1 is a simulation of one-dimensional transport in a semi-infinite column with a constant concentration boundary condition. For this problem, flow is assumed to be unidirectional and a contaminant is assumed to be introduced at a constant concentration along the entire upgradient boundary. The analytical solution to this problem (Ogata 1961) is

\[
\frac{C}{C_0} = 0.5 \left\{ \text{erfc} \left( \frac{x - vt}{2\sqrt{D}t} \right) + \exp \left( \frac{vx}{D} \right) \text{erfc} \left( \frac{x + vt}{2\sqrt{D}t} \right) \right\},
\]

Eq. 4.4

where \( v = \frac{K}{\theta} \cdot \frac{dh}{dl} \) is the average velocity of the ground water and \( D = \alpha v \) is the dispersion coefficient.

The major variables and grid choices are enumerated in Table 4.6. Four cases were simulated, and are characterized by the cell Peclet number \( (Pe = \Delta x/\alpha) \). The four cases are for \( Pe = 2, 5, 50 \) and infinite, respectively, and correspond to values of dispersivity, \( \alpha \) of 5 meters, 2 meter, 0.2 meters, and 0.0 meters. Computed values of \( C/C_0 \) are plotted in Figure 4.10 at elapsed times of 25 and 50 days and are compared to the analytical solutions using the equations derived by Ogata and Banks (1961). The absolute average errors for the four cases at 50 days are 0.23, 0.26, 1.21 and 0.00\%.
Figure 4.10: Comparison of analytical and numerical solutions for Problem 1.1
Table 4.6: Grid dimensions and input parameters for model testing simulations.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Simulation Qualitative Dispersion Simulation</th>
<th>Problem 1.1 1-D Constant Concentration</th>
<th>Problem 1.3 2-D Constant Point Source Fine Mesh</th>
<th>Problem 1.3 2-D Constant Point Source Medium Mesh</th>
<th>Problem 1.3 2-D Slug Source Coarse Mesh</th>
<th>Problem 1.4 Radial Transport from an Injection Well</th>
</tr>
</thead>
<tbody>
<tr>
<td>Grid</td>
<td>41 × 2 × 2</td>
<td>40 × 2 × 2</td>
<td>39 × 20 × 2</td>
<td>39 × 10 × 2</td>
<td>13 × 5 × 2</td>
<td>49 × 11 × 2</td>
</tr>
<tr>
<td>Δx</td>
<td>5 ft</td>
<td>5 m</td>
<td>60 m</td>
<td>60 m</td>
<td>180 m</td>
<td>variable</td>
</tr>
<tr>
<td>Δy</td>
<td>5 ft</td>
<td>10 m</td>
<td>15 m</td>
<td>30 m</td>
<td>60 m</td>
<td>5 m</td>
</tr>
<tr>
<td>Δz</td>
<td>5 ft</td>
<td>10 m</td>
<td>33.5 m</td>
<td>33.5 m</td>
<td>33.5 m</td>
<td>5 m</td>
</tr>
<tr>
<td>Conductivity, $K_x$</td>
<td>2.82 × 10^{-2} cm/s</td>
<td>10 m/day</td>
<td>1.86 × 10^{-2} cm/s</td>
<td>1.86 × 10^{-2} cm/s</td>
<td>1.86 × 10^{-2} cm/s</td>
<td>0.1 cm/s</td>
</tr>
<tr>
<td>Conductivity, $K_y$</td>
<td>2.82 × 10^{-2} cm/s</td>
<td>10 m/day</td>
<td>1.86 × 10^{-2} cm/s</td>
<td>1.86 × 10^{-2} cm/s</td>
<td>1.86 × 10^{-2} cm/s</td>
<td>0.1 cm/s</td>
</tr>
<tr>
<td>Dispersivity, $\alpha_z$</td>
<td>0.6 ft</td>
<td>2.5, 1.0, 0.1, 0.0 m</td>
<td>21.3 m</td>
<td>21.3 m</td>
<td>21.3 m</td>
<td>4 m</td>
</tr>
<tr>
<td>Dispersivity, $\alpha_T$</td>
<td>0.6 ft</td>
<td>-</td>
<td>4.3 m</td>
<td>4.3 m</td>
<td>4.3 m</td>
<td>1 m</td>
</tr>
<tr>
<td>Porosity, $\theta$</td>
<td>0.4</td>
<td>0.25</td>
<td>0.35</td>
<td>0.35</td>
<td>0.35</td>
<td>0.35</td>
</tr>
<tr>
<td>Gradient, $\partial h/\partial t$</td>
<td>0.01</td>
<td>0.01</td>
<td>0.01</td>
<td>0.01</td>
<td>0.01</td>
<td>0.0231</td>
</tr>
<tr>
<td>Injection Rate, $Q$</td>
<td>Not Applicable</td>
<td>Not Applicable</td>
<td>0.433 gpm</td>
<td>0.433 gpm</td>
<td>0.433 gpm</td>
<td>Not Applicable</td>
</tr>
<tr>
<td>Initial Concentration, $C_0$</td>
<td>10 mg/l</td>
<td>1.0 mg/l</td>
<td>5000 g/cm$^3$</td>
<td>5000 g/cm$^3$</td>
<td>5000 g/cm$^3$</td>
<td>400 mg/m$^3$</td>
</tr>
</tbody>
</table>

(1 m$^3$/day = 0.1835 gpm)
Often, when numerical models are set to simulate conditions with sharp fronts of contamination, as in the very low and no dispersion cases, there will be some overshoot and oscillation near the front. Huyakorn et al. (1984), used this scenario to test a code called SEFTRAN, and noted large oscillations in the numerical solution of the Pe = 50 and infinite cases. Figure 4.11 shows the numerical oscillations in the SEFTRAN solution. The average absolute difference between the analytical solutions and the two SEFTRAN cases shown are 5.6 and 6.6%, respectively.

4.3.1.1. Problem I.1 Supplemental One-Dimensional Transport at a 45 Degree Angle to the Grid Orientation.

In §4.1.1. a slug of contaminant was allowed to advect and disperse with flow at a 45 degree angle to the grid orientation (flow is from the lower left to the upper right). The results of that simulation showed that in that case, numerical dispersion dominated the solution. In order to quantify this numerical dispersion, flow at an angle to the grid has been tested in a one-dimensional case with a constant concentration boundary. The simulation is set up on the same 41 × 41 grid that was used in §4.1.1, with all the same input parameters, except that the lower left hand corner of the model grid was set to have a 10 mg/L constant concentration boundary. In addition, a triangular section of the model domain in the lower left hand corner was set to have an initial concentration of 10 mg/L. In this manner, the advancing contaminant front is linear and behaves in a manner similar to that seen in the previous section.

The simulation was performed for two cases, αL = αT = 0.0 ft, and αL = 0.6 ft, αT = 0.0001 ft. Contaminant concentrations were monitored at two points, 40.7 and 76.0 ft downstream of the initial contaminant front. The analytical solution given in §4.3.1 was fit to the numerical solutions using the longitudinal dispersivity as a fitting parameter, to provide a quantitative estimate of the numerical dispersion added to the model. The results of the two simulations and fitting the analytical solutions to the numerical solutions are shown in Figure 4.11c. According to the fitting shown, the no dispersion
Figure 4.11: Comparison of analytical and numerical solution for SEFTRAN.
Figure 4.11c: Advevtively dominated flow at a 45 degree angle to the grid orientation.
numerical solution matches the analytical solution for $\alpha_L = 0.5$ ft, and the numerical solution with $\alpha_L = 0.6$ ft matches the analytical solution for $\alpha_L = 1.1$ ft. This implies that flow at an angle to the grid orientation adds a consistent amount of longitudinal numerical dispersion to the simulation. In this case that amount is 0.5 ft, or 1/10 of the grid spacing. The numerical dispersion added in these simulations is small, and can be accounted for by adjusting the input parameters. This is consistent with the observation in §4.2.1 of a numerical dispersion of approximately 8-11% of the grid spacing in a radial flow case.

4.3.2. Problem I.3 Transport from a Continuous Point Source in a Uniform Two-Dimensional Flow Field.

Problem I.3 tests the accuracy of dispersivity in the longitudinal and transverse directions. The implementation of this problem makes use of the symmetry that is defined in the problem. Only one half of the domain is modeled, as shown in Figure 4.12. The contamination is introduced via an injection well located at the appropriate location.

Three grids were used in this simulation, so that the sensitivity to mesh size could be determined. The grid choices are labeled as Coarse, Medium, and Fine meshes, corresponding to grid cells of $180 \text{ m} \times 60 \text{ m}$, $60 \text{ m} \times 30 \text{ m}$, and $60 \text{ m} \times 15 \text{ m}$, respectively. All grid and simulation parameters are given in Table 4.6.

![Figure 4.12: The X-axis is a line of symmetry for the contaminant plume. It is also a flow line, and therefore can be considered an impermeable boundary.](image)
FLOTRAN simulates a mass flux along with some addition of water to the system (either by a constant flux boundary, or by an injection well). The addition of mass in this problem was accomplished by using an injection well at a very low flow rate. It was very important in this case not to disturb the flow patterns, so that almost all the lateral dispersion of the contaminant is produced by dispersion. A low flow rate was chosen for this reason. This problem was simulated using two identical layers, with identical boundary conditions, including the injection well. In this case, to get an equivalent mass flux of 704 grams/(meter-day), the two wells were each injecting water contaminated at 5000 mg/L at a flow rate of $1.36 \times 10^{-5}$ m$^3$/s. The above injection rate and concentration yields a total mass flux of 352 grams/(meter-day), however since the injection is along an impermeable boundary, the mass flux simulates twice that much, with half of the total dispersing in the $+y$-direction, and the other half in the $-y$-direction. Inspection of the head output shows that the presence of the injection well causes minimal mounding.

Results of the simulation are shown in Figures 4.13 - 4.15 for the Coarse, Medium, and Fine meshes, respectively. Snapshots of concentrations are taken at times of 500, 1000, 2000, and 2800 days. The analytical solution derived by Hunt (1978) and Wilson and Miller (1978) is also plotted in Figures 4.13 - 4.15 for comparison. Values for the analytical solution are taken from Huyakorn et al. (1984). As expected, the fine mesh shows the best agreement between analytical and numerical solutions. The average absolute differences between the analytical solution and the FLOTRAN solution for the Coarse, Medium, and Fine grids are 11.1, 5.5, and 2.3%, respectively. Decreasing the grid size, and therefore, the Peclet number, increases the accuracy of this simulation significantly.
Figure 4.13: Concentration distributions along the x-axis showing a comparison of numerical and analytical solutions for Problem I.3 with the Coarse mesh.

Figure 4.14: Concentration distributions along the x-axis showing a comparison of numerical and analytical solutions for Problem I.3 with the Medium mesh.
Figure 4.15: Concentration distributions along the x-axis showing a comparison of numerical and analytical solutions for Problem I.3 with the Fine mesh.
Dimensionless variables are calculated and used in the plots according to the following formulas

\[ x_D = x/(2\alpha_L), \quad \text{Eq. 4.5} \]

\[ y_D = y/(2\alpha_L), \quad \text{Eq. 4.6} \]

\[ C_D = 2\pi\sqrt{\alpha_L\alpha_T} \frac{vC}{Q C_0}, \quad \text{Eq. 4.7} \]

where \( v \) is the background seepage velocity, \( Q \) is the injection rate, \( \alpha_L \) and \( \alpha_T \) are the longitudinal and transverse dispersivities, respectively, and \( C \) and \( C_0 \) are the 'present' and initial concentrations, respectively.

4.3.2.1. Problem 1.3 Supplemental Transport from a Continuous Point Source in a Uniform Two-Dimensional Flow Field at a 45 Degree Angle to the Grid Orientation.

As a final test of the code running at an angle to the grid orientation, a run similar to those in §4.3.2 was performed with the flow at a 45 degree angle. This simulation was run on the same 41 \times 41 grid used in §4.1.1, but with an injection well located 25\sqrt{2} feet from the lower left corner of the grid (in cell 6,6). For this simulation, dispersivity values of \( \alpha_L = 7.6 \text{ ft} \) and \( \alpha_T = 0.76 \text{ ft} \) were used. The simulation was allowed to achieve steady state conditions, and the steady state version of the analytical solution presented in Huyakorn et al. (1984) is fit to the resulting plume to give a qualitative measure of the numerical dispersion.

Figure 4.16a shows the numerical solution to the problem and the fitted and unfitted analytical solutions. The unfitted solution is higher along the centerline of the plume than the numerical solution. Figure 4.16b shows a profile along the centerline of the numerical solution, the unfitted and the fitted analytical solutions. For this simulation, the measure of the goodness of fit was the average of the absolute differences between the numerical and analytical solutions over half the model area (where the
Figure 4.16: Concentrations around an injection well in a uniform flow field.
concentration was significant). The fitted solution uses $\alpha_L = 7.6$ ft and $\alpha_T = 1.1$ ft. Using these fitting parameters, the error was 0.012 units of dimensionless concentration (see Equation 4.7). The error using $\alpha_L = 7.6$ ft and $\alpha_T = 0.76$ ft was 0.042 units. Based on the fitted dispersivity values, flow at an angle adds about 0.4 ft (about 1/10 the grid spacing) to the transverse dispersivity in this case.

4.3.3. Problem I.4 Transport of a Slug of Contaminant in a Uniform Flow Field.

This problem, like Problem I.3, tests advection and dispersion in a uniform flow field, however the source of contamination is changed in this problem to a slug of contaminant, instead of a continuing source. This problem tests the code in two ways: (1) it tests the ability to trace a slug as it flows downgradient, and as it disperses in two dimensions, and (2) it tests the ability of the code to simulate a case in which the longitudinal and transverse dispersivities are different. (Huyakorn et al., 1984)

Sauty (1980) presented a general analytical solution to this problem. The solution is presented as follows (Huyakorn et al., 1984)

$$C_R(a, t_R') = \frac{K}{t_R'} \exp \left( -\frac{a^2 + t_R'^2}{4t_R'} \right),$$

Eq. 4.8

where

$$t_R' = \sqrt{a^2 + 4} - 2,$$

$$t_{Rmax} = \sqrt{a^2 + 4} - 2,$$

$$a = \left( \frac{x_R^2 + y^2}{\alpha_L \alpha_T} \right)^{1/2},$$

and $x_R$ is defined as

$$x_R = \frac{x}{\alpha_L}, \quad \text{when } x > 0, \text{ and }$$

$$x_R = \frac{(|x| + 2v t/\phi)/\alpha_L, \quad \text{when } x < 0.}$$

In Equation 4.8, $v$ is the background seepage velocity and $C_R = C(x, y, t)/C_{max}$, where $C_{max}$ is the maximum concentration at time $t$. $C_{max}$ is given by
\[
C_{max} = \frac{m}{4\pi \phi \alpha_L \sqrt{\alpha_L \alpha_T}} f(x_R, a),
\]
Eq. 4.9

where
\[
f(x_R, a) = \frac{1}{x_R t_{R_{max}}} \exp \left( -\frac{x_R (1 - t_{R_{max}})^2}{4 t_{R_{max}}} - \frac{a^2 - x_R^2}{4 x_R t_{R_{max}}} \right),
\]

and
\[
t_{R_{max}} = \left( 1 + \frac{4}{x_R^2} + \frac{a^2 - x_R^2}{x_R^2} \right)^{1/2} - \frac{2}{x_R}.
\]

In this scenario, the contaminant is introduced into the system at \(x = y = 0\), and allowed to flow downstream. This simulation is symmetrical about the \(x\)-axis and can be run on half of the domain, omitting the \(-y\) direction.

The simulation was done on a variable grid, which models the upper half of the \(x-y\) plane (see Figure 4.12). The layout of the grid is shown in Figure 4.17. The contaminant source is located in the cell centered on \((0, 0)\). This was done for a reason similar to the reasoning behind the grid conversion from BIOPLUME II to FLOTTRAN given in § 4.1.3.1. The model used by Huyakorn et al. (1984), SEFTRAN, is a mesh centered model, unlike FLOTTRAN and BIOPLUME II. SEFTRAN applies boundary conditions and calculates concentrations at the edges of the cells, instead of the centers. This causes the conversion from SEFTRAN to FLOTTRAN to be somewhat awkward. In the SEFTRAN model, the well is located at \((0, 0)\), which is along the edge of a cell. Other input values are listed in Table 4.6.

Huyakorn et al. (1984) state that the time discretization used in SEFTRAN was as follows, \(\Delta t_0 = 1\) day, and \(\Delta t_i = 1.2 \Delta t_{i-1}\), with a maximum of 50 days, and choose to compare numerical and analytical results at \(t = 3.96, 10.59\) and \(16.59\) days. This is in error, because the times selected cannot be produced by the given series. The time discretization scheme that they used is \(\Delta t_0 = 0.1\) day, and \(\Delta t_i = 1.2 \Delta t_{i-1}\), with a maximum of 2 days. This scheme gives the proper series of times.
Figure 4.17: Grid layout for FLOTRAN simulation of Problem I.4.

Figure 4.18: Concentrations along the x-axis showing comparisons of the numerical and analytical solutions to Problem I.4.
The analytical solution is compared to the numerical solution given by FLOTRAN in Figure 4.18. At \( t = 3.96 \) days, the numerical solution differs slightly from the analytical solution, especially at the center of mass of the solute plume. At the two later times, there is very good agreement between the analytical and numerical solutions. This behavior is expected, since the analytical solution is for a problem involving a point source, and the numerical solution involves a 25 m\(^2\) source. In such a case, one would expect the solutions to agree better at later time steps. The errors calculated for this simulation are the average absolute errors divided by the maximum concentration at a given time. For \( t = 3.96, 10.59 \) and 16.59 days, the calculated errors are 0.86, 0.68, and 0.48\%, respectively.

The difficulty with the time discretization inspired another type of test. In this test, the simulation was run without forcing the time steps given above. FLOTRAN calculates time steps based on the criteria given in Equations 3.6 and 3.7. The user may force smaller time steps by requiring a printout at any given time. In this case, only \( t = 3.96 \) days was forced. The resulting concentration profile is not shown in a figure, but the maximum simulated concentration at 3.96 days is over 30\% higher than the analytical solution.

### 4.3.4. Problem 1.5 Transport in a Radial Flow Field Created by an Injection Well.

Problem 1.5 consists of modeling the dispersion of solute from a fully penetrating well in a two-dimensional confined aquifer. The two major assumptions in this problem are that there is no background gradient and that the flow field is radial and at steady state. Objectives of this problem are to test the code when there is longitudinal dispersion in a nonuniform flow field, and to test the accuracy of the code when the dispersivity is small (and thus, the Peclet number is high).

Ogata (1958) derived a general solution to this problem, but it involves integrals that are too complicated to evaluate analytically (Huyakorn et al., 1984; p. 91, Equation
4.18). Hoopes and Harleman (1966) derived an approximation to the Ogata solution that can be solved analytically. This solution is

\[
\frac{C}{C_0} = \frac{1}{2} \operatorname{erfc}\left[\left(\frac{r^2}{2} - \frac{Qt}{2\pi b\theta}\right)\left(\frac{4}{3} \alpha_L r^3\right)^{1/2}\right],
\]

Eq. 4.10

where \( r \) is the distance from the well, \( Q \) is the injection rate, \( t \) is the time since injection of contaminated water began, \( b \) is the thickness of the aquifer, \( \theta \) is the porosity, and \( \alpha_L \) is the longitudinal dispersivity. It is assumed that the flow field is at steady state when the injection of contaminated water begins.

The basic set up of the simulation is given in Table 4.6. The symmetry of the situation allowed for it to be modeled in only the first quadrant. A well was located at cell (1,1), and the \( x = 0 \) and \( y = 0 \) boundaries were set to be Neumann type boundaries, with a flux of zero (no flow boundaries). This is possible since the equipotential lines are perpendicular to the \( x \)- and \( y \)-axes. Those axes are, in essence, no flow boundaries. The \( x = L \) and \( y = L \) boundaries were set to be Dirichlet type boundary conditions with a constant head of 100 m. This is equivalent to simulating an area 4 times the size, with the same \( \Delta x \) and \( \Delta y \), and with the well in the center of the domain. Since the model is simulating one fourth of the area, the pumpage entered into the model is one-fourth of the pumpage that one will enter into the analytical solution. Table 4.6 states that the pumpage in this case is 6.25 m³/d, which equates to an 'actual' pumpage of 25 m³/d.

The simulation is repeated for three values of longitudinal dispersivity, \( \alpha_L = 0.3 \) m, 0.15 m, and 0.015 m, corresponding to Peclet numbers, \( Pe = 3.33, 6.67, \) and 66.67, where \( Pe = \Delta x / \alpha_L \). Results of the simulation are presented, along with a plot of the Hoopes and Harleman approximation to the analytical solution, on Figure 4.19. For \( \alpha_L = 0.3 \) m, results from SEFTRAN are also shown on the graph, and it can be seen that neither numerical model agrees with the analytical approximation. The average absolute errors for the FLOTRAN \( \alpha_L = 0.3 \) m, 0.15 m, and 0.015 m, and SEFTRAN \( \alpha_L = 0.3 \) m cases are 3.6, 2.8, 3.6, and 2.9%, respectively. Huyakorn et al. attribute this disagreement to
Figure 4.19: Concentration snapshots in the vicinity of an injection well.
the fact that Equation 4.10 is an approximation to the true solution. Hoopes and Harleman also note differences between results given by numerical solutions and Equation 4.10.

The reader should also note that as the dispersivity decreases (and the cell Peclet number increases) the numerical solution becomes less reliable. To test this, two mesh refinements were done for the lowest dispersivity case. Values of $\Delta x = 0.5$ m and 0.25 m ($Pe = 33.33$ and $16.67$) were chosen. The results are shown in Figure 4.20. The average absolute errors calculated for these simulations are 3.1, 1.8, and 1.8% for $\Delta x=1.0$, 0.5, and 0.25 ft, respectively. Two observations can be made as the mesh size decreases, (1) the shape of the concentration front steepens, and more closely approximates the shape of the analytical solution, and (2) the crossover point, where the numerical solution and analytical solutions are at the same concentration at the same location, occurs at a relative concentration closer to 0.5. The first effect is caused by the cell Peclet number, however, the second seems to be an effect of the geometry of the problem. Remember that symmetry arguments were used to show that the first quadrant of the model domain could be used to model the entire domain. FLOTTRAN is a cell centered model, and as such, it calculates all concentrations in the center of the model cells, and it places all wells at the center of the model cells. This causes a break in the symmetry which is assumed to model these types of problems. The no flow boundary, instead of passing through the well, passes a distance $\Delta x/2$ from the well, or 0.5 m in this case. This is illustrated very simply in Figure 4.21.
Figure 4.20: Effects of reducing $\Delta x$, and therefore, the Peclet number are shown.

Figure 4.22: Effect of reducing the size of the cell including the injection well are shown.
To illustrate how this can affect the results of the simulation, a separate model run was done with a variable grid. The cell containing the well was reduced in size to \((0.25 \text{ m})^2\). The cells along the \(x\)- and \(y\)-axes were \(0.25 \text{ m} \times 1.0 \text{ m}\) rectangles, and all other cells were \((1.0 \text{ m})^2\) squares. The resulting model grid would have a shape similar to the area in the first quadrant of Figure 4.21 (the area above and to the left of the \(x\)- and \(y\)-axes). In the new model, however, the origin is shifted to the center of the cell containing the well. There is still asymmetry, however the no flow boundaries in this simulation are only 0.125 m from the well and the results of the simulation are much closer to the analytical solution. The average absolute error in this simulation is 1.2\%, which is less than 1/3 the error of the original simulation for \(\alpha_L = 0.3 \text{ m}\). Based on the runs shown in Figure 4.22, the accuracy of this approximation increases with the ratio of the distance from the well to the distance between the well and the no flow boundary.

4.4. Level III Testing — Field Validation.

Level III testing involves applying the model to a field site. "Comparison of modeling results with field data allows an assessment to be made as to whether observed hydrogeologic conditions are represented adequately in the simulation study. In addition, the flow and transport results of the models constructed can be calibrated on the basis of observed field data." (Huyakorn et al., 1984)
4.4.1. Areal Simulation of Water Flow and Chloride Transport.

This testing scenario involves using FLOTTRAN to simulate the ground water flow and contaminant transport at a section of the Canadian Forces Base Borden Landfill site. Two previous simulations of this site have been performed. The first simulation was by Sykes (1982), and the second was by Huyakorn et al. (1984), as a testing scenario for SEFTRAN. A detailed site history and description is available in Huyakorn et al. (1984).

In brief, there is a landfill at the CFB Borden, from which contaminants had been leaching for up to 36 years at the time of the study in 1976. Under the landfill is an unconfined sandy aquifer which ranges in thickness from about 75 ft near the landfill, to about 20 ft approximately 1/2 mile downgradient of the landfill. The sandy aquifer is bounded on the bottom by a silty clay aquitard. From water level elevation data, it has been determined by Sykes (1982) that a flow line passes through the landfill. This line, called A–A', was taken to be one of the boundaries of the study area, and is treated as a no flow boundary in the modeling. Figure 4.23 shows the layout of the model grid, with the aforementioned no flow boundary at the top of the model area. The study area was divided into $16 \times 9 \times 5$ rectangular blocks for the modeling effort. Since the thickness of the aquifer is variable, the blocks below the aquifer are set to a low conductivity to simulate an impermeable area. The variation in thickness used in the modeling is shown in Figure 4.23. The heavy lines separate areas of different thickness.

The landfill is simulated as a contaminant source leaching chloride to the aquifer. It is assumed to be leaching at a constant water flux and constant chloride concentration. Values of these and other parameters used by Sykes (1982) are given in Table 4.7, while the grid spacings are given in Table 4.8.
Figure 4.23: Model grid for Borden Landfill and surrounding area. The landfill is bounded by the dashed line. Ground water flow is generally from left to right.
Table 4.7: Parameters used in the analysis of ground water flow and chloride transport at the Borden Landfill. (From Huyakorn et al., 1984).

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Horizontal hydraulic conductivity, $K_{xx}$</td>
<td>6.22 m/d</td>
</tr>
<tr>
<td>Horizontal hydraulic conductivity, $K_{yy}$</td>
<td>6.22 m/d</td>
</tr>
<tr>
<td>Vertical hydraulic conductivity, $K_{zz}$</td>
<td>3.11 m/d</td>
</tr>
<tr>
<td>Infiltration rate on landfill area, $I^*$</td>
<td>0.366 m/yr</td>
</tr>
<tr>
<td>(Chloride contaminated water)</td>
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<td>Infiltration rate on remaining ground surface, $I$</td>
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<td>Longitudinal dispersivity, $\alpha_L$</td>
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<tr>
<td>Transverse dispersivity, $\alpha_T$</td>
<td>0.25, 1.0, and 5.0 ft</td>
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<tr>
<td>Leachate chloride concentration, $C_{O}$</td>
<td>400.0 mg/L</td>
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Table 4.8: Spacing used for the Borden Landfill simulation. (From Huyakorn et al., 1984).

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Figure 4.24 shows the water levels measured June, 1979, and the water levels predicted by Sykes (1982) using a code described in Intercomp (1976). The upper boundary of the area shown in Figure 4.24 is A-A', the no-flow boundary. Figure 4.25 shows the water levels predicted by FLOTRAN for June, 1979. Constant head boundary
Figure 4.24: Measured versus simulated water levels for June, 1979 (meters above MSL). Adapted from Sykes *et al.*, 1982.
Figure 4.25: Water surface elevations at the Borden Landfill for June, 1979 predicted by FLOTRAN.
conditions for FLOTRAN were chosen to match the water levels shown in Figure 4.24. Inspection of Figures 4.24 and 4.25 shows good agreement between the water level calculations done by Sykes and with FLOTRAN. The simulation assumes that the flow conditions are at steady state at June, 1979 conditions.

Once the flow had been modeled, the solute transport could be considered. Three cases were simulated, because of the variability in the dispersivity at the site. They correspond to the following values of longitudinal and transverse dispersivity

Case I: \( \alpha_L = 25 \text{ ft}, \quad \alpha_T = 0.25 \text{ ft} \),
Case II: \( \alpha_L = 25 \text{ ft}, \quad \alpha_T = 1.0 \text{ ft} \),
Case III: \( \alpha_L = 25 \text{ ft}, \quad \alpha_T = 5.0 \text{ ft} \).

Figure 4.26 shows the measured chloride concentrations along the line A–A’ in August, 1978. The chloride concentrations show a bimodal distribution, implying that the source varied with time. The chloride sinks toward the bottom of the aquifer, but does not penetrate the silty clay aquitard below the aquifer. No similar plots of measured data are available for a plan view. Figures 4.27 and 4.28 show the simulated chloride concentrations after a 36 year simulation for case I. These figures show the concentration contours along several cross sections of the model area, and the effects of transverse and vertical dispersion on the contaminant plume. Figure 4.27 shows vertical slices along A–A’ (a), and parallel to A–A’ (b–e), while Figure 4.28 shows plan views near the water surface (a), and at depths of 15, 25, 37.5, and 60 feet (b–e). Near the landfill and directly downstream of it, chloride concentrations vary from 300 mg/L down to 10 mg/L, while in the vertical slice 250 ft away from the edge of the landfill (Figure 4.27d), the concentration never reaches 150 mg/L, and 37.5 feet below ground surface (Figure 4.28d), the concentration also never reaches 150 mg/L.

The dashed lines in Figures 4.27ff represent the edge of the low conductivity area used to force a variable thickness aquifer. In the vertical slices, the area below the dashed lines is low conductivity, while in the plan views the area to the right of the dashed line is
Figure 4.26: Measured Chloride Concentrations at the Borden Landfill in August, 1978.
Vertical concentration profiles. The dashed line represents the bottom of the model aquifer for that cross section.

Longitudinal Dispersivity = 0.25 ft.

Figure 4.27: Case I, vertical slice views of simulated concentration contours after 36 years.
Concentration contours (mg/l). The area to the right of the dashed line is not part of the model aquifer.

Longitudinal Dispersivity = 0.25 ft.

Figure 4.28: Case I, plan views of simulated concentration contours after 36 years.
low conductivity. The contaminant spreads downward and transversely away from the landfill as it flows downstream, and is seemingly unaffected by the presence of a low permeability area. This will be discussed more below.

Figure 4.29 presents vertical slice views at A-A’ for cases I, II and III from (a) the FLOTRAN simulation and (b) the simulation by Sykes (1982). The vertical dispersion is much more variable in the FLOTRAN simulation than in the Sykes simulation. Unfortunately, Sykes does not specifically state the vertical dispersivity values used in the simulation. Since this is the case, it is assumed that the vertical dispersivities were the same as the transverse dispersivities. This assumption may be the cause of the sensitivity to vertical dispersivity.

Figure 4.30 shows plan views near the water surface for cases I, II, and III from (a) the FLOTRAN simulation, and (b) the simulation by Sykes. From Figure 4.30a, one can see that increasing the transverse dispersivity causes an increase in the horizontal spread of the contaminant and a decrease in the maximum concentration from $362 \, \text{mg/L}$ in Case I, to $294 \, \text{mg/L}$ in Case II, to $215 \, \text{mg/L}$ in Case III in the FLOTRAN run. Figure 4.30b shows similar maximum concentrations of just over $200 \, \text{mg/L}$ for all three cases as predicted by Sykes. The lower transverse dispersivity reduces the spread of the contaminant by an appreciable amount in the FLOTRAN runs, while it hardly affects the simulation (in comparison) on the code Sykes used.

One will notice that the contaminant disperses into the low conductivity area in each of the FLOTRAN simulations (Figures 4.27a-e and 4.29a). This is because of the averaging scheme used by the numerical model. As can be seen in Figure 4.29b, the Intercomp code that Sykes used has similar qualities. The contaminant will disperse into the first, and possibly second layer past the ‘edge’ of the aquifer. In this case, there are only one or two grid blocks which are ‘outside’ the aquifer, so this spreading is very severe. The only way to reduce this effect is to increase the number of grid blocks such that there are ‘buffer’ areas. To test this, a simulation was set up using a $32 \times 18 \times 10$
(a) Vertical slice view of chloride concentrations after 36 years of simulation by FLOTRAN.

(b) Vertical slice view of chloride concentration after 36 years as simulated by Sykes.  
(Adapted from Sykes, 1982)

Figure 4.29: Vertical slice concentration profiles for Problem III.2. Vertical scale is exaggerated.
(a) Plan view of chloride concentrations after 36 years of simulation by FLOTRAN.

(b) Plan view of chloride concentrations simulated by Sykes. (Adapted from Sykes, 1982).

Figure 4.30: Plan views of chloride concentrations calculated for Problem III.2.
grid. All the input files were appropriately modified and the simulation was run. Figure 4.31 shows the resulting set of vertical slices corresponding to Case I, as shown in Figure 4.27. The contamination concentrations simulated in this run follow the aquifer boundaries more closely than those in the $16 \times 9 \times 5$ simulation. The overlap into low permeability areas still exists, and cannot be avoided with this numerical method, but increasing the number of grid blocks in the low permeability area reduces the simulated ‘dispersion’ of contaminant into a low conductivity area, such as clay or bedrock.

Because of the difficulties that arise when a variable thickness aquifer is simulated with the brick method used here, the author of FLOTRAN decided to implement a general geometry code which allows the user to vary the shapes of the individual model elements. In order to test that feature, it will be applied to the Borden Landfill case here, for Case I, $\alpha_T = 0.25$ ft.

First, an interpolated map of aquifer thicknesses was created from available data. These thicknesses then divided into five equal parts; each layer is the same thickness at a given x-y location. The layer thicknesses vary from about 15 ft near the landfill to about 4 ft near point A’. These were the only changes necessary to implement this feature of the code.

The resulting contaminant plume is shown in Figure 4.32. The area shown in this figure is 10% larger than the model grid due to the software used to contour the concentrations.

Figure 4.32a shows a plan view of the concentrations near the water table. The concentrations in the leading edge are higher in this simulation than in either of the other simulations. This is in large part because the entire mass of contaminant is now confined to the aquifer. No contaminant mass is allowed to get out of the aquifer bottom into the ‘clay’ where it travels very slowly, because the aquifer bottom is now modeled as a strict no-flow boundary.
Vertical concentration profiles. The dashed line represents the bottom of the model aquifer for that cross section.

**Longitudinal Dispersivity** = 0.25 ft.

Figure 4.31: Case I, vertical slice views of simulated concentration contours after 36 years. This simulation was performed on a 32 x 18 x 10 grid.
(a) Plan view of contaminant concentrations near the water table.

(b) Vertical slice view of contaminants along A-A'.

Figure 4.32: Borden Landfill simulation results using the general geometry modification to model variable aquifer thickness.
Figure 4.32b shows a vertical slice along A–A'. Comparison of this figure with Figure 4.26 shows that the maximum depth of contaminant is similar to the observed depths (about 30 feet), and that the modeled contaminant concentrations downstream of the landfill are higher than observed.

4.5. Summary of Testing Results.

Four types of testing were performed on FLOTRAN, qualitative testing, testing in radially dominated flow regimes, quantitative testing against analytical solutions, and testing against another code at a 'field' site.

Three qualitative simulations were performed. In the first, FLOTRAN seems to work well when the grid is oriented along the direction of flow. When the grid is at an angle to the direction of flow, a large amount of numerical dispersion is introduced into the solution. In the second, the retardation which is caused by sorption works as one would expect, slowing the advection and dispersion processes. In the third, biodegradation is compared with BIOPLUME II. FLOTRAN seems to produce more dispersion than BIOPLUME II, however the contaminant plumes and oxygen depleted areas are of a similar size and shape. In addition, FLOTRAN outperforms BIOPLUME II in mass balance.

Two simulations were performed in radially dominated flow regimes. The first, recharge/recovery from a single well shows that FLOTRAN performs well except in the no dispersion case. In this case, the difficulty seems to be related to the numerical dispersion seen in the diagonal dispersion test. The second of these tests, a recharge/recovery pair showed very good results. The observed concentrations in the recovery well were lower than those predicted by the semi-analytical solution, but the two breakthrough curves were almost identically shaped.

Four situations with analytical solutions were simulated. In the first, one dimensional flow with a constant concentration source, FLOTRAN performed
exceptionally well, matching the analytical solution almost exactly. In the second, two
dimensional dispersion from a continuous point source in a uniform flow field, FLOTRAN
performed well when the mesh size was fine enough. Poor performance with coarser
 grids is not unexpected. In the third of these tests, two dimensional dispersion from a
slug source in a uniform flow field, FLOTRAN also performed well, matching the
analytical solution nicely. The last of these tests was transport in the radial flow field
around an injection well. FLOTRAN's performance in this simulation is not as good as in
the other simulations, especially in the low dispersivity case. This case also shows the
need for care when simulating a well at the corner of a model grid.

Two additional simulations were performed with flow at a 45 degree angle to the
grid orientation. The first of these, one-dimensional flow from a constant concentration
boundary, showed that flow at a 45 degree angle creates numerical dispersion on the
order of 1/10 the grid size in the direction of flow. The second, transport around an
injection well in a uniform two dimensional flow field, shows that flow at an angle adds a
similar amount of numerical dispersion transverse to the direction of flow.

The final test was a three dimensional simulation of chloride contamination at the
Canadian Forces Base Borden landfill. FLOTRAN performed well in this test, with final
chloride concentrations very similar to those simulated by another program, and matching
fairly well with observed data. One interesting observation about three dimensional
groundwater modeling is the fact that these models will show large concentrations in low
permeability areas where the ground water should not penetrate. This is due to the fact
that modeling dispersion is generally by some sort of averaging among cells. In order to
reduce the effects of dispersion into low permeability areas, one must have a 'buffer' area
around the low permeability area. This buffer area cannot, however, be a very thin model
layer, because that would reduce the time step size dramatically (see Equation 3.6 for
details). Modeling the Borden Landfill with a variable thickness grid using the general
geometry modification allows the user to avoid the problems of mass leaving the system
through the lower 'boundary' of the aquifer. The resulting plume has a similar shape, but since the mass cannot 'escape' through the bottom of the aquifer, the downgradient concentrations are higher.
Chapter 5. Modeling a TCE Plume in Arizona.

5.1. Background and Objectives for Current Modeling.

As a final test, FLOTRAN is used to model TCE contamination at a site in Arizona. In late 1981, Phoenix, Arizona officials found (TCE) in two of the city water supply wells (ADWR, 1990). Following this discovery further sampling was performed, and due to high levels of contamination, the area was placed on the National Priorities List by the United States Environmental Protection Agency (EPA) in 1984. It is known as the North Indian Bend Wash (NIBW) Superfund site. As a part of the Remedial Investigation / Feasibility Study (RI/FS), the Arizona Department of Water Resources (ADWR) modeled the flow conditions at the site using MODFLOW. Contaminant transport was also modeled in order to evaluate several remediation scenarios.

The current effort in this research is to model contaminant transport at the site with an emphasis on determining the conditions in the subsurface during the time period from 1957 to 1981. To accomplish this, a new model is formulated in two different steps. Flow conditions are modeled with MODFLOW for the time period from 1957 to 1978. The results from the flow simulation are used to create flow fields in FLOTRAN which are then used in the contaminant transport modeling. The main objectives of the new flow and contaminant transport modeling are: (1) to provide a complex field test of FLOTRAN and (2) to determine where the contamination in the water supply wells could have originated.

Both of the simulations incorporate the geophysical data used in the ADWR MODFLOW simulation. The area modeled is 66 square miles (see Figure 5.1). The flow simulation requires pumpage data from 1957 to 1978, as well as an estimation of the boundary conditions and recharge. The contaminant transport is performed on an area approximately 1/3 of the area modeled by the ADWR. This area is chosen to include all
Figure 5.1: North Indian Bend Wash model area. The entire area is modeled in the ADWR MODFLOW model, and the contaminant transport model area is also shown. The mountains and buttes shown are modeled as impermeable areas.
the contaminated wells in the area. The ADWR MODFLOW model simulates ground water flow in the North Indian Bend Wash region, surrounding the contaminated aquifers. Figure 5.1 shows the ADWR model area, the FLOTRAN model area, and the NIBW Superfund site. The FLOTRAN model area is chosen to allow modeling on a finer grid, and includes all the contamination in the area. Since the contaminant transport uses a different grid arrangement, the geophysical data is interpolated to the new grid for contaminant modeling.

In order to best utilize the available data and previous modeling efforts, the framework of the ADWR MODFLOW model is utilized. It is necessary to change out the pumpage, recharge, and boundary conditions to create as accurate an estimate of water levels as is possible. This estimate of water levels is then used as a basis for modeling the transport of contaminants using FLOTRAN.

5.2. Previous Modeling Efforts.

Following the discovery of TCE in city water wells, sampling was performed on area water wells to confirm the existence of ground water contamination, and to determine its extent. (City of Phoenix [COP], 1984) In 1984, the EPA placed the area on the National Priorities List and initiated the North Indian Bend Wash RI/FS, which was designed to define ground water flow patterns, determine the vertical and lateral extent of contamination, estimate the volume of ground water impacted, determine potential sources of contamination, and obtain data with which to complete the Feasibility Study.

The ADWR developed a ground water flow and contaminant transport simulation in 1988 to suggest possibilities for remediation at the site. Ground water flow was modeled using MODFLOW. Contaminant transport modeling performed was solely intended to evaluate possible remediation scenarios and will not be discussed here. The original ADWR flow model was calibrated for the time period between January, 1983
and April, 1988. The simulated water levels provided a close match to measured water levels (ADWR, 1990).

The ADWR studies of the system to date have been aimed at characterization of the contamination as it was at the time of the study, and preparation for eventual remediation of the contaminated aquifers. This study attempts to simulate the initial contamination of the aquifers and determine the source of the TCE which was detected in the city water supply wells, an important issue not addressed by the ADWR models.

5.2.1. Hydrogeological Background.

The Indian Bend Wash area is underlain by three alluvial aquifers, hereafter called the Upper Alluvium Unit (UAU), Middle Alluvium Unit (MAU), and Lower Alluvium Unit (LAU). The LAU is actually underlain by a fourth unit called the Red Unit, but these units are combined here and in the ADWR modeling. The three units are underlain by a bedrock which slopes steeply downward from buttes to the west (ADWR, 1990). The LAU was modeled as if its lowest elevation was 900 ft below mean sea level (~900 ft MSL). Figure 5.2 shows several cross sections of the elevations of the bottoms of the three alluvium units. The cross sections can be located by the corresponding letters on Figure 5.1. This complex three dimensional system presents a challenge for the application of MODFLOW and FLOTAN.
Figure 5.2: Ground surface elevation, elevations of bottoms of LAU, MAU and UAU (from ADWR MODFLOW model).
5.2.2. Upper Alluvium Unit.

The UAU is the youngest alluvial deposit in the IBW area. It ranges in thickness from 100 to 250 feet in the area of concern. Heavy ground water pumpage has dewatered the UAU in the area to the north and west of the NIBW Superfund area. Where the UAU is not dewatered, it is an unconfined aquifer. The ADWR (1990) used the following reported hydraulic properties for the UAU in their MODFLOW model:

- Specific yield: 0.2,
- Porosity: 0.3,
- Hydraulic conductivity: 234 ft/day,
- Vertical Hydraulic Conductivity: 0.13 ft/day.

5.2.3. Middle Alluvium Unit.

This unit underlies the UAU in most of the study area. It is a confined aquifer which ranges in thickness from 100 to 900 ft. The ADWR (1990) determined the following aquifer properties for use in their MODFLOW model of the site:

- Average Storage Coefficient: $5 \times 10^{-4}$,
- Specific Storage: $6 \times 10^{-5}$ /ft (volume of water released / ft of aquifer medium / ft change in head)
- Average Specific Yield: 0.05,

The average porosity was estimated to be about 0.40. Due to the fact that the pores in sediments may be nonconnected, or dead end, and fluids flowing through the sediment may not pass through all of the pore space, an effective porosity of 0.10 was used in the model. The effective porosity of unconsolidated sediments is generally considered to be more closely approximated by the specific yield than the total porosity, therefore a value of 0.10 was chosen by the ADWR (1990) as being a reasonable value for the model. (Todd, 1964) The ADWR (1990) also performed pump tests and
calculated values for hydraulic conductivities. The conductivities calculated are spatially varying, ranging from 5 ft/day to 23 ft/day, typical of a good sand aquifer. Calculated vertical hydraulic conductivities range from 0.002 ft/day to 0.035 ft/day.

5.2.4. Lower Alluvium Unit.

The LAU underlies the MAU and UAU, and ranges in thickness from about 100 to over 1400 feet. The bottom of the modeled LAU is in contact with bedrock. In some areas, a minimum of −900 ft MSL was chosen (see Figure 5.2) because no wells are completed below that depth in the study area. Very little field data existed for the LAU when the ADWR model was being developed, so most of the hydrogeologic parameters are estimated or assumed. The storage coefficient, specific storage, specific yield and porosity are given the same values as in the MAU. In the model, the hydraulic conductivity is input as an array of values ranging from 3.3 ft/day to 23.0 ft/day, and vertical conductivity is assumed to be the same as that of the MAU.

According to the ADWR MODFLOW inputs, the bedrock under the LAU slopes at a grade which reaches as high as 0.43 ft/ft, and averages 0.11 ft/ft, not including the area which is artificially flat at −900 ft MSL. The high slopes of the bedrock under the NIBW Superfund site add to the difficulties surrounding the spill of a dense, non-aqueous phase liquid (DNAPL), such as TCE. Non aqueous phase liquids (NAPLS) are generally hydrocarbons which do not readily dissolve in water. As such, large volumes of free phase NAPLS will often remain in the subsurface after a spill. DNAPLS by definition are denser than water and will sink to the lowest possible point in an aquifer. Bedient et al. (1994) note that TCE is often present at waste sites in a DNAPL form due to its density effects and other chemical properties. If a DNAPL were to reach the bedrock, it would flow down the slope, contaminating an ever larger area of the aquifer. (Fetter, 1993) In this case, the slope of the bedrock is perpendicular to the direction of ground water flow, so the DNAPL would flow downhill, not downstream, and could create a large zone of
contamination. For a more detailed discussion of NAPLs, see Chapter 11 of Bedient et al. (1994).

5.2.5. Time Discretization.

The ADWR model simulates the time from January, 1983 to April, 1988. The time is divided up into eleven stress periods, each of which is run for two time steps. The first stress period is four months long, from January, 1983 to April, 1983, and each of the others is 6 months long, either from May to October of one year, or from November of one year to April of the next.

5.2.6. Water Budget — Recharge and Pumpage.

An extensive survey of ground water inflow and outflow components was performed by the ADWR for this modeling project (ADWR, 1990). Recharge to the aquifer system was considered by all of the following pathways: stream channels; agriculture; business and industrial zones; mountain fronts, natural desert, and bare earth construction areas; irrigated residential, desert, residential apartments, and trailers; green areas; ponds; and canals and laterals. The model grid was split up into these categories and each grid block was assigned a recharge based on data about its category(ies).

Based on the above criteria, the estimated recharge over most of the model area is approximately 1 ft/year, except at and around the Salt River. Figure 5.3a shows the applied recharge for the first time step of the ADWR model (1983). In order to have some color variation in the 0 - 3 ft/year range, only 0 - 25 ft/year contours are shown. Inside the Salt River, the maximum recharge is 117 ft/year, with most areas in the center of the river having approximately 100 ft/year of recharge. The majority of the model area (aside from the Salt River) has constant recharge values in the range of 0 - 3 ft/year.

The recharge values for the other time steps are the same as for time step 1 except for in the area under the Salt River, which is high (> 100 ft/yr) for three time periods in
Figure 5.3: Recharge in the ADWR MODFLOW model, (a) for early 1983 and (b) average recharge over the entire simulation (1983 - 1988). The recharge shown in red is 25 ft/year, since a larger range would make the lower level (0 - 3 ft/year) color variations too slight to be useful. Therefore, the recharge in (a) which is greater than 25 ft/year is not shown.
which the Salt River flowed, and low (< 15 ft/yr) for all other time periods. Figure 5.3b shows the recharge averaged over all 11 time steps.

In addition to recharge, the ADWR researched total water withdrawals from extraction wells in the NIBW area. There are many water supply wells in the NIBW area, pumping water for a variety of uses, including domestic, industrial, and agricultural. Over the years, this pumpage has greatly affected the water levels and the direction of ground water flow in the area. As such, the proper determination of pumpages is important to correctly simulate water surface elevations.

5.2.7. ADWR MODFLOW Model Grid.

The site was modeled with a variable 17 × 31 × 3 grid with spacings of 1/4, 1/2, and 1 mile. The modeled area is 6 miles in the east-west direction (x) and 11 miles in the north-south direction (y). A plan view of the grid and model area is shown in Figure 5.4. The area outlined by the double line is the area for which contaminant transport modeling has been done. The areas to the left of the grid where there are no grid lines are actually inactive cells in the MODFLOW simulation. These inactive cells represent Mummy Mountain, Camelback Mountain, the Papago Buttes and Tempe Butte (North to South), areas in which the bedrock breaks the ground surface. These mountains and buttes are shown on Figure 5.1. The bold area represents the UAU, which has been totally dewatered to the north and west due to heavy pumpage. The three alluvium units vary in thickness from about 100 to more than 1400 feet, as depicted in Figure 5.2.

5.2.8. Contamination at the NIBW Site.

Figure 5.5a-c shows the 1989 TCE concentrations used in the ADWR contaminant transport modeling for the UAU, MAU, and LAU. The area shown is the 4 × 5 mile contaminant transport model area shown in Figure 5.1. The concentrations for
Figure 5.4: 17 x 31 grid used in MODFLOW simulation. All the constant head boundaries are applied in the top layer (UAU). The wells are those applied to the 1957 - 1978 time period.
Figure 5.5: Representative interpolated TCE concentration for 1989 in model cell, (µg/L), for indicated alluvial unit. * = COS 71, 0 = COS 72 (water supply wells). (Adapted from ADWR, 1990.)

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Upper Alluvial Unit

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Middle Alluvial Unit

Figure 5.5b
Figure 5.5c

Figure 5.5 continued: Representative interpolated TCE concentration for 1989 in model cell, (µg/L), for indicated alluvial unit. * = COS 71, ◊ = COS 72 (water supply wells). (Adapted from ADWR, 1990.)
1989 were used to determine the efficacy of the remediation schemes proposed by the ADWR.

The city water wells in which TCE was first detected are indicated on this map. They are both located just south of Thomas Rd., and west of Hayden Rd. These wells are known as COS 71 and COS 72, and were owned by the City of Phoenix in 1981 and later sold to the City of Scottsdale (COS). The highest concentrations of TCE in the vicinities of COS 71 and COS 72 are in the MAU.

5.3. Modeling of Flow from 1957 to 1978 — MODFLOW.

Most of the basic hydrogeologic data from the original MODFLOW simulation was kept intact, including the aquifer top and bottom elevations, vertical leakance values, hydraulic conductivities, and porosity. This leaves pumpages, recharge, initial heads, and boundary conditions to be determined for the model of the years 1957 to 1978.

5.3.1. Determination of Pumpages.

The Arizona Department of Water Resources provided a printout of yearly total pumpages from many wells for the period of interest. (ADWR, unpublished data) This information is combined with pumpage data from three maps which show total pumpage over the years 1957 - 1966, 1967 - 1977 and 1978 - 1985. Based on the data available, the area was modeled in multiple year time steps, averaging the pumpage data over each time period. The time steps are as follows: 1957 - 1960; 1961 - 1965; 1966 - 1970; 1971 - 1975; 1976 - 1978. Since the pumpages are being averaged over multi-year intervals, the resulting water surfaces will also be ‘average’ water surfaces. The calculated water surfaces provide for an estimate of average ground water flow in the model area.

Many of the wells are screened over more than one alluvial unit, which complicated the task of assigning pumpages to model layers. Assigning pumpages to different alluvium units was accomplished by using the following system. First priority
was given to the ratio of pumpages given in the ADWR MODFLOW model, if there was a pumping well in that grid block. Second priority was given to finding well screening data and estimating the elevation of the aquifer boundary, if this was available. Last, if there was no data on which to base a decision, the pumpage was assumed to be evenly divided between the aquifers it penetrated. Some data was usually available to determine an approximate depth for the well, and thus to determine which aquifers that the well penetrated. Pumpages in the MODFLOW simulation area are detailed in Table 5.1.

Inspection of Table 5.1 shows a large variation in flow rates from the wells in the model area. In the following section, 'plan view cell' refers to all model grid blocks that are at the same x-y location, a 'well block' refers to simulating pumping from a single grid block in a single layer, and a 'well' refers to all well blocks in a single plan view cell. In Table 5.1, wells which are in the same plan view cell are listed next to each other, with the MODFLOW cell listed as the same for both wells. These values are for total pumpage from a well and are not split up into the pumpages from the UAU, MAU, and LAU. There are 121 wells shown in Table 5.1. Several of these wells are located in the same plan view cell, so that there are 88 different plan view cells represented (See Figure 5.4), and 153 different well blocks. Many of the wells are screened over more than one aquifer, and must therefore be modeled as more than one well.

5.3.2. Determination of an Average Recharge.

As shown in Figure 5.3a, recharge in the NIBW area is highly variable. Since the recharge may vary by over two orders of magnitude, its effects must be considered in the overall model. There is no specific recharge data available for the time span being studied, so the recharge used is an average of the recharge for the 5 year period modeled by the ADWR (1990). As stated above, the majority of the recharge values are estimated from land use data, and are assumed to be constant from year to year. The only area with
Table 5.1: Pumpages used in MODFLOW and FLOTRAN simulations.

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Table 5.1: Pumpages used in MODFLOW and FLOTRAN simulations.

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Table 5.1: Pumpages used in MODFLOW and FLOTRAN simulations.

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* Removed from simulation due to edge effects.
varying recharge is the Salt River. Since the Salt River does not flow every year, an average of the recharge values from all eleven stress periods of the ADWR model is used. The ADWR model includes two stress periods with rainfall which produced a large amount of infiltration from the Salt River, in the southern portion of the model area, as well as several stress periods with little or no infiltration from the Salt River. The average recharge used in the 1957 - 1978 model is depicted in Figure 5.3c. Comparison of Figure 5.3c with Figure 5.3a shows that in the area away from the Salt River, the recharge is exactly the same for the 'averaged' values and for the individual time steps.

5.3.3. Determination of Boundary Conditions and Initial Heads.

Boundary conditions can greatly affect the results of a ground water simulation. A Dirichlet type (constant head) boundary represents an area of horizontal recharge to the aquifer from an upgradient source, or possibly from a lake or river, while a Neumann type (no-flow) boundary condition represents an impermeable boundary. Neumann boundaries can represent either a boundary with an impermeable barrier, such as bedrock, or a streamline, since there is no flow across a streamline.

The boundary conditions are for the most part retained from the ADWR model (1990). Specifically, the UAU is modeled with a constant head boundary along the southern portion of the east boundary and in the southwest corner. (See Figure 5.4) The former of these is one of the major sources of water in the ADRW model, while the latter is a sink. These boundary conditions include the assumption that the UAU is dewatered on the north and west portions. The bold line on Figure 5.4 shows the boundary of the UAU. The dewatered portions of the UAU to the northwest are modeled as impermeable cells. The MAU and LAU are both modeled with impermeable boundaries along all sides. A major complicating factor in the boundaries is the presence of three buttes/mountains along the western boundary of the model area. These are areas where the bedrock breaks through to the land surface. Of course, there are no aquifers in this
area, and they are modeled as impermeable boundaries in all three layers. In Figure 5.2, these areas appear as aquifer boundaries that are off of the scale above the rest of the model boundaries.

The ADWR (1990) developed a map (Figure 5.6) showing an estimate of historical water levels (before pumpage had dewatered the northwest portion of the model area) from historical sources. This map indicates that the ground water was generally flowing from the north - northeast toward the southwest corner of the model area. In the absence of recharge and pumpage, these heads were reproduced on the ADWR MODFLOW grid. The boundary conditions for this simulation are essentially constant head around all four edges of the model. On the west edge, the presence of the buttes complicates the boundaries, so that the constant head cells are not all along the edge of the grid. The results are shown in Figure 5.7. All three alluvium units are shown in Figure 5.7, for comparison. The water levels in the three alluvium units are very close (never more than 5 ft. apart). These water levels are taken to be the initial heads for the ensuing MODFLOW simulations. Some error is introduced here, because there was pumpage prior to 1957 which is not simulated.

5.4. Results of MODFLOW Simulations.

Figures 5.8a-c show the calculated water levels in each aquifer in 1970. The UAU flows mostly from east to west, becoming dewatered in the northwest portions of the model area. The MAU flows from the outside toward the center, where the majority of the pumping wells are located. The LAU flows mostly toward the center also. The basic pattern of flows is similar to that modeled by the ADWR (1990), Figure 5.9a-c.

All five stress periods show similar behavior, with cones of depression around active pumping wells. The ground water isoelevation contours shown are on 5 ft. intervals, with every fifth contour in bold. Labels for selected contours are indicated. The water levels in the simulation gradually decrease in time, showing that there is more
Figure 5.6: 1900 water surface elevations in the Indian Bend Wash area. Adapted from ADWR (1990).
Figure 5.7: Estimated water levels in 1900 -- MODFLOW simulation. All three aquifers are shown on this figure. Contours are at five foot intervals, and bold contours are at even 25 foot intervals.
Figure 5.8: NIBW water levels in 1970 in the UAU, MAU, and LAU, as calculated by MODFLOW. Contours are at 5 ft. intervals, and bold contours are on even 25 ft. intervals. The highest and lowest bold contours are labeled.
Figure 5.9: NIBW water levels in late 1984 in the UAU, MAU, and LAU, as calculated by MODFLOW. Contours are at 5 ft. intervals, and bold contours are on even 25 ft. intervals. The highest and lowest bold contours are labeled.
outflow than inflow in the system, however the decrease is slow. This decrease in water levels is consistent with the observation that the northwest portion of the UAU has been dewatered by the beginning of the ADWR study (1983). Table 5.2 shows the minimum and maximum water levels in the NIBW study area for the MODFLOW simulation from 1900 to 1978. Table 5.2: Minimum and Maximum Water Levels for the NIBW MODFLOW simulation.

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5.5. FLOTRAN Simulation of a Portion of the NIBW Area.

FLOTRAN was used to model a 4 × 5 mile rectangle including the NIBW Superfund site. Figure 5.1 shows the area to be used for the FLOTRAN model in comparison to the MODFLOW model area and the boundaries of the NIBW Superfund site. The 4 × 5 mile rectangle is discretized into a 32 × 40 × 1 grid, as discussed in the following section.

5.5.1. Choice of Model Domain for FLOTRAN Modeling.

As stated in § 5.2.7, initial data suggests that two wells, COS 71 and COS 72, were pumping mostly from the MAU and that most of the contamination is in the MAU. Therefore, to simplify the FLOTRAN modeling, ground water flow and contaminant transport are considered in the MAU only. The 4 × 5 mile tract was chosen because it encompasses all of the major suspected source areas, and to provide for a smaller mesh than the minimum 1/4 × 1/4 mile mesh used in the MODFLOW simulation. For this
simulation, a slightly non-uniform grid was used. (The grid is essentially uniform $1/8 \times 1/8$ mile squares, except for the boundary cells, which are $1/16 \times 1/8$ mile squares. These cells are shown as regularly sized cells in Figure 5.10. This was done so that in case a comparison with BIOPLUME II was desired, it could be achieved with as little alteration of input files as possible. See § 4.1.3.1 for details.) Figure 5.10 shows the $32 \times 40 \times 1$ grid used for the application of FLOTRAN to this site, probable source areas, and the locations of area water supply wells. Values for the variable aquifer thickness are determined by interpolation from the ADWR MODFLOW model.

5.5.2. Sources of TCE Contamination.

Figure 5.11 shows the suspected sources in the NIBW Superfund area. The bold line is the boundary of the NIBW Superfund site. The six suspected source areas are industrial sites with known or suspected use of trichloroethylene between the 1950s and 1980s.

Based on Figure 5.5 and other source information, Source Area 1 and Source Area 2 were assumed to be the only sources of contamination in the MAU. These two TCE contamination sources were simulated as wells injecting contaminated water at a rate of 0.2 cfs per site. The injected water was assumed to be contaminated at 1% of the solubility of TCE in water, or 11,000 µg/L (parts per billion). This equates to a mass loading of 1964 kg TCE / yr / source area. The CRC Handbook of Chemistry and Physics (1986) quotes a value of 1.46 kg/L as the density of TCE. Using this value, the contamination simulated is equivalent to the release of about 1346 liters of pure TCE per year at each source, all of which gets dissolved in the ground water.

Source information indicates that the industry at Source Area 1 began operation in 1961, while the industry at Source Area 2 began operation in 1957. It is assumed that groundwater contamination begins in the initial year of operation at each plant, and continues at a constant rate throughout the model time period. Source Area 1 is about the
Source Area 1
Source Area 2
Source Area 2 Injection Wells
Area of Recharge From UAU to MAU
Location of COS 71
Location of COS 72
Location of Extraction Well
Figure 5.11: Boundaries and possible sources in the NIBW Superfund site. The heavy line is the boundary of the NIBW Superfund Site.
size of one grid cell, so it is simulated as an injection well at that cell. (See Figure 5.10) Based on a site map (Figure 5.12), it is assumed that the contamination at Source Area 2 is spread out over the rectangle shown in Figure 5.10. Each of the four cells included in the rectangle which is simulated as Source Area 2 is given a flow rate of 0.05 cfs, for a total of 0.2 cfs for the source.

5.5.3. Aquifer characteristics.

All aquifer characteristics were interpolated from values used in the ADWR MODFLOW simulation using a function in MATLAB by The MathWorks. The ADWR simulation included values for the elevation of the top of the MAU, the elevation of the bottom of the MAU and the hydraulic conductivity of the MAU for each point on the 31 × 17 × 3 MODFLOW grid. These values were interpolated to the 32 × 40 × 1 grid used in the FLOTRAN simulation. Other aquifer parameters used were a constant porosity of 0.1 and dispersivities of 100 ft (longitudinal) and 10 ft (transverse) (ADWR, 1990).

The accuracy of the variable thickness modification to FLOTRAN was tested here by observing the difference between the flow fields calculated with a constant thickness of 400 ft for the MAU and variable thicknesses interpolated from the ADWR simulation. The effects of variable thicknesses were observed by looking at the cones of depression around wells in areas where the constant thickness was greater than, approximately equal to, and less than the variable thickness. As expected, the depths of the cones of depression were inversely proportional to aquifer thickness.
Figure 5.12: Plan view of Source Area 2, showing possible entry points for TCE contamination of the subsurface.
5.5.4. Pumpage.

Pumpage data is gleaned from the same sources as are used for the MODFLOW simulation, and are also averaged over the same time periods, 1957-1960; 1961 to 1965; 1966 to 1970; 1971 to 1975; and 1976 to 1978. Total pumpages for wells are given in Table 5.1. A portion of this pumpage was applied to the MAU only for those wells which penetrate the MAU.

5.5.5. Boundary Conditions.

Boundary conditions for the FLOTRAN simulation were taken from the appropriate MODFLOW time periods. Constant head boundary conditions were applied on all four sides, with the heads interpolated from the values calculated by MODFLOW.

The presence of buttes and mountains along the western edge of the MODFLOW model area causes some problems in converting from MODFLOW to FLOTRAN grids. A small area of the FLOTRAN grid in the southwest corner is impinged by the Papago Buttes and Tempe Butte. (See Figures 5.1 and 5.4.) This area is not treated as no-flow in the FLOTRAN simulation, since it is relatively small and far from the sources. The butte area is given hydrologic parameters equal to those in the areas immediately east of the butte.

5.5.6. Vertical Flow From the UAU to the MAU.

Initially, there was no plan to simulate flow between the alluvium units in the FLOTRAN simulation. Inspection of the assumed vertical leakances used by the ADWR indicates that what recharge exists from the UAU to the MAU and from the MAU to the LAU is probably fairly uniform. Therefore, ignoring leakances should not change flow directions or velocities significantly. (Note: Vertical leakances used in MODFLOW are calculated by dividing the vertical hydraulic conductivity by the distance between the centers of the layers. The resulting vertical leakance (units of l/time) can be multiplied
by the head difference between the layers to give a value of flow per unit area between the layers.)

Initial results showed a marked difference in flow patterns between the MODFLOW and FLOTRAN simulations. There seemed to be a shortage of water in the southwest area of the FLOTRAN simulation. Investigation of the cause showed that the assumption to ignore vertical flow from the UAU to the MAU, and from the MAU to the LAU was in error. In order to include this in the FLOTRAN simulation, the vertical leakage values from the MODFLOW simulation were multiplied by the difference in the heads between the two aquifers. These values were then interpolated using the same scheme presented for the boundary conditions, and were used as vertical recharge values in the FLOTRAN model. Inclusion of vertical flow greatly improved the matching of flow patterns.

In addition, inspection of 1991 water level data indicates that there is a large source of recharge into the MAU centered approximately 1/2 mile north of Source Area 2. In June, 1991 this recharge is reflected in the ground water mound shown in Figure 5.13. This mound is evident in ground water elevation contours from February to September, 1991. The two wells which are inside the mound were installed in late 1987, so this data was apparently not available for the ADWR modeling effort. Based on this evidence, a source of additional recharge to the MAU is applied to an area which would be inside the mound in Figure 5.13. The area on which the additional recharge is applied is shown in Figure 5.11.

Figure 5.14 shows September 1991 TCE concentrations in the MAU. The area of the ground water mound (north of Source Area 2) shows no TCE contamination, confirming the existence of a hydraulic barrier in this area. Figure 5.5b, however, shows some contamination in the area, indicating that the ground water mound may not be present in the area at all times. In addition, ground water samples tested in 1981 - 1982 showed that COS 72 (to the east) was consistently contaminated to a higher level than
Figure 5.13: September, 1991 water surface elevations at the North Indian Bend Wash Superfund site.
Figure 5.14: September, 1991 TCE concentrations in the middle alluvium unit under the NIBW Superfund site.
was COS 71. This indicates that there may have been a major shift in ground water flow directions between the early 1980's and the early 1990's.

In order to create a 5 ft ground water mound in the MAU, a recharge of 27.95 ft/yr was applied to the appropriate area (see Figure 5.10). This is compared to a maximum of 0.36 ft/yr calculated from the maximum leakances used in the ADWR model and assuming a 50 ft head difference between the UAU and MAU. To create a mound this large, the vertical conductivity should be much higher than estimated by the ADWR. Seasonal variations in the height of the mound have been noted, so a yearly average would be expected to be smaller than the maximum. Therefore, the amount of recharge ultimately used in the model was 17.60 ft/yr, about 2/3 of what would be required to create a 5 ft ground water mound.

Figure 5.15a-c shows the modeled ground water elevations in 1957 - 1960 with no recharge, 17.60 ft/yr, and 27.95 ft/yr of recharge.

5.5.7. Flow Calibration.

Figure 5.16a-d shows the piezometric head elevations calculated by FLOTRAN for the last 4 time periods (1957 - 1960 is shown in Figure 5.15b). Comparisons of Figure 5.16b with the outlined areas of Figures 5.8b show that the flow regimes are very similar for the 1966-1970 time period. Note that the flow in the FLOTRAN simulation area is generally from southeast to northwest in the MODFLOW simulation. The other time steps show similar behavior. The ground water mound discussed in § 5.5.6 is the only major difference.

5.5.8. Time Discretization.

As stated above, the simulation was run for five time periods (1957 - 1981), with average pumpages for each time period. The pumpage data is moderately complete from 1957 to 1978, however the first samples of TCE contaminated water were taken in 1981.
Figure 5.15: Ground water elevations estimated by FLOTTRAN for 1957 to 1960 time period. The three cases are (a) no additional recharge, (b) additional recharge of 17.60 ft/yr, and (c) additional recharge of 27.95 ft/yr, over the area shown in Figure 5.10.
Figure 5.16: Water surface elevations calculated by FLOTTRAN for 1961 - 1981. Flow from 1961 to 1965 is simulated assuming that the additional recharge to create the mound is absent. The last three time steps include the additional recharge at $1.7 \times 10^{-5}$ cm/s
In order to arrive at an estimate of the extent of contamination in 1981, the last time step is extended through that year, with the assumption that there are no changes in pumpage, recharge, or boundary conditions between the end of 1978 and the end of 1981.

5.6. Assumptions in the FLOTRAN Contaminant Transport Simulation.

Many preliminary runs were made to test the effects of changing different input parameters on the final contaminant plumes. The final runs had several assumptions about subsurface conditions. Among these assumptions were that the ‘ground water mound’ discussed in §5.5.6 did not exist from 1957 - 1965. Evidence shown in Figures 5.5b and 5.14 indicates that the ground water mound shown in Figure 5.13 is not constant, possibly changing in height dramatically over time. Since the mound appears to grow larger over time, it was removed from the first two time periods entirely.

The presence of the large ground water mound also indicates that the UAU/MAU vertical leakance values used in the ADWR MODFLOW model are lower than actual leakances. The given UAU/MAU leakance values ranged from 0.022/year to 0.22/year. In order to increase the overall UAU/MAU leakances, the vertical leakances from the UAU to the MAU used were made more uniform by increasing the low leakance values to be equal to the medium-low range values (everything less than 0.066/year was increased to 0.066/year) and a few of the medium-low range leakance values were increased to a medium range value (0.066/year to 0.11/year). The range of leakances, originally 0.022 to 0.22/year, was changed to 0.066 to 0.22/year. The leakance values from the MAU to the LAU were unchanged.

In addition, since the Salt River’s recharge effects were totally ignored in the calculations of boundary condition, water levels in the southwest corner of the MODFLOW model area drop off more than would be expected. To remedy this, the constant head boundary conditions were altered slightly, increasing four constant head cells in that area by 2 - 8 feet.
5.7. Results of FLOTRAN Contaminant Transport Simulation

Simulated TCE concentrations in the years 1960, 1965, 1970, 1975, 1978, and 1981 are shown in Figure 5.17a-e. The plume emanating from Source Area 1 moves generally to the west. Ground water velocities in this area are very low, and there are three wells near that site which pumped quite heavily from 1957 - 1978. (See Table 5.1, FLOTRAN cells (5, 8), (7, 5), and (9, 4).) These wells probably removed a significant amount of TCE from the subsurface. The plume in the MAU extending from Source Area 2 travels northwest, avoiding the 'mound' then extends northward toward the two water wells COS 71 and COS 72.

The simulated TCE concentration in the two water supply wells in 1981 is estimated at 292 µg/L for COS 72 and 36.5 µg/L for COS 71. Actual concentrations in COS 72 and COS 71 in November, 1981 were 350 µg/L and 100 µg/L, respectively. (Ferrari, 1984) Figure 5.18 shows the simulated TCE concentration in the two water wells plotted against the year of the simulation. According to the model results, the contamination in COS 72 has been greater than 5 µg/L since approximately 1971.

As shown in Figure 5.11, COS 71 and COS 72 are not located in the centers of their model cells, but along the western edges. To account for this, the concentrations reported for the FLOTRAN simulations at COS 71 and COS 72 are average concentrations of the cells to the east and west of the wells.

5.8. Sensitivity Analysis.

The sensitivity of the model to variation in several of the aquifer parameters was observed. The following parameters were varied to determine the effect on the model: porosity, dispersivity, hydraulic conductivity, the shape of the source for Source Area 2, and the recharge which creates the 'mound' discussed in § 5.5.6. The parameters were varied to determine which exerted the most significant effects on the outcome of the model.
Figure 5.17: Concentrations estimated by FLOTRAN for (a) 1960, (b) 1965, (c) 1970, (d) 1975, and (e), 1981. Contours are at 200 μg/L intervals. Maximum concentrations in the two plumes are given in Table 5.4.
Figure 5.17: Concentrations estimated by FLOTAN, continued.
Figure 5.18: TCE Concentrations in the City Water Wells
The model responded significantly to a 50% increase in the porosity (from 0.1 to 0.15). The main result of this variation was an 18-25% reduction in the lengths of the two plumes, based on the extent of the 200 μg/L contour. Overall, the shape of the plumes were not changed, as would be expected. Changing the porosity does not affect the hydraulic gradients, so the shape of the plume should not change significantly. A decrease of porosity by 33% (such that $\theta_{hi} = 1.5 \theta_{norm}$ and $\theta_{norm} = 1.5 \theta_{low}$) results in 20-25% longer plumes. In addition, the concentrations at COS 71 and COS 72 are increased by about a factor of two. Since the concentration gradients are so large in this simulation and the receptor wells are at the very edge of the plume from Source Area 2, a small increase in the length of the plume has a large effect on these concentrations. The plumes are slightly longer in the $\theta_{low}$ simulation, and the plume from Source Area 2 has nearly the same maximum concentration (within 4%). There is, however, no reason to expect the porosity to fall below 0.1, especially not as low as 0.066.

Multiplying each of the variable the hydraulic conductivity values by 1.5 reduced the size of the cones of depression around the extraction wells in the model, while not significantly affecting the regional hydraulic gradients. The increase in hydraulic conductivity directly affected the ground water velocity, thus extending the length of the plume. The increase in velocity also increases the dispersion coefficient ($D = \alpha v$). As a result, the plume extending from Source Area 2 is longer, but is also more spread out, with a lower maximum concentration (from 2430 μg/L to 1720 μg/L). The contamination around Source Area 1 is more spread out toward the west, and has the maximum concentration reduced in half (from 960 μg/L to ~450 μg/L). Decreasing the hydraulic conductivity by 33% (similar to porosity) results in a much slower moving and more compact contaminant plume. Maximum concentrations are much higher at both source areas, increasing by about 50%.
Increasing the aspect ratio ($\alpha_f/\alpha_l$) from one tenth to three tenths while keeping the longitudinal dispersivity constant at 100 ft causes very little change in the two contaminant plumes. The maximum concentration is reduced by less than 1% from Source Area 2, and about 4% from Source Area 1. Reducing the longitudinal dispersivity from 100 ft to 10 ft, and the transverse from 10 ft to 1 ft increases the maxima in the two plumes slightly (1 - 3%), and results in slightly more compact plumes.

The shape of Source Area 2 is not known very well. Figure 5.12 shows several wells which could be sources. Changing the shape of Source Area 2 from a rectangle to a square centered over the industrial site had very little effect on the overall simulation. The resulting contaminant plume has a slightly different shape, and a much higher maximum (about 50% higher), since the injection wells are a square instead of a rectangle. The concentrations at the two city water wells are slightly lower (~20%), since the closest source well is slightly farther away, but overall the effect is minor.

The presence of the ground water mound discussed in § 5.5.6 has a major effect on the plume from Source Area 2. Without the mound, the plume heads almost due north, to the west of the two city water wells. The concentrations in the two city water wells is very similar to that predicted by including the mound for the last three time steps. On its path to the north, however, the TCE travels through where the mound would be. Including the mound slows the northward progress of the contamination, and shifts it to the west.

5.9. Summary of NIBW Contaminant Transport Modeling.

Contaminant transport in a portion of the Middle Alluvium Unit for the years 1957 - 1981 was simulated using FLOTRAN. Ground water elevations, and therefore velocities, were calculated in multi-year time steps using pumping data supplied by the Arizona Department of Water Resources, and a modification of a ground water flow model developed by the ADWR in the late 1980s. The pumping data, along with vertical
recharge from the Upper Alluvium Unit and to the Lower Alluvium Unit calculated by the modified MODFLOW model, provided a series of five steady-state flow fields with which contaminant transport calculations were performed. Two sources of trichloroethylene contamination were placed in the aquifer thus simulated, and contaminant transport was simulated.

FLOTRAN is capable of modeling flow in three space dimensions, however for this site, only two dimensions were used. Modeling contaminant transport in the NIBW in three dimensions would be extremely complex, due to the interconnections between the three aquifers, and due to the numerical dispersion between vertical model cells discussed in § 4.4.1. In order to avoid numerical ‘cross-contamination,’ the model would require two or three extra vertical layers between each aquifer, for a total of 7-9 vertical layers to simulate a three aquifer system. These extra layers would be very difficult to characterize, and not enough is known about the subsurface to adequately carry this out. Further complicating the matter of three dimensional modeling are the three separate TCE plumes in the UAU, two possibly separate plumes in the MAU, and a plume in the LAU.

As is stated in § 5.5.2, this simulation was performed assuming that Source Areas 1 and 2 are the only sources of contamination that affect the water wells COS 71 and COS 72. There are other possible sources of contamination, which could not be included in this model. In addition to the MAU, COS 72 also penetrates the LAU, and there is some TCE present in that aquifer. The source of the TCE contamination in the LAU is not certain. It is suspected that this contamination may be resulting from contaminated water flowing down an well which is screened over all three aquifers near Source Area 2. This well was used for extracting water for agricultural use until about 1970, when it was shut down. If the contamination in the LAU is due to this well, it most likely would not have begun to spread until about 1970, which would likely limit the contribution that contamination from this well could have to COS 71 and COS 72 in 1981. There are also other industries in the NIBW area, however these industries are either farther from the
city water wells than Source Areas 1 and 2, or evidence shows that contamination from these sites is limited to the UAU.

In conclusion, modeling of contaminant transport at the NIBW with FLOTTRAN shows a possible avenue for contamination of two city water wells COS 71 and COS 72 with trichloroethylene. The model produces concentrations at the water wells which are within a factor of two of observed concentrations in November, 1981. The model is sensitive to changes in the hydraulic conductivity and porosity, and is somewhat sensitive to the presence of the ground water mound north of Source Area 2.
Chapter 6. Overall Results and Conclusions.

Numerical models are widely used to simulate ground water flow and contaminant transport. In order to use a model with confidence, the user must know that it has been tested and will perform correctly in everything from a simple situation with an analytical solution to a complex field site. In order to test the performance of the three dimensional ground water flow and contaminant transport model, FLOTRAN, a series of test simulations was designed. The simulations fall into five basic test categories: (1) qualitative comparisons, (2) radially dominated flow, (3) comparisons with analytical solutions, (4) comparison with a previously modeled field site, and (5) modeling a new, complex field site.

6.1. Overall Testing Results.

A summary of the results of testing within each of the five test categories follows. In each case, a brief description of the simulation is given, along with the results.

6.1.1. Qualitative Test Results.

Three qualitative tests were performed, including a grid orientation test, a sorption test, and a biodegradation test. In the grid orientation test, FLOTRAN gave both encouraging and discouraging results. Referring back to Figures 4.2a and 4.2c, one can see the results for advection and dispersion of a slug of contaminant in a uniform flow field with dispersion turned on, and for a no dispersion case. When the flow is along the grid orientation, both simulations are extremely well-behaved. In the no-dispersion case, the entire contaminant slug remains inside a single cell. On the other hand, when the flow direction is at a 45 degree angle to the grid orientation, numerical dispersion becomes large, even when FLOTRAN is simulating a zero dispersion case.
In the sorption test, the expected result of adding a retardation factor of 2 is for all the transport processes to slow by a factor of 2. As discussed in §4.1.2, Figure 4.3 shows that the contaminant slug with retardation at 100 days is the same shape and is in the same location as the contaminant slug without retardation at 50 days. The maximum concentrations in the two plumes are equal.

The last qualitative test is a comparison of FLOTRAN and BIOPLUME II with biodegradation. The two models give very similar results in this test. Referring to Figures 4.5 and 4.6, the hydrocarbon and oxygen plumes around a contaminated injection well in a uniform flow field are shown. The plumes are of similar length, although the FLOTRAN plume is more disperse than the BIOPLUME II plume. FLOTRAN's biodegradation calculations using fast equilibrium parameters match reasonably well with those of BIOPLUME II. In addition, FLOTRAN's mass balance errors were less than $10^{-5}$%, while BIOPLUME II's were around 2 - 7%.

6.1.2. Radially Dominated Flow Test Results.

Two radially dominated flow tests were performed, recharge/recovery from a single well, and a recharge/recovery doublet. Both of these tests were performed on very coarse grids under high stress conditions. In §4.2.1, the first of these simulations is discussed. In this simulation, contaminated water was injected into a well and then removed from the same well. Figure 4.6 shows the simulated contaminant concentration at the well along with the analytical solution. In three of the four cases simulated, numerical dispersion is significant, increasing the time required to remove the contamination from the aquifer.

§4.2.2 details the recharge/recovery doublet simulation, in which contaminated water is injected into one well and recovered from another. Figures 4.8 and 4.9 show the resulting breakthrough curves given by FLOTRAN, the USGS. Method of Characteristics model, and the semi-analytical model RESSQ. Both FLOTRAN and MOC show
concentration breakthrough to the extraction well at about the same time as predicted by RESSQ, but while FLTRAN shows a smooth rise in concentrations, the MOC simulation shows large fluctuations in concentration. Due to model edge effects, FLTRAN has difficulty with the simulation, however when the model domain was enlarged, the FLTRAN simulation results improved dramatically.

6.1.3. Results of Comparisons with Analytical Solutions.

Four different tests of problems with analytical solutions were performed, including one-dimensional transport from a constant concentration boundary, transport from a continuous point source in a uniform two dimensional flow field, transport of a contaminant slug in a uniform two dimensional flow field, and transport in the radial flow field around an injection well. The first of these simulations (see §4.3.1) tests one dimensional flow for four different values of dispersivity, from zero to a moderately high value (5 ft). Figure 4.10 shows the results for the four values of dispersivity. The FLTRAN simulations match the analytical solution very closely in all four cases. Another code, SEFTRAN, tested with the same simulation shows numerical oscillations when the dispersivity is low (Figure 4.11). Modeling the same situation at a 45 degree angle produced breakthrough curves which, when fit to the analytical solution, show that the 45 degree angle adds numerical longitudinal dispersivity approximately equal to 1/10 of the grid cell size.

The second of these tests, transport from a continuous source in two dimensions, included a mesh refinement trial. The code was tested using three different meshes: Coarse, Medium, and Fine. FLTRAN matched the concentrations along the x-axis very closely using the Fine mesh, but underestimated the concentrations using the Coarse and Medium meshes (See Figures 4.13 - 4.15 in §4.3.2). Modeling this scenario at a 45 degree angle produced steady state results which, when fit to the analytical solution show
that the 45 degree angle adds numerical transverse dispersivity approximately equal to 1/10 of the grid cell size.

The third of the tests with analytical solutions, transport of a slug of contaminant in a two dimensional flow field, is very similar to the second, without the mesh refinement analysis. Concentration snapshots at three times are given in §4.3.3, Figure 4.17. FLOTRAN overestimates the maximum concentration at the earliest time step by about 3%, and matches the later two time steps to within 1%. In addition to this test, the time discretization scheme used by FLOTRAN (see Equations 3.6 and 3.7) was also tested. For this simulation, the time step size chosen by FLOTRAN’s internal criteria is too large. The results of this test overshoot the analytical solution by over 30% at t = 3.96 days.

The last of the tests with analytical solutions is a simulation of transport from an injection well (see §4.3.4). This test is performed with three different values of dispersivity. Snapshots of the concentrations after 20 and 40 days (Figure 4.19) show that the FLOTRAN solution lags behind the analytical solution. Reducing the size of the grid blocks improves the agreement between solutions, especially in the low dispersivity case (Figure 4.20). In the high dispersivity case, simply reducing the size of the grid block which includes the well improves the results dramatically (Figure 4.21).

6.1.4. Results of a Comparison with a Previously Modeled Field Site.

In §4.4.1, FLOTRAN is compared with a model used by Sykes (1982) to model contamination at the Canadian Forces Base Borden Landfill. This model is used as a benchmark for comparison with FLOTRAN, based on work by Huyakorn et al. (1984). The 16 × 9 × 5 model grid is the same as was used in the Sykes model (Figure 4.23). Flow conditions were calibrated to the observed water levels and the water surface elevations used in the Sykes model, and are shown in Figures 4.24 and 4.25. Figure 4.29 shows chloride concentrations at 36 years in a vertical slice (A-A’) beginning below the landfill as calculated (a) by FLOTRAN and (b) by Sykes’ model. Three different cases are
shown, with varying transverse dispersivity values. The concentrations calculated by FLOTRAN show a larger sensitivity to transverse (vertical) dispersivity than those calculated by Sykes' model. Figure 4.30 shows chloride concentrations just below the water table for the same three simulations. Again, the FLOTRAN runs show more transverse spread of the chloride. In addition to these runs, a mesh refinement run was performed to determine the effects of 'dispersion' into the low conductivity areas below the modeled aquifer. Figures 4.31 and 4.27 show that the chloride will 'disperse' into the first model cell at the edge of the aquifer. Thus refining the mesh confines the chloride to an area closer to the actual aquifer.

The first of the above cases was also modeled with a variable thickness aquifer, which eliminates the problem of mass escaping the model area. When this was done, the concentrations simulated downgradient of the landfill were higher, because the contaminant was not allowed to move out of the aquifer.

6.1.5. Results of Modeling at a Complex Field Site.

Chapter 5 discusses the final test, in which FLOTRAN was used to model trichloroethylene contamination at the North Indian Bend Wash Superfund site in Arizona. Along with testing FLOTRAN, the modeling effort was designed to determine the extent of contamination in the NIBW area prior to discovery of TCE in two city water wells in 1981. An existing regional ground water flow model (for 1983 - 1988) using MODFLOW was adapted to model regional flow conditions for the three aquifer system in the 66 square mile area surrounding the NIBW site for 1957 - 1981. These flow conditions were used as a starting point for modeling contaminant transport in a 20 square mile subsection of the middle of the three aquifers with FLOTRAN. Figure 5.1 shows the NIBW MODFLOW model area, the FLOTRAN model area, and the boundary of the NIBW Superfund Site. One of the features accounted for by the contaminant transport model is the existence of a ground water mound in the center of the model area,
apparently created by a hydraulic connection between the upper aquifer (UAU) and the middle aquifer (MAU). Figure 5.13 shows several possible source areas and the two contaminated wells. Two of these sources are included in the model: Source Area 1, to the north of the wells, and Source Area 2, to the southeast.

Flow conditions in the MAU during the simulation period are generally toward the northwest in the FLOTRAN model area. Figure 5.8b shows the flow conditions calculated by MODFLOW for 1970. These heads were then used to create matching flow conditions in FLOTRAN, as shown in Figure 5.16b. The contaminant transport calculated using these flow conditions (Figure 5.17a-e) has TCE flowing from Source Area 2 toward the contaminated water supply wells, and TCE from Source Area 1 flowing north and east, away from the wells.

6.2. Conclusions.

In the course of testing the groundwater flow and contaminant transport model FLOTRAN, several observations have been made, and are listed below.

1. When simulating biodegradation, advection, and dispersion, FLOTRAN produces output similar to BIOPLUME II, with no oscillations and much better mass balance.

2. In the radially dominated flow tests, FLOTRAN outperforms BIOPLUME II, except for a test with very low dispersivity.

3. In the tests with analytical solutions, FLOTRAN matches the analytical solutions and shows no signs of oscillation.

4. When the flow is at a large angle to the grid orientation, numerical effects add to the apparent dispersivity by about 1/10 of the grid cell size. These effects are exaggerated in the case of a slug of contaminant flowing at a large angle to the grid.
5. In the three dimensional Borden Landfill simulation, FLOTTRAN performed acceptably in ‘brick’ mode, and performed very well using the general geometry modification written by Dawson in 1995.

6. FLOTTRAN can easily and accurately simulate a variable thickness aquifer using the general geometry modification.

7. On the complex simulation of TCE transport in Arizona, FLOTTRAN performed well, accounting for the ground water mound, variable flow rates, variable recharge, and steep concentration gradients.

8. Varying the pumpages between time steps greatly affects the direction and rate of ground water flow in the NIBW area.

9. Model results strongly suggest that Source Area 2 is the source of the TCE in the two city water wells.

10. Model results also suggest that significant (>5 μg/L) TCE contamination existed in a water supply well (COS 72) for approximately ten years before it was discovered in November, 1981.

6.3. Recommendations.

Based on the results of this testing and on the author’s observations during the months spent working with the program, FLOTTRAN is a very useful code. The code correctly simulates advection, dispersion, sorption and biodegradation, and only has small numerical error. Creating an input file for a FLOTTRAN simulation is about as difficult as for BIOPLUME II.

In the future, the input structure of FLOTTRAN could be revised to provide for consistency in the input units. In addition, a standard output file should be created which
echoes all the inputs, in order to help the user determine the location of input errors. 

FLOTTRAN is also capable of modeling transient flow situations, however this option has been turned off in the current version. Transient flow simulation should be reinstalled and tested.
Bibliography.


Appendix — Program Input and Output.

Various inputs are required for FLOTRAN. They include a mesh on which to perform calculations, iteration parameters, aquifer parameters, boundary conditions and solute parameters. The following sections describe the input variables used in FLOTRAN. These input variables are not given in the order required by FLOTRAN.

Mesh Input and Iteration Parameters.

Following is a list of inputs and descriptions.

- \( N_x, N_y, N_z \): Number of grid blocks in the x, y, and z directions.
- \( L_x, L_y, L_z \): Length of model domain in the x, y, and z directions.
- \( \text{imesh} \): 'u' indicates uniform mesh, 'n' indicates nonuniform mesh.
- \( \text{file 'mesh'} \): For nonuniform mesh, file 'mesh' includes the values of \( x_1, \ldots, x_{N_x+1}, y_1, \ldots, y_{N_y+1}, \) and \( z_1, \ldots, z_{N_z+1} \) as described in Figure 3.1.
- \( \text{iconln} \): Units of \( L_x, L_y, L_z \), and entries in file 'mesh.'
- \( \text{nsteps} \): Maximum number of time steps.
- \( \text{factor} \): Time step multiplier, cfl, see Equation 3.6.
- \( \text{kprint} \): Print a standard output every kprint time steps.
- \( \text{kcont} \): Print an output suitable for contouring every kcont time steps.
- \( \text{itim} \): Units of time used in time inputs.
- \( \text{nprint} \): Number of times at which the user wishes to force output to be printed.
- \( \text{tprint} \): Array of times at which the user wishes to force output to be printed.
- \( \text{tinit}, \text{tfinal} \): Initial and final simulation times.
- \( \text{idisp} \): Calculate dispersion every idisp time steps. '0' indicates a no dispersion simulation.
- \( \text{numobs} \): Number of observation wells in the model.
- \( \text{iobs}, \text{jobs}, \text{kobs} \): Location of the observation well (repeated numobs times).

Aquifer Parameters.

Following is a list of inputs and descriptions.

- \( \text{theta} \): Aquifer porosity.
idisp Calculate dispersion every idisp time steps. ‘0’ indicates a no dispersion simulation.

$\alpha_m, \alpha_L, \alpha_{T1}, \alpha_{T2}$ Molecular diffusion constant, longitudinal and transverse dispersivities. ($\alpha_{T1}$ is perpendicular to the direction of flow and parallel to the ground surface, while $\alpha_{T2}$ is perpendicular to both.)

$K_x, K_y, K_z$ Hydraulic conductivities in the x, y, and z directions, respectively. These parameters may be given constant values by assigning a flag input variable to a value of 0, and entering the constant conductivity on the next line, or variable values by assigning a flag input variable the value of 1, and entering a filename to use for the conductivity values on the next line.

**Boundary Conditions.**

Following is a list of inputs and descriptions required for each boundary.

ibndx, ibndy, ibndz Enter ‘d’ for Dirichlet, ‘n’, for Neumann, or ‘m’ for mixed Dirichlet and Neumann boundary conditions.

ivar Enter ‘c’ for constant boundary condition along the boundary, or ‘v’ for variable. If mixed boundary conditions are chosen, ‘ivar’ is not used.

value or filename If ivar = ‘c’, this is the value of the boundary condition (head for Dirichlet or flux for Neumann). If ivar = ‘v’, or ibndx = ‘m’, this is the name of the file in which the variable or mixed boundary conditions are stored. Variable boundary conditions are read as a $N_x \times N_y, N_x \times N_z$, or $N_y \times N_z$ array, depending on the boundary.

**Solute Parameters.**

Following is a list of input required for each solute component and descriptions.

ncmp Number of solute components to be modeled.

$C_0$ Initial constant concentration of the solute.

ret Retardation factor, $R_p$.

pexp Freundlich isotherm exponent (disabled).

irestrt Is this a restart (y/n)? If yes, the next line lists the name of a file which contains initial concentration data.

The following input is required for each boundary.

iread If iread = 0, the following line contains a concentration which is given to all water entering the model domain from that boundary. If iread $\neq 0$, the following line lists a filename which contains variable concentration data.
Biodegradation Parameters.

Following is a list of input required for biodegradation and descriptions.

<table>
<thead>
<tr>
<th>Variable</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>ireact</td>
<td>If ireact = 'y', read biodegradation input parameters from the file 'in.reac.'</td>
</tr>
<tr>
<td>k</td>
<td>Hydrocarbon utilization rate per unit mass of microorganisms.</td>
</tr>
<tr>
<td>K_c</td>
<td>First order decay rate of natural organic carbon.</td>
</tr>
<tr>
<td>C</td>
<td>Natural organic carbon concentration.</td>
</tr>
<tr>
<td>F</td>
<td>Ratio of oxygen to hydrocarbon consumed.</td>
</tr>
<tr>
<td>Y</td>
<td>Yield (g cells produced / g hydrocarbon consumed).</td>
</tr>
<tr>
<td>K_h</td>
<td>Hydrocarbon half-saturation constant.</td>
</tr>
<tr>
<td>K_o</td>
<td>Oxygen half-saturation constant.</td>
</tr>
<tr>
<td>nsmall</td>
<td>Number of iterations to perform.</td>
</tr>
</tbody>
</table>

Output Given by Model.

FLOTRAN prints most of its run-time output to the screen, but this can be saved to a file if desired. Screen outputs include an echo of most input values, and then during the run, at each computed time step, the time, time step size, and error balance are printed, along with the maximum and minimum concentrations. Other outputs are saved to files, including the computed heads (once only for steady state) and the concentration of each modeled solute at each user selected time step (given in tprint). Both of these are in a format suitable for contouring. Also output is the final concentration of solute in a format suitable for use as a ‘restart’ file. Other outputs are a file containing concentrations at the observation wells at each selected time step (one per solute), and a file containing mass balance errors at each selected time step.